EFFECTS OF ELECTROMAGNETIC FIELDS ON THE PERFORMANCE OF MOLECULAR COMMUNICATIONS

A Dissertation Submitted to
the Graduate School of Engineering and Sciences of
İzmir Institute of Technology
in Partial Fulfillment of the Requirements for the Degree of

DOCTOR OF PHILOSOPHY

in Electronics and Communication Engineering

by
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December 2022
İZMİR

ACKNOWLEDGMENTS

First and foremost, I am extremely grateful to my supervisor, Prof. Dr. Barış ATAKAN. His invaluable advice, continuous support, and patience encouraged me in my academic research. I would also like to express my sincere gratitude to Dr. Abdurrahman GÜMÜŞ and Dr. Erdal UZUNLAR for their kind help, support, and guidance during my Ph.D. study. I am also grateful to Prof. Dr. Cüneyt GÜZELİŞ and Assoc. Prof. Dr. Burhan GÜLBAHAR for sparing their valuable time and their valuable comments on my thesis.

I am grateful to my friends Ali KALAYCI, Fulya METE, Erdem OKUR, and Sibel OKAN for their precious support in every step of my academic and daily life.

I would also like to thank Assoc. Prof. Dr. Leyla ÇELEBİ GÜLSEREN. Without her tremendous understanding and encouragement over the past few years, it would be impossible for me to complete my study.

Last but not least, I am grateful for my mother. Her love and guidance made me the strong and independent woman I am today.

ABSTRACT

EFFECTS OF ELECTROMAGNETIC FIELDS ON THE PERFORMANCE OF MOLECULAR COMMUNICATIONS

This thesis analyzes molecular communication (MC) systems' performance under electromagnetic fields. The aim of the thesis is to model and study molecular behavior under electromagnetic fields (EMF).

The thesis starts with the theoretical explanation of classic electromagnetism. The directional and thermal changes are the main effects of EMF on particles. The directional effects of EMF are studied with regard to electromagnetic forces. The applied electromagnetic forces are presented for different types of particles. The effect of EMF on magnetically susceptible particles is analyzed in particular. Furthermore, molecular movement is analyzed by considering four fundamental forces on diffusing molecules under EMF. The energy transfer between EMF and particles is studied to understand the thermal effects of EMF.

An MC scheme that transmits information with magnetically susceptible molecules is studied in the second part of the thesis. The molecular type and the configuration of EMF are studied to understand the effect of EMF on the diffusion rate. The effects of magnetic field gradient (MFG) and concentration gradient magnetic force (CGMF) are analyzed to model the change in the diffusion rate and concentration of magnetically susceptible molecules.

The last part of the thesis focuses on molecular dynamics under EMF. The effect of thermal changes on the molecular reaction rate and binding kinetics is modeled with reaction-diffusion systems. The specific reaction rate constant is analyzed to determine the effect of temperature change caused by the EMF. The movement of molecules is modeled by Langevin's diffusion model. The probability distribution functions of the molecule's velocity and displacement are studied to understand and model the molecular behavior under EMF. Moreover, the mean-squared displacement is employed to analyze the diffusion type under EMF.

ÖZET

ELEKTROMANYETİK ALANLARIN MOLEKÜLER HABERLEŞME BAŞARIMINA ETKİSİ

Bu tez, elektromanyetik alan altında moleküler haberleşme (MH) sistemlerinin performansının analizine odaklanmaktadır. Bu tezin amacı, elektromanyetik (EM) alan altında moleküler davranışı modellemek ve incelemektir.

Tez, elektromanyetizmanın teorik açıklaması ile başlamaktadır. EM alanın parçacıklar üzerindeki ana etkileri hareket yönü ve termal değişiklikler olarak kabul edilir. EM alanın hareket yönüne etkisi EM kuvvetler açısından incelenmektedir. Uygulanan elektromanyetik kuvvetler farklı parçacık türleri için de anlatılmaktadır. EM alanın manyetik parçacıklar üzerindeki etkisi ayrıntılı olarak analiz edilmektedir. Ayrıca, moleküllerin EM alan altındaki hareketleri maruz kaldıkları dört temel kuvvet dikkate alınarak analiz edilmektedir. EM alanın termal etkilerini anlamak için EM alan ve parçacıklar arasındaki enerji transferi incelenmektedir.

Tezin ikinci bölümünde, manyetik molekülleri kullanarak bilgi aktaran MH sistemleri incelenmektedir. EM alanın difüzyon hızı üzerindeki etkisini anlamak için moleküllerin tipi ve EM alanın konfigürasyonu incelenmektedir. Manyetik moleküllerin difüzyon hızı ve konsantrasyonundaki değişimi modellemek için manyetik alan gradyan ve konsantrasyon gradyan manyetik kuvvetlerinin etkileri analiz edilmektedir.

Tezin son kısmı, EM alan altında moleküler dinamiklere odaklanmaktadır. Termal değişikliklerin moleküler reaksiyon hızı ve bağlanma kinetiği üzerindeki etkisi, reaksiyon-difüzyon sistemleri ile modellenmektedir. EM alanın neden olduğu sıcaklık değişiminin etkisini belirlemek için spesifik reaksiyon hız sabiti analiz edilmektedir. Moleküllerin hareketi Langevin'in difüzyon modeli ile modellenmektedir. Molekülün hızının ve pozisyonunun olasılık dağılım fonksiyonları, EM alanın altında moleküler davranışı anlamak ve modellemek için analiz edilmektedir. Ayrıca, EM alan altında difüzyon tipini analiz etmek için moleküllerin ortalama karesel pozisyonları kullanılmaktadır.

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LIST OF ABBREVIATIONS

MC . . . . . Molecular Communication
EMF . . . . . Electromagnetic Field
CGMF . . . . . Concentration Gradient Magnetic Force
ELF-EMF . . . . . Extremely-Low Frequency Electromagnetic Field
DC . . . . . Direct Current
AC . . . . . Alternating Current
SMF . . . . . Static Magnetic Field
MRI . . . . . Magnetic Resonance Imaging
MNP . . . . . Magnetic Nanoparticles
OOK . . . . . On-Off Shift Keying
CSK . . . . . Concentration Shift Keying
MoSK . . . . . Molecular Shift Keying
ISI . . . . . Inter-Symbol Interference
MRI . . . . . Magnetic Resonance Imaging
SAR . . . . . Specific Absorption Rate
RRE . . . . . Reaction Rate Equation
CME . . . . . Chemical Master Equation
MSD . . . . . Mean-Squared Displacement

CHAPTER 1

INTRODUCTION

1.1. Molecular Communication

The definition of communication is exchanging information in several forms. Each species has its own method. We, humans, communicate by speaking, writing, and hand gestures. What we all have in common is employing several types of molecules and nanoparticles to communicate. Every process in our bodies is carried out by molecules communicating between cells. Several types of ions are employed for communication at the cellular level. These ions pass through gap junctions on the cell membrane and are received by the receptors on the receiver cell. For instance, calcium (Ca^{+2}) signaling is an effective signaling mechanism in cells. It has roles in vital cellular processes like cell metabolism, proliferation, and contraction. Ca^{+2} ions have rapid binding kinetics, making them a convenient molecule for communication. Therefore, they are widely employed in cells like astrocytes and muscle cells (Source: Barros et al., 2015; Kuran et al., 2012; Sneyd et al., 1994). Figure 1.1 represents a simple Ca^{+2} signaling over a gap junction at the cell membrane.

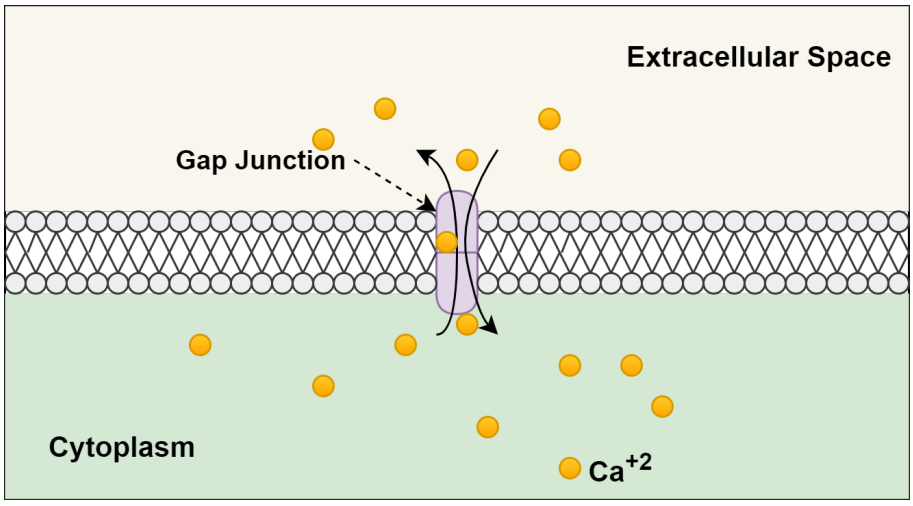

Figure 1.1. Calcium signaling model (Source: Levin et al., 2017)

Molecular communication is also present in unicellular organisms. A prokaryote-like bacteria employ molecules to sense its surrounding. The bacterial community regulates its gene expression by emitting molecules to the environment and adjusting themselves according to the density of molecules. This process is called quorum sensing (Source: Miller et al., 2001). MC can be employed in various ranges/scales. Ca^{+2} signaling is an example of a microscale communication scheme. Macroscale (cm to m scale) communication is also present in nature. Animals like ants and insects depend on pheromones to orient in nature. They navigate and adjust according to these chemical signals (Source: Billen and Morgan, 2019).

Scientists try to imitate and interpret nature to better understand it and its principles. From the viewpoint of communication engineering, MC is a branch that tries to model molecular communication methods in nature and utilize them for communicating on various scales. Inspired by nature, MC employs molecules rather than electromagnetic waves as information carriers. Therefore, it is carried out in environments such as aqueous and gaseous, where molecules can move freely. Understanding the behavior of molecules in such environments requires the contribution of various research fields. Therefore, MC benefits from natural sciences and interdisciplinary areas like biophysics and biochemistry. In communication engineering, the scale of the system highly affects communication methods and performance. MC is studied on different scales as well. The range of communication determines the scale of the communication system. We see that communication in nature is performed in various ranges from nm to m. If the range is between nm to cm, it is a short to mid-range communication and denotes a microscale MC system. Though miniaturization of components employed in communication systems is challenging, developments in nanotechnology made it possible to produce devices on the nanoscale. These devices are named nanomachines. They are biocompatible machines that act on a specific stimulus. They can be created artificially or biologically. Biocompatible nanomachines and nanorobots are examples of artificially produced nanomachines. Furthermore, motor proteins and genetically engineered cells are examples of biological nanomachines (Source: Bogunia-Kubik and Sugisaka, 2002; Hiyama et al., 2007; Novotnỳ et al., 2020). MC is a proper communication method for nanomachines. It can be employed in a simple communication system design that includes single transmitter and receiver nanomachines. A simple MC model is presented in Figure

1.2. In this figure, TX and RX correspond to a transmitter and receiver, respectively. TX emits molecules to the channel, and diffusing molecules perform passive MC. On the other hand, TX can perform active MC by carrying molecules over a filament.

