

MOLECULAR CODE DIVISION MULTIPLE ACCESS:
GAUSSIAN MIXTURE MODELING

by

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Abstract

Communications between nano-devices is an emerging research field in nanotechnology. Molecular Communication (MC), which is a bio-inspired paradigm, is a promising technique for communication in nano-network. In MC, molecules are administered to exchange information among nano-devices. Due to the nature of molecular signals, traditional communication methods can't be directly applied to the MC framework. The objective of this thesis is to present novel diffusion-based MC methods when multi nano-devices communicate with each other in the same environment. A new channel model and detection technique, along with a molecular-based access method, are proposed in here for communication between asynchronous users.

In this work, the received molecular signal is modeled as a Gaussian mixture distribution when the MC system undergoes Brownian noise and inter-symbol interference (ISI). This novel approach demonstrates a suitable modeling for diffusion-based MC system. Using the proposed Gaussian mixture model, a simple receiver is designed by minimizing the error probability. To determine an optimum detection threshold, an iterative algorithm is derived which minimizes a linear approximation of the error probability function. Also, a memory-based receiver is proposed to improve the performance of the MC system by considering previously detected symbols in obtaining the threshold value. Numerical evaluations reveal that theoretical analysis of the bit error rate (BER) performance based on the Gaussian mixture model match simulation results very closely.

Furthermore, in this thesis, molecular code division multiple access (MCDMA) is proposed to overcome the inter-user interference (IUI) caused by asynchronous users communicating in a shared propagation environment. Based on the selected molecular

codes, a chip detection scheme with an adaptable threshold value is developed for the MCDMA system when the proposed Gaussian mixture model is considered. Results indicate that the MCDMA system is a promising approach to reduce interference created by asynchronous nodes in multi-user MC systems. Meanwhile, the receiver is modified by exploiting previously detected chips to eliminate the ISI. The performance evaluations via computer simulations show that the memory-based receiver, which considers previously detected chips in detection procedure, outperforms the memory-less receiver.

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Dedication

*To my supportive family,
Hossein, Parvin and Mohammad kia,
Without whom none of my success would be possible.*

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List of Abbreviation and Symbols

ASK	Amplitude Shift Keying
BER	Bit Error Rate
BMI	Brain Machine Interface
CSK	Concentration Shift Keying
DFE	Decision Feedback Equalizer
DNA	Deoxyribonucleic Acid
ISI	Inter-Symbol Interference
IUI	Inter-User Interference
M-MCDMA	Multi-Molecular Code Division Multiple Access
MAP	Maximum A Posteriori
MCDMA	Molecular Code Division Multiple Access
MC	Molecular Communication
MIMO	Multiple Input Multiple Output
ML	Maximum Likelihood
MMSE	Minimum Mean Square Error
MoNo	Molecular Code Distance Function
MoSK	Molecular Shift Modulation
MTSK	Molecular Transition Shift Keying
OOK	On-Off Keying
PIC	Parallel Interference Cancellation
PPM	Pulse Position Modulation
QMoSK	Quadruple Molecular Shift Keying
SER	Symbol Error Rate

SM	Spatial Multiplexing
LTI	Linear and Time-Invariant
α	Fraction of molecular energy
$\alpha^{(k)}$	Fraction of molecular energy regarding k th user
$\bar{I}_{m\text{IUI}}$	Expectation of IUI
$\delta(\cdot)$	Dirac delta function
η	Viscosity of the aqueous medium
\hat{d}_m	Detected symbol
$\hat{N}_m^a(t)$	Number of received molecules absorbed by active receiver
$\hat{N}_m^p(t)$	Number of received molecules measured by passive receiver
\hat{q}_{jk}	Detected chip sequence of k th user
λ	Threshold value
$\lambda_{\text{op}}^{\text{G}}$	The optimum threshold of Gaussian modeling
$\lambda_{\text{op}}^{\text{GM}}$	Threshold value of Gaussian mixture modeling
λ_a	Auto-correlation of code set
λ_c	Cross-correlation of code set
\mathbf{X}_{R}	Receiver position
\mathbf{X}_{T}	Transmitter position
$\mathbf{X}(t)$	Molecule position
μ	Mean
ρ_a	Radius of the active receiver
ρ_p	Radius of the passive receiver
σ^2	Variance

τ_k	Delay time of k th user
$\{d_i\}_{i=0}^{\infty}$	Symbol sequence
$C(\mathbf{X}, t)$	Expected molecular concentration
C_k	Code set of k th user
D	Diffusion coefficient
E_k	Energy of impulse response regarding k th user
E_r	Total molecular energy
$h(t)$	Expected impulse response of diffusion channel
$h_a(t)$	Expected impulse response of active receiver
$h_k(t)$	Expected impulse response of k th channel
$h_p(t)$	Expected impulse response of passive receiver
I	Number of previous transmitted symbols
$I_{m\text{ISI}}$	Total ISI element
$I_{m\text{IUI}}$	Total IUI component
K	Number of active users
k_B	Boltzmann constant
L	Code length
l'	Number of previously detected symbol
M	Number of molecules emitted per symbol "1"
M_k	Number of molecules released from k th user
$n(t)$	Noise process
$N_m^a(t)$	Expected number of received molecules absorbed by active receiver
$N_m^p(t)$	Expected number of molecules measured by the passive receiver
P_m^a	Probability of a molecule being absorbed

P_m^p	Probability of a molecule arriving within passive receiver
p_0	The probability of sending symbol “0”
p_1	The probability of sending symbol “1”
P_e	The probability of error
q_{jk}	Chip sequence of k th user
r_d	Distance between transmitter and receiver
r_k	Distance between k th user and receiver
R_m	Radius of the messenger molecule
$s_k(t)$	Input signal of k th channel
s_m	Total desired molecular signal
T	Temperature
T_c	Chip duration
T_s	Symbol duration
V_R	Spherical volume of the passive receiver
w	Code weight
$x(t)$	Expected response of channel to periodic emission
$y(t)$	Received molecular signal
y_m	Total received molecular signal
$z(t)$	Diffusion channel response to one shot transmission

Chapter 1

Introduction

Inspired from interactions among biological systems, molecular communication (MC) is proposed as a new communication paradigm that enables the transmission of information via the emission, diffusion and reception of molecules [1]. MC is considered a promising paradigm for implementing nano-networks; in which simple nano-devices interconnect to perform complex tasks [2]. Furthermore, MC provides a bio-compatible, energy efficient and non-toxic solution in interacting with micro-organisms especially for biological applications [3]. However, due to the unique characteristics of the MC channel [4]; most techniques applied in traditional communication requires reconsideration to make them feasible for MC system. Therefore, this thesis aims to present novel guidelines for channel modeling, receiver design and detection methods that can be applied to MC systems.

This chapter provides a short introduction on the objective and outline of this thesis. Previous literature on nano-networks, from nano-electromagnetic waves to molecular communication are reviewed in Section 1.1. Furthermore, the molecular system model and noticeable applications of MC are discussed in Section 1.1. Section 1.2 studies the reaming challenges and unsolved issues of this field, followed by the key contributions presented in this work. Finally Section 1.3 outlines the organization of this research thesis.

1.1. HISTORY AND BACKGROUND

1.1 History and Background

Nanotechnology is the science and technology that enables the manipulation of matter for the development of nano-scale devices. The concept of nanotechnology was first envisioned by the famous physicist Richard Feynman on his talk entitled “There’s Plenty of Room at the Bottom” in 1960 [5]. Later on, Eric Drexel presented the idea of implementing nano-scale devices [6] (e.g. nanomachines) and ever since noticeable attempts have been realized to manufacture such machines for various nanotechnology applications [1–4]. Due to the small size and energy constraints, a single nano-device has limited capabilities where it can only perform simple tasks such as computing, sensing and actuation [1]. In addition, nano-networking allows nano-devices to interconnect and share information [2, 7], to expand their potentials in function and complexity. Though, since nanomaterials show unique properties in nano range, the physical channel is different from the protocols developed in conventional wireless networks. In this regard, a novel communication framework is required to enable nano-networking. Therefore, how nano-devices exchange information in a network has recently become the main challenge among researchers.

In literature two approaches have been proposed for nano-networking [8] (i) nano-electromagnetic communication [9–16] and (ii) molecular communication (MC) [4, 7, 17]. In the following, Section 1.1.1 and Section 1.1.2 thoroughly investigates both alternatives, respectively.

1.1.1 Nano-Electromagnetic Communication

Nano-electromagnetic communication is defined as the transmission and reception of electromagnetic radiation from nano-level elements [9]. In nano-electromagnetic

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communication, current methods in traditional electromagnetic networks are revised in order to fit them into nano-level range. Recent progress in electronic nano-materials and graphene substances (e.g. carbon nano-tubes) has led to the development of nano-batteries [10] and even nano-scale antennas that radiate nano-electromagnetic waves in the terahertz band [11,12].

Some work have addressed the issues and challenges remaining in this field. By employing nano-electromagnetic communication in wireless nano-sensor networks (WNSN), [13] refers to channel modeling in the terahertz band, current manufacturing techniques and nano-sensor components. Furthermore in [14], carbon nanotube sensor networks (CNSN) are studied that are similar to the conventional sensor networks in wireless communication. Here, the obstacles of nano-electromagnetic communication are discussed in terms of network functionality and realization. A terahertz propagation model is achieved in [15] where the channel capacity is investigated when molecular absorption is considered. In addition, [16] presents models that considers the scattering effect of nano-electromagnetic waves on graphene-based substances.

Although noticeable work have focused on the feasibility of adopting nano-electromagnetic communication to nano-networks; recent research has identified that terahertz wave damages the DNA molecule and seems to effect gene expression [18]. Therefore, nano-electromagnetic communication isn't a suitable technique for nano-networking, since most applications for nano-communication involves interacting with biological systems (e.g. organs, cells).

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1.1.2 Molecular Communication

Molecular Communication (MC) is proposed as the most promising paradigm for interconnection among nano-devices [1,3,4,17,19–22] which is inspired from biological mechanisms viewed in nature. In MC, information is encoded in molecular patterns rather than electromagnetic waves in conventional networks. Since MC is originated from nature, it expects to provide a feasible, bio-compatible and energy efficient platform for communicating with nano-level environment [4]. Calcium signaling [23], molecular motors (e.g. kinesin, myosin) [3,24] and DNA hybridization [25] are one of the few important mechanisms performed in nature that use MC techniques. Once messenger molecules are released, they propagated in the fluidic medium (e.g. through free diffusion, flow or guided paths) till they reach a specific destination.

From the authors knowledge, MC was first introduced in 2005 with the aim of accomplishing a bio-compatible communication framework for nano-networking [3]. In [1,2], the concepts of MC for designing nano-networks and possible applications in nanotechnology are highlighted. A complete review of previous works on MC is presented in the book entitled “Molecular Communication” [17]; where existing biological models in nature and human body followed by a mathematical modeling of the MC channel is investigated. Also unique features of the MC channel compared to traditional communication is discussed in [4,22].

Since the concepts of traditional communication can't be directly employed to MC, a new design framework is required to model the MC system. In the following, Section 1.1.2.1 describes a basic system model for MC, while potential application of this field are addressed in Section 1.1.2.2.

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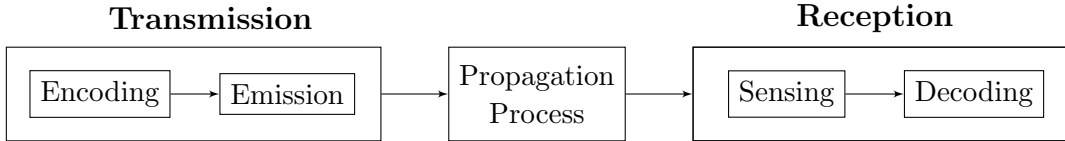


Figure 1.1: Block diagram of the molecular communication system

1.1.2.1 Molecular Communication System Model

As shown in Fig. 1.1, a basic MC system consists of three general phases: transmission, propagation and reception. In the following paragraphs each process is described in more detail.

Transmission is the stage where molecules as message carriers are encoded and released in the propagation environment. At the transmitter, information can be encoded in three main forms for the receiver to detect.

(I) The most common form of modulation is *concentration shift keying (CSK)* [26,27], which is similar to amplitude shift keying (ASK) modulation in wireless communication. In CSK, messages are encoded in concentration or number of molecules; where only one type of molecules is employed. (II) Another technique is *pulse position modulation (PPM)*, in which information is encoded in different time shifts of the transmitted signal when one type of molecules is used [19,28]. (III) *Molecular shift keying (MoSK)* [26], is an orthogonal modulation technique which messages are encoded in the concentration of different types of molecules. Compared to CSK, system performance significantly improves for MoSK; while fewer molecules are transmitted. Note that, the complexity of the receiver structure increases in MoSK, since it requires to distinguish multiple kinds of molecules from each other.

Once the transmitter encodes the information according to one of the aforementioned modulation techniques, molecules are released into the propagation environment.

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Propagation is the phase during which molecules move from the transmitter to the receiver through a fluidic medium. In literature two general types of propagation processes are proposed that categorizes the MC system: (i) *Diffusion-based MC* and (ii) *Flow-based MC*.

- *Diffusion-based MC* is the simplest and most fundamental type of propagation, where molecules diffuse freely; while no external energy is required for transportation [3]. Diffusion-based MC is considered in [29–36] where molecules propagated randomly from high to low concentration based on their Brownian motion [19, 37]. Moreover the challenges in modeling and simulating the diffusion-based MC system is presented in [38–40]. One of the most important and common examples of diffusion-based MC in nature is calcium signaling [23], in which calcium ions as messenger molecules diffuse till they arrive within the cytoplasm of a cell.
- In *flow-based MC* (also known as active transportation), the released molecules are guided by currents or flows to their destination, similar in hormonal communication through the blood stream [1]. This flow or flux aids the propagation process compared to a medium that is only governed by the laws of diffusion. Considerable works have been presented for channel modeling of flow-based MC in [41–45]. An example of this flow-based MC is the chemotaxis-based technique presented in [46, 47], where flagellated bacteria contained information encoded in DNA molecules are released to glide towards the destination.

Reception is accomplished by measuring the received molecular concentration present within the receiver sensing area and decoding the information. The receiver

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structure can be either passive or active depending on the how it functions. A passive receiver is designed to simply observe the received molecular signal [32–36]. In other words, molecules remain in the medium and aren't absorbed. Meanwhile, once molecules hit the surface of an active receiver, they are instantly absorbed and vanished from the medium [48, 49]. In the decoding process a chemical reaction may occur that either includes the production of new molecules, the performance of a simple task or the production of another signal [4, 20, 36, 50, 51]. A ligand-binding receiver model is presented in [20, 50, 51] where the receiver produces a reaction when molecules bind to the receiver surface.

1.1.2.2 Potential Applications

MC is a distinctive candidate and a possible tool for interacting with biological systems and microorganisms, due to its bio-stability, energy efficiency and feasibility at the nano and even micro range [1–4]. Thus, MC has the potential to significantly impact various interdisciplinary applications such as biology and healthcare, environmental and industrial areas [17]. In the following paragraphs, a brief description for each application is discussed.

Biomedical and healthcare is one of the most essential applications of MC which influences nanotechnology for diagnosis and therapy techniques [1, 2, 17]. In biomedical, MC benefits the development of small-scale systems such as lab-on-the-chip for analyzing biological samples for disease detection [52, 53]. Furthermore, MC provides novel methods for regenerating tissues and organs by producing new molecular patterns [54]. MC also may provide a molecular or chemical means of interacting with the human brain instead of using current electrical devices in brain machine

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interface (BMI) [55].

For healthcare and biomedicine applications, MC has the potential to revolutionize monitoring techniques and performing therapy [56–61]. In targeted drug delivery, MC provides alternate methods to improve therapy performance on a targeted site (e.g. diseased cells or tumor); while simultaneously reducing the drug effect on healthy organs [58–60]. In [60], a particulate drug delivery system is proposed where MC is used to model the propagation of drug particles in the cardiovascular network. Moreover, MC provides molecular imaging to monitor cellular functions for example cancer cells to gather information for early diagnosis [61]. The concept is to diagnose cancer cells by measuring the concentration of a specific type of molecules (e.g. fluorescence) that are released when attached to the cancer cells. Meanwhile, nano-devices can communicate in a network by adopting MC to enhance the detection of a tumor in the body.

Environmental applications includes monitoring the substances of a contaminated environment such as controlling water pollution and air pollution [1, 17, 62–64]. Nano-networking based on MC provides a solution for nano-devices to interconnect in order to quickly identify the toxicity source in air or water.

Industrial applications includes producing functional materials such as foods products and smart fabrics that are adaptable to the changes encountered in the environment [1, 4, 17, 65–68]. In food science, nano-devices could employ MC to identify when a plant needs nutrients or water and deliver nutrients or vitamins to increase the quality [65, 66]. MC may also provide novel approaches to sense and control the growth of bacteria in medical apparel and hospital devices [67]. Furthermore, MC is a good solution for developing microbial organisms; for example bacterial biofilms [68]

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to treat organic waste.

1.2 Research Challenges, Objectives and Contribution

The main objective of this work is to investigate and develop a practical framework for MC system to allow nano-communication. This thesis focuses on diffusion-based MC system, where the released molecules diffuse randomly from the transmitter to the receiver. Although, diffusion-based is studied as the most basic type of MC; many challenges and unsolved issues remain in channel modeling and detection techniques for single-user and multi-user scenarios [4, 38]. In the following, Section 1.2.1 discusses the channel modelings proposed in literature for diffusion-based MC systems. In Section 1.2.2 a summary of previous works on detection methods, receiver design and channel coding are reviewed, followed by the main contributions of each chapter in this thesis. Moreover, the published achievements of this research are presented in Section 1.2.3.

1.2.1 Channel Modeling

Similar to conventional communication, channel modeling is one of the most fundamental aspects of designing a diffusion-based MC system, in terms of signal propagation and noise sources. Early literature have studied the MC channel from an information theoretical perspective [19, 28, 69–71]; where the capacity and information rate of the diffusion channel are obtained, regardless of considering the noise effect. In addition, a design of an in vitro MC system is described in [72] by considering the effects of noise in evaluating the maximum information rate.

In [38, 39], the unique characteristics of the expected impulse response regarding

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the diffusion channel in terms of the propagation delay, amplitude and transfer function are investigated. For the first time in [20], a physical end-to-end model of the MC system is proposed based on a ligand-binding receiver; where the transmission, propagation and reception processes are mathematically modeled according to gain and delay. From the same authors, the corrupting noise sources caused due to the random molecular movement are systematically investigated in [73]. By adopting CSK modulation scheme, authors in [73] confirm that the received signal in diffusion-based MC follows a Poisson distribution with a mean and variance equal to the expected received signal at each instant time. In this regard, a closed form expression of the channel capacity regardless of the type of modulation is determined in [74]; which compared to previous works considers noise assumptions and inter-symbol interference (ISI). Similarly, for a ligand-binding receiver noise analysis and channel capacity are derived in [50] and [51], respectively. An alternate stochastic channel model is presented in [75] that considers particle dynamics and noise effects according to the Markov process. In a recent work [76], a Langevin approach is introduced for mathematically modeling the noise caused by Brownian motion.

- **In chapter 2, the diffusion channel is mathematically modeled by Fick's diffusion law and Brownian motion. Here, the expected molecular concentration in time and space is described by Fick's second law of diffusion. Meanwhile, Brownian motion is adopted to systematically model the random nature in molecular movement as a signal-dependent additive noise. For one shot transmission, the channel response of the diffusion-based MC system are developed for both passive and active receiver designs according to the aforementioned**

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models.

1.2.2 Detection Techniques, Receiver Design and Channel Coding

Particle diffusion is a gradual process, which results molecules to fail reaching the destination at the intended time. Thus, the late arrival of molecules causes inter-symbol interference (ISI) at the receiver location. Recovering the emitted information that is distorted by ISI is a challenging issue encountered in diffusion-based MC systems. In this regard, previous literature have addressed various detection techniques and receiver designs [26, 32–34, 48, 77–82], followed by channel coding methods [83–85] to overcome the ISI caused by sequential transmission.

An early work characterized ISI in terms of communication range, pulse-width, and data rate among a pair of communication nodes based on CSK modulation [77]. In [78], a closed form expression for ISI is derived according to wave theory, where the ISI is approximated by considering the effect of only one previous time slot. In [26], ISI is evaluated for various modulation techniques, which MoSK modulation is concluded more resilient to ISI compared to CSK modulation.

In the presence of noise and ISI many research have been employed to design receivers that are capable of restoring transmitted data; while maintaining low complexity in computation and structure [32–34, 48, 81, 82]. Viterbi algorithm is proposed in [79] to design an optimum receiver when MoSK modulation is adopted for diffusion-based MC system. Similarly in [32], sequence detection techniques based on maximum-a-posteriori (MAP) and maximum likelihood (ML) criterion's, followed by a decision feedback equalizer (DFE) and minimum mean square error (MMSE) are presented for on-off keying (OOK) modulation. An information theoretical approach

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is proposed in [80] that obtains an optimal detection technique based on maximum mutual information and ML sequence detector by using Reduced-State Viterbi algorithm. By considering the effect of ISI and noise, previous transmissions are considered for one, two and three dimensional MC model when one molecule is transmitted to represent symbol 1 [80]. In addition, enzymes are adopted in [33] to degrade the undesired molecules remaining in the medium to improve system performance. A novel modulation method referred to as Zebra-CSK is introduced in [81] that periodically emits two types of messenger molecules in subsequent symbol duration based on CSK modulation. Meanwhile, each type of molecule acts as an inhibitor for the other kind, reducing the ISI effect from the previous time slot [81]. Two detection techniques, namely, amplitude detection and energy detection are proposed in [34] for a pulse-based modulation scheme; where they are compared in terms of delay, amplitude (energy) and pulse width. In a recent work, a closed form expression for the probability of error based on [34] are derived when ISI and noise sources are considered [82]. Additionally, molecular transition shift keying (MTSK) is proposed as a power adjustment method in [48] for mitigating the ISI effect by linking the receiver and transmitter together. Also, the error probability and optimal threshold is derived by considering MMSE equalizer and DFE designs in the decoding process.

Channel codes have also been proposed as an alternate solution to overcome the ISI caused by residual molecules [83–85]. A type of error correction codes (e.g. block codes) are introduced in [83] for an absorbable receiver structure that aims to improve the system performance. Since the Hamming distance paradigm can not be applied for code design in MC systems, a molecular code distance function (MoNo) for efficient code design is investigated in [84]. From the same authors, ISI-free codes are proposed

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in [85] that offer good system performance while maintaining low complexity.

The aforementioned literature have demonstrated solid and extensive work for overcoming ISI and noise sources in designing single-user MC systems. Although, almost all have approximated the received molecular signal to follow a Gaussian distribution when an infinite stream of sequential data is emitted (due to simplicity) [26, 32–34, 48, 77–82]. However for the first time, this thesis confirms that Gaussian is not an acceptable model to achieve optimal detection performance. Hence, the objective is to design a novel statistical model for the received molecular signal in order to deal effectively with ISI.

- **In chapter 3 Gaussian mixture distribution is proposed for modeling the received molecular signal when a sequence of molecules are released at the transmitter. By using OOK modulation, Gaussian mixture modeling considers previous transmissions to contribute in the decision making process. Subsequently, a simple detection algorithm is developed that minimizes the probability of error in order to determine the optimum threshold value. Based on Gaussian mixture model, a type of memory-based receiver is also proposed that eliminates the impact of ISI by considering previously detected symbols in decision process.**

In a nano-network where multiple nano-devices are interacting with each other through the emission, diffusion and reception of molecules, inter-user interference (IUI) is inevitable. Since the environment is shared among multiple nodes, IUI arises and challenges the detection of information. Thus, reducing the IUI to enhance system performance and reliability is essential.

1.2. RESEARCH CHALLENGES, OBJECTIVES AND CONTRIBUTION

Though canceling IUI is a key challenge in designing diffusion-based MC networks, only few existing works have investigated this issue [26, 35, 36, 49, 78]. In [78], a closed form expression is derived for the IUI that analyzes signal propagation in diffusion channel by adopting wave theory. The same authors extended their work and evaluated the the IUI based on both CSK and MoSK modulation schemes [26]. Multiple input multiple output (MIMO) techniques to improve system performance in the presence of IUI was first introduced in [35]. The concepts of diversity and spatial multiplexing (SM) methods are explored and an approximation for the probability of error is obtained [35]. In [49], a decision threshold is computed using MAP criterion when two transmitters are communicating synchronously with a single receiver. The error probability is derived when only the ISI effect from one previous transmission duration is considered [49]. Moreover, a diffusion-based MC model is presented in [36] that deals with IUI as continuous external noise source and calculates the expected bit error rate for various cases (e.g. assuming Binomial, Poisson and Gaussian distribution for the received molecular signal). In the presence of advection (flow), [36] employs enzymes to diminish the interfering molecules causing IUI and ISI.

Though aforementioned literature have presented considerable work regarding the challenges encountered in multiple communication for diffusion-based MC systems; non have actually provided any solution to reduce the IUI effectively. Thus, another key contribution of this thesis is proposing a well justified method to maintain high system performance when a number of active nano-devices are communicating in a shared medium. In the following paragraph the fundamental objective and approach of chapter 4 is presented:

- **The other core contribution of this thesis is introducing molecular**

1.2. RESEARCH CHALLENGES, OBJECTIVES AND CONTRIBUTION

code division multiple access (MCDMA) scheme to overcome the IUI effect caused by several active users while transmuting information asynchronously. In MCDMA, each user is assigned to a molecular code sequence that are designed to degrade the asynchronous IUI. These codes selected such that the auto-correlation and cross-correlation of the codes are bounded by small specific values. Furthermore, an optimal chip detection method is evaluated that determines an adaptable threshold based on Gaussian and Gaussian mixture modeling for the MCDMA system. The proposed receiver efficiently restores the data sent from each user by minimizing the effect of the IUI, ISI and noise.

1.2.3 Publication

Two following conference papers have been accepted as the achievements of this thesis till now.

- **”Receiver Design for Diffusion-based Molecular Communication: Gaussian Mixture Modeling”** accepted to IEEE International Conference on Communications, ICC 2016.
- **”Molecular Code Division Multiple Access in Nano Communication Systems”** accepted to IEEE Conference on Wireless Communications and Networking, WCNC 2016.

1.3. THESIS OUTLINE

1.3 Thesis Outline

The remaining chapters of this thesis is organized as follows. In chapter 2, the diffusion channel model of the MC system is described according to Fick's law and an additive Brownian noise for both passive and active receiver structures.

Chapter 3 introduces Gaussian mixture distribution as an acceptable approach for modeling the received molecular signal in diffusion-based MC system. A novel detection algorithm is presented that calculates the optimal threshold value by minimizing the probability of error. Furthermore, a memory-based receiver is designed that considers previously detected symbols in obtaining the optimal threshold value in order to mitigate the ISI effect.

In chapter 4, molecular code division multiple access (MCDMA) is proposed as a distinctive method to overcome the asynchronous IUI produced from communicating in a shared propagation environment. A chip detection receiver is developed for the MCDMA system when Gaussian and Gaussian mixture modeling are employed in determining the optimal threshold. In addition, the performance of the MCDMA system is compared for a memory-less and memory-based receiver.

In chapter 5 conclusions and possible future works in this research are presented.

Chapter 2

Channel Modeling for Diffusion-based Molecular Communication

Designing a molecular communication (MC) system requires a channel modeling that is capable of describing the propagation of molecules through a fluidic environment. Depending on the transportation mechanism, there are two types of MC systems proposed in literature [1]: diffusion-based and flow-based. Since molecular diffusion is the simplest form of data transmission, most literature have presented channel models for diffusion-based MC systems [20, 50, 51, 73–76]; where molecules move randomly from high to low concentration. Noise analysis have also been considered in diffusion-based MC systems by studying random particle movement [19, 20, 50, 73, 76].

The objective of this chapter is to study the mathematical model of diffusion channel based on (1) Fick’s diffusion law [86] and (2) Brownian motion [37]. While Fick’s diffusion law simply refers to the expected received molecular signal; Brownian motion models the random molecular movement in terms of an additive noise, when an instant release of molecules are emitted. Moreover, the signal response of the diffusion-based MC system is developed for both passive and active receiver designs. The channel modeling presented in this chapter is considered the most common model used in literature [32–34, 36, 48, 49, 73, 79–81, 83].

The reminder of this chapter is presented as follows: in Section 2.1 signal propagation in diffusion channel is derived for passive and active receivers according to Fick’s diffusion law and Brownian motion.

2.1. DIFFUSION CHANNEL MODEL

2.1 Diffusion Channel Model

Similar to designing any communication system, first the characterization of the communication channel must be investigated in terms of signal propagation. In a diffusion-based MC system, information transmission is mainly accomplished by a thermally activated diffusion process of messenger molecules. In this mechanism, molecules propagate independently from high (e.g. transmitter) to low (e.g. receiver) concentration in an aqueous environment. Since communication is governed solely by means of the laws of free diffusion, the molecular movement is systematically subject to Fick's diffusion law [86] and Brownian motion [37].

In the following, Section 2.1.1 describes Fick's diffusion law to observe the expected response of the propagation channel and Section 2.1.2 studies the statistical characteristics of the molecular movement by referring to Brownian motion. Furthermore, channel modeling is presented for two types of reception processes, namely *passive* and *active* receivers.

Note that, before proceeding to the next section, the following assumptions are considered in this thesis for modeling the diffusion-based MC system:

- The communication environment is considered 3-dimensional with an infinite boundary which is indexed through the Cartesian axes x , y and z .
- The size of the transmitter is assumed negligible and is approximated as a point source that contains an endless supply of messenger molecules.
- The information molecules are identical and indistinguishable from each other, which the collisions and electrostatic forces among them are neglected.

2.1. DIFFUSION CHANNEL MODEL

- Depending on the type of receiver (passive or active), it is assumed that the reception process (observing or absorbing) operates perfectly without any complication.

2.1.1 Fick's Diffusion law

In physics, Fick's second law of diffusion describes the variation of the molecular concentration with respect to time when molecules undergo the diffusion process [86]. According to Fick's law, the "expected" molecular concentration, denoted by $C(\mathbf{X}, t)$, at time t and location $\mathbf{X} = (x, y, z)$ is expressed by the following differential equation,

$$\frac{\partial C(\mathbf{X}, t)}{\partial t} = D\nabla^2 C(\mathbf{X}, t) \quad (2.1)$$

where $\nabla^2 C(\mathbf{X}, t)$ is the sum of the second derivative of $C(\mathbf{X}, t)$ in 3-dimensional space. Here, D is the constant diffusion coefficient that is expressed as

$$D = \frac{k_B T}{6\pi\eta R_m} \quad (2.2)$$

where k_B is the Boltzmann constant ($k_B = 1.38 \times 10^{-23}$ J/K) and T is the absolute temperature in kelvin (K). The viscosity of the diffusive medium is denoted as, η and R_m is the radius of the messenger molecules that are assumed identical in size and shape. Note that, in this dissertation these parameters have been selected for a homogeneous water-based environment in average body temperature with insulin as the messenger molecules [87].

In order to determine the expected molecular concentration, the equation given in (2.1) can be solved under certain conditions. Depending on the type of reception

2.1. DIFFUSION CHANNEL MODEL

process (e.g. either passive or active), the initial and boundary conditions are defined differently. In this regard, Section 2.1.1.1 considers a passive receiver; while Section 2.1.1.2 employs an active receiver with an absorbing surface.

2.1.1.1 Passive Receiver

For computing the expected molecular concentration, the partial differential equation defined in (2.1) is solved by considering the following initial condition,

$$C(\mathbf{X}_T, t = 0) = M\delta(\mathbf{X}_T) \quad (2.3)$$

which denotes that an instant impulse of M number of molecules released from the transmitter point source located at $\mathbf{X}_T = (x_T, y_T, z_T)$. Here, $\delta(\cdot)$ is defined as the Dirac delta function. Therefore, the expected molecular concentration is obtained as

$$C(r, t) = \frac{M}{\sqrt{(4\pi Dt)^3}} \exp\left(-\frac{r^2}{4Dt}\right), \quad (2.4)$$

where $r = |\mathbf{X} - \mathbf{X}_T|$ is the Euclidean distance between the point \mathbf{X} and transmitter location. In addition, for a receiver centered at $\mathbf{X}_R = (x_R, y_R, z_R)$, the “expected” scaled (by M) impulse response becomes

$$h_p(t) = \frac{M}{\sqrt{(4\pi Dt)^3}} \exp\left(-\frac{r_d^2}{4Dt}\right), \quad (2.5)$$

where $r_d = |\mathbf{X}_R - \mathbf{X}_T|$ is the Euclidean distance between the transmitter and center of receiver. Since, (2.5) is derived under no terms specifying the boundary of the reception site; this type of receiver is referred to as passive [3, 32–36]. A passive

2.1. DIFFUSION CHANNEL MODEL

receiver is simply an observer that measures the molecular concentration (or number of molecules) arriving within the reception area; thus, molecules remain in the fluidic medium forever. For simplicity, $h_p(t)$ is referred to as the expected impulse response of the passive receiver.

Here, (2.5) is evaluated based on the consistency of concentration throughout the reception space. That is, the molecular concentration measured within the receiver's volume are assumed equivalent to that measured at the center of the receiver [33, 36]. This assumption is fairly true when r_d is far greater than the receiver's radius, denoted as ρ_p . Therefore when $\rho_p < r_d$, the expected number of molecules counted till time t , denoted by $N_m^p(t)$, is expressed as

$$N_m^p(t) = V_R h_p(t) \quad (2.6)$$

in which $V_R = \frac{4}{3}\pi\rho_p^3$ is the volume of the passive receiver.

2.1.1.2 Active Receiver

In some literature [3, 48, 49] the receiver is considered to have an absorbable surface which is also referred to as an active receiver. Here, it is assumed that once molecules hit the receiver surface, they are absorbed and disappeared from the medium. In [48], the impulse response of the active receiver is mathematically derived from (2.1) under the following boundary conditions,

$$(1) \quad \lim_{\mathbf{x} \rightarrow \infty} C(\mathbf{X}, t) = 0 \quad (2) \quad \frac{\partial C(\mathbf{X}, t)}{\partial \mathbf{X}} = wC(\mathbf{X}, t) \quad \text{for} \quad |\mathbf{X}| = \rho_a \quad (2.7)$$

2.1. DIFFUSION CHANNEL MODEL

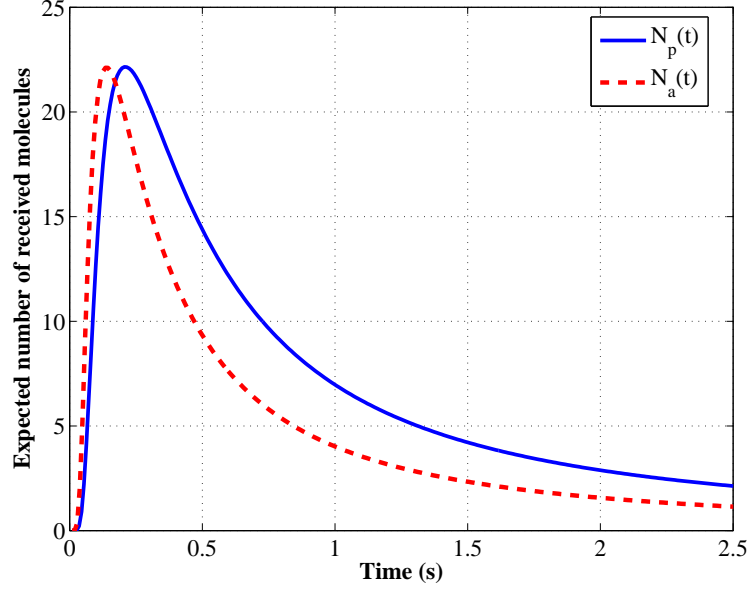


Figure 2.1: The expected number of received molecules measured by the passive and active receiver.

where the first condition reflects the assumption that for very far distances (especially further than r_d), the effect of molecular concentration is neglected. In the second term when the rate of reaction, denoted as w , approaches infinity, the boundary condition signifies that every collision leads to an absorption. Thus, the molecular concentration is zero at the absorbing surface with radius ρ_a . According to (2.7) when $w \rightarrow \infty$, the response of (2.1) to (2.3) becomes [48]

$$h_a(t) = \frac{M\rho_a}{r_d} \operatorname{erfc} \left(\frac{r_d - \rho_a}{\sqrt{4Dt}} \right), \quad (2.8)$$

where $h_a(t)$ is the expected number of molecules that are absorbed by the receiver after transmission time t has passed.