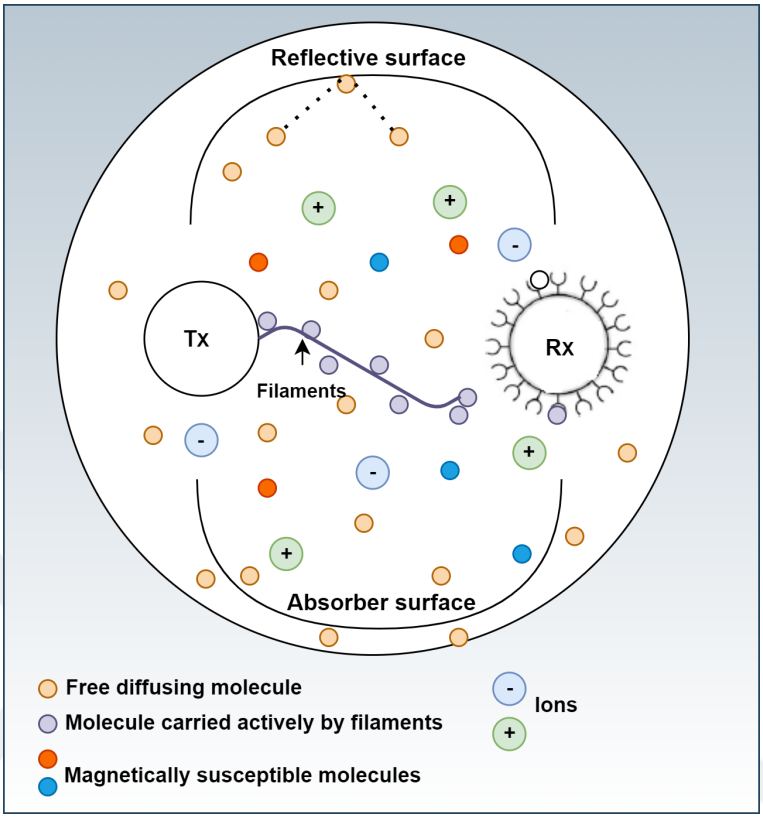

Figure 1.2. A simple molecular communication system

Nevertheless, it can be employed in a more complex setting with multiple nanomachines to perform more sophisticated tasks (Source: Akyildiz et al., 2008; Atakan et al., 2012). Various structures of nanomachines are utilized in biomedical and environmental applications. For instance, they can be employed as nanomedicine in targeted drug delivery systems. A good example of a biomedical application of nanomachines is presented in (Source: Chahibi et al., 2014). This study employs antibodies as information carriers for targeted drug delivery. A drug delivery system model is designed to consider antibodies' biological and geometrical properties. In addition, a network of nanomachines can be constructed for a targeted drug delivery system where nanomachines communicate with each other to avoid the healthy cells and deliver the drug to the diseased cells (Source: Atakan et al., 2012). Furthermore, environmental applications of MC include pollution control and monitoring the environment for contamination. Much like an insect using its

olfactory sensors to recognize its environment, an electronic nose sensing and locating the odor in the environment is modeled in (Source: Marques and De Almeida, 2000). The proposed system can be employed in robotics as a chemical sensor and robotic guide.

In addition to the microscale systems, MC is also studied in macroscale. The range of communication changes from cm to m in macroscale systems. Though one might think that MC is not suitable for macroscale applications because of the lifespan of molecules/chemical trails, the environmental conditions might require or benefit from MC. For instance, MC might perform better in environments where electromagnetic signals experience significant diffraction or attenuation (Source: Guo et al., 2015; Stojanovic, 2003). Furthermore, the performance of MC at the macroscale can be improved by channel modeling, network designs, modulation techniques, and external factors. In (Source: Farsad et al., 2013), a basic macroscale MC system is designed that includes a sprayer and an alcohol sensor. In this system, alcohol molecules are employed as information carriers, and the propagation of molecules is supported by a fan behind the sprayer. The sprayer is the transmitter, the alcohol sensor is the receiver, and the fan is the external factor employed to enhance molecular movement. A new approach to macroscale MC systems is introduced in (Source: Gulec and Atakan, 2020a) where emitted alcohol molecules are modeled as liquid droplets. And by doing so, the nonlinearity in the channel is addressed. The effect of this nonlinearity on the distance estimation between transmitter and receiver is investigated. Furthermore, the trajectory of a molecule in a macroscale experimental MC setup is presented. An end-to-end macroscale channel model is proposed in (Source: Gulec and Atakan, 2020b), where information-carrying molecules are modeled as droplets for a realistic approach.

1.2. Molecular Communication under Electromagnetic Fields

An electromagnetic field is caused by moving electric charges. EMF can be created naturally or artificially. For instance, Earth has its magnetic field caused by the materials in its core. Earth's rotational movement accelerates these materials and creates a magnetic field. Like most things, we also learned how to create and utilize EMF. Technological developments throughout history have increased the use of EMF. Thus, electromagnetic field exposure has increased as well. Cell phones, computers, and

appliances are the essentials of daily life (Source: Yalçın and Erdem, 2012). Moreover, they produce EMF and expose us to magnetic fields. Organisms create magnetic fields via the motion of charged molecules (Source: Cifra et al., 2011; Trushin, 2003). These magnetic fields can be employed in several ways. For instance, endogenous fields are created by cells to perform the inter or intramolecular communication (Source: Adams and Levin, 2013; Fröhlich and McCormick, 2010; Funk, 2015; Tseng and Levin, 2013). Since our bodies employ MC on every scale, understanding the effects of EMF on MC is important to assess the biological risks of magnetic exposure.

EMF is present in our daily life in several frequency ranges via manufactured safety, health, and household devices. Mainly, three types of magnetic fields are studied in the literature: static magnetic fields, extremely low-frequency electromagnetic fields (ELF-EMF), and pulse-modulated magnetic fields. Static magnetic fields do not vary with time and result from a direct current (DC). Geomagnetic fields are examples of static magnetic fields (Source: Rosch and Markov, 2004). ELF-EMF is produced by alternating current (AC) and varies with time. It is effective in the frequency range of 0 to 300 Hertz. Power lines (50-60 Hz) and domestic appliances are examples of ELF-EMF. Pulse-modulated EMF is produced at radio frequencies between 100 kHz and 300 GHz and employed in medical imaging devices.

Generally, negative effects are expected as a result of magnetic field exposure. However, magnetic fields can be manipulated constructively in wound healing or drug therapy applications (Chahibi and Akyildiz, 2014; Pesce et al., 2013). For instance, the effect of the magnetic field on the cell membrane permeability is studied in (Source: Nguyen et al., 2017). Red blood cells are exposed to a high frequency (18 GHz) EMF. Results indicate that a high-frequency alternating EMF causes an energy dissipation near the cell membrane and affects the cell membrane stability. This alteration in the cell membrane permeability yields an increase in nanoparticle consumption, which may be interpreted as an increase in the information rate of MC. Hence, this type of alteration in cell membrane permeability can be employed in drug delivery applications. In (Source: Lucia et al., 2017), a biochemical thermodynamic approach is introduced to reduce cell proliferation. The proposed method specifies the frequency of applied ELF-EMF to reduce cell proliferation for specific cell lines. Meaning of that ELF-EMF affects the molecular communication dynamics in cell proliferation explicitly.

Nevertheless, the negative effects of magnetic field exposure cannot be ignored. In (Source: Nava et al., 2018), ELF-EMF with the intensity of 4.5 millitesla and a frequency of 120 Hz is applied to the rats for 50 minutes daily. An increase in liver cancer is observed through quantum measurement techniques. In (Source: Rezaei-Tavirani et al., 2018), the effect of ELF-EMF on protein dynamics is investigated. Rats are exposed to ELF-EMF at a 50 Hz frequency with different intensities (0.5 and 1 mT), and the effect on the hippocampus is observed. The proteomic analysis is employed to evaluate gene regulation and protein expression. As a result, the expression of proteins in cytoskeletal and metabolic processes is downregulated. In addition to ELF-EMF exposure, higher-frequency magnetic fields are studied as well. In (Source: Bourdineaud et al., 2017), EMF with 900 MHz frequency is applied to earthworms with different exposure durations. As a result of gene expression analysis, up-regulation is observed in the expression of stress response proteins. Furthermore, several studies indicate that EMF affects many cellular processes such as gene transcription (Source: Bodamyali et al., 1998; Nikolova et al., 2005), gene expression (Source: Bourthoumieu et al., 2013; Remondini et al., 2006) and protein synthesis (Source: Bersani et al., 1997; Gerner et al., 2010; Han et al., 1998; Kwee et al., 2001). Understanding these various responses of cells to magnetic field exposure improves the way we comprehend and mimic nature. New MC models, simulations, and experiments provide an adequate platform for studying the biological effects of EMF.

The effect of EMF on molecules is studied in several aspects (Source: Funk et al., 2009). They can affect the molecular systems thermally or non-thermally. The thermal effect of EMF is caused by energy absorption in the exposed area. The non-thermal effects of EMF are caused by the electric and magnetic forces that change the orientation of molecules. Frequency, exposure time, intensity, and modulation type of the field are significant properties of electromagnetic fields and determine the characteristics of the field's effect on molecules. In addition to the field properties, the effect of magnetic field exposure depends on the condition of the biological environment, molecule, and molecular system. The theory behind the electromagnetic field effect on molecular systems is limited due to its complexity. Even with the assumptions of a homogeneous and thermally stable environment, the computation of molecular states is hard to calculate. The stochastic nature of molecular motion causes this. Various algorithms have been developed to reduce the complexity of these systems. However, one cannot achieve that

by preserving the exactness of the algorithm.

In MC systems under EMF, the type of the molecule is a significant parameter for the effect of EMF on the molecule. Since EMF exerts forces on molecules, molecule type determines the molecule's response to the EMF. The molecules that are employed as information carriers in an MC system can be uncharged, charged, or magnetically susceptible (Source: Nakano et al., 2013). A simple example of such a system is given in Figure 1.3.

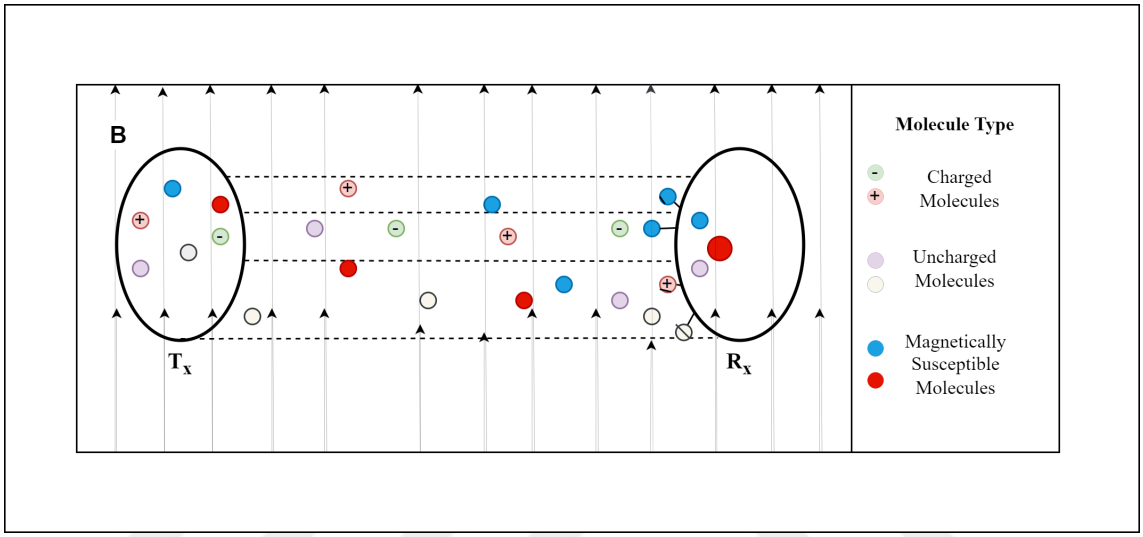

Figure 1.3. Molecular communication system under EMF (Source: Nakano et al., 2013)

Though EMF exerts forces on uncharged molecules, they are not easily affected by the EMF. The strength of the EMF needs to be high to alter the movement of the molecule (Source: Franchetti et al., 2021; Lemeshko et al., 2013). On the other hand, charged molecules can be affected by the EMF more quickly compared to uncharged molecules. The force that the EMF applies affects the movement range of the molecules (Source: Moggia et al., 1997). Magnetically susceptible molecules are affected by the EMF regarding their magnetizability. The magnetic moment of the molecule changes under the EMF and results in several levels of magnetization. There are three types of magnetically susceptible molecules. Ferromagnetic molecules are magnetic materials that have magnetic properties without the presence of an EMF. They can be magnetized even with low magnetic field strength. Paramagnetic molecules/materials present magnetic properties under the EMF. Magnetic fields attract paramagnetic molecules. On the other

hand, diamagnetic molecules are repelled by the magnetic fields (Source: Aharoni et al., 2000). These different features of molecules present different possibilities in MC design and performance.

Theory and simulation in MC schemes can help to a certain extent because the biological environment conditions are theoretically challenging and complex to define. However, experiments by biologists, doctors, and geneticists have been carried out to see the effect of EMF on several types of tissues, cells, organs, and DNA. There are various perspectives regarding magnetic field exposure in biology or genetics. The response of a cell to a magnetic field depends on the cell state. If the cell is in proliferation, it is more vulnerable to the effects of magnetic fields. Field exposure can affect cell signaling mechanisms, gene expression, protein secretion, and inter or intracellular molecular communication. The evaluation criteria changes depending on the examined biological environment. Hence, most of the studies assume perfect conditions to analyze molecular systems.

The molecular movement under EMF is complex due to the nature of molecules, environmental conditions, and size of the MC system. The size and random movement of molecules make the system stochastic. Furthermore, the environmental condition of the channel affects molecular behavior as well. Though biologists or chemists conduct experimental studies, it is an open research field that needs improvements in theory and simulation. An interdisciplinary approach is needed to understand, model, and represent the cells' and molecules' behavior under EMF. This thesis focuses on two main aspects of electromagnetic field effects on molecules and the performance of an MC system. Since EMF exposure changes the thermal conditions of the environment, the effect of thermal change on molecular movement and molecular binding kinetics are investigated. Furthermore, the effects of EMF on molecular movement are researched. Any change in the molecules' diffusion rate can affect the information rate. Therefore, several parameters like the molecule type, magnetic field strength, and channel conditions are considered to understand the changes in the diffusion rate of molecules.

1.3. Thesis Outline

This section consists of each chapter's summaries and presents the thesis's outline as follows. The classic theory of electromagnetism and electromagnetic forces are presented in Chapter 2. The electric and magnetic fields are described by Maxwell's equations. Electromagnetic wave results from the continuous induction of electric and magnetic fields. The combination of these induced fields creates the EMF. EMF interacts with particles through electromagnetic forces and energy transfer. The effects of electromagnetic forces on different types of particles are presented in this chapter. The effect of electromagnetic forces varies for different types of particles. The electric and magnetic properties of particles are significant in determining the effect of electromagnetic forces. Stationary and moving particles also experience different forces. A charged, stationary particle is affected by the electric force governed by Coulomb's law. Magnetic fields apply magnetic forces on charged, moving, or magnetically susceptible particles. Furthermore, the effect of transferred energy is studied to examine the thermal changes in the exposed area. The temperature increase and distribution research is presented for different tissue types. Principal forces on diffusing molecules under an EMF are also represented. The driving force for diffusion and viscous drag caused by the medium is studied as the primary forces on diffusing molecules. The magnetic field gradient and concentration gradient magnetic force are analyzed to determine the effect of magnetic fields on diffusing molecules. The total effect of principal forces on magnetically susceptible molecules is considered separately for diamagnetic and paramagnetic molecules.

Chapter 3 focuses on the MC systems that employ magnetically susceptible molecules as information carriers. Magnetically susceptible molecules are appropriate for an externally controllable MC system. The control of such systems is managed by EMFs. The EMF's strength, configuration, and distribution are significant parameters in the control of MC systems. The strength of EMF determines the applied electromagnetic force's magnitude. EMF can be configured as parallel or perpendicular to the medium. The direction of the field affects the direction of the applied force. The distribution of EMF can be uniform or non-uniform. The non-uniform distribution of EMF results in magnetic field gradients. In addition to electromagnetic forces, magnetic field gradient force is applied to the molecules under a non-uniform EMF. The magnetic susceptibility of molecules

is significant in determining the extent of the magnetic field gradient force. According to their susceptibility, molecules are attracted or repelled by magnetic field gradients. The molecular movement is altered by magnetic field gradient force. Hence, molecules' concentration and distribution change under magnetic field gradients. The heterogeneity of molecules affects the magnetic energy of the system. As a result, a concentration gradient magnetic force is introduced to the system for the conservation of energy. The magnetic properties and distribution of molecules determine the change in the system's magnetic energy. Therefore, the magnitude and direction of the concentration gradient magnetic force depend on the molecules' magnetic features. The directional effects of concentration gradient magnetic force on molecules' diffusion are studied to evaluate the change in the diffusion rate and coefficient. The concentration of molecules is analyzed for diamagnetic and paramagnetic molecules. Finally, the MC system's information rate is studied under concentration gradient magnetic force.

The effect of EMF on molecular communication is studied in Chapter 4. The temperature change in the environment and the directional change in the molecular movement are considered the main effect of EMF on molecular behavior. Moreover, diffusion type and characteristics are also studied. A reaction-diffusion system can be employed to model an MC system. The rate of chemical reactions depends on temperature. Therefore, the reception rate of MC may be affected by the increase or decrease in temperature. The specific reaction rate constant is studied to understand the effect of temperature change on the chemical reactions and reception rate of MC. The chapter also focuses on molecular behavior under EMF. The change in the molecule's velocity and displacement is considered to model the molecular movement under EMF. Furthermore, the mean-squared displacement of molecules is calculated to understand the type of diffusion performed by molecules. In Chapter 5, the thesis is summarized, and concluding remarks are represented.

CHAPTER 2

ELECTROMAGNETIC FIELDS

2.1. Introduction

In this chapter, we focus on the classical theory of EMF and the effects of EMF on particles and diffusing molecules. We begin with the definition and governing equations of EMF in Section 2.2. Electric and magnetic fields comprise the EMF. An electric field encloses charged particles. A magnetic field is characterized by moving electric charges and magnetic materials. Though many scientists have contributed to the electromagnetism theory, Maxwell has comprehensively defined classic electromagnetism. This comprehensive definition consists of four fundamental equations describing electric and magnetic fields and their relation. Gauss's law for electricity defines the proportional relation between the net electric charge and the electric field over an enclosed surface. Furthermore, Gauss's law for magnetic fields states that the magnetic flux over a Gaussian surface is zero because there can be no net magnetic charge enclosed by the surface. Faraday and Ampere-Maxwell's law relates electric and magnetic fields to electric and magnetic flux. The classification of EMFs according to their frequency, energy, and waveform is discussed as well.

In Section 2.3, electromagnetic forces on particles are studied inclusively. Charged particles experience three types of forces. If charged particles are not moving, i.e., static, they act on each other depending on their charge and the distance between them. The resulting force is the electrostatic force governed by Coulomb's law. If charged particles are moving, a magnetic force acts on them because of the imposed magnetic field. The magnetic force depends on the charge and the velocity of the particle. Lorentz's force describes the combination of these forces. In Section 2.3.1, magnetization is discussed in order to understand the force that EMF applies depending on the magnetizability of a particle. The interaction between magnetically susceptible molecules and magnetic field gradients are studied to this extent. Effective forces on diffusing molecules under EMF are

presented in Section 2.4. In addition to the electromagnetic forces, diffusing molecules experience different forces due to diffusion, environment, and external factors. The effect of diffusion is due to the random movement of molecules (Source: Cussler, 2009). The viscous properties of the aqueous environment create a drag force that affects molecular movement. Furthermore, convection could be introduced to the system naturally or by an external factor. The electromagnetic forces that affect the molecules depending on their electric and magnetic properties are discussed in Sections 2.4.1 and 2.4.2. The conclusion of the chapter is presented in Section 2.5.

2.2. Classic Theory of Electromagnetic Fields

I happened to have discovered a direct relation between magnetism and light, also electricity and light, and the field it opens is so large, and I think rich.

-Michael FARADAY [1]

The simplest definition of the electromagnetic field is made by Faraday when he wrote these words to C.F. Schoenbein in (Source: Faraday and Schönbein, 1899). As he has foreseen, EMF is a vast research area that needs further discoveries even today. In classic physics, a combination of an electric and magnetic field caused by static and moving charges is a basic definition for electromagnetic fields (Source: Feynman et al., 1965). The theory of EMF stems from the Maxwell equations that define the electric and magnetic fields. Maxwell's equations define classic electromagnetism comprehensively (Source: Fitzpatrick, 2010). The set of Maxwell's equations is given as

$$\nabla \cdot \mathbf{E} = \frac{\rho}{\varepsilon_0} \qquad \text{Gauss's Law} \tag{2.1}$$

$$\nabla \cdot \mathbf{B} = 0 \qquad \text{Gauss's Law for Magnetism} \tag{2.2}$$

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t} \qquad \text{Faraday's Law of induction} \tag{2.3}$$

$$\nabla \times \mathbf{B} = \mu_0 \mathbf{J} + \mu_0 \varepsilon_0 \frac{\partial \mathbf{E}}{\partial t} \qquad \text{Ampere-Maxwell Law} \tag{2.4}$$

[1] *Küster, F. W. (1900). The Letters of FARADAY and SCHOENBEIN, 1836 – 1862. With Notes, Comments, and References to contemporary Letters edited by GEORG WA KAHLBAUM and FRANCIS V. DARBISHIRE. 376 Seiten mit 2 Portraits. Preis 15 fr.(Basel, BENNO Schwabe; London, WILLIAMS and NORGATE, 1899.).*

where $\mathbf{E}$ is the electric field, ρ is the volume charge density, ε_0 is the vacuum permittivity, $\mathbf{B}$ is the magnetic flux density, c is equal to the speed of light, μ_0 is the permeability of free space and, $\mathbf{J}$ is the electric current density.

Eq. 2.1 represents the relationship between a static electric field and an electric charge. Eq. 2.2 states that the net flow of the magnetic flux over a closed surface is equal to zero. Eq. 2.3 describes Faraday's law of induction. Faraday's law states that a time-varying magnetic field induces an electric field, and the opposite is also valid for a time-varying electric field. Ampere's circuital law with Maxwell's correction, i.e., Eq. 2.4 defines the generation of magnetic fields by electric current and varying electric field. The solution of Maxwell's equations results in an electromagnetic wave. This electromagnetic wave represents the relation between electric and magnetic fields governed by Maxwell's equations. The variation in magnetic flux induces an electric field, i.e., Faraday's law of induction. Similarly, varying electric flux induces a magnetic field, i.e., Ampere-Maxwell law (Source: Halliday et al., 2013). These fields are induced continuously and result in an electromagnetic wave, as shown in Figure 2.1.

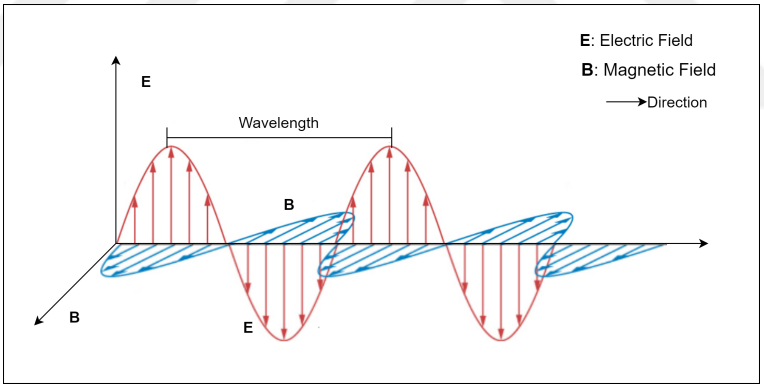

Figure 2.1. Electromagnetic wave (Source: Halliday et al., 2013)

The frequency, waveform, and energy of EM wave characterize the field. These properties are directly related to the intensity of the EMF. Furthermore, different frequency ranges and waveforms indicate different intensities and types of EMF. Hence, they play a significant part in the utilization and application of EMF. EMF can be employed in various areas, such as household appliances, industrial, communication, and medical systems (Source: Halliday et al., 2013).