Note that, $h_p(t)$ refers to the expected molecular concentration; meanwhile $h_a(t)$ denotes the expected number of received molecules. In addition, it is true to define

2.1. DIFFUSION CHANNEL MODEL

$N_m^a(t) = h_a(t)$. Fig 2.1 illustrates $N_m^p(t)$ and $N_m^a(t)$ when $r_d = 10 \mu\text{m}$ and $\rho_p = \rho_a = 2 \mu\text{m}$. The number of molecules released at the transmitter for the passive receiver is selected as $M = 10^6$; though for the active receiver $M = 10^4$. The difference between the number of emitted molecules for both cases relates to the second boundary condition defined in (2.7). Since molecules tend to diffuse from high to low concentration, this process occurs faster when the molecular concentration is zero at the receiver surface (active receiver). Hence compared to passive receiver, the same maximum amplitude is achieved for the active receiver with less number of emitted molecules.

2.1.2 Brownian motion

The movement of molecules through a homogeneous environment is via Brownian motion. Though Fick's law deals with the expected molecular concentration, Brownian motion is the result of random collisions among diffusing messenger particles with the fluids molecules [37]. This random behavior makes it difficult to predict the exact location of molecules; thus causing uncertainty in the measured molecular concentration at the reception site.

Brownian motion is mathematically modeled by the Wiener process, a continuous-time stochastic process with independent Gaussian increments [37, 88]. According to the Wiener process, for a small time duration of Δt , the movement of each emitted molecule follows a Gaussian distribution with zero mean and a variance defined as $2D\Delta t$. In other words, the location of a molecule, $\mathbf{X}(t)$, after Δt time duration

2.1. DIFFUSION CHANNEL MODEL

changes randomly as follows,

$$\mathbf{X}(t + \Delta t) = \mathbf{X}(t) + \sqrt{2D\Delta t} \mathcal{N}(\mathbf{0}_{3 \times 3}, \mathbf{I}_{3 \times 3}), \quad (2.9)$$

where $\mathcal{N}(\mathbf{0}_{3 \times 3}, \mathbf{I}_{3 \times 3})$ is a 3-by-3 Diagonal matrix, where its diagonal elements represent the normal distribution with zero mean and variance 1. Since it is assumed that a molecule moves independently in each direction with a Gaussian distribution; according to (2.9) the probability density function (pdf) of the diffusing molecule located at $\mathbf{X} = (x, y, z)$ viewed till time t can be expressed as

$$f(r, t) = f(x, t)f(y, t)f(z, t) = \frac{1}{\sqrt{(4\pi Dt)^3}} \exp\left(-\frac{r^2}{4Dt}\right). \quad (2.10)$$

where $r^2 = x^2 + y^2 + z^2$. Hence, the probability of each molecule arriving at time t within the passive receiver is evaluated by integrating (2.10) over the reception volume as follows

$$P_m^p = \int_{r_d}^{r_d + \rho_p} \int_0^{2\pi} \int_0^\pi r^2 f(r, t) \sin \theta \, d\theta d\phi dr. \quad (2.11)$$

where for simplicity $P_m^p(t)$ is replaced by P_m^p . Note that, generally there is no closed form solution for (2.11). However, previously it was assumed that the receiver is sufficiently far from the transmitter, especially compared to the receiver radius ($\rho_p < r_d$). Thus, the molecular concentration can be approximated uniform throughout the receiver volume and equal to that measured at the center. According to this assumption there is no need to integrate over the volume and (2.11) is simplified to

$$P_m^p = V_R f(r_d, t) = \frac{V_R}{\sqrt{(4\pi Dt)^3}} \exp\left(-\frac{r_d^2}{4Dt}\right) \quad (2.12)$$

2.1. DIFFUSION CHANNEL MODEL

where as mentioned earlier V_R is the passive receiver volume. Since, all messenger molecules are presumed to move independently from each other, they all reach the passive receiver with probability P_m^p . Therefore when M molecules are released at the transmitter, the number of received molecules till time t , denoted as $\hat{N}_m^p(t)$, follows a Binomial distribution

$$\hat{N}_m^p(t) \sim \mathcal{B}(M, P_m^p). \quad (2.13)$$

Note that, under the condition where M is selected large enough such that $\mathbb{E}[\hat{N}_m^p(t)] \geq 10$, the binomial distribution can be approximated with the Gaussian distribution. Hence, (2.13) is replaced by

$$\hat{N}_m^p(t) \sim \mathcal{N}(MP_m^p, MP_m^p(1 - P_m^p)), \quad (2.14)$$

By substituting P_m^p from (2.12) to (2.14), the mean value of $\hat{N}_m^p(t)$ becomes

$$\mu_p = \frac{MV_R}{\sqrt{(4\pi Dt)^3}} \exp\left(-\frac{r_d^2}{4Dt}\right). \quad (2.15)$$

where comparing to the expression in (2.6), μ_p is equal to the expected number of received molecules, $N_m^p(t)$, derived from Fick's second law of diffusion. In this regard, (2.14) can be rewritten as,

$$\hat{N}_m^p(t) \sim \mathcal{N}(N_m^p(t), N_m^p(t)\left(1 - \frac{N_m^p(t)}{M}\right)). \quad (2.16)$$

Moreover for an active receiver, the probability of a molecule being absorbed by the

2.1. DIFFUSION CHANNEL MODEL

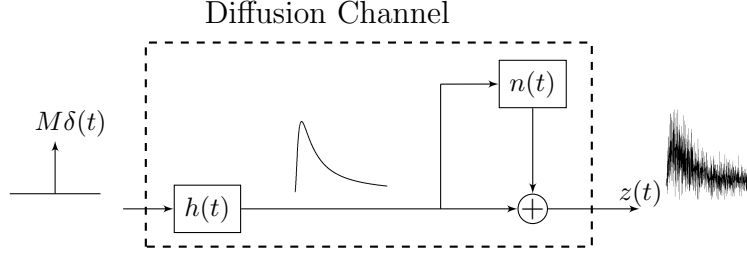


Figure 2.2: Diffusion channel model

receiver surface within time t is determined as follows [48, 49]

$$P_m^a = \frac{\rho_a}{r_d} \operatorname{erfc} \left(\frac{r_d - \rho_a}{\sqrt{4Dt}} \right). \quad (2.17)$$

Similar to the passive receiver, for the transmission of M molecules, the absorbed number of messenger molecules follows a Gaussian distribution analogous to (2.14); by substituting P_m^a from (2.17). Therefore the following expression is derived,

$$\hat{N}_m^a(t) \sim \mathcal{N}(N_m^a(t), N_m^a(t)(1 - \frac{N_m^a(t)}{M})), \quad (2.18)$$

where $N_m^a(t) = MP_m^a = h_a(t)$.

According to the results derived in Sections 2.1.1 and 2.1.2 the diffusion channel is modeled as shown in Fig. 2.2; similar to [32–34, 36, 48, 49, 73, 79–81, 83]. In Fig. 2.2, the output of the diffusion channel to an instant release of molecules, denoted as $z(t)$, is expressed as

$$z(t) = h(t) + n(t) \quad (2.19)$$

where $h(t)$ is the “expected” impulse response, regardless of the type of receiver (could be either $h_p(t)$ or $h_a(t)$) that models the deterministic behavior of the diffusion channel. Meanwhile, $n(t)$ is the additive noise due to the Brownian motion which

2.1. DIFFUSION CHANNEL MODEL

models the random characteristic of molecular movement. In this regard, based on the expressions determined in the aforementioned sections, $n(t)$ and $z(t)$ for a passive receiver are respectively characterized as follows

$$\begin{aligned} n(t) &\sim \mathcal{N}\left(0, \frac{h_p(t)}{V_R}(1 - P_m^p)\right), \\ z(t) &\sim \mathcal{N}\left(h_p(t), \frac{h_p(t)}{V_R}(1 - P_m^p)\right). \end{aligned} \quad (2.20)$$

Note that, here the parameters are selected such that $P_m^p < 0.0002$ which will result in $(1 - P_m^p) \simeq 1$. Therefore, the above expression can be rewritten as follows

$$\begin{aligned} n(t) &\sim \mathcal{N}\left(0, \frac{h_p(t)}{V_R}\right), \\ z(t) &\sim \mathcal{N}\left(h_p(t), \frac{h_p(t)}{V_R}\right). \end{aligned} \quad (2.21)$$

Additionally, for an active receiver $n(t)$ and $z(t)$ are respectively obtained as

$$\begin{aligned} n(t) &\sim \mathcal{N}\left(0, h_a(t)(1 - P_m^a)\right) \\ z(t) &\sim \mathcal{N}\left(h_a(t), h_a(t)(1 - P_m^a)\right) \end{aligned} \quad (2.22)$$

Here, the parameters are selected such that $P_m^a < 0.04$ in which the value $1 - P_m^a$ can be ignored in (2.23). In this regard, (2.23) is approximately rewritten as

$$\begin{aligned} n(t) &\sim \mathcal{N}\left(0, h_a(t)\right) \\ z(t) &\sim \mathcal{N}\left(h_a(t), h_a(t)\right) \end{aligned} \quad (2.23)$$

Here $z(t)$ refers to the number of absorbed messenger molecules rather than concentration. Note that, the channel model presented in Fig. 2.2 is well known model

2.1. DIFFUSION CHANNEL MODEL

commonly used in literature [32–34, 36, 48, 49, 73, 79–81, 83]. Also, according to Fick’s diffusion law described in (2.1) by the linear differential equation, since the diffusion coefficient is a constant value, the channel is a linear and time-invariant (LTI) system.

Chapter 3

Receiver Design: Gaussian Mixture Modeling

Inter-symbol interference (ISI) is considered one of the most challenging issues in designing a diffusion-based MC system. Since particle diffusion is a gradual process, some molecules fail reaching the receiver at the intended time. In other words, for sequential data transmission the receiver not only senses the effects of the current transmission, it holds information on previously emitted molecular signals. Hence, for a low signaling interval, ISI arises and influences recovering the transmitted information.

In literature various channel models and receiver designs are proposed to overcome the ISI effect for signal detection [26, 32, 77–80], [33, 48, 81–85]. For the first time, ISI is characterized in [77] for a diffusion-based MC system; and [78] adopts wave theory to study the ISI effect. In [80], information theoretic approach are presented that proposes an optimal detection scheme by considering all previous transmissions for a one-dimensional MC system. In [32, 48, 79], different types of detection techniques (e.g., Viterbi algorithm, decision feedback, ...) are adopted to reduce the molecular noise and ISI effect. Though these types of receivers are too complex to implement for communication between nano-devices. Channel coding schemes are introduced in [83–85] to enhance system performance in the presence of ISI. Various types of modulation techniques for ISI mitigation are proposed and compared in [26, 81, 82]. Furthermore, a recent study, adopts enzymes to degrade the undesired molecules

3.1. MOLECULAR SYSTEM MODEL

remaining in the medium to reduce the ISI [33].

In this chapter Gaussian mixture model is proposed for the received molecular signal when on-off keying (OOK) modulation is used in diffusion-based MC systems. It is demonstrated that for sequentially emitted molecules, the observed molecular signal at the reception site follows a Gaussian mixture distribution; where, previous transmissions are considered in the decision making. Theoretical analysis of the Gaussian mixture modeling is compared with the result of computer simulations for both passive and active receivers. Furthermore, a simple detection algorithm is developed which determines the optimum threshold value based on Gaussian mixture modeling. To mitigate the ISI effect caused by residual molecules, a memory-based receiver is also proposed in this chapter. Consequently, the system performance is enhanced by employing previously detected symbols.

In the reminder of this chapter, Section 3.1 presents the system model of the diffusion-based MC system followed by a passive receiver structure in Section 3.2. Gaussian and Gaussian mixture modeling are developed in Section 3.2.1 where the receiver is considered memory-less. Furthermore, a type of memory-based receiver is developed in Section 3.2.2 via Gaussian mixture modeling. Also, the Gaussian and Gaussian mixture modeling is established in Section 3.3 for an active receiver. The performance of the MC system is evaluated by computer simulations in Section 3.4; comparing results for passive and active receivers.

3.1 Molecular System Model

Fig. 3.1 illustrates a diffusion-based molecular communication (MC) system consisting of a transmitter, messenger molecules, diffusion channel, and a receiver. The

3.1. MOLECULAR SYSTEM MODEL

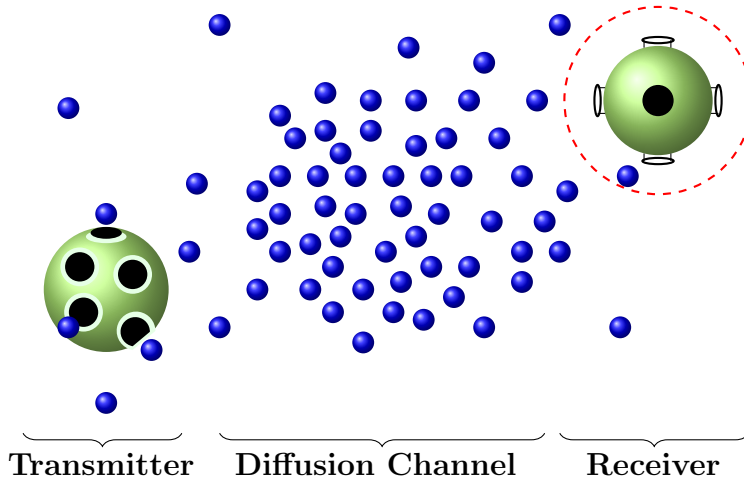


Figure 3.1: Diffusion-based MC system

transmitter is responsible for embedding the information in the concentration of molecules by adopting OOK modulation scheme. Here, the transmitter releases M number of molecules to represent symbol “1”; while no molecule is emitted to signify “0”. Meanwhile, the arrived molecules at the reception cite are measured and information is decoded according to the variation of molecular concentration.

Fig. 3.2 depicts the block diagram of the diffusion-based MC system regardless of the receiver type (either passive or active). According to Fig. 3.2, the expected response of the diffusion channel to periodic data emission, denoted by $x(t)$, is given as

$$x(t) = \sum_{i=0}^{\infty} d_i h(t - iT_s), \quad (3.1)$$

where $\{d_i\}_{i=0}^{\infty}$ and T_s are the symbol sequence and the duration between transmitted symbols, respectively. At the reception location, the total received molecular signal

3.1. MOLECULAR SYSTEM MODEL

caused by the transmitted data sequence $\{d_i\}$ is expressed as follows

$$\begin{aligned} y(t) &= x(t) + n(t) \\ &= \sum_{i=0}^{\infty} d_i h(t - iT_s) + n(t). \end{aligned} \tag{3.2}$$

where $n(t)$ is the signal-dependent additive noise. In chapter 2, it was discussed that $n(t)$ modeled by Brownian motion. It was shown that if the number of received molecules is large enough $n(t)$ approximately follows a Gaussian distribution with zero mean and variance proportional to the expected number of molecules.

The transmission of sequential molecular impulses, causes the system to encounter inter-symbol interference (ISI) due to the infinite signal duration of $h(t)$ as illustrated in Fig. 2.1 (either $h_p(t)$ or $h_a(t)$). That is, if a new impulse is emitted before the molecular concentration becomes negligibly low at the receiver, the effects of both current and previous transmissions are measured. Therefore, the response to the currently emitted impulse is distorted with the previous transmissions if the signaling interval is low. Although increasing T_s eliminates the ISI, the transmission rate will decrease significantly which is undesirable for communication in MC systems. In order to deal effectively with the ISI, this chapter aims to design a receiver by presenting a suitable statistical model for the received molecules.

Though both passive and active receivers are denoted important models in MC systems, Section 3.2 considers the passive receiver; while Section 3.3 presumes an active receiver.

3.2. PASSIVE RECEIVER DESIGN

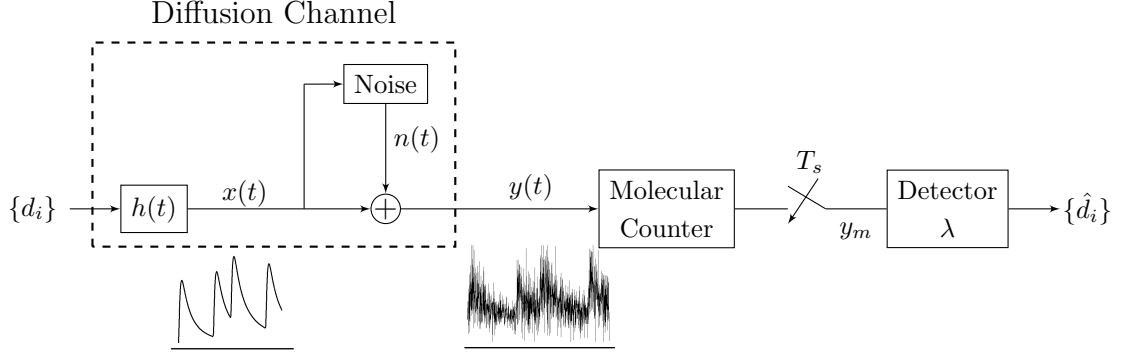


Figure 3.2: Block diagram of the diffusion-based MC system

3.2 Passive Receiver Design

In nano-networks, simple structures are required in implementing communication elements that are able to perform computationally efficient tasks at nano-scale. Here, a passive receiver is considered that simply measures the number of molecules inside the reception space within time T_s .

According to Fig. 3.2, by defining $y_m(t)$ as the received molecular concentration up to time $(m + 1)T_s$, with m as the time index, (3.2) can be rewritten as

$$\begin{aligned}
 y_m(t) &= y(t)|_{t < (m+1)T_s} \\
 &= d_m h_p(t - mT_s) + \sum_{j=0}^{m-1} d_j h_p(t - jT_s) + n_m(t),
 \end{aligned} \tag{3.3}$$

where $h_p(t)$ is the expected impulse response of the passive receiver defined in (2.5). In (3.3), the first, second and third terms are respectively the desired signal, the ISI component and the noise element when $t \in (0, (m + 1)T_s)$. Additionally, the total

3.2. PASSIVE RECEIVER DESIGN

observed molecules during the m th time interval is given as

$$y_m = \int_{mT_s}^{(m+1)T_s} y_m(t) dt = \underbrace{E_r d_m \alpha_0}_{s_m} + \underbrace{E_r \sum_{j=0}^{m-1} d_j \alpha_{m-j}}_{I_{m\text{ISI}}} + n_m \quad (3.4)$$

where s_m , $I_{m\text{ISI}}$ are the total desired signal and ISI components, respectively. Here, $n_m = \int_{mT_s}^{(m+1)T_s} n_m(t) dt$ denotes the overall noise element measured at the m th time duration. Furthermore, E_r is the total molecular energy (related to the number of received molecules) at distance r for a passive receiver. In [34], E_r is defined as follows

$$E_r = \int_0^{\infty} h_p(t) dt = \frac{M}{4\pi D r_d}, \quad (3.5)$$

Also, α_i is a fraction of E_r in time duration $t \in (iT_s, (i+1)T_s)$ given as

$$\alpha_i = \frac{1}{E_r} \int_{iT_s}^{(i+1)T_s} h_p(t) dt \quad (3.6)$$

where $0 \leq \alpha_i \leq 1$ and $\sum_{i=0}^{\infty} \alpha_i = 1$.