EMFs are divided into three main categories depending on their frequency and waveform. Static magnetic fields (SMF) are created by direct currents. Hence, they do not

vary with time. SMFs do not change with time, but the magnetic field intensity changes according to the field distribution. A non-uniform magnetic field causes magnetic field gradients (Source: Waskaas, 2021). Magnets are a good example of SMFs. Another example is the Earth's magnetic field, as shown in Figure 2.2. All creatures experience the effect of SMFs due to Earth's magnetic field (Source: Dini and Abbro, 2005; Zhang, Yarema, and Xu, Zhang et al.).

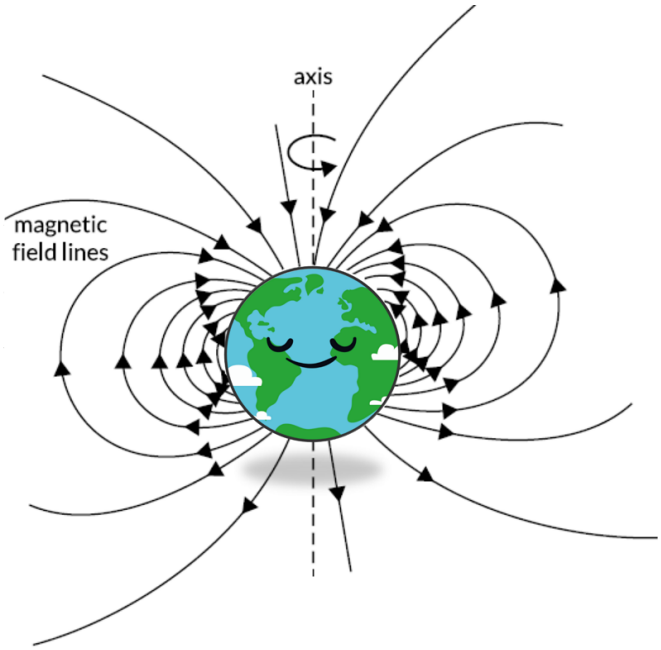

Figure 2.2. Electromagnetic Field of Earth

Another type of EMF results from alternating current. AC EMFs are generated by sine waves and vary with time. The household appliances operate on power lines at 50 and 60 Hz and produce an ELF-EMF. Cell phones, radio, and television broadcasting employ higher frequency (1800 - 1900 MHz) EMFs. Furthermore, another time-varying magnetic field is produced by pulse-shaped signals. Pulse-modulated EMFs are employed in therapeutic applications and medical imaging devices.

EMF exerts forces on charges in the environment that change according to their electric and magnetic properties. The interaction between the environment and the EMF varies for different types of EMF. Moreover, the effects of EMF depend on its frequency, intensity, and waveform. Therefore, the classic theory and classification of EMF are studied to understand the EMF's effects on particles.

2.3. Electromagnetic Forces

Electromagnetic forces are the combination of forces applied to a particle by an electric and magnetic field. The electrical and magnetic properties of the particles are significant in determining the magnitude and direction of the forces. The interaction between charged particles is formulated by Coulomb's law given by

$$\vec{F} = \frac{1}{4\pi\varepsilon_0}\frac{q_1 q_2}{r^2}\vec{r} \tag{2.5}$$

where ε_0 is permittivity of free space, r is the distance between charged particles, q_1 and q_2 are the charges of the particles. The electric force depends on the charges and the distance between the particles. Coulomb's law is fundamental to understanding the interaction between electric fields and particles. As stated in Eq. 2.1, charge density produces an electric field proportional to the permittivity of free space. The produced electric field interacts with a charged particle by exerting a force on it. The magnitude of the force can be negative or positive according to the charges. If they have the same charge, particles repel each other. On the other hand, the particles with different charges attract each other (Source: Huray, 2011). This relation is presented in Figure 2.3.

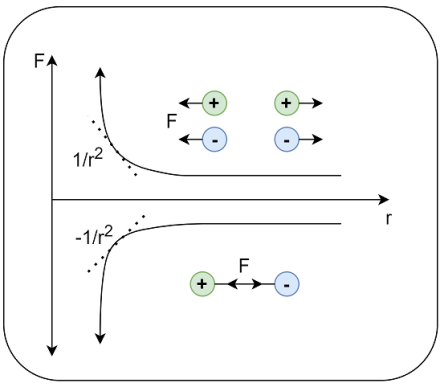

Figure 2.3. Coulomb's Law (Source: Huray, 2011)

Every material contains bound or free, positive and negative charges. Conductors have many free charges as opposed to insulators (dielectrics) that include bound charges.

The electric force affects positive and negative charges in opposite directions, resulting in an electric dipole. For a conducting material, free charges move in opposite directions due to the force applied by an electric field. Moreover, the electric field produced by these charges modifies the applied field. Since dielectric materials include bound charges, positive and negative charges inside charged particles align under an electric field. The electric dipole moment, i.e., $\vec{p}_i$ induced by the separation of positive and negative charges, is represented in Figure 2.4.

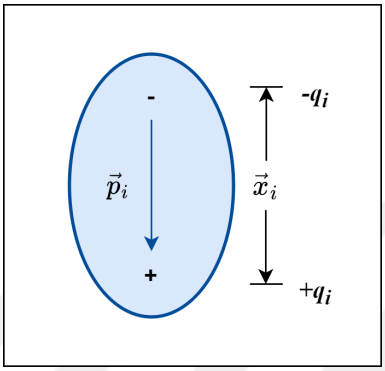

Figure 2.4. Electric dipole moment, $\vec{p}_i$, induced in a dielectric by positive and negative charges, $+q_i$ and $-q_i$, separated with a distance x_i (Source: Huray, 2011)

The electric dipoles of a dielectric are oriented randomly. Under an electric field, these dipoles align because of the applied forces. The alignment of permanent dipoles of a dielectric under an electric field is presented in Figure 2.5.

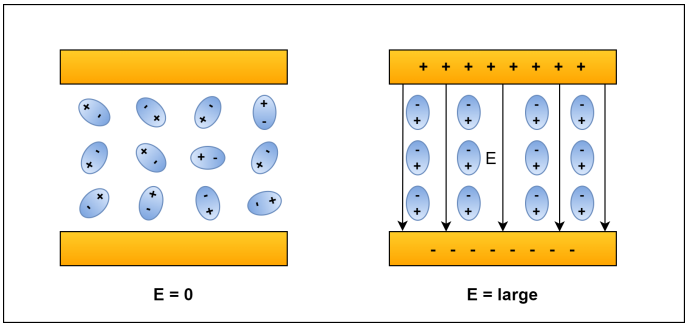

Figure 2.5. Alignment of permanent electric dipoles under electric field (Source: Huray, 2011)

Since charges in the material also creates an electric field, the total effect of the electric field is determined by the polarizability of the material and the effect of electric

forces on the charges. The material is polarized in proportion to its dielectric constant, i.e., relative permittivity, defined as

$$\varepsilon_r = \frac{\varepsilon}{\varepsilon_0} \tag{2.6}$$

where ε is the permittivity of the material and ε_0 is the permittivity of free space. The electric field affects both static and moving charges. Furthermore, the effect of the electric field increases the velocity of a free charge and the collision probability of particles. As the number of particles increases, the force that each particle experiences change depending on the particles' positions. Nevertheless, all charges produce an electric field and experience an electric force; magnetic field and magnetic forces can only be produced or experienced by moving charges (Source: Greenebaum and Barnes, 2018).

Magnetic force that affects a moving charged particle under an EMF is formulated as

$$\vec{F_B} = q\vec{v} \times \vec{B} \tag{2.7}$$

where B is the magnetic flux density, q is the particle's charge, and v is the particle's velocity. According to Eq. 2.7, a particle does not experience any magnetic force if it is not charged or moving (Source: Huray, 2011). The effect of the magnetic field on particles is analogous to the effect of the electric field. In this case, the magnetic field creates magnetic dipoles in accordance with their magnetizability, i.e., permeability. The effect of magnetic fields on the particles will be studied further in section 2.3.1.

The combination of electric and magnetic forces results in an electromagnetic force defined by Lorentz (Source: Huray, 2011). Lorentz's force is significant in modeling the movement of charged molecules and defined by

$$\vec{F} = q\vec{E} + q\vec{v} \times \vec{B} \tag{2.8}$$

where q is particle's charge, E is the electric field, B is the magnetic flux density, and v is the particle's velocity. In (Source: Abdoli and Sharma, 2021), the effect of Lorentz force on charged diffusing particles is studied under a uniform and non-uniform magnetic field. Though the Lorentz force does not affect passive diffusing particles, the magnetic field strength and homogeneity affect the active diffusing particles. The behavior of actively diffusing charged particles under a non-uniform external magnetic field is studied in

(Source: Vuijk et al., 2020). The Lorentz force and magnetic field gradient affect the particle movement and raise a flux that leads to an inhomogeneous system.

A particle under EMF experiences various forces. The type of these depends on the electrical and magnetic properties of the particle. Furthermore, the characteristic features of EMF contribute to the effect. A charged or magnetically susceptible particle experiences the effect of EMF differently. While the force on a charged particle is proportional to its charge and velocity, the EMF distribution and magnetic properties are more substantial for a magnetically susceptible particle. The acting forces on molecules are significant in determining the behavior of molecules in the medium. In addition to electromagnetic forces, molecules are affected by other forces while diffusing. These forces need to be considered in analyzing an MC system under EMF.

2.3.1. Magnetization

The magnetic field is derived from Faraday's and Ampere-Maxwell's laws. These laws indicate the relation between electric and magnetic fields. Eqs. 2.3 and 2.4 state that a moving charge and varying electric field induce a magnetic field. In a similar way, a time-varying magnetic field conducts a time-varying electric field. The interaction dynamics of the electric and magnetic fields with particles are also alike. The polarization and magnetization of particles result in electric and magnetic dipoles. Similar to an electric field created by a point charge, magnetic poles produce magnetic fields. These magnetic fields point from a negative magnetic pole to a positive magnetic pole. A good example of a magnetic moment is the magnetic dipole moment of a permanent magnet, as represented in Figure 2.6.

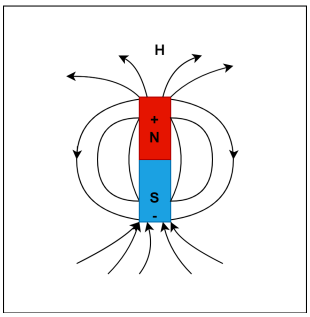

Figure 2.6. The magnetic dipole moment of a permanent magnet (Source: Stöhr and Siegmann, 2006)

The magnetic moment of a particle is comprised of the magnetic moments of unpaired electrons. The orbital movement of electrons with respect to a center defines the magnetic moment. The magnetic moment of an electron that orbits with respect to a center at a distance is defined as

$$m = -\frac{e\mu_0}{2}(r \times v) \tag{2.9}$$

where e is the charge of the electron, r is the radius of orbital movement, v is the electron's velocity and μ_0 is the permeability of free space. The magnetic moment alongside the classical momentum is depicted in Figure 2.7.

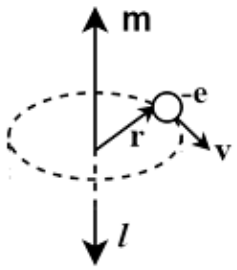

Figure 2.7. The magnetic moment of an electron (Source: Stöhr and Siegmann, 2006)

The classical angular momentum of an electron with mass m_e is given by

$$l = m_e(r \times v) \tag{2.10}$$

and relates to the magnetic moment as given in

$$m = -\frac{e\mu_0}{2m_e}(r \times v)\, l \tag{2.11}$$

The change in the particle's magnetic moment is defined as magnetization. Compass is a good example to understand the relationship between magnetic moments and magnetization. We know that a needle under an external magnetic field aligns with the magnetic poles. The underlying cause of this is the needle conserving its angular momentum.

The needle already has a magnetic moment caused by its electron spins. The external magnetic field changes the magnetic moment, and the needle moves back and forth to preserve its angular momentum. This difference between the permanent and induced magnetic moments is the magnetization of the needle. When we use a compass, we can see the needle's movement to align along the Earth's magnetic field (Source: Stöhr and Siegmann, 2006).

The relation between EMF and magnetization of a particle is defined by

$$M = \chi H \tag{2.12}$$

where H is the magnetic field strength and χ is the volume magnetic susceptibility of the particle. Magnetic susceptibility is a constant that defines the extent of magnetization. The magnetizability changes depending on the magnetic properties of particles.

The change in the magnetic moment of a diamagnetic particle due to an EMF is small. The value of χ is smaller than 0 for diamagnetic molecules. Moreover, the change in the magnetic moments is present only under the EMF. The effect of EMF on diamagnetic particles is in the opposite direction of the EMF. Therefore, diamagnetic particles are repelled by the EMF and move to the weak magnetic field gradients. For a paramagnetic molecule, χ is greater than 0. A considerable change occurs in the magnetic moment of a paramagnetic particle under the EMF. The magnetic moment of paramagnetic particles aligns with the magnetic field. Hence, paramagnetic particles move towards the strong magnetic field gradients. Diamagnetic and paramagnetic particles are magnetized while a magnetic field is present. Ferromagnetic particles present magnetic properties without an EMF, and their magnetic susceptibility is much greater than 0 (Source: Waskaas, 1993).

The EMF strength and the magnetization of the particles are directly related to the magnetic force. The magnetization of a particle is especially important when there is a non-uniform EMF. The inhomogeneous distribution of EMF creates magnetic field gradients. Magnetically susceptible molecules are attracted or repelled by magnetic field gradients. The force applied by the magnetic field gradient affects the particles on different levels depending on their magnetizability. Furthermore, the change in the magnetic energy of the system introduces a concentration gradient magnetic force. The diffusion rate of the magnetically susceptible molecules increases or decreases depending on their

magnetizability. Therefore, magnetization is significant in understanding the interaction between molecules and EMF. This will be further discussed in Chapter 3.

2.4. Principal Forces on Diffusing Molecules Under Electromagnetic Field

In molecular communication, molecules diffuse in the communication channel. The channel properties depend on the physical, chemical, and biological properties of the aqueous or gas in the medium. These properties of the channel affect the forces that are applied to the information-carrying molecules. To begin with, the thermal fluctuations in the environment cause a random dispersal and lead to the diffusion of molecules. Diffusion is the driving force for molecular movement (Source: Renn, 2005). The classical theory of diffusion is derived by Adolf Fick. Fick's diffusion model describes the diffusion flux in relation to the concentration gradient of molecules. According to this model, molecules diffuse from a high to a low concentration in proportion to a concentration gradient (Source: Crank, 1979). For a simple one-dimensional movement of molecules, the diffusion equation is derived as

$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2} \tag{2.13}$$

where x is the molecule's position, D is the diffusion coefficient, and C is the concentration of diffusing substance. The diffusion coefficient is a constant proportion that depends on the molecular characteristics and is defined by

$$D = \frac{kT}{6\pi a\eta} \tag{2.14}$$

where k is the Boltzmann's constant, T is the temperature in Kelvin, η is the viscosity of the aqueous solution, and a is the radius of the molecule. The thermal condition of the system, viscous properties of the medium, and the size and geometry of the molecule are significant for the molecule's diffusion characteristics. Molecules may be imposed by

many other forces during their random movement. Therefore, the effect of electromagnetic forces needs to be considered with the other forces acting on molecules. Diffusion is the leading force for molecular movement. In addition, molecular movement may change depending on the viscous drag and natural convection. Furthermore, molecules are affected by forced convection, Lorentz's force, and magnetic field gradients under the EMF.

Every molecule inside an aqueous environment is affected by the viscous drag. The viscosity of the fluid causes the viscous drag force. In simpler terms, viscosity is the stubbornness of the fluid to a change in the environment. A famous example of different viscosities is the comparison of water and honey. Water is an easy-going liquid and changes its shape quickly. On the other hand, honey is stubborn and sticky. It does not want to change. Therefore, the viscosity of the honey is greater than water. Hence, honey introduces more drag force to a particle moving inside of it. Viscous drag is a natural and important part of molecular movement. The drag force experienced by a spherical molecule in a viscous fluid is defined by Stoke's law and given as

$$F_v = 6\pi\eta a v \tag{2.15}$$

where η is the viscosity of the fluid in the medium, a is the molecule's radius, and v is the molecule's velocity. The velocity, shape, and size of the molecule determine the viscous drag force. Furthermore, the viscosity of the medium affects the diffusion coefficient of the molecule, as seen in Eq. 2.14. The molecule's diffusion coefficient decreases when the viscosity increases. Molecules are imposed to a greater drag force. In (Source: Krafcik et al., 2015), magnetic nanoparticles are employed to deliver drugs to the lungs. The contribution of viscous drag and gravity are considered in the analysis of a targeted drug delivery system. The convenience of the drug delivery system is assessed by the strength of the viscous drag in the environment. Since the viscosity of the air in the lungs is much smaller than blood, the drug delivery system suppresses the viscous and gravitational forces.

Convection is another force that acts on molecules. Convection is a flow that is generated naturally or by an external factor. Natural convection occurs in thermal or density changes in the fluid (Source: Gebhart and Pera, 1971). Gravity is a natural factor

that generates convection. As the difference between densities increases, the convection becomes rapid. On the other hand, viscous fluids and dispersion of the thermal gradient decrease the convection. In addition to natural causes, convection can be created by external forces as well (Source: Egan et al., 2008). A thermal gradient that is caused by the EMF exposure creates forced convection (Source: Zhu et al., 2007). The strength of the flow in forced convection can be greater than in natural convection.

Nevertheless, EMF exposure causes other external forces. The electric and magnetic fields affect charged or magnetically susceptible molecules in various ways. Lorentz's force is a fundamental force that an EMF causes. It affects both moving and stationary charged molecules. Thermal or directional effects of Lorentz's force are studied for ion movement and binding kinetics (Source: Muehsam and Pilla, 1996). Ion movement under a static or time-varying magnetic field is modeled by the Langevin-Lorentz equation (Source: Moggia et al., 1997; Blackman et al., 1990; D'Inzeo et al., 1993; Oliveri et al., 2004). Briefly, these studies state that the Lorentz force significantly affects ions' velocity and binding kinetics due to thermal and directional changes. Furthermore, the range of molecular movement is reduced (Source: Kinouchi et al., 1988).

In addition to the diffusion and viscous drag, magnetically susceptible molecules are affected by magnetic field gradient and concentration gradient magnetic forces. The magnetic moments of magnetically susceptible molecules are altered under EMF. Hence, the magnetic energy of the magnetically susceptible molecules changes. The magnetic energy of a magnetic moment under an EMF is defined in (Source: Stöhr and Siegmann, 2006) and given as

$$E = -m \cdot H \tag{2.16}$$

where m is the magnetic moment and H is the magnetic field strength. Therefore, the magnetic energy of a magnetically susceptible molecule depends on the EMF strength, the molecule's magnetic moment, and magnetic properties. Furthermore, the configuration of the EMF is significant in determining the direction and strength of the applied force. Generally, two types of EMF configurations are studied in the literature. EMFs are parallel or perpendicular to the medium. According to the direction of the field and the molecule's magnetic properties, the direction of the electromagnetic force is determined. In the case of a parallel magnetic field, convection is introduced to the medium. A perpendicular magnetic field produces a magnetic force parallel to diffusion. The direction and

magnitude of this force depend on the EMF distribution and the molecule's magnetic susceptibility (Source: Rabah et al., 2004). A non-uniform EMF results in a magnetic field gradient, and a magnetic field gradient force is introduced to the system. Since the EMF is perpendicular to the medium, the magnetic field gradient force is parallel to the diffusion. Furthermore, the direction of the applied force depends on the molecule's magnetic properties. The magnetic field gradient force is defined in (Source: Rabah et al., 2004) and given by

$$\vec{F}_M = \frac{\chi C B}{\mu_0} \nabla \vec{B} \tag{2.17}$$

where χ is the magnetic susceptibility of a molecule, B is the magnetic flux density, C is the concentration of magnetically susceptible molecules, and μ_0 is the vacuum permeability. As seen in Eq. 2.17, magnetic field gradient force changes in proportion to the magnetic susceptibility of the molecule. According to their magnetic susceptibility, molecules are attracted or repelled by the magnetic field. The magnetic field gradient force is either opposed or in the same direction as diffusion.

The change in the magnetic energy of the system causes another force that depends on the magnetic properties and the concentration gradient of magnetically susceptible molecules. The magnetic energy of the system increases or decreases depending on the alignment of magnetically susceptible molecules' magnetic moments. Therefore, a magnetically driven flux is established to decrease or increase the magnetic energy of the system. The molecular flux is caused by the concentration-gradient magnetic force and is parallel to diffusion. The magnetic susceptibility of the molecule is significant to determine the direction and magnitude of the concentration-gradient magnetic force (Source: Zablotskii et al., 2021). The concentration-gradient magnetic force is given as

$$\vec{F}_{CGMF} = \frac{\chi B^2}{2\mu_0} \vec{\nabla} C \tag{2.18}$$

where χ is the magnetic susceptibility of the molecule, B is the magnetic flux density, μ_0 is the vacuum permeability, and C is the concentration of magnetically susceptible molecules. The direction of the concentration gradient magnetic force depends on the diffusion flux and the magnetic susceptibility of the molecules. Since the magnetic susceptibility of paramagnetic molecules is greater than zero, their magnetic moment aligns

with the EMF and increases the magnetic energy of the system. Therefore, a concentration gradient magnetic force affects the molecules in the opposite direction of the diffusion to decrease the magnetic energy of the system. However, the magnetic susceptibility of diamagnetic molecules is smaller than zero, and their magnetic moment is in the opposite direction of EMF, the magnetic energy of the system decreases. Therefore, a concentration gradient magnetic force is introduced to the system in the same direction as diffusion. As a result, the diffusion rate of the molecules changes (Source: Zablotskii et al., 2021).

A molecule moving in a medium may experience all of the previously mentioned forces depending on the environmental conditions and molecular characteristics. Diffusion and viscous drag are fundamental forces for molecular movement. Naturally, the effective forces on diffusing molecules are not limited to these. The environmental conditions, the electrical and magnetic properties, and the geometry of molecules are significant parameters to determine the total effect of the applied forces. These forces represent the variety of EMF's effects on molecular movement. A thermal change that EMF introduces may cause a natural or forced convection and affect molecular movement. Furthermore, the velocity of the molecules may be affected by the thermal changes or Lorentz's force. A non-uniform magnetic field results in a magnetic field gradient and a concentration gradient magnetic force that changes the diffusion rate of molecules.