In order to recover the transmitted information from ISI and noise, here the maximum-a-posterior (MAP) principle is adopted at the receiver. According to the MAP criterion, the receiver detects $\{d_i\}_{i=0}^{\infty}$ by maximizing the conditional probability distribution function (pdf) of $f(d_m|y_m)$ [89], given as follows

$$\hat{d}_m = \underset{d_m \in (0,1)}{\operatorname{argmax}} f(d_m|y_m) \quad (3.7)$$

3.2. PASSIVE RECEIVER DESIGN

where \hat{d}_m is the detected symbol. The OOK modulation scheme is used, to make a decision on \hat{d}_m by performing the following test

$$P\{d_m = 1\}f(y_m|d_m = 1) \underset{\hat{d}_m=1}{\overset{\hat{d}_m=0}{>}} P\{d_m = 0\}f(y_m|d_m = 0). \quad (3.8)$$

According to (3.8), the goal is to model the conditional pdf of y_m . One of the most used model for $f(y_m|d_m)$ is Gaussian distribution [26,32–34,48,77–82]. Though Gaussian distribution can be a good model for the received molecules in one shot of transmitted molecule. This model is not suitable for the received signal when a sequence of molecular shots are transmitted, due to the random phenomenon of molecular motion occurred in the diffusive channel. In this paper, we propose Gaussian mixture distribution for $f(y_m|d_m)$ instead of Gaussian to have a better statistical model, when the impact of previous transmitted symbols $\{d_i\}_{i=0}^{m-1}$ are considered in detecting d_m .

In the following, Sections 3.2.1 and 3.2.2 develop Gaussian mixture modeling for memory-less and memory-based receivers, respectively. An algorithm is derived that determines the optimum threshold based on Gaussian mixture for both scenarios. In the memory-based receiver, previously detected symbols are considered in the detection algorithm to reduce the ISI effect. While, in the memory-less receiver, d_m is detected only by observing y_m .

3.2.1 Memory-less Receiver

In this section a memory-less receiver is considered that has no knowledge on previously detected symbols in the decision making process. Since the detection algorithm

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for Gaussian mixture distribution is partially dependent on Gaussian modeling, Section 3.2.1.1 briefly deals with Gaussian modeling. Afterwards Section 3.2.2.1 thoroughly describes Gaussian mixture modeling for a memory-less receiver.

3.2.1.1 Gaussian Modeling

In this subsection, $f(y_m|d_m)$ is assumed to follow Gaussian distribution for a memory-less receiver. According to the OOK modulation, the two hypotheses tests H_0 and H_1 are given as

$$\begin{aligned} H_0 : \quad f(y_m|d_m = 0) &\sim \mathcal{N}(\mu_0, \sigma_0^2), \\ H_1 : \quad f(y_m|d_m = 1) &\sim \mathcal{N}(\mu_1, \sigma_1^2), \end{aligned} \tag{3.9}$$

where μ_0 and μ_1 are determined as follows

$$\mu_0 = \mathbb{E}[y_m|d_m = 0] = \bar{I}_{m\text{ISI}}, \tag{3.10}$$

$$\mu_1 = \mathbb{E}[y_m|d_m = 1] = E_r\alpha_0 + \mu_0, \tag{3.11}$$

where $\bar{I}_{m\text{ISI}}$ is the expectation of the ISI. For a passive receiver, σ_0^2 and σ_1^2 are defined as $\sigma_i^2 = \frac{\mu_i}{V_R}$ for $i = \{0, 1\}$ according to (2.21). In addition, for symbol detection the MAP rule can be simplified to

$$\hat{d}_m = \begin{cases} 1, & y_m \geq \lambda, \\ 0, & y_m < \lambda. \end{cases} \tag{3.12}$$

where λ is the threshold value. To obtain the optimum threshold for Gaussian modeling, the error probability is minimized with respect to λ . In this regard, the error

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probability, denoted by P_e , is expressed as

$$P_e = p_0 Q\left(\frac{\lambda - \mu_0}{\sigma_0}\right) + p_1 \left[1 - Q\left(\frac{\lambda - \mu_1}{\sigma_1}\right)\right]. \quad (3.13)$$

where $p_1 = P\{d_m = 1\}$ and $p_0 = 1 - p_1$ are the probability of sending symbol “1” and “0”, respectively. Thus, the optimum threshold for Gaussian modeling, $\lambda_{\text{op}}^{\text{G}}$, by solving $\frac{\partial P_e}{\partial \lambda} = 0$ (under the condition that $\lambda \geq 0$) becomes

$$\lambda_{\text{op}}^{\text{G}} = \sqrt{\mu_0 \mu_1 \left[1 + \frac{1}{V_R(\mu_1 - \mu_0)} \ln\left(\frac{p_0^2 \mu_1}{p_1^2 \mu_0}\right)\right]}. \quad (3.14)$$

where μ_0 is given as

$$\begin{aligned} \mu_0 &= \mathbb{E} \left[E_r \sum_{j=0}^{m-1} d_j \alpha_{m-j} \right] = E_r \sum_{j=0}^{m-1} \mathbb{E}[d_j] \alpha_{m-j} \\ &= p_1 E_r (1 - \alpha_0), \end{aligned} \quad (3.15)$$

and μ_1 is evaluated from (3.11) by substituting μ_0 from (3.15). Note that, the threshold should be a positive value, otherwise it is set to be zero ($\lambda_{\text{op}}^{\text{G}} \geq 0$).

3.2.1.2 Gaussian Mixture Modeling

In diffusion-based molecular communications, all previous transmitted symbols $\{d_i\}_{i=0}^{m-1}$ contribute in the decision making process due to late arrival of some molecules at the reception site. By considering I previous symbols that make the most contributions in y_m ; $f(y_m|d_m)$ can be presented as

$$f(y_m|d_m) = \sum_{d_{m-1}^{m-I} \in \Omega} P\{d_{m-1}^{m-I}\} f(y_m|d_m, d_{m-1}^{m-I}) \quad (3.16)$$

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where $d_i^j = (d_i, d_{i-1}, \dots, d_j)$ for $j \leq i$. Here, $P\{d_{m-1}^{m-I}\}$ indicates the probability of transmitted d_{m-1}^{m-I} and Ω is the set of all possibilities for d_{m-1}^{m-I} . It is assumed that the transmitted symbols are independent and have identical distributions (iid) such that $p_1 = P\{d_i = 1\}$ and $p_0 = 1 - p_1$. In (3.16), $P\{d_{m-1}^{m-I}\}$ can be expressed as

$$P\{d_{m-1}^{m-I}\} = p_1^{K_n} p_0^{I-K_n} \quad (3.17)$$

where K_n and $I - K_n$ denote the number of “1” and “0” symbols in d_{m-1}^{m-I} . Here, the index n is the decimal representation of d_{m-1}^{m-I} in binary number. According to (3.16), $f(y_m|d_m)$ is modeled as Gaussian mixture distribution and the two hypothesis tests are expressed as follows

$$\begin{aligned} H_0 : f(y_m|d_m = 0) &\sim \sum_{n=0}^{2^I-1} p_1^{K_n} p_0^{I-K_n} \mathcal{N}(\mu_n, \sigma_n^2), \\ H_1 : f(y_m|d_m = 1) &\sim \sum_{n=2^I}^{2^{I+1}-1} p_1^{K_n} p_0^{I-K_n} \mathcal{N}(\mu_n, \sigma_n^2) \end{aligned} \quad (3.18)$$

where $n = \sum_{j=0}^I d_{m-j} 2^{I-j}$ corresponds to the binary representation of $d_{m-1}^{m-I} = (d_m, d_{m-1}, \dots, d_{m-I})$ and $K_n = \sum_{j=1}^I d_{m-j}$. In (3.18), $\{\mu_n\}_{n=0}^{2^{I+1}-1}$ and $\{\sigma_n^2\}_{n=0}^{2^{I+1}-1}$ are obtained as,

$$\begin{aligned} \mu_n &= E_r \sum_{j=0}^I d_{m-j} \alpha_j + p_1 E_r \left(1 - \sum_{j=0}^I \alpha_j \right) \\ \sigma_n^2 &= \frac{\mu_n}{V_R} \quad \text{for } n = \{0, 1, \dots, 2^{I+1} - 1\} \end{aligned} \quad (3.19)$$

where $\mu_0 < \mu_1 < \dots < \mu_{2^L-1}$ for $L = 2^I$. Fig. 3.3 shows the conditional pdf's of $f(y_m|d_m)$ of a memory-less receiver for $I = 1$. The receiver detects d_m (between

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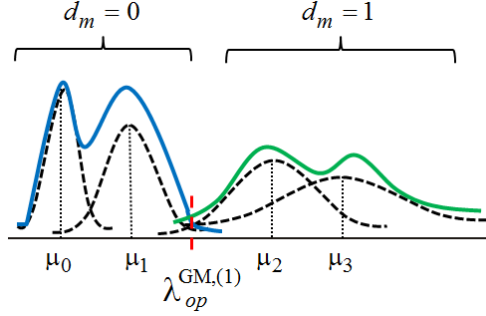


Figure 3.3: The conditional pdf of Gaussian mixture modeling for memory-less receiver by setting $I = 1$.

“0” and “1”) by comparing y_m to a threshold value (similar to (3.12)). To derive the optimum threshold for Gaussian mixture model, the error probability is expressed as

$$\begin{aligned}
 P_e &= \sum_{n=0}^{2^I-1} p_1^{K_n} p_0^{I-K_n+1} Q\left(\frac{\lambda - \mu_n}{\sigma_n}\right) \\
 &+ \sum_{n=2^I}^{2^{I+1}-1} p_1^{K_n+1} p_0^{I-K_n} \left[1 - Q\left(\frac{\lambda - \mu_n}{\sigma_n}\right)\right].
 \end{aligned} \tag{3.20}$$

Determining the optimum threshold requires minimizing the error probability. In this regard, the derivative of (3.20) with respect to λ is given as follows

$$\begin{aligned}
 \frac{\partial P_e}{\partial \lambda} &= - \sum_{n=0}^{2^I-1} \frac{p_1^{K_n} p_0^{I-K_n+1}}{\sigma_n \sqrt{2\pi}} \exp\left[-\frac{1}{2} \left(\frac{\lambda - \mu_n}{\sigma_n}\right)^2\right] \\
 &+ \sum_{n=2^I}^{2^{I+1}-1} \frac{p_1^{K_n+1} p_0^{I-K_n}}{\sigma_n \sqrt{2\pi}} \exp\left[-\frac{1}{2} \left(\frac{\lambda - \mu_n}{\sigma_n}\right)^2\right].
 \end{aligned} \tag{3.21}$$

Clearly, deriving the optimum threshold by solving $\frac{\partial P_e}{\partial \lambda} = 0$ is not straightforward. As a solution, a linear approximation is applied for the exponential component in (3.21) based on Taylor’s series. Hence, at a given point $\lambda = \lambda_t$, the exponential element is

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approximated as

$$\begin{aligned} \exp \left[-\frac{1}{2} \left(\frac{\lambda - \mu_n}{\sigma_n} \right)^2 \right] &\cong \\ \exp \left[-\frac{1}{2} \left(\frac{\lambda_l - \mu_n}{\sigma_n} \right)^2 \right] &\left\{ 1 + \frac{\lambda_l (\lambda_l - \mu_n)}{\sigma_n^2} - \left(\frac{\lambda_l - \mu_n}{\sigma_n} \right) \lambda \right\} \end{aligned} \quad (3.22)$$

by substituting (3.22) in (3.21), a closed form expression is achieved for $\frac{\partial P_e}{\partial \lambda}$. Thus, the solution to the linear approximation of $\frac{\partial P_e}{\partial \lambda} = 0$, denoted by $\lambda = \lambda_{l+1}$, becomes

$$\lambda_{l+1} = - \frac{\sum_{n=0}^{2^I-1} \frac{p_1^{K_n} p_0^{I-K_n+1}}{\sigma_n} B(n, l) - \sum_{n=2^I}^{2^{I+1}-1} \frac{p_1^{K_n+1} p_0^{I-K_n}}{\sigma_n} B(n, l)}{\sum_{n=0}^{2^I-1} \frac{p_1^{K_n} p_0^{I-K_n+1}}{\sigma_n} A(n, l) - \sum_{n=2^I}^{2^{I+1}-1} \frac{p_1^{K_n+1} p_0^{I-K_n}}{\sigma_n} A(n, l)}. \quad (3.23)$$

where $A(n, l)$ and $B(n, l)$ are defined as follows

$$\begin{aligned} A(n, l) &= \exp \left[-\frac{1}{2} \left(\frac{\lambda_l - \mu_n}{\sigma_n} \right)^2 \right] \left\{ - \left(\frac{\lambda_l - \mu_n}{\sigma_n} \right) \right\} \\ B(n, l) &= \exp \left[-\frac{1}{2} \left(\frac{\lambda_l - \mu_n}{\sigma_n} \right)^2 \right] \left\{ \frac{\lambda_l (\lambda_l - \mu_n)}{\sigma_n^2} + 1 \right\} \end{aligned} \quad (3.24)$$

By replacing λ_l with λ_{l+1} in (3.24), one can repeat the same aforementioned process. A step by step procedure is presented in Algorithm 1, to obtain the threshold value for Gaussian mixture modeling, denoted by $\lambda_{\text{op}}^{\text{GM}}$. In Algorithm 1, I refers to the number of previous symbols considered in modeling $f(y_m|d_m)$; while $\varepsilon \ll 1$. According to the derived threshold value, the expression for probability of error is achieved by substituting $\lambda = \lambda_{\text{op}}^{\text{GM}}$ in (3.20). In addition, as seen in (3.16), $f(y_m|d_m)$ is modeled as Gaussian mixture distribution based on a combination of 2^I Gaussian distributions

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Algorithm 1 Calculating Threshold Value for Memory-less Receiver

1. Choose $I \geq 1$ and $\lambda_0 = \lambda_0^{(I)}$
 2. Set $l = 0$
 3. Compute λ_{l+1} from (3.23)
 4.
 - if** $\lambda_{l+1} - \lambda_l < \varepsilon$ **then**
 - $\lambda_{\text{op}}^{\text{GM},(I)} = \lambda_{l+1}$
 - else**
 - $l \leftarrow l + 1$
 - go to step 3
 - end if**
-

(I -order). The initial value of the I -order model, denoted as $\lambda_0^{(I)}$, is selected from the final result in the ($I-1$)-order model; such that $\lambda_0^{(I)} = \lambda_{\text{op}}^{\text{GM}(I-1)}$. Note that, for $I = 1$, the initial value of λ is chosen based on the optimum threshold determined from the Gaussian model, $\lambda_0^{(1)} = \lambda_{\text{op}}^{\text{G}}$.

3.2.2 Memory-based Receiver

In this section, the case in which $f(y_m|d_m)$ is modeled based on knowing l' previously detected symbols, also referred as “memory-based receiver” is considered. The receiver holds information of l' previously detected symbols, such that $\hat{d}_{m-l'}^{m-1} = (\hat{d}_{m-1}, \dots, \hat{d}_{m-l'})$ is substituted instead of $d_{m-l'}^{m-1} = (d_{m-1}, \dots, d_{m-l'})$ in modeling $f(y_m|d_m)$. Furthermore, it is straightforward that maximizing $f(y_m|d_m)$ with respect to $d_{m-l'}^{m-1} = \hat{d}_{m-l'}^{m-1}$ is similar to maximizing $f(y_m|d_m, d_{m-l'}^{m-1} = \hat{d}_{m-l'}^{m-1})$.

In the following, Section 3.2.2.1 and Section 3.2.2.2, develops the detecting algorithms of a memory-based receiver based on Gaussian and Gaussian mixture distributions for $f(y_m|d_m, d_{m-l'}^{m-1} = \hat{d}_{m-l'}^{m-1})$, respectively.

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3.2.2.1 Gaussian Modeling

In this subsection, Gaussian distribution is considered in modeling $f(y_m | d_m, d_{m-l'}^{m-1} = \hat{d}_{m-l'}^{m-1})$ for a l' -based receiver. In order to perform the test given in (3.8), the two hypotheses H_0 and H_1 are expressed as

$$\begin{aligned} H_0 : \quad & f(y_m | d_m = 0, d_{m-l'}^{m-1} = \hat{d}_{m-l'}^{m-1}) \sim \mathcal{N}(\mu_0, \sigma_0^2), \\ H_1 : \quad & f(y_m | d_m = 1, d_{m-l'}^{m-1} = \hat{d}_{m-l'}^{m-1}) \sim \mathcal{N}(\mu_1, \sigma_1^2), \end{aligned} \quad (3.25)$$

where μ_0 is determined by

$$\mu_0 = E_r \sum_{l=1}^{l'} \hat{d}_{m-l} \alpha_l + p_1 E_r \left(1 - \sum_{l=0}^{l'} \alpha_l \right), \quad (3.26)$$

Also μ_1 is computed from (3.11) by substituting the given μ_0 in (3.26). The optimum threshold value λ_{op}^G (which depends on $\hat{d}_{m-l'}^{m-1}$) is obtained from (3.14) by adopting the new determined μ_0 and μ_1 in this subsection.

3.2.2.2 Gaussian Mixture Modeling

In this subsection, a memory-based receiver for Gaussian mixture modeling is considered when l' previously detected symbol are saved at the receiver. Here without loss of generality, a one-memory-based receiver ($l' = 1$) is designed by setting $I = 2$. Note that, the results given in the following can be simply extended for l' -memory-based

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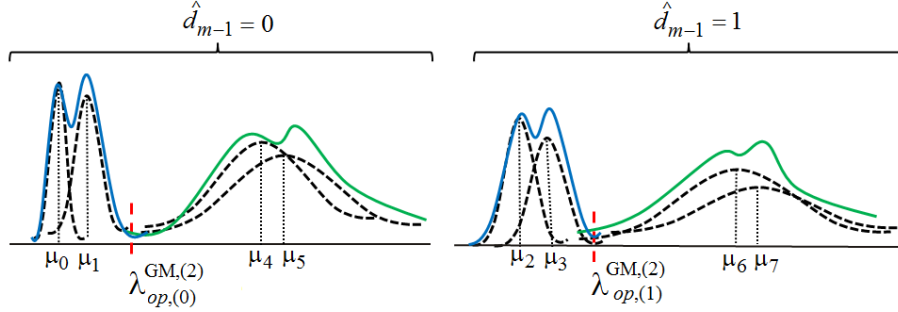


Figure 3.4: The conditional pdf of Gaussian mixture modeling for one-memory-based receiver by setting $I = 2$.

receiver and any I as long as $I \geq l'$. In this regard, the four hypotheses test become

$$\begin{aligned}
 H_1 &: f(y_m | d_m = 0, \hat{d}_{m-1} = 0) \sim p_0 \mathcal{N}(\mu_0, \sigma_0^2) + p_1 \mathcal{N}(\mu_1, \sigma_1^2), \\
 H_2 &: f(y_m | d_m = 0, \hat{d}_{m-1} = 1) \sim p_0 \mathcal{N}(\mu_2, \sigma_2^2) + p_1 \mathcal{N}(\mu_3, \sigma_3^2), \\
 H_3 &: f(y_m | d_m = 1, \hat{d}_{m-1} = 0) \sim p_0 \mathcal{N}(\mu_4, \sigma_4^2) + p_1 \mathcal{N}(\mu_5, \sigma_5^2), \\
 H_4 &: f(y_m | d_m = 1, \hat{d}_{m-1} = 1) \sim p_0 \mathcal{N}(\mu_6, \sigma_6^2) + p_1 \mathcal{N}(\mu_7, \sigma_7^2),
 \end{aligned} \tag{3.27}$$

where the two hypotheses $\{H_1, H_3\}$ decide about d_m for $\hat{d}_{m-1} = 0$; while $\{H_2, H_4\}$ are considered in detecting d_m when $\hat{d}_{m-1} = 1$. Here, $\{\mu_n\}_{n=0}^7$ can be obtained from (3.19) when $d_{m-1} = \hat{d}_{m-1}$. Fig. 3.4 indicates $f(y_m | d_m, \hat{d}_{m-1})$ for one-memory-based receiver by setting $I = 2$. Since there are two sets of hypotheses, the receiver requires two levels of threshold in order to make a decision about d_m . The probability of error for $\hat{d}_{m-1} = 0$ and $\hat{d}_{m-1} = 1$ are defined as $P_e^{(0)}$ and $P_e^{(1)}$, respectively. Therefore, for $I = 2$ the aforementioned error probabilities are defined as

$$\begin{aligned}
 P_e^{(0)} &= p_0^2 Q\left(\frac{\lambda - \mu_0}{\sigma_0}\right) + p_1 p_0 Q\left(\frac{\lambda - \mu_1}{\sigma_1}\right) \\
 &+ p_1 p_0 \left[1 - Q\left(\frac{\lambda - \mu_4}{\sigma_4}\right)\right] + p_1^2 \left[1 - Q\left(\frac{\lambda - \mu_5}{\sigma_5}\right)\right].
 \end{aligned} \tag{3.28}$$

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$$\begin{aligned}
P_e^{(1)} &= p_0^2 Q\left(\frac{\lambda - \mu_2}{\sigma_2}\right) + p_1 p_0 Q\left(\frac{\lambda - \mu_3}{\sigma_3}\right) \\
&+ p_1 p_0 \left[1 - Q\left(\frac{\lambda - \mu_6}{\sigma_6}\right)\right] + p_1^2 \left[1 - Q\left(\frac{\lambda - \mu_7}{\sigma_7}\right)\right].
\end{aligned} \tag{3.29}$$

A similar procedure presented in Section 3.2.1.2 is adopted here for obtaining the optimum thresholds. In Fig. 3.4, $\lambda_{op,(0)}^{\text{GM},(2)}$ and $\lambda_{op,(1)}^{\text{GM},(2)}$ are the optimum threshold values for one-memory-based receiver with $I = 2$. By minimizing $P_e^{(0)}$ and $P_e^{(1)}$ with respect to λ and applying (3.20), the following threshold values are achieved,

$$\lambda_{l+1,(0)} = -\frac{\frac{p_0^2 B(0,l)}{\sigma_0} + \frac{p_1 p_0 B(1,l)}{\sigma_1} - \frac{p_1 p_0 B(2,l)}{\sigma_2} - \frac{p_1^2 B(3,l)}{\sigma_3}}{\frac{p_0^2 A(0,l)}{\sigma_0} + \frac{p_1 p_0 A(1,l)}{\sigma_1} - \frac{p_1 p_0 A(2,l)}{\sigma_2} - \frac{p_1^2 A(3,l)}{\sigma_3}}. \tag{3.30}$$

$$\lambda_{l+1,(1)} = -\frac{\frac{p_0^2 B(4,l)}{\sigma_4} + \frac{p_1 p_0 B(5,l)}{\sigma_5} - \frac{p_1 p_0 B(6,l)}{\sigma_6} - \frac{p_1^2 B(7,l)}{\sigma_7}}{\frac{p_0^2 A(4,l)}{\sigma_4} + \frac{p_1 p_0 A(5,l)}{\sigma_5} - \frac{p_1 p_0 A(6,l)}{\sigma_6} - \frac{p_1^2 A(7,l)}{\sigma_7}}. \tag{3.31}$$

where $A(n, l)$ and $B(n, l)$ for $n = \{1, \dots, 7\}$ are obtained from (3.24) for the initial point $\lambda_{l,(0)}$ and $\lambda_{l,(1)}$, respectively. Afterwards, the same process is repeated for replacing $\lambda_{l,(0)}$ with $\lambda_{l+1,(0)}$ as shown in Algorithm 2. Algorithm 2 determines $\lambda_{op,(0)}^{\text{GM},(2)}$ and $\lambda_{op,(1)}^{\text{GM},(2)}$; which is equivalent to the procedure of deriving λ_{op}^{G} for memory-less receiver when $I = 1$. Note that the total probability of error $P_e \geq p_0 P_e^{(0)}|_{\lambda=\lambda_{op,(0)}^{\text{GM},(2)}} + p_1 P_e^{(1)}|_{\lambda=\lambda_{op,(1)}^{\text{GM},(2)}}$ is a lower bound of error probability due to assuming that the previously detected symbols are detected correctly. Generally, the developed process in above can be easily extended for memory-based receiver for $l' > 1$ and $I \geq l'$.

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Algorithm 2 Calculating Threshold Value for One-memory-based Receiver

1. For $I = 2$ ($I \geq l'$) choose $\lambda_{0,(0)} = \lambda_{0,(0)}^{(2)}$ and $\lambda_{0,(1)} = \lambda_{0,(1)}^{(2)}$
 2. Set $l = 0$
 3. Compute $\lambda_{l+1,(0)}$ from (3.30)
 4. Compute $\lambda_{l+1,(1)}$ from (3.31)
 5.
 - if** $\lambda_{l+1,(0)} - \lambda_{l,(0)} < \varepsilon$ **then**
 - $\lambda_{\text{op},(0)}^{\text{GM},(2)} = \lambda_{l+1,(0)}$
 - else**
 - $l \leftarrow l + 1$
 - go to step 3
 - end if**
 - if** $\lambda_{l+1,(1)} - \lambda_{l,(1)} < \varepsilon$ **then**
 - $\lambda_{\text{op},(1)}^{\text{GM},(2)} = \lambda_{l+1,(1)}$
 - else**
 - $l \leftarrow l + 1$
 - go to step 3
 - end if**
-

3.3 Active Receiver Design

In this section, an active receiver is considered that is responsible for absorbing the received number of molecules. The results accomplished for the passive receiver in Section 3.2 can be applied to the active receiver with some modifications. In this regard, the following changes are made for the active receiver:

(I) In (3.3), $h_p(t)$ is replaced by $h_a(t)$, the expected impulse response of the active receiver; which is defined in (2.8). Due to this modification, the total molecular energy for an active receiver becomes $E_r = h_a(t)|_{t=0}^{\infty}$. Moreover, (3.6) is replaced by $\alpha_i = \frac{1}{E_r} h_a(t)|_{t=iT_s}^{(i+1)T_s}$ for $i = 0, 1, \dots$

(II) By replacing $h_p(t)$ with $h_a(t)$, $y(t)$ is referred to as the number of received molecules (not the received concentration). Therefore, the distribution of $y(t)$ becomes $y(t) \sim \mathcal{N}(x(t), x(t))$, according to (2.23). This new adjustment will effect

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the evaluation of the threshold value. For example, in Gaussian modeling where the receiver is memory-less, $\lambda_{\text{op}}^{\text{G}}$ is obtained as

$$\lambda_{\text{op}}^{\text{G}} = \sqrt{\mu_0 \mu_1 \left[1 + \frac{1}{(\mu_1 - \mu_0)} \ln \left(\frac{p_0^2 \mu_1}{p_1^2 \mu_0} \right) \right]}. \quad (3.32)$$

where μ_0 and μ_1 are respectively defined in (3.10) and (3.11) by substituting E_r from part (I) for an active receiver. Note that, $\sigma_i^2 = \mu_i$ for $i = \{0, 1\}$ is considered in deriving (3.32).

Section 3.2.1 and Section 3.2.2 can be extended to the active receiver by adopting part (I) and (II) for Gaussian and Gaussian mixture modeling.

3.4 Performance Evaluation

In this section, the performance of the diffusion-based MC system based on bit error rate (BER) is evaluated by computer simulations and compared to theoretical analysis. In Section 3.4.1, the BER performance of the passive receiver is examined for Gaussian and Gaussian mixture modeling. The results of memory-less receiver are also compared with memory-based receiver. Furthermore, Section 3.4.2 considers

Table 3.1: System parameters used for numerical and simulation results

Parameters	Value
Viscosity of the fluid (η)	$0.001 \frac{\text{kg}}{\text{s m}}$
Temperature	310K
Radius of messenger molecules(r_m)	2.5 nm
Diffusion coefficient(D)	$79.4 \frac{\mu\text{m}^2}{\text{s}}$
Distance between transmitter and center of receiver (r_d)	$10 \mu\text{m}$
Passive receiver radius (ρ_p)	$1 \mu\text{m}$
Active receiver radius (ρ_a)	$1 \mu\text{m}$

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the proposed detection algorithm for an active receiver. Theoretical analysis of BER along with simulation results are presented and investigated under different scenarios for active memory-less and memory-based receivers.

3.4.1 Passive Receiver Performance Evaluation

To evaluate the performance of the passive receiver, a series of parameters are defined to characterize the physical channel of the MC system according to OOK modulation. It is assumed that the diffusion medium is a homogeneous water-based environment with parameters listed in Table 3.1. The diffusion coefficient is set to $D = 79.4 \frac{\mu\text{m}^2}{\text{s}}$ for insulin messenger molecules [87]. The distance between the transmitter and the center of the receiver is $r_d = 10\mu\text{m}$; with a receiver radius set to $\rho_p = 1\mu\text{m}$. Note that, r_d is selected large enough compared to ρ_p for achieving uniform concentration inside the receiver volume. Furthermore, results are given for $\alpha_0 = 0.4$ which indicates that 40% of the energy (in this case concentration) is received in $t \in (0, T_s)$. In addition, from [34] T_s is determined as follows

$$\int_0^{T_s} h_p(t)dt = \alpha \frac{M}{4\pi D r_d} \quad \longrightarrow \quad T_s = \frac{r_d^2}{4D \operatorname{erfc}^{-1}(\alpha_0)^2}, \quad (3.33)$$

where erfc^{-1} is the inverse complementary error function. According to the selected parameters, the symbol duration, for this system is $T_s = 0.9$ s. Thus, the transmission rate becomes $R_s = \frac{1}{T_s} = 1.11 \frac{\text{symbol}}{\text{s}}$, which is decreased by increasing the distance between the transmitter and receiver.

The precision and accuracy of Gaussian mixture modeling compared to Gaussian are investigated by adopting Monte Carlo simulations. The BER performance of the

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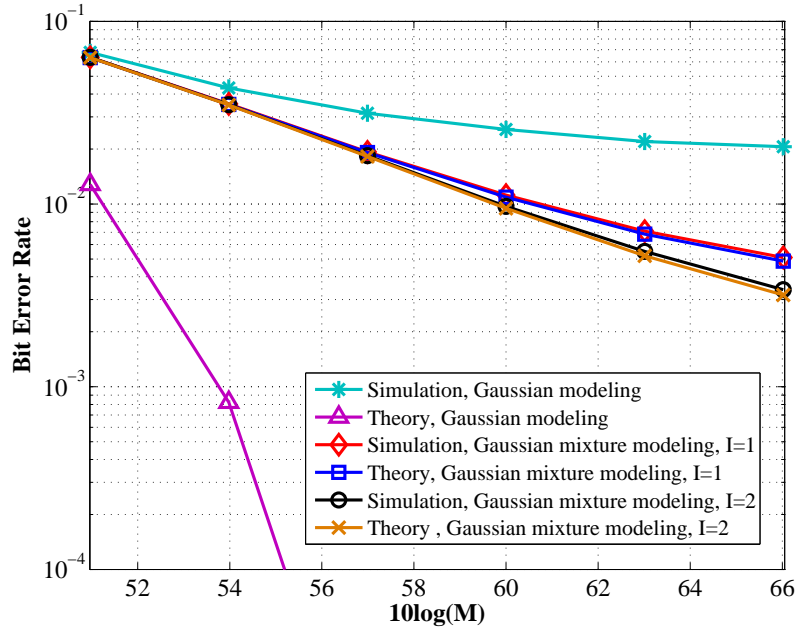


Figure 3.5: Comparison among simulation and theory results of (i) Gaussian and (ii) Gaussian mixture models (when $I = 1$, $I = 2$) for a passive memory-less receiver.

optimum receiver is evaluated with respect to $10 \log M$ for both memory-less and memory-based receiver when $p_1 = p_0 = 0.5$.

Fig. 3.5 illustrates the BER performance of the diffusion-based MC system when both Gaussian and Gaussian mixture models are considered in memory-less receiver. Comparing Gaussian mixture modeling for $I = 1$ and $I = 2$ indicates that simulation results follow the outcomes of the developed theory very closely. Therefore, one can conclude that $f(y_m|d_m)$ follows Gaussian mixture distribution when a sequence of molecular signals are emitted in diffusion-based MC systems. Moreover, in Fig. 3.5 the BER drops as I is increased especially for large values of M . Clearly, the precision of the Gaussian mixture modeling enhances as more previously transmitted symbols are considered. Note that, the theoretical performances showed in Fig. 3.5 (and also

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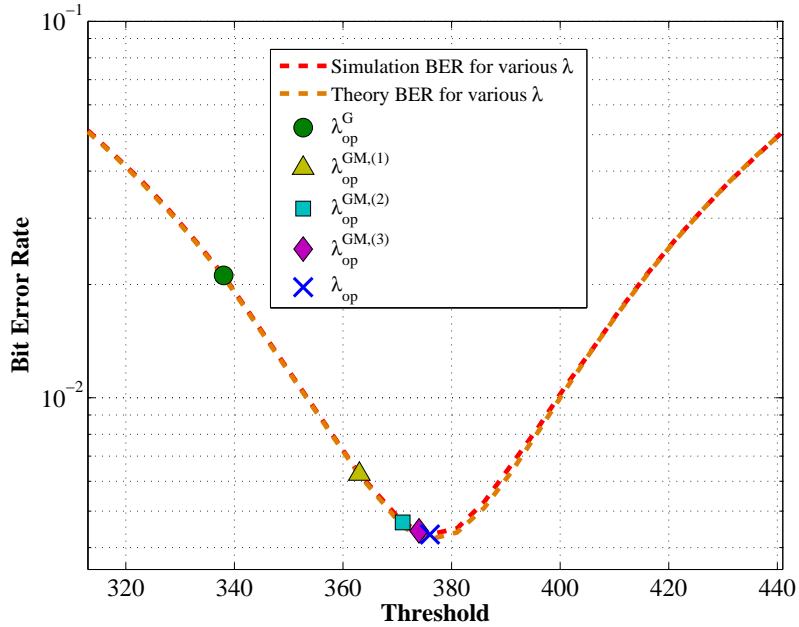


Figure 3.6: Simulation and theoretical results of a passive memory-less receiver for different values of threshold by setting $10 \log M = 63$.

in the following figures) are obtained when the precise error probability (P_e in (3.25)) is expressed by I^* previously transmitted symbols such that $\sum_{i=0}^{I^*} \alpha_i > 0.9$.

Fig. 3.6 depicts the system performance based on simulation and theoretical results for various values of threshold. Selecting $10 \log M = 63$, Fig. 3.6 shows that the proposed detected algorithm determines the optimum threshold which here is achieved for $I > 3$. Note that, for small values of released molecules the optimum threshold is achieved when few transmitted symbols are considered in decision making. Fig. 3.6 designates that Gaussian mixture distribution is an acceptable model for obtaining threshold value in diffusion-based MC system.