2.4.1. Principal forces on Paramagnetic Molecules

The effect of EMF changes according to molecules' physical and chemical properties. EMF interacts with free or bound electrons inside the molecules. The spin of electrons causes the magnetic moment. The net change in the molecule's magnetic moment defines its magnetizability (Source: Stöhr and Siegmann, 2006). The number and configuration of paired and unpaired electrons also affect the magnetizability of the molecule. Paramagnetic molecules include unpaired electrons and have net magnetic moments. The paired and unpaired electrons are represented in Figure 2.8.(A). The magnetic moment of a paramagnetic molecule does not have any particular direction without an EMF. Under an EMF, paramagnetic molecules' magnetic moment aligns in the same direction as EMF (Source: Stöhr and Siegmann, 2006). Figure 2.8.(B) represents the alignment of

paramagnetic molecules with a net magnetic moment.

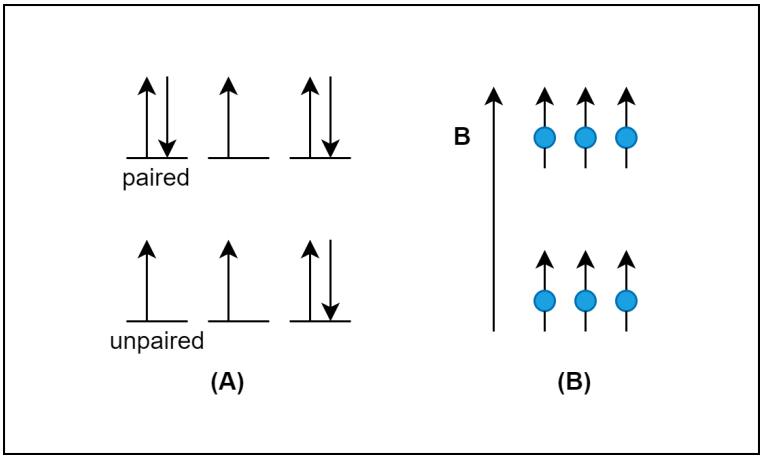

Figure 2.8. The electron pairing (A) and alignment (B) of a paramagnetic molecule (Source: Lehner, 2010)

A simple model of a paramagnetic molecule placed in a medium is presented in Figure 2.9. A magnetic field and concentration gradient are assumed in the medium. Every molecule moves from a high concentration to a lower concentration. The diffusion flux from high to lower concentration is represented as J_D. The viscous drag introduced by the medium is presented as F_v. The viscous drag always opposes the net diffusion flux. In this scenario, we assume the net movement of molecules is in the direction of J_D. The magnetic field gradient is presented with the field lines. As the distance between field lines decreases, the strength of the magnetic field gradient increases. Since the magnetic field is perpendicular to the medium, the force applied by a non-uniform magnetic field is parallel to the diffusion. The magnetic field attracts a paramagnetic molecule, and the magnetic field gradient force, i.e., Eq. 2.17, is in the same direction as diffusion. The effect of these forces increases the concentration of molecules in the direction of diffusion. Hence, the number of collisions between molecules increases. The increased molecular interactions and EMF changes the magnetic moment of the paramagnetic molecules. As a result, the magnetic energy of the system changes. Therefore, a concentration gradient magnetic force, i.e., Eq. 2.18, arises in the opposite direction of the diffusion to decrease the magnetic energy of the system.

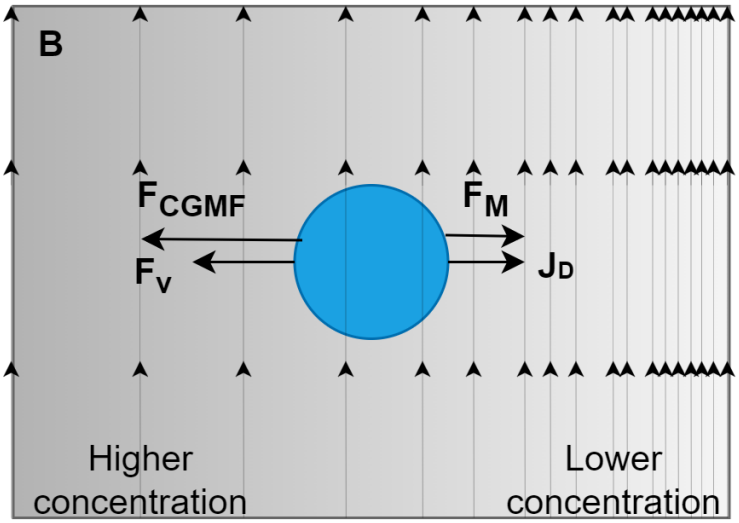

Figure 2.9. Effective forces on a paramagnetic molecule under an EMF (Source: Hinds et al., 2001)

The diffusion rate of the paramagnetic molecule changes due to the applied forces. The properties of the magnetic field and the magnetically susceptible molecules are significant to determine the total effect of the forces. The magnetic field distribution and strength affect the magnetic field gradient force, i.e., F_M, and the concentration gradient magnetic force, i.e., F_{CGMF}. The change in the magnetic energy of the system is proportional to the magnetic field strength. Therefore, the magnetic field strength is significant in determining the direction and strength of the concentration gradient magnetic force. The change in the magnetic energy decreases the diffusion rate of a paramagnetic molecule. In an MC system that employs a paramagnetic molecule, the information rate is expected to change due to the changes in the diffusion coefficient and rate of change in the molecular flux.

2.4.2. Principal Forces on Diamagnetic Molecules

All molecules have diamagnetic attributes. Diamagnetic molecules include paired electrons and do not have a net magnetic dipole moment. The effect of EMF on the magnetic dipole moment of a diamagnetic molecule is weak due to the bound electrons. Nonetheless, diamagnetic molecules are repelled by EMF. However, the applied force is much smaller than that of the force applied to a paramagnetic molecule (Source:

Lehner, 2010). Figure 2.10.(A) represents the bound and paired electrons in a diamagnetic molecule. Under a non-uniform EMF, the magnetic moment of diamagnetic molecules is parallel and opposes the direction of the field gradient, as presented in Figure 2.10.(B).

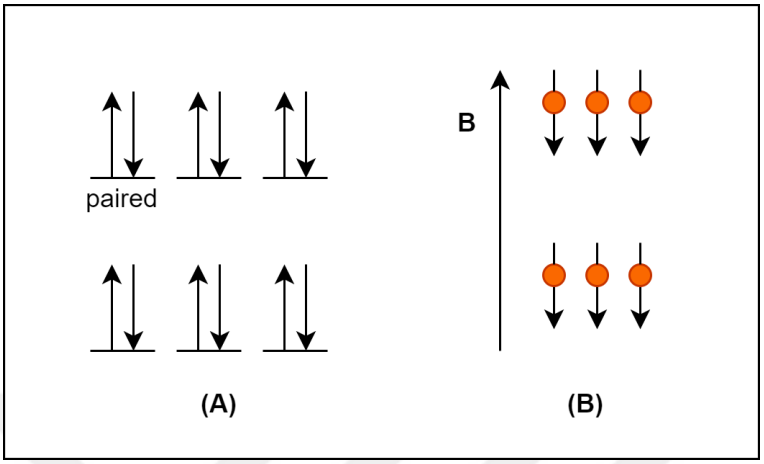

Figure 2.10. The electron pairing (A) and alignment (B) of a diamagnetic molecule (Source: Lehner, 2010)

The effect of principal forces on a diamagnetic molecule is modeled as represented in Figure 2.11. Diamagnetic molecules diffuse from a high to a low concentration, and the diffusion flux is represented with J_D. The previous scenario is also assumed for diamagnetic molecules. Therefore, viscous drag opposes the diffusion flux. Magnetic field gradient repels diamagnetic molecules. Hence, the resulting magnetic gradient force is still parallel but in the reverse direction and opposes the diffusion. Hence, diamagnetic molecules move towards a higher concentration. The increased number of collisions between molecules and the external field affects the magnetic moment of diamagnetic molecules. The alterations in molecules' magnetic moments affect the system's magnetic energy. Therefore, a molecular flux occurs in the system by the concentration gradient magnetic force that is parallel and in the same direction as diffusion.

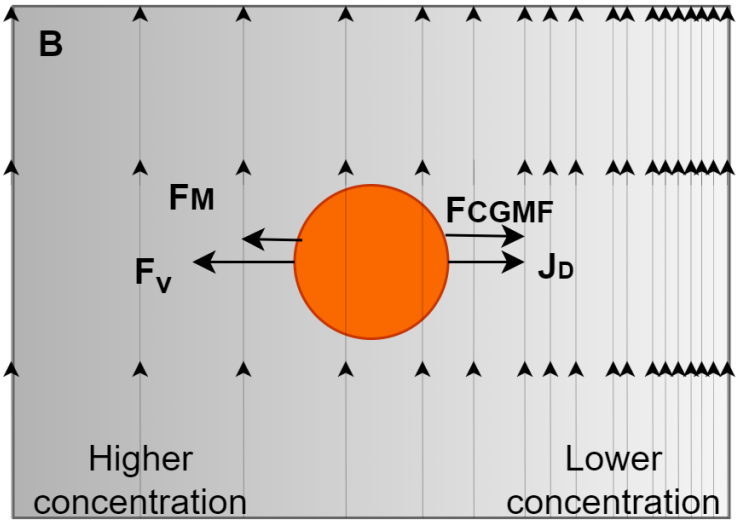

Figure 2.11. Effective forces on a diamagnetic molecule under an EMF (Source: Hinds et al., 2001)

The total effect of forces differs for a diamagnetic molecule. The magnetic properties of the molecule affect the direction of the magnetic field gradient and concentration gradient magnetic force. Therefore, the diffusion rate of a diamagnetic molecule is increased by the applied forces. Since the magnetizability of diamagnetic molecules is small, the effect of EMF on the diffusion rate of diamagnetic molecules is smaller.

2.5. Conclusion

This chapter presents the theory of EMF as in classical physics. The foundation of this theory is formed by Maxwell's equations. The set of four equations provides a basis for various inventions such as electric motors, microwave ovens, radar, transmitters, and receivers. EMF is utilized in many ways depending on its frequency, waveform, and energy.

Molecules that are exposed to EMF are affected by electromagnetic forces. Electromagnetic forces depend on molecules' electric and magnetic properties, such as electric charge and magnetic susceptibility. Furthermore, the EMF's strength, direction, and distribution significantly contribute to the applied forces.

Molecular communication systems employ diffusing molecules as information carriers. Therefore, a comprehensive analysis of molecules' behavior provides insight

into molecular movement under EMF. Diffusion and viscous drag are fundamental for molecules moving through an aqueous environment. Furthermore, external factors such as an EMF create additional forces to molecular movement. The total effect of these forces changes the diffusion rate of molecules. Any alteration in the molecular movement may affect the information rate of an MC.

CHAPTER 3

MOLECULAR SYSTEMS UNDER ELECTROMAGNETIC FIELDS

3.1. Introduction

MC employs various types of molecules to encode and transmit information. The design and performance of the MC system depend on the molecular type, medium, and external factors. The molecule's type and physical properties are significant in determining the information encoding scheme. Information can be encoded into one or more types of molecules. Moreover, the concentration and release time of molecules can also be employed as an information encoding scheme. The channel characteristics affect the molecular movement and information rate. The forces, i.e., viscous drag, experienced by molecules depend on the chemical characteristics of the aqueous or gas in the medium. Furthermore, the homogeneity of the medium also affects diffusion. Therefore, the transmitter and receiver need to be designed to mitigate the channel effects and improve the performance of MC. The transmission of molecules is performed by a modulation scheme suitable for the requirements of MC.

The propagation of molecules in the medium is related to the molecule's size, geometry, type, and diffusion coefficient. The electric and magnetic properties of molecules also affect the transmission and reception processes. The chemical and physical properties of the medium may alter the propagation of charged or magnetically susceptible molecules. Furthermore, external factors such as an EMF affect the movement of molecules.