Fig. 3.7 compares the system behavior of the (i) memory-less, (ii) one-memory and (iii) two-memory-based receivers. The simulation and theoretical analysis are

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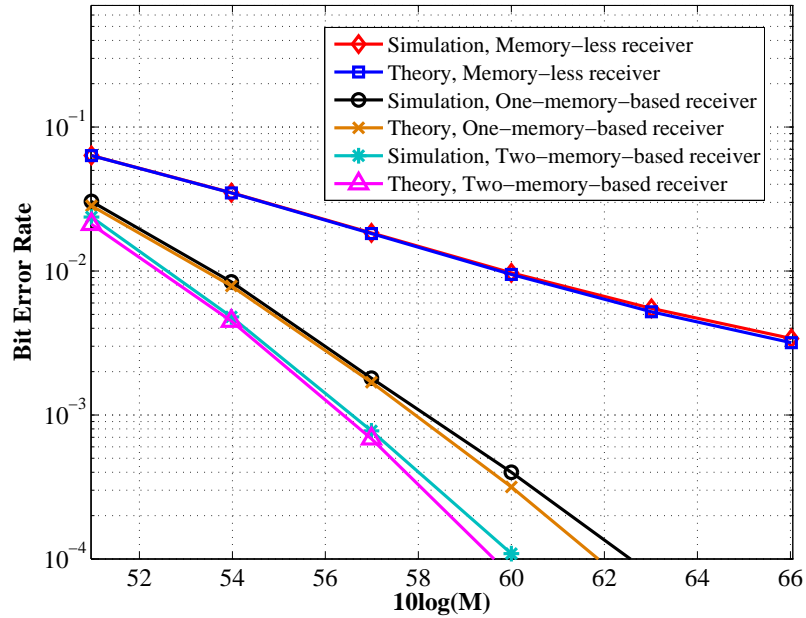


Figure 3.7: The BER performance of the Gaussian mixture modeling when $I = 2$ for passive (i) memory-less, (ii) one-memory and (iii) two-memory-based receivers.

evaluated based on Gaussian mixture modeling by setting $I = 2$. Note that, according to Fig. 3.7 system performance significantly improves as the receiver's memory is increased; especially for one-memory-based receiver (compared to memory-less). This is due to eliminating a major part of the ISI by considering previous detected symbols in obtaining the threshold value. Furthermore, the results confirm that theory indicates a lower bound of BER compared to simulation for one and two-memory-based receivers. This is due to assuming previous detection's are correct in theoretical analysis for memory-based receivers. In other words in Fig. 3.7, the gap between simulation and theory increases when more previous detected symbols are considered at the receiver.

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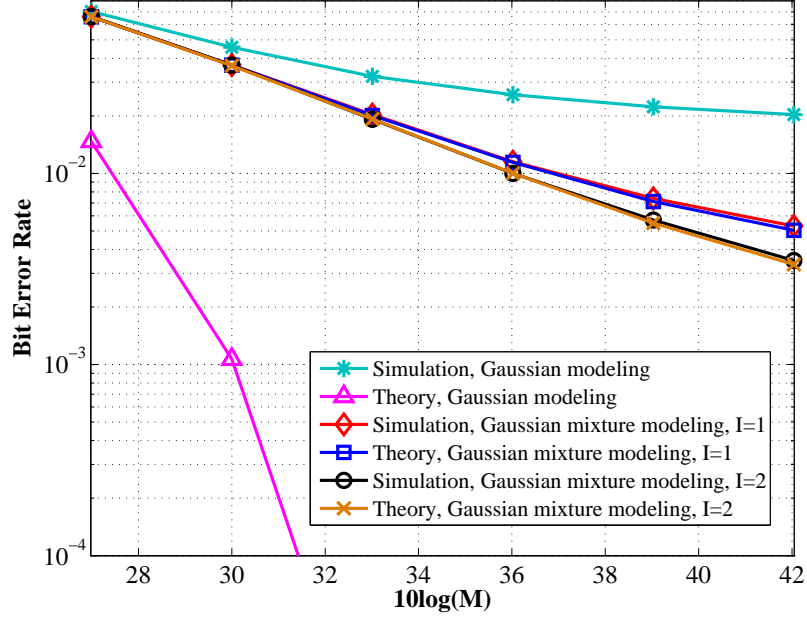


Figure 3.8: Comparison among simulation and theory results of (i) Gaussian and (ii) Gaussian mixture models (when $I = 1$, $I = 2$) for an active memory-less receiver.

3.4.2 Active Receiver Performance Evaluation

In this section, the BER performance of the proposed detection algorithm is evaluated for an active (absorbing) receiver based on Gaussian mixture modeling. For computer simulations, parameters are given presented in Table 3.1; where the radius is selected as $\rho_a = 1 \mu\text{m}$. Similarly, for setting $\alpha_0 = 0.4$, T_s is derived as follows

$$T_s = \frac{(r_d - \rho_a)^2}{4D \operatorname{erfc}^{-1}(\alpha_0)^2}, \quad (3.34)$$

where based on the selected parameters, $T_s = 1.4 \text{ s}$. Note that, the rest of the parameters are chosen equivalently to Section 3.4.1.

Fig. 3.8 compares the Gaussian and Gaussian mixture results of a memory-less

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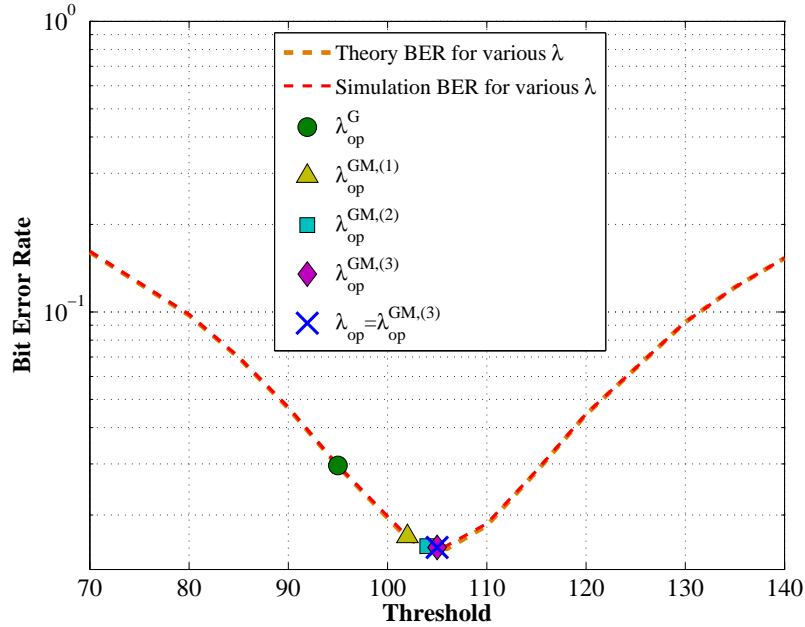


Figure 3.9: Simulation and theory results of an active memory-less receiver for different values of threshold by setting $10 \log M = 34$.

receiver with an absorbing surface. Theoretical and simulation results match very well based on Gaussian mixture for $I = 1$ and $I = 2$; despite Gaussian modeling. Hence, the results indicate that the Gaussian mixture is an acceptable model for $f(y_m|d_m)$ also for an active receiver design. According to Fig. 3.8, the BER performance enhances as more previously transmitted symbols are considered at the receiver. Fig. 3.9 shows the BER performance of the MC system for various threshold values with a memory-less receiver. The minimum of the error probability occurs for $I = 3$ by selecting $10 \log M = 34$ when the receiver is assumed active. Compared to Fig. 3.6, similar results are accomplished in Fig. 3.9 for an active receiver by emitting fewer number of molecules.

Fig. 3.10 shows the performances of (i) memory-less, (ii) one-memory and (iii) two-memory-based receivers based on Gaussian mixture modeling with $I = 2$. Fig. 3.10

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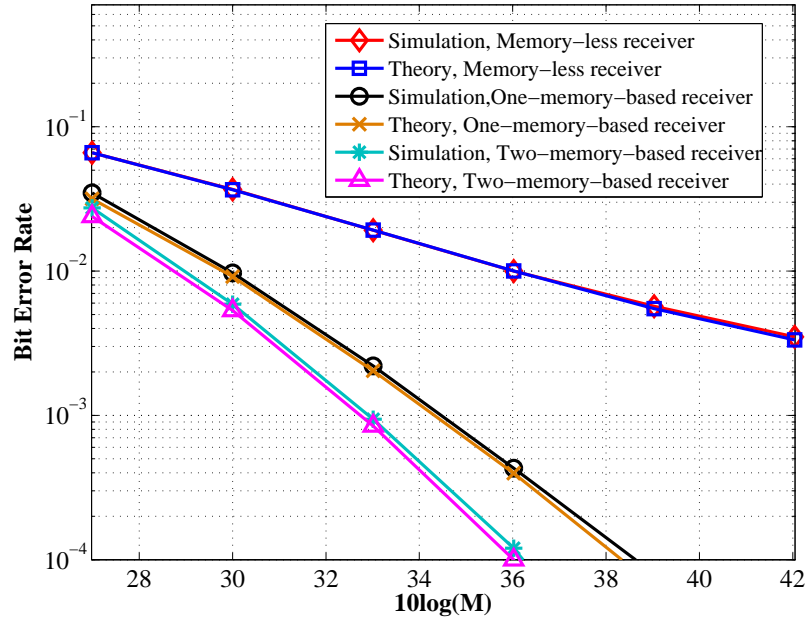


Figure 3.10: The BER performance of the Gaussian mixture modeling when $I = 2$ for active (i) memory-less, (ii) one-memory and (iii) two-memory-based receivers.

indicates that saving detected symbols at the receiver decreases the ISI effect, concluding improvement in system performance. Furthermore, by increasing the memory of the receiver, Fig. 3.10 confirms that theoretical analysis determines a lower bound for the BER performance. Note that, the BER performance of the active receiver based on Gaussian mixture modeling for both memory-less and memory-based receivers are identical to the results given for a passive receiver. However, for a limited source of messenger molecules an active receiver is more notable for designing MC systems [1, 4].

Chapter 4

Molecular Code Division Multiple Access (MCDMA)

In MC nano-networks, multiple nano-devices are required to communicate in a shared fluidic environment. The main purpose is to provide communication links with high reliability among active users. Since the communication environment is shared among multiple nodes, inter-user interference (IUI) arises and challenges the detection of information. Therefore, it is essential to cancel or to reduce the impact of IUI in multi-user diffusion-based MC systems.

Few research have investigated the effect of IUI in multi-user MC systems [26, 35, 36, 49, 78]; where in all transmitters are considered to send data synchronously. In [26, 78], wave theory is employed to derive a closed form expression for IUI for both CSK and MoSK modulation schemes. In [35], MIMO techniques are explored to improve system performance. In [49], a decision threshold is computed when the effect of one previous transmission is considered when two transmitters are communicating synchronously with a single receiver. Moreover, in [36] enzymes are adopted to diminish the interfering molecules causing IUI and ISI.

In this chapter, a MC system using molecular code division multiple access (MCDMA) is proposed as an approach that operates in the presence of IUI. The users are asynchronous with each other in the MCDMA system and a signature/code sequence selected from a set of molecular codes is assigned to each of them. This code set is similar to optical codes [90], and is selected such that the auto-correlation and

4.1. MCDMA SYSTEM MODEL

cross-correlation of the codes are bounded by small specific values.

Moreover, a chip detection scheme similar to that discussed in chapter 3 is proposed for the MCDMA system. Gaussian mixture modeling is applied in determining an optimal threshold by considering previously transmitted chips when multiple nodes are communication. Though the system encounters high levels of IUI, the proposed modeling method efficiently restores the data sent from each user by minimizing the effect of the IUI, ISI and noise. It is also shown that the performance of the proposed MCDMA system is improved as the memory length is increased in the chip detection method at the receiver.

The remainder of this chapter is organized as follows: Section 4.1 presents the diffusion-based MCDMA model. In Section 4.2 a simple passive receiver design is developed based on chip detection scheme. Gaussian and Gaussian mixture modeling in the presence of IUI is studied in Section 4.2.1 and Section 4.2.2, respectively. The performance of the MCDMA system for different scenarios based on Gaussian and Gaussian mixture method are evaluated by computer simulations in Section 4.3.

4.1 MCDMA System Model

The diffusion-based MC system consisting of multiple transmitters and multiple receivers is illustrated in Fig. 4.1 when OOK modulation is adopted for particle transmission. Once a receiver synchronizes itself with its own transmitter, while it is asynchronous with other transmitters; information is decoded according to the molecular concentration present within the receiver volume. Since multiple users communicate in the same medium, inter-user interference (IUI) is inevitable. To reduce the IUI effect, for the first time molecular code division multiple access (MCDMA) scheme

4.1. MCDMA SYSTEM MODEL

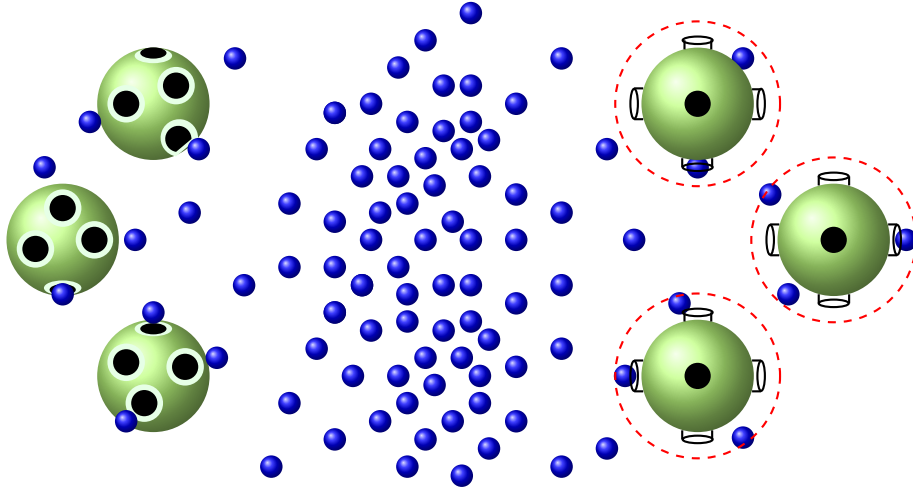


Figure 4.1: Multi-user diffusion-based MC system

is proposed in this thesis that allows several users to transmit information asynchronously. Each user is assigned to a molecular based code sequence (analogous to optical codes [90]), that are designed to overcome the asynchronous IUI. These codes patterns are a set of binary sequences that are quasi-orthogonal; in other words they are designed to have good auto-correlation and cross-correlation. Since molecules are used in this coding scheme, they are referred to as molecular codes. The most significant aspect of MCDMA is allowing users to communicate asynchronously, thus making it a considerable solution for nano-communication systems.

Fig. 4.2 shows the block diagram of the transmitter structure for the MCDMA system. Without loss of generality, here it is assumed that K number of users (transmitters) are active, which they are all communicating with the same receiver. According to Fig. 4.2, the input signal to the k th channel, denoted by $s_k(t)$, is expressed as follows,

$$s_k(t) = \sum_{i=0}^{\infty} \sum_{l=1}^L d_{ik} c_{lk} \delta(t - lT_c - iT_s - \tau_k), \quad (4.1)$$

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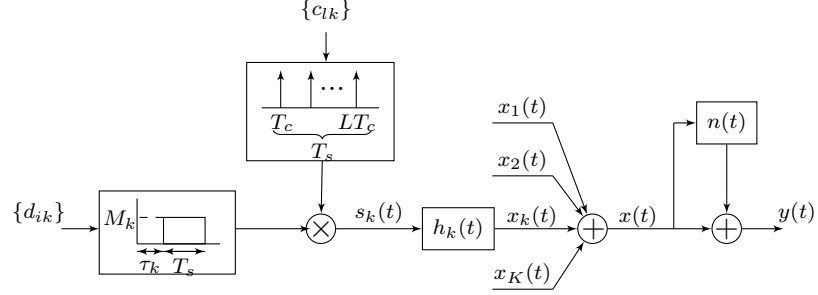


Figure 4.2: Block diagram of the MCDMA transmitter structure.

where T_s and T_c are the symbol and the chip duration, respectively. In (4.1), τ_k is the delay time of the k th transmitter, since the transmitters are asynchronous. Note that, τ_k is a random variable that follows a uniform distribution such that $\tau_k \in (0, T_s)$. Furthermore, $\{d_{ik}\}_{i=0}^{\infty}$ and $\{c_{lk}\}_{l=1}^L$ are respectively the k th symbol stream and code signature. Due to using OOK modulation, $d_{ik} \in \{0, 1\}$. The code sequences defined in (4.1) are selected from a code set $C_k = (c_{1k} \ c_{2k} \ \dots \ c_{Lk})$ where $c_{lk} \in \{0, 1\}$. In MCDMA, the k th transmitter sends its specific code sequence, C_k , to represent data “1” and sends nothing to represent data “0”. The code set is specified by $(L, w, \lambda_a, \lambda_c)$; where L indicates the code length and $w = \sum_{l=1}^L c_{lk}$ is the code weight. Here λ_a and λ_c are respectively the maximum value for the auto-correlation and cross-correlation of the code set which are defined as,

$$\begin{aligned} \sum_{l=1}^L c_{lk} c_{l \oplus l', k} &\leq \lambda_a, \\ \sum_{l=1}^L c_{lk} c_{l \oplus l', k'} &\leq \lambda_c, \quad k \neq k'. \end{aligned} \tag{4.2}$$

where $l' \in \{\mathbb{N} | l' \neq 0 \pmod{L}\}$ and \oplus indicates the mod L addition operator [91].

4.2. CHIP DETECTION BASED RECEIVER

In Fig. 4.2, the expected response of the channel to the k th transmitter is expressed as,

$$x_k(t) = \sum_{i=0}^{\infty} \sum_{l=1}^L d_{ik} c_{lk} h_k(t - lT_c - iT_s - \tau_k). \quad (4.3)$$

where $h_k(t)$ is the expected impulse response of the k th diffusion channel. Therefore, the total received signal- comprised from the summation of the received signals from K active users- becomes,

$$\begin{aligned} y(t) &= \sum_{k=1}^K x_k(t) + n_k(t) \\ &= \sum_{k=1}^K \sum_{i=0}^{\infty} \sum_{l=1}^L d_{ik} c_{lk} h_k(t - lT_c - iT_s - \tau_k) + n(t), \end{aligned} \quad (4.4)$$

where $n(t) = \sum_{k=1}^K n_k(t)$ is the total additive noise process generated from the K active users communicating asynchronously. Note that, this noise is a random process approximated with Gaussian increments dependent to the average of the received signal as investigated in chapter 2.

In the following, section 4.2 presents a chip detection scheme for a passive receiver based on Gaussian and Gaussian mixture modeling. The process of chip detection derived in the following is similarly employed for an active receiver. Thus, in order to avoid repetition only passive receiver is considered in this chapter.

4.2 Chip Detection based Receiver

In this section a passive receiver similar to the design described in chapter 3 is considered that functions based on chip detection method. Fig. 4.3 depicts the structure of the receiver model which basically measures the molecular concentration present

4.2. CHIP DETECTION BASED RECEIVER

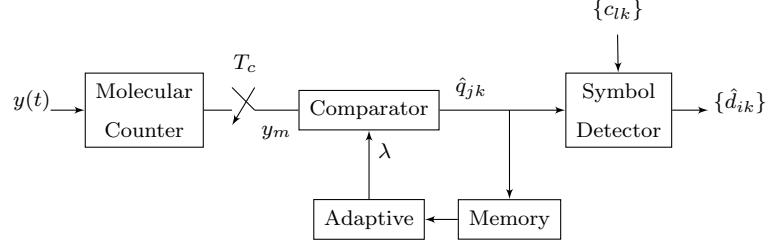


Figure 4.3: MCDMA receiver structure with a memory-based detector.

within the reception space. Since here the receiver is considered passive, according to (2.6) the impulse response of the k th channel is defined as

$$h_k(t) = \frac{M_k}{\sqrt{(4\pi Dt)^3}} \exp\left(-\frac{r_k^2}{4Dt}\right), \quad (4.5)$$

where r_k is the Euclidean distance from the k th transmitter to the center of the receiver. Here, for simplicity r_k and $h_k(t)$ are used instead of the notations r_{d_k} and $h_{p_k}(t)$, respectively. In (4.5), M_k is the number of molecules released abruptly by the k th transmitter at time instants of T_c to denote chip 1. Furthermore, equation (4.4) can be rewritten as

$$y(t) = \sum_{k=1}^K \sum_{j=0}^{\infty} q_{jk} h_k(t - jT_c - \tau_k) + n(t). \quad (4.6)$$

where q_{jk} is the chip regarding the k th transmitter which is defined as $q_{jk} = d_{ik} c_{lk}$ such that $j = iL + l$.

Since the main goal is to detect q_{jk} ; the receiver synchronizes itself with the transmitter whose chips are going to be detected. Note that, due to $\lambda_a < w$, the procedure of synchronization is straightforward. Without loss of generality, it can be assumed that the receiver is detecting the chips of the first user ($k = 1$); thus, $\tau_1 = 0$.

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Moreover for $t \leq (m + 1)T_c$ where m is the time index; $y(t)$ can be expressed as,

$$\begin{aligned}
 y(t) = & q_{m1}h_1(t - mT_c) + \sum_{j=0}^{m-1} q_{j1}h_1(t - jT_c) \\
 & + \sum_{k=2}^K \sum_{j=0}^m q_{jk}h_k(t - jT_c - \tau_k) + n_m(t),
 \end{aligned} \tag{4.7}$$

where the first terms refers to the desired signal, and the second and third are ISI and IUI elements, respectively. In (4.7), $n_m(t)$ is the added noise component of the received signal. According to Fig. 4.3, the molecular counter measures the total received concentration at time within each m th time duration, denoted by y_m , is determined as follows

$$\begin{aligned}
 y_m = \int_{mT_c}^{(m+1)T_c} y(t)dt = & \underbrace{E_1 q_{m1} \alpha_0^{(1)}}_{s_m} + \underbrace{E_1 \sum_{j=0}^{m-1} q_{j1} \alpha_{m-j}^{(1)}}_{I_{m\text{ISI}}} + \underbrace{\sum_{k=2}^K E_k \sum_{j=0}^m q_{jk} \alpha_{m-j}^{(k)}}_{I_{m\text{IUI}}} + \underbrace{\int_{mT_c}^{(m+1)T_c} n_m(t)}_{n_m}
 \end{aligned} \tag{4.8}$$

where s_m , $I_{m\text{ISI}}$, $I_{m\text{IUI}}$ and n_m are respectively the total desired signal, ISI, IUI and noise observed within the m th time interval. In (4.8), E_k is the energy of the expected k th impulse response for a passive receiver. Similar to (3.8) in chapter 3, E_k is expressed as,

$$E_k = \frac{M_k}{4\pi D r_k}, \tag{4.9}$$

Moreover, $\alpha_i^{(k)}$ in (4.8) refers to a fraction of E_k that has reached the receiver in time duration $t \in (iT_c - \tau_k, (i + 1)T_c - \tau_k)$; which is defined as follows

$$\alpha_i^{(k)} = \frac{1}{E_k} \int_{iT_c - \tau_k}^{(i+1)T_c - \tau_k} h_k(t)dt, \tag{4.10}$$

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where $0 \leq \alpha_i^{(k)} \leq 1$ and $\sum_{i=0}^{\infty} \alpha_i = 1$. In (4.10), since τ_k follows a uniform distribution, $\alpha_i^{(k)}$ is also a random variable.

For chip detection, the receiver employs MAP criterion to distinguish the transmitted chips $\{q_{m1}\}$ by maximizing the conditional pdf, $f(q_{m1}|y_m)$. In this regard, the following test is performed,

$$P\{q_{m1} = 1\}f(y_m|q_{m1} = 1) \underset{\hat{q}_{m1}=1}{\overset{\hat{q}_{m1}=0}{>}} P\{q_{m1} = 0\}f(y_m|q_{m1} = 0), \quad (4.11)$$

where \hat{q}_{m1} is the detected chip. To detect \hat{q}_{m1} , $f(y_m|q_{m1})$ is approximately modeled as Gaussian distribution for simplicity. By referring to the central limit theorem [89], some literature [26, 35, 36, 49, 78] have considered Gaussian distribution in modeling $f(y_m|q_{m1})$ under the assumption that the ISI and IUI for all users are independent from each other. Though, chapter 3 showed that Gaussian mixture distribution is an acceptable model for the received molecules, when the system experiences high levels of ISI. In addition, Gaussian and Gaussian mixture modeling are investigated in Section 4.2.1 and Section 4.2.2 to compare system performance based on the MCDMA technique. Furthermore, memory-less and memory-based receiver are assumed to obtain an optimal threshold value for both modeling schemes.

4.2.1 Gaussian Modeling for MCDMA System

In this subsection, all previous transmissions are approximated as a single Gaussian distribution for modeling y_m . By considering the receiver memory-less (no knowledge

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on previous detected chips), the two hypotheses H_0 and H_1 are made as follows,

$$\begin{aligned} H_0 : \quad f(y_m | q_{m1} = 0) &\sim \mathcal{N}(\mu_0, \sigma_0^2), \\ H_1 : \quad f(y_m | q_{m1} = 1) &\sim \mathcal{N}(\mu_1, \sigma_1^2), \end{aligned} \quad (4.12)$$

where the mean values, μ_0 and μ_1 are obtained as

$$\mu_0 = \mathbb{E} [y_m | q_{m1} = 0] = \bar{I}_{m\text{ISI}} + \bar{I}_{m\text{IUI}}, \quad (4.13)$$

$$\mu_1 = \mathbb{E} [y_m | q_{m1} = 1] = E_1 \alpha_0^{(1)} + \mu_0. \quad (4.14)$$

Here, $\bar{I}_{m\text{ISI}}$ and $\bar{I}_{m\text{IUI}}$ are the expectation of the ISI and IUI, respectively. In (4.12), for a passive receiver, σ_0^2 and σ_1^2 are defined as $\sigma_i^2 = \frac{\mu_i}{V_R}$ for $i = 0, 1$, according to (2.19) given in chapter 2. In addition, the MAP rule for chip detection can be simplified to

$$\hat{q}_{m1} = \begin{cases} 1, & y_m \geq \lambda, \\ 0, & y_m < \lambda. \end{cases} \quad (4.15)$$

where λ denotes the threshold value. The intention is to obtain an optimal threshold value that improves system performance of the MCDMA system. A convenient approach is to minimize the probability of error with respect to λ . In this regard, the probability of error, denoted by P_e , is expressed as,

$$P_e = p_0 Q \left(\frac{\lambda - \mu_0}{\sigma_0} \right) + p_1 \left[1 - Q \left(\frac{\lambda - \mu_1}{\sigma_1} \right) \right], \quad (4.16)$$

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where p_0 and p_1 are the probability of sending chip “0” and chip “1”, respectively. By solving $\frac{\partial P_e}{\partial \lambda} = 0$ for $\lambda \geq 0$; the optimal threshold is derived as follows,

$$\lambda_{op}^G = \sqrt{\mu_0 \mu_1 \left[1 + \frac{1}{V_R(\mu_1 - \mu_0)} \ln \left(\frac{p_0^2 \mu_1}{p_1^2 \mu_0} \right) \right]}. \quad (4.17)$$

where λ_{op}^G is denoted as the optimal threshold based on Gaussian modeling. Note that, the threshold must be a positive value since it illustrates the molecular concentration. From (4.12) and (4.17), it is clear that λ_{op}^G depends on $\bar{I}_{m\text{ISI}}$; which relates to previously detected chips. For a memory-less receiver, μ_0 is derived as follows

$$\mu_0 = p_1 E_1 (1 - \alpha_0^{(1)}) + \bar{I}_{m\text{ISI}}. \quad (4.18)$$

where the first term represents the expectation of ISI. Take into account that $\{q_{jk}\}_{j=0}^{\infty}$ for all $k = 1, \dots, K$ is presumed to have independent and identical distributions (iid) such that $p_1 = P\{q_{jk} = 1\}$, for all j and k . Since μ_1 is achieved from μ_0 according to (4.14); hence, the optimal threshold is independent of previously detected chips when the receiver is memory-less. However, for the case where the receiver is memory-based, l' previously detected chips (\hat{q}_{j1} for $j = m - l', \dots, m - 1$) are employed in the decision making process. In this regard, $2^{l'}$ number of optimum threshold levels are computed from (4.17), according to the following mean values,

$$\begin{aligned} \mu_n = & E_1 q_{m1} \alpha_0^{(1)} + E_1 \sum_{j=m-l'}^{m-1} \hat{q}_{j1} \alpha_{m-j}^{(1)} \\ & + p_1 E_1 \left(1 - \sum_{l=0}^{l'} \alpha_l^{(1)} \right) + \bar{I}_{m\text{IUI}}, \end{aligned} \quad (4.19)$$

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where $n = \sum_{j=0}^{l'} q_{m-j,1} 2^{l'-j}$ corresponds to the binary representation of $\{q_{j1}\}_{j=m}^{m-l'} = (q_{m1}, \dots, q_{(m-l')1})$ such that $n = 0, 1, \dots, 2^{l'+1} - 1$. Note that at each detecting symbol, by substituting $q_{j1} = \hat{q}_{j1}$ for $j = m-1, \dots, m-l'$, n can be obtained when $q_{m1} = 0$ and 1. Furthermore, the mean values given in (4.18) and (4.19) are dependent on $\bar{I}_{m\text{IUI}}$; which is expressed as

$$\bar{I}_{m\text{IUI}} = \mathbb{E} \left[\sum_{k=2}^K E_k \sum_{j=0}^{m-1} q_{j1} \alpha_{m-j}^{(k)} \right] = p_1 \sum_{k=2}^K E_k \sum_{j=0}^m \mathbb{E} \left[\alpha_{m-j}^{(k)} \right]. \quad (4.20)$$

Note that $\bar{I}_{m\text{IUI}}$ is not straightforward to evaluate; since $\alpha_{m-j}^{(k)}$ is random for each user due to τ_k , according to (4.10). Considering the definitions in (4.10) and (4.5); with some manipulations $\mathbb{E} \left[\alpha_i^{(k)} \right]$ is given as follows

$$\begin{aligned} \mathbb{E} \left[\alpha_i^{(k)} \right] &= \mathbb{E} \left[\frac{1}{E_k} \int_{iT_c - \tau_k}^{(i+1)T_c - \tau_k} \frac{M_k}{\sqrt{(4\pi Dt)^3}} \exp\left(-\frac{r_k^2}{4Dt}\right) dt \right] \\ &= \mathbb{E} \left[\operatorname{erfc} \left(\frac{r_k}{\sqrt{4((i+1)T_c - \tau_k)D}} \right) \right] - \mathbb{E} \left[\operatorname{erfc} \left(\frac{r_k}{\sqrt{4(iT_c - \tau_k)D}} \right) \right]. \end{aligned} \quad (4.21)$$

To determine the first and second term given in (4.21), the random element should be considered. Since τ_k is denoted to follow a uniform distribution, the pdf becomes

$$f(\tau_k) = \begin{cases} \frac{1}{T_s}, & 0 \leq \tau_k \leq T_s, \\ 0, & \text{otherwise.} \end{cases} \quad (4.22)$$

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In this regard, the first term in (4.21) is calculated as

$$\begin{aligned} \mathbb{E} \left[\operatorname{erfc} \left(\frac{r_k}{\sqrt{4((i+1)T_c - \tau_k)D}} \right) \right] &= \frac{1}{T_s} \int_0^{T_s} \operatorname{erfc} \left(\frac{r_k}{\sqrt{4((i+1)T_c - \tau_k)D}} \right) d\tau_k \\ &= \frac{r_k^2}{2DT_s} \int_{x_1}^{x_2} \frac{\operatorname{erfc}(x)}{x^3} dx \end{aligned} \quad (4.23)$$

where $x_1 = \frac{r_k}{\sqrt{4((i+1)T_c)D}}$ and $x_2 = \frac{r_k}{\sqrt{4((i+1)T_c - T_s)D}}$. In order to obtain the above expression, the following integrals are adopted

$$\int \operatorname{erfc}(ax)x^{-n} dx = -\frac{\operatorname{erfc}(ax)}{(n-1)x^{(n-1)}} - \frac{2a}{(n-1)\sqrt{\pi}} \int \frac{1}{x^{(n-1)}} \exp(-a^2x^2) dx \quad (n \geq 2) \quad (4.24)$$

$$\int \frac{1}{x^2} \exp(-x^2) dx = -\frac{\exp(-x^2)}{x} - \sqrt{\pi} \operatorname{erf}(x) \quad (4.25)$$

Thus, for this case since $n = 3$ and $a = 1$, the integral given in (4.23) becomes

$$\mathbb{E} \left[\operatorname{erfc} \left(\frac{r_k}{\sqrt{4((i+1)T_c - \tau_k)D}} \right) \right] = -\frac{r_k^2}{2T_s D} \left[\frac{\operatorname{erfc}(x)}{2x^2} - \frac{\exp(-x^2)}{\sqrt{(\pi)x}} - \operatorname{erf}(x) \right] \Bigg|_{x_1}^{x_2} \quad (4.26)$$

Similarly, the second term in (4.21) is determined as aforementioned. Therefore, the closed form expression for $\bar{I}_{m\text{IUI}}$ is derived as follows,

$$\bar{I}_{m\text{IUI}} = \frac{p_1}{2T_s D} \sum_{k=1}^K E_k r_k \sum_{j=0}^m \sum_{i=1}^4 (-1)^i \left[\frac{\operatorname{erfc} \left(\frac{r_k}{\sqrt{4F_i D}} \right)}{\frac{r_k^2}{2F_i D}} - \operatorname{erf} \left(\frac{r_k}{\sqrt{4F_i D}} \right) - \frac{\exp \left(-\frac{r_k^2}{4F_i D} \right)}{r_k \sqrt{\frac{\pi}{4F_i D}}} \right] \quad (4.27)$$

where $F_1 = (m-j)T_c$, $F_2 = F_1 - T_s$, $F_3 = F_4 - T_s$ and $F_4 = F_1 - T_c$. Depending on the type of receiver, the optimal detection based on Gaussian modeling is achieved by employing the derived ISI and IUI expressions.

4.2. CHIP DETECTION BASED RECEIVER

4.2.2 Gaussian Mixture Modeling for MCDMA System

Gaussian mixture distribution is considered in this section for modeling $f(y_m|q_{m1})$ when multiple active users are communicating asynchronously. As discussed in chapter 3, I previous transmissions which have the most influence on the received molecular concentration are applied to achieve the optimal threshold. In addition, the two hypothesis tests H_0 and H_1 for chip detection based on Gaussian mixture modeling are performed as

$$\begin{aligned} H_0 : f(y_m|q_{m1} = 0) &\sim \sum_{n=0}^{2^I-1} p_1^{O_n} p_0^{I-O_n} \mathcal{N}(\mu_n, \sigma_n^2), \\ H_1 : f(y_m|q_{m1} = 1) &\sim \sum_{n=2^I}^{2^{I+1}-1} p_1^{O_n} p_0^{I-O_n} \mathcal{N}(\mu_n, \sigma_n^2) \end{aligned} \quad (4.28)$$

where n is the decimal representation of $\{q_{i1}\}_{i=m-1}^{m-I}$ in binary digit. Here, O_n and $I - O_n$ denote the number of “1” and “0” chips corresponding to $\{q_{i1}\}_{i=m-1}^{m-I} = (q_{m1}, \dots, q_{(m-I)1})$, respectively. Note that, the receiver is assumed memory-less in the above test. The mean values, $\{\mu_n\}_{n=0}^{2^{I+1}-1}$ given in (4.28) are derived as follows

$$\mu_n = E_1 \sum_{j=0}^I q_{(m-j)1} \alpha_j^{(1)} + p_1 E_1 \left(1 - \sum_{j=0}^I \alpha_j^{(1)} \right) + \bar{I}_{m\text{IUI}} \quad \text{for } n = \{0, 1, \dots, 2^{I+1} - 1\} \quad (4.29)$$

where $\bar{I}_{m\text{IUI}}$ is defined in (4.27). Note that, the mean values evaluated for the MCDMA system in (4.29) are shifted by $\bar{I}_{m\text{IUI}}$ compared to (3.19). In general, the results concluded in chapter 3 in Section 3.2.1.2 for a memory-less receiver, including the detection algorithm can be applied for the MCDMA system by substituting the

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mean values defined in (4.29). Furthermore memory-based receiver has been thoroughly studied in Section 3.2.2.2 for Gaussian mixture. Hence, to avoid unnecessary repetition the same procedure is adopted for MCDMA by considering the IUI impact derived in (4.27).

After chip detection (either based on Gaussian or Gaussian mixture modeling), the symbol detector in Fig. 4.3 makes a decision on the transmitted symbol \hat{d}_{i1} . Since the the code pattern is known at the receiver, the following test is performed,

$$(\hat{q}_{iL+1,1}c_{11} + \hat{q}_{iL+2,1}c_{21} + \dots + \hat{q}_{iL+L,1}c_{L1}) \stackrel{\hat{d}_{i1}=0}{\neq} \stackrel{\hat{d}_{i1}=1}{=} w \quad (4.30)$$

where w and $C_1 = (c_{11} \ c_{21} \ \dots \ c_{L1})$ are the code weight and the code sequence of the first user, respectively. Note that, depending on which k th user the receiver is linked, the aforementioned test can be employed to detect d_{ik} of the k th users.

4.3 Performance Evaluation

Numerical and simulation results are presented in this section to investigate the performance of the MCDMA system based on the proposed chip detection method. Here the environmental parameters are selected as listed in Table (3.1) given in chapter 3. In the following, by adopting Monte Carlo simulation, the symbol error rate (SER) analysis of the MCDMA system is evaluated for various cases.