The characteristic features of molecules, i.e., chemical, physical or magnetic properties, can be employed as an external control mechanism in the transmission and reception processes. An MC system that employs acids, bases, and hydrogen ions is proposed in (Source: Farsad and Goldsmith, 2016). The information is encoded and transmitted

by the concentration of hydrogen ions. The concentration of hydrogen ions is controlled by emitting acid or base to the communication medium. The chemical reactions between acids, bases and hydrogen ions result in increases or decreases in the concentration of ions. The emission of acids and bases affects the pH level in the communication medium. Therefore, the receiver is designed to measure the pH level of the concentration of hydrogen ions. Furthermore, a charged and moving molecule can be manipulated by Lorentz force exerted under an EMF.

A magnetic force is applied to the magnetically susceptible molecules under an EMF. The magnetic susceptibility, i.e., paramagnetic, diamagnetic, or ferromagnetic, the spatial distribution, and the strength of the field affect the applied magnetic forces. A non-uniform electromagnetic field applies a magnetic field gradient force to the magnetically susceptible molecules. Furthermore, the magnetic energy of the system changes due to the magnetization of molecules. As a result, a concentration gradient magnetic force arises in the medium. The magnetic forces and the change in the magnetic energy of the system may increase or decrease the molecules' diffusion rate. Therefore, the strength and distribution of the EMF, the type, and the concentration of molecules can be utilized in manipulating molecules under an EMF.

Generally, the magnetic manipulation of molecules is employed in biomedical applications. The utilization of bio-nanomachines provides a more personalized approach to the diagnosis and treatment of diseases. Nano-sized, biocompatible particles are employed in various medical applications, such as the non-invasive detection of diseases and enhancing the accuracy of imaging techniques employed in the diagnosis. A non-invasive biopsy method is proposed in (Source: Patil et al., 2015). Since the biopsy of brain tumors is difficult, magnetic resonance imaging (MRI) is employed to diagnose brain cancer. In (Source: Patil et al., 2015), a new nanoimaging contrast agent is developed for the MRI. The magnetic properties of contrast agents enhance image accuracy. Therefore, the diagnosis of brain tumors can be accomplished by a non-invasive procedure. Furthermore, the magnetically steered nanorobots can be employed as MRI accuracy enhancement agents (Source: Martel et al., 2009). Externally controllable nanomachines are promising developments for targeted drug delivery systems. The size and biocompatibility of nanomachines are appropriate for such systems. Furthermore, the external control of nanomachines is an advantage for accurately delivering drugs. An artificial nanomachine

is developed in (Source: Zhang et al., 2009). The study indicates that magnetic nanorobots can be guided inside the water with a weak, rotating magnetic field. The magnetic control of the nanomachines results from the interaction between MF and the magnetic part of the nanomachine. In addition to the targeted drug delivery systems, the manipulation of magnetically labeled cells is utilized in tissue repair. In (Source: Kanczler et al., 2010), the gene expression in human bone marrow stromal cells is upregulated by activating magnetically labeled receptors on the cell membrane. A targeted tissue repair scheme is provided by the remote control of magnetically labeled cells.

In this chapter, an MC system that employs magnetically susceptible molecules is analyzed under an EMF. A binary communication scheme is modeled where the information is encoded and transmitted by the concentration of magnetically susceptible molecules. The magnetic properties of molecules provide control over the diffusion rate under an EMF. The magnetic field gradient and concentration gradient magnetic force alter the diffusion rate of magnetically susceptible molecules. Hence, the information rate of the MC changes. In Section 3.2, the molecular movement is studied under the magnetic field gradients. The effect of magnetic field gradient force is analyzed for paramagnetic and diamagnetic molecules. In Section 3.4, the concentration gradient magnetic force is studied to understand the effect of EMF on the diffusion rate of magnetically susceptible molecules. The conclusion of the chapter is presented in Section 3.5.

3.2. Molecular Diffusion under Magnetic Field Gradients

A magnetic field gradient is defined by the variation of the magnetic field across space. The strength of MFG changes depending on the distribution of MF. The non-uniform distribution of MF creates a suitable external control scheme for molecular systems. A comprehensive analysis of MFG on molecular mechanisms is presented in (Source: Zablotskii et al., 2016). Since most of the biological cells and tissues present diamagnetic attributes, a high MFG is considered to evaluate the effect of MF on cellular mechanisms. MFG exerts a magnetic gradient force on cells in the medium. The applied force affects cells according to their electrical and magnetic properties. For instance, every cell has a resting membrane potential regulated by the ion movement through the membrane. The effect of MFG alters the ion movement and depolarizes or hyperpolarizes

the membrane potential. Changes in the movement and concentration of ions inside and outside the cell affect many cellular processes like cell differentiation or death. Furthermore, the gap of a gated ion channel can be affected by the high MFG. The exposure time, strength, and distribution of MF are significant properties to determine the effect of MFG on cellular processes. In addition to the characteristics of MF, the effect of MFG also depends on the cell's type, state, and magnetic properties.

The effect of magnetic field gradient force is utilized in the external control of molecular systems. In (Source: Zablotskii et al., 2010), magnetically labeled nanoparticles (MNP) are employed in the design of targeted drug and gene delivery systems. The MF configuration, the MFG distribution, and the magnetic gradient force are studied to improve the performance and reliability of the system. An externally controllable MC system is proposed in (Source: Wicke et al., 2018). The system employs MNP to transmit binary information symbols. The external control of MNP is established by a magnet placed under the channel. The MF created by the magnet induces a magnetic drift and guides the particles in the diffusion direction. Therefore, molecular movement is modeled as diffusion with drift. The information is modulated with on-off keying. Moreover, the channel is designed as a two-dimensional and bounded medium to resemble a microfluidic channel. The impulse response is derived for the proposed channel. Furthermore, the symbol error rate is calculated to assess the performance of MC under MF. The analysis indicates that MF improves the system's performance. The drift induced by MF decreases the symbol error rate and increases the probability of MNP reaching the receiver.

An MF exerts a force on magnetically susceptible molecules' magnetic moment. This force is defined by

$$\overrightarrow{F} = \nabla \left(\overrightarrow{m} \cdot \overrightarrow{H} \right) \tag{3.1}$$

where m is the magnetic moment of the magnetically susceptible molecules and H is the magnetic field strength. In a uniform MF, the net force on the magnetic dipole moment is zero. However, molecules experience torque that is defined as

$$\overrightarrow{T} = \overrightarrow{m} \times \overrightarrow{H} \tag{3.2}$$

In a non-uniform MF, i.e., MFG, the net force on the magnetic dipole moment depends

on the gradient of MF. The magnitude of the force changes and affects the movement of molecules in accordance with their magnetic properties. The effect of uniform and non-uniform MF on a magnetic dipole moment is represented in Figure 3.1 (Source: Stöhr and Siegmann, 2006). Figure 3.1.(A) represents a magnetic moment, m, under a uniform MF. The forces applied to the magnetic dipoles of the magnetic moment, m, are equal to each other under a uniform MF. Therefore, torque is applied to the magnetic moment. Figure 3.1.(B) represents a magnetic moment under a magnetic field gradient. In this case, the net force applied to the magnetic moment is not zero. Therefore, a magnetic field gradient force is applied to the magnetic moment and changes the molecule's movement. The alteration in the molecular movement is proportional to the molecule's magnetic susceptibility and the magnetic field gradient.

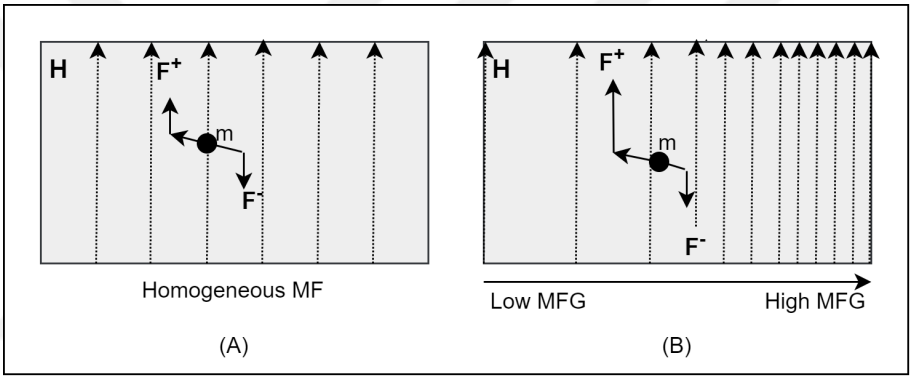

Figure 3.1. Force on a magnetic dipole moment in a uniform (A) and non-uniform (B) magnetic field (Source: Stöhr and Siegmann, 2006)

MFG force depends on MF's strength, molecules' magnetic properties, and concentration. An MF parallel to the medium causes convection and affects molecular movement. A perpendicular MF exerts an MFG force on molecules. The magnetic susceptibility of molecules affects the magnitude and direction of the MFG force. According to the molecule's magnetic properties, the MFG force opposes or is in the same direction as the molecular movement. Paramagnetic molecules move toward high MFG. However, diamagnetic molecules are repelled by high MFG. Figure 3.2 represents systems with magnetically susceptible molecules. As the distance between field lines decreases, the intensity of MFG increases. Figure 3.2.(A) represents the random distribution of molecules without MFG. Figure 3.2.(B) represents the distribution of molecules under MFG. Since the direction of MFG force depends on the magnetic susceptibility of molecules, the

concentration of paramagnetic molecules increases in the direction of the MFG. On the other hand, the concentration of diamagnetic molecules increases towards low MFG.

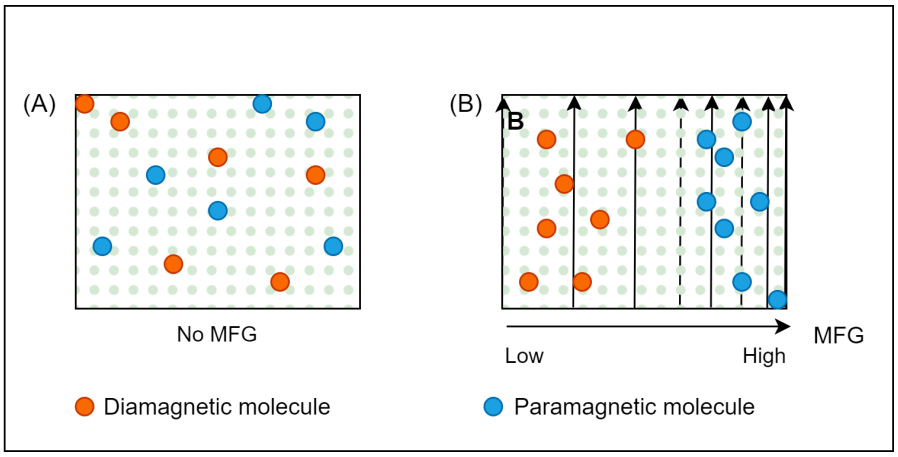

Figure 3.2. Distribution of paramagnetic and diamagnetic molecules without (A) and with (B) MFG

Mainly, MFG is utilized in the external control of molecular systems. The non-uniform distribution of MF provides manipulation of molecules depending on their magnetic properties. Systems that include magnetically susceptible molecules have magnetic energy. Magnetic energy is defined by the net magnetic moment and the strength of MF. The forces applied by MF affect the magnetic moment of molecules. Furthermore, the strength of MF varies according to its distribution. Therefore, the magnetic energy of a system that includes magnetically susceptible molecules changes under MFG. As a result, magnetically driven molecular flux is generated and provides control over the diffusion rate of molecules.