In the first case, $K = 2$ transmitters are considered active in the medium, that are located at the same distance $r_1 = r_2 = 10 \mu\text{m}$ from the center of the receiver. Here, the radius of the spherical receiver is configured as $\rho_p = 1 \mu\text{m}$. Results are configured

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by setting $\alpha_0^{(1)} = 0.5$ such that 50% of the energy is received in $t \in (0, T_c)$. Similar to (3.33), T_c is determined as follows

$$T_c = \frac{r_1^2}{4D \operatorname{erfc}^{-1}(\alpha_0^{(1)})^2}, \quad (4.31)$$

where according to the selected parameters, $T_c = 0.66$ s based on $k = 1$, since the information of the first transmitter is assumed to be detected. Also, each transmitter is presumed to release the same number of molecules, $M_1 = M_2 = M$. Here, the selected code set for $K = 2$ is characterized as $(5, 2, 1, 1)$ (with $L = 5$, $w = 2$, $\lambda_a = 1$ and $\lambda_c = 1$), where $C_1 = \{1, 1, 0, 0, 0\}$ and $C_2 = \{1, 0, 1, 0, 0\}$ are the code sequences for the first and second transmitter, respectively. Note that, in all cases the SER performance are given with respect to $10 \log M$. In this case, simulation results are averaged over different values of τ_2 , where they are randomly occurred.

In order to verify the impact of CDMA in MC systems, Fig. (4.4) shows the SER performance when the information is transmitted with and without coding. Here, results are compared for (i) memory-less, (ii) one-memory and (iii) two-memory-based receiver; where chip detection is employed by adopting Gaussian modeling. According to Fig. (4.4), the proposed code set with $L = 5$ is capable of reducing the IUI at the receiver when users are asynchronous. However, for the uncoded scenario when $\tau_2 \in (0, 5T_c)$, the results indicate that the SER performance is very poor regardless of the type of receiver (i.e. memory-less, ...). Thus compared to the uncoded case, it can be concluded that for asynchronous communication, MCDMA is a distinctive candidate that achieves high system performance. Furthermore, increasing receiver memory improves the SER performance significantly especially for one-memory-based receiver. Note that, based on the selected code set for two active users, $p_1 = 0.2$; while

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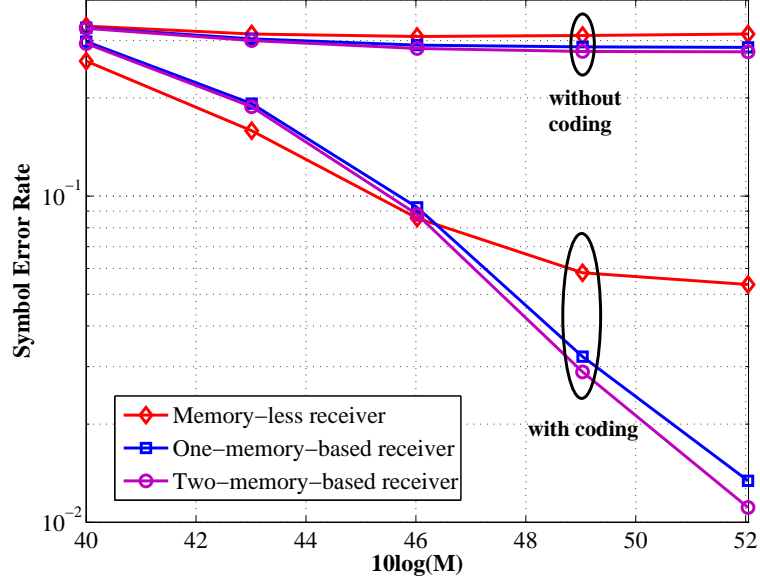


Figure 4.4: Symbol error rate performance of the chip detection method for (i) memory-less (ii) one-memory-based and (iii) two-memory-based receiver when information is sent with and without coding for $K = 2$ and $L = 5$.

for the uncoded scenario, $p_1 = 0.5$.

Moreover, MCDMA technique is evaluated when $K = 4$ transmitters are considered active and communicating asynchronously in the shared environment. Similarly, for $K = 4$ each transmitter is positioned at the same distance $r_k = 10\mu m$ (for $k = 1, \dots, 4$) from the center of the receiver, where all transmitters are required to emit equal number of molecules. The code sequences of $K = 4$ active users are selected from a $(10, 2, 1, 1)$ code set. These code signatures are given as $C_1 = \{1, 1, 0, 0, 0, 0, 0, 0, 0, 0\}$, $C_2 = \{1, 0, 1, 0, 0, 0, 0, 0, 0, 0\}$, $C_3 = \{1, 0, 0, 1, 0, 0, 0, 0, 0, 0\}$ and $C_4 = \{1, 0, 0, 0, 1, 0, 0, 0, 0, 0\}$. Furthermore, τ_k (for $k = \{2, 3, 4\}$) are selected randomly from $(0, 10T_c)$, where all possibility values have been considered for simulation analysis. Fig. 4.5 illustrates the performance of the MCDMA system based on

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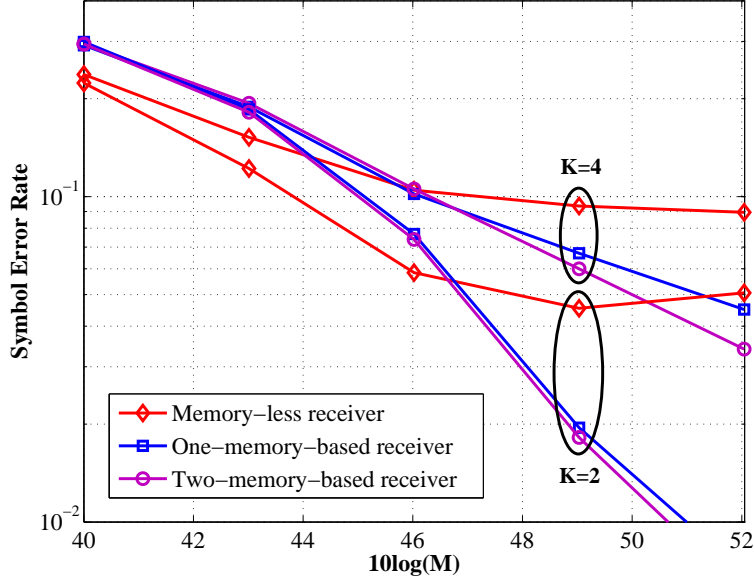


Figure 4.5: Symbol error rate performance of the MCDMA system when $K = 2$ and $K = 4$ transmitters are active for (i) memory-less (ii) one-memory-based and (iii) two-memory-based receiver by setting $L = 10$.

the proposed chip detection scheme for two scenarios: when (i) $K = 2$ and (ii) $K = 4$ transmitters are sending data asynchronously. For $K = 2$, C_1 and C_2 are used as the transmitted code pattern. According to the selected code set, the probability of sending chip “1” is $p_1 = 0.1$. As seen in Fig. 4.5, the IUI effect decreases as the number of released molecules is increased. Also, the system performance depends on the number of active users; which decreases for $K = 4$ compared to $K = 2$. Furthermore, comparing Fig. 4.4 and Fig. 4.5 concludes that the impact of inter-user interference reduces as the code length is increased.

Since the SER performance of the memory-less receiver is low for small values of M , the probability of error in one and two memory-based receiver increases for low values of M . This is due to the false detection of previous chips that causes error

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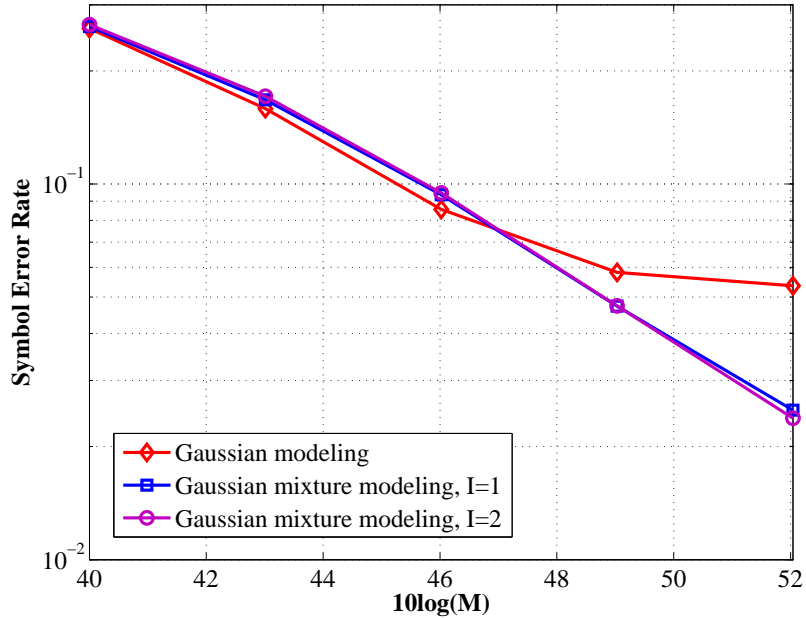


Figure 4.6: Simulation performance of the MCDMA system when (i) Gaussian and (ii) Gaussian mixture modeling (by setting $I = 1$, $I = 2$) are considered for a memory-less receiver with $K = 2$ and $L = 5$.

propagation. This phenomenon is vividly observed in Fig. 4.5 for $K = 2$. Section 4.2.2 investigated Gaussian mixture distribution for modeling the received number of molecules in MCDMA systems. In this part, simulation analysis is presented for a memory-less receiver when $K = 2$ users are active are with $L = 5$.

Fig. 4.6 depicts SER performance of the MCDMA system when Gaussian and Gaussian mixture modeling is employed. Comparing Gaussian and Gaussian mixture modeling for $I = 1$ and $I = 2$, indicates that for large values of M the SER is improved, particularly for $I = 1$. Since the graph for $I = 2$ follows $I = 1$ very closely; it can be concluded that by considering only one previously transmitted chip in threshold value is enough to obtain the optimal performance. Thus, according to Fig. 4.6 the proposed Gaussian mixture distribution is the acceptable model for the

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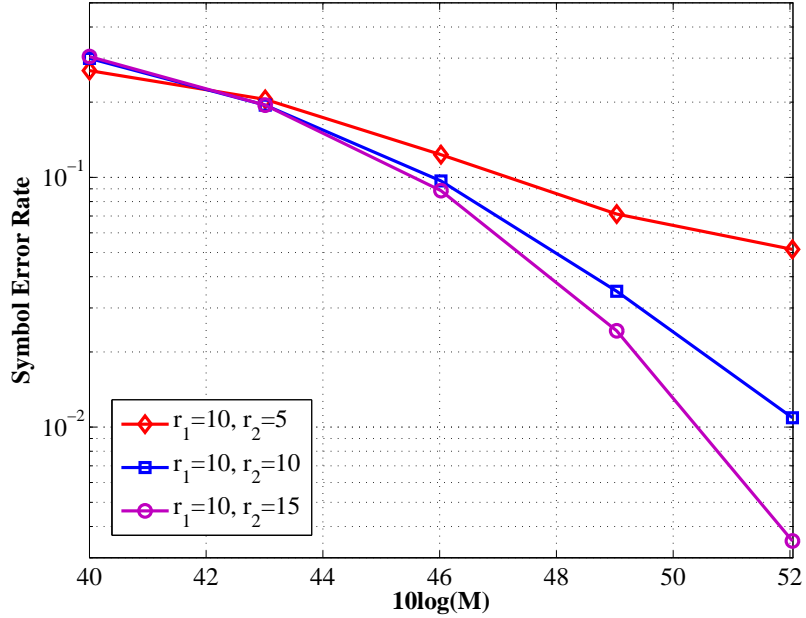


Figure 4.7: Symbol error rate performance of MCDMA system for $r_1 = 10 \mu\text{m}$, while (i) $r_2 = 5 \mu\text{m}$ (ii) $r_2 = 10 \mu\text{m}$ and (iii) $r_2 = 15 \mu\text{m}$ when $K = 2$. Simulation is performed for one-memory-based receiver according to Gaussian mixture modeling with $I = 2$ and $L = 5$.

received molecular signal in MCDMA system.

In the aforementioned scenarios the distance between transmitter and the receiver where considered the same for all users. Though this segment aims to examine the effect of IUI, when the interfering user is located at different locations from the center of the receiver. For $K = 2$ active users present within the fluidic medium, the three following cases are employed: (i) $r_1 = 10 \mu\text{m}$ and $r_2 = 5 \mu\text{m}$, (ii) $r_1 = 10 \mu\text{m}$ and $r_2 = 10 \mu\text{m}$, and also (iii) $r_1 = 10 \mu\text{m}$ and $r_2 = 15 \mu\text{m}$. Additionally, the transmitters are releasing the same number of molecules. Meanwhile, the receiver is synchronized with the first user to detect the transmitted information. The chosen code pattern here is $(5, 2, 1, 1)$, for $L = 5$ code length.

Fig. 4.7 shows the SER performance of the MCDMA systems for different values of

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r_2 . Chip detection is adopted for one-memory-based receiver, in which the threshold value is calculated according to Gaussian mixture modeling by setting $I = 2$. Clearly, results verify that as r_2 increases, the impact of IUI on the fixed user (first user) is significantly reduced. In other words, the best performance is achieved when $r_2 = 15 \mu\text{m}$ as seen in Fig. 4.7.

Chapter 5

Summary and Conclusions

This thesis presents molecular communication (MC) as a promising framework that enables nano-devices to interconnect via the emission, diffusion and the reception of molecules. Compared to traditional data transmission, (e.g, electromagnetic waves), MC is more bio-compatible and energy efficient in designing nano-scale devices for future health and environmental applications. Since conventional methods don't apply to nano-communication, the focus of this research is to propose novel channel modeling and detection techniques for single-user and multiple-user scenarios in diffusion-based MC system.

In this chapter, Section 5.1 provides a summary of the research achievements and Section 5.2 discusses potential future works.

5.1 Summary

The following paragraphs summarizes the accomplishments in each chapter of this thesis for designing an efficient diffusion-based MC network.

In chapter 2, the characteristics of the diffusion channel is modeled by Fick's diffusion law and Brownian motion. In this chapter it is shown that the expected impulse response of the diffusion channel is derived from solving Fick's second law. Meanwhile, the random nature in molecular movement is mathematically described as an additive noise. For an instant release of molecules (e.g. one shot transmission) the received molecular signal approximately follows Gaussian distribution when both

5.1. SUMMARY

passive and active receiver models are considered.

In chapter 3, Gaussian mixture distribution is proposed in modeling the received molecular signal. In Gaussian mixture model previous transmissions are considered in the decision making process when a stream of data is transmitted. Analytically, an iterative algorithm is developed to determine a threshold value that minimizes a linear approximation of the error probability, based on the Gaussian mixture model. For both passive and active receiver models, theory results of the Gaussian mixture followed simulation results very closely. Thus, indicating that Gaussian mixture distribution is a suitable model for the received number of molecules, compared to Gaussian modeling. Furthermore, a type of memory-based receiver for Gaussian mixture modeling is designed that significantly improves the bit error rate (BER) performance of the system by eliminating the inter-symbol interference (ISI).

In chapter 4, molecular code division multiple access (MCDMA) is proposed as a method for communication among nano-devices that share the same propagation environment. Molecular codes have been employed to overcome inter-user interference (IUI) when users are asynchronous such that each user transmits its signal without synchronizing with other users. A chip detection-based receiver is developed for both Gaussian and Gaussian mixture modeling, where an adaptable threshold is used to make decision between “1” (on) and “0” (off) hypotheses by counting the received molecules. Results showed that the optimal and adaptive threshold of the proposed multi-user molecular communication system is achieved when previous emissions are considered in decision process. Moreover, the symbol error rate (SER) performance of the MCDMA system has been evaluated for memory-less and memory-based receivers with a passive structure. Results indicate that MCDMA is a distinctive solution for

5.2. FUTURE WORK

asynchronous communications, which is capable of reducing the impact of the IUI based on the selected codes. In addition, simulation signified that the performance of the memory-based receiver has been improved when previously detected chips are considered in computing the threshold value.

The achievements of this thesis have been accepted in the International Conference on Communication (ICC 2016) and the Wireless Communication and Networking Conference (WCNC 2016), till now.

5.2 Future Work

This thesis aimed to provide basic methods for designing diffusion-based MC system; from channel modeling and receiver design for single-user case (e.g. Gaussian mixture modeling), to proposing MCDMA in overcoming the asynchronous IUI when multiple users are communicating in a shared environment. However, to implement nano-networks there still remains some issues that need to be addressed especially in multi-user scenario.

Though MCDMA offers various benefits like efficient asynchronous access and secure communication in diffusion-based MC systems, there are some limitations regarding the IUI effect. In the following, potential alternatives for improving the MCDMA system to mitigate the IUI under special cases are proposed.

- **Multi-Molecular Code Division Multiple Access (M-MCDMA)**

The code signature designed for MCDMA systems are a set of binary sequences that are quasi orthogonal, having good auto and cross-correlations. However, as the number of active users (K) or code weight (w) is increased, the length of the sequence (L) increases rapidly in order to gain high system performance.

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Increasing L limits the data rate and causes it to drop significantly.

A promising approach to increase the transmission rate when large number of users are communicating, is adopting various types of molecules in designing new code sequences. In this method which is referred to multi-molecular code division multiple access (M-MCDMA), each user transmits a code word with a specific kind of molecule. This technique is able to effectively decrease the IUI effect, without using long code patterns. Note that, to achieve good system performance in M-MCDMA the selected group of molecules are required to be orthogonal; in other words they don't combine with each other. Furthermore, it is assumed that the receiver is able to efficiently distinguish the received molecules for every type of them.

- **Multi-user Detection Techniques**

Detection techniques also play an important role in eliminating the IUI effect in the MCDMA system. In chapter 4, a basic correlator was adopted for symbol detection. Although this detector is simple to implement, the IUI decreases the performance; thus, the number of users should be limited in a nano-network. One of the promising approaches to enhance system performance of the MCDMA is employing multi-user detection techniques [92]. Specifically parallel interference cancellation (PIC) can be proposed as a solution when downlink or uplink scenarios are used. The concept of the PIC method is to extract the data of non-desired users and removing them from the received signal. Although this method faces computational complexities, it is capable of removing the IUI. Note that, even removing the IUI effect of one user (e.g. the nearby user) can have an extreme impact on system performance.

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- **Modulation Techniques**

This thesis only focused on On-Off keying (OOK) modulation technique. The proposed communication methods can be extended to other modulation techniques such as concentration shift keying (CSK), quadruple molecular shift keying (QMoSK) and pulse position modulation (PPM) [26].

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