3.3. Concentration Gradient Magnetic Force

Various types of electric and magnetic fields are studied to understand the effect of these on living mechanisms (Source: Lei et al., 2020; Zablotskii et al., 2018; Blank and Goodman, 2002; Funk and Monsees, 2006). Electric fields are one of the first fields studied and employed in biology to understand and control living mechanisms. The rate of change in the electric field force is known to affect several cellular processes like membrane voltage, ion channel fluxes, and proliferation (Source: Levin, 2012; Tosen-

berger et al., 2015; Blackiston et al., 2009; Levin, 2014). Electric fields and gradients have several utilization areas like wound healing, targeted drug delivery, and inter or intracellular communication (Source: Levin et al., 2017; Pietak and Levin, 2017; McCaig et al., 2005; Ryan et al., 2021).

The effects of magnetic fields are also studied for molecular movement and biological mechanisms. In (Source: Kinouchi et al., 1988), the effects of static magnetic fields on particles in solutions are studied by considering the Lorentz force and Maxwell stress applied to the particles. It is stated that the magnetic field does not alter the movement of the particle unless the magnetic field strength is high. Similar to the electric field gradients, the rate of change in the magnetic field strength also causes a magnetic field gradient. Magnetically susceptible molecules are affected by MFG depending on their magnetic properties.

A magnetically susceptible molecule is magnetized under an MF. The magnetic susceptibility and permeability of the molecule determine the extent of the magnetization. The magnetic moment of the molecule changes due to magnetization. The net magnetic moment of a magnetically susceptible molecule and the strength of MF determine the energy of a system with magnetically susceptible molecules. Therefore, a change in the magnetic moment of molecules affects the system's magnetic energy. The change in the magnetic energy is proportional to the magnetization that is induced by the field, i.e., Eq. 2.12 (Source: Jackson, 1999). According to the magnetic susceptibility of the molecule, the magnetic energy increases or decreases. Hence, a molecular flux is induced to change the system's energy. This flux creates a concentration gradient of magnetically susceptible molecules. The concentration gradient of magnetically susceptible molecules results in a concentration gradient magnetic force. The magnitude and direction of the CGMF are proportional to the molecule's magnetic susceptibility and EMF's strength (Source: Zablotskii et al., 2013, 2016). The volume density of the concentration gradient magnetic force is given as

$$\vec{f} = \frac{\chi B^2}{2\mu_0}\vec{\nabla}C \tag{3.3}$$

where χ is the magnetic susceptibility of the molecule, B is the magnetic flux density, μ_0 is the vacuum permeability, C is the molar concentration of molecules, and ∇ is the gradient operator. In (Source: Zablotskii et al., 2021), the molecular movement under the

concentration gradient magnetic force is modeled as diffusion with drift and defined by

$$\frac{\partial C}{\partial t} = D\nabla^2 C - \left(\vec{\nabla} \cdot C\vec{u}\right) \tag{3.4}$$

where C is the molar concentration and $\vec{u}$ is the velocity of molecules. By substituting $u = \frac{D\vec{f}}{k_B T}$ into Eq. 3.4, we obtain

$$\frac{\partial C}{\partial t} = D_{eff}\nabla^2 C \tag{3.5}$$

where D_{eff} is the effective diffusion coefficient of molecules and defined as

$$D_{eff} = D\left(1 - \frac{\chi B^2}{2\mu_0 RT}\right) \tag{3.6}$$

$$= D\left(1 - \beta\right) \tag{3.7}$$

where D is the diffusion coefficient of a free molecule i.e., Eq. 2.14, $R = 8.31(J/Kmol)$ is the gas constant and $\beta = \frac{\chi B^2}{2\mu_0 RT}$. Since the magnetic field strength and the magnetic susceptibility of the molecules affect the diffusion coefficient, the diffusion rate of the molecules is expected to change with CGMF.

The extent of magnetization is different for paramagnetic and diamagnetic molecules. The magnetization of paramagnetic molecules is greater than diamagnetic molecules due to the unbound electrons. The alteration in the magnetic moment of paramagnetic molecules increases the magnetic energy of the system. Therefore, molecular flux arises in the opposite direction of diffusion to decrease the magnetic energy of the system. On the other hand, the change in the magnetic moment of diamagnetic molecules decreases the magnetic energy of the system. Hence, the magnetically driven molecular flux is induced in the same diffusion direction. The diffusion rate of molecules changes until the system reaches a steady state.

The change in the diffusion rate is expected to affect the concentration of information-carrying molecules. In (Source: Atakan and Akan, 2010), the concentration of molecules

is given as

$$Q_t = \frac{Q}{(4\pi D_{eff} t)^{3/2}} exp\left(-\frac{d^2}{4D_{eff}t}\right) \tag{3.8}$$

where d is the distance between transmitter and receiver, Q is the initial concentration of the magnetically susceptible molecules in the medium. The change in the diffusion coefficient caused by the concentration gradient magnetic force affects the concentration of information-carrying molecules inside a molecular communication channel. The concentration of magnetically susceptible molecules between transmitter and receiver NMs is simulated for different effective diffusion coefficients of magnetically susceptible molecules. The simulation parameters are represented in Table 3.1. Since diffusion coefficient cannot be negative, the effective diffusion coefficient is calculated when $\beta = 0.5$ for paramagnetic molecules and $\beta = -0.5$ for diamagnetic molecules.

Table 3.1. Simulation parameters for the concentration of magnetically susceptible molecules

Diffusion coefficient (D)	$10^{-6}(m^2/s)$
Distance between NMs (d)	$[0, 1]cm$
Permeability of free space (μ_0)	$4\pi \times 10^{-7}(H/m)$
Effective diffusion coefficient of magnetically susceptible molecules (D_{eff})	$D \times (1 - \beta)$
Gas constant (R)	$8.31(J/K \times mol)$
Temperature (T)	298 (K)
Boltzmann's constant (k)	$1.38 \times 10^{-23}(J/K)$

The concentration of paramagnetic molecules is presented in Figure 3.3. Due to the concentration gradient magnetic force, paramagnetic molecules' diffusion coefficient and concentration decrease. On the other hand, the diffusion coefficient and concentration of diamagnetic molecules increase under CGMF.

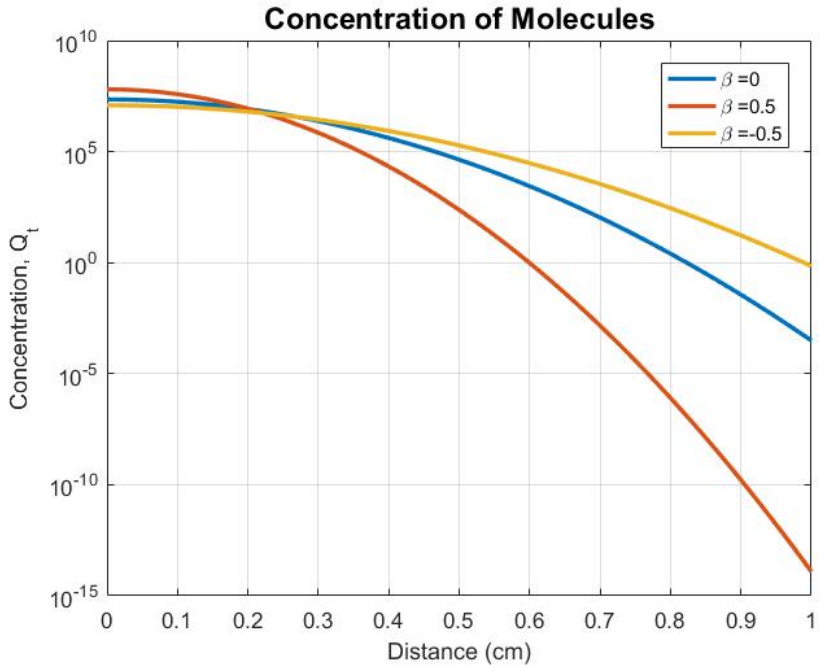

Figure 3.3. Concentration of magnetically susceptible molecules versus distance (cm) at $t = 1s$ for molecules with $D = 1\mu m^2/s$ from initial position $d_0 = 0$ under CGMF where $\beta = 0$ (no CGMF), $\beta = 0.5$ (paramagnetic molecules under CGMF) and $\beta = -0.5$ (diamagnetic molecules under CGMF)

The energy of a system under MF that consists of magnetically susceptible molecules is determined by the net magnetic moment of the molecules and MF's strength. The magnetization of paramagnetic and diamagnetic molecules affects the net magnetic moment. Therefore, the magnetic energy decreases or increases by introducing a concentration gradient magnetic force to the system. Since CGMF affects the molecule's velocity, the molecular movement under CGMF is modeled as diffusion with drift. The diffusion coefficient of molecules changes due to the alteration in the molecule's velocity. Since CGMF depends on the molecule's magnetic susceptibility, MF's strength, and the concentration gradient of molecules, the molecule's diffusion coefficient also changes proportionally to these parameters. Therefore, the magnetic field and concentration gradient magnetic field force introduces a drift to the system to conserve the magnetic moment, i.e., the magnetic energy of the system.

3.4. Molecular Communication under Concentration Gradient Magnetic Force

The MC system studied in this thesis employs magnetically susceptible molecules as information carriers. The proposed model considers a binary communication scheme defined in (Source: Atakan, 2013) and employs magnetically susceptible molecules as information carriers. The transmitter emits molecules for bit 1 and no molecules for bit 0. The transmission of bit 1 starts with emitting molecules to the medium. If the receiver obtains the molecules within the slot duration, the reception is complete, and bit 1 is successfully transmitted. In the transmission of bit 0, the transmitter does not emit any molecule. The receiver receives no molecules within the slot duration for a successful bit 0 reception. Molecules are assumed to perform normal diffusion under CGMF. Therefore, molecular movement is modeled with Brownian motion. The time delay experienced by molecules in the medium is given by

$$f(t) = \frac{d}{\sqrt{4\pi D_{eff} t^3}} e^{-\frac{d^2}{4D_{eff}t}}, \quad t > 0 \tag{3.9}$$

where d is the distance between transmitter and receiver and D_{eff} is the effective diffusion coefficient of molecule under CGMF. And the cumulative distribution function for the time delay is given as

$$F(t) = Erfc\left(\frac{d}{2\sqrt{D_{eff}t}}\right), \quad t > 0 \tag{3.10}$$

The delay experienced by molecules affects the probability of successful reception of molecules at the receiver. Therefore, the change in the diffusion coefficient of molecules affects the transmission and reception probabilities.

In the binary communication scheme, bit 1 is transmitted with the probability β_n, and bit 0 is transmitted with $(1 - \beta_n)$ at slot n. A molecule that is transmitted at slot n may not reach the receiver in the specified slot duration. However, molecules still diffuse until they reach the receiver. Therefore, any molecule transmitted in previous slots may

reach the receiver in slot n. The probability of a previously transmitted molecule reaching the receiver in slot n is defined as

$$\lambda_{nk} = \beta_k \left[F\left((n-k+1)\,\tau \right) - F\left((n-k)\,\tau \right) \right], \quad k < n \tag{3.11}$$

where k is the previous slot number defined as $k \in \{1, 2, \cdots\cdots, n-1\}$, β_k is the probability of transmitting a molecule that does not reach the receiver in slot k. The molecules transmitted in slot k but received at slot n introduce noise to the system. The total noise at slot n is defined as

$$Z_n = \sum_{k=1}^{n-1} \Gamma_{n,k} \tag{3.12}$$

where $\Gamma_{n,k} \sim Bernoulli\left(\lambda_{nk}\right)$ and defines the molecules emitted at slot k is received i.e., λ_{nk} or not received i.e., $(1-\lambda_{nk})$ by receiver at slot n. Therefore, the channel output can be defined as

$$Y_n = G_n + Z_n \tag{3.13}$$

where G_n is the input that defined by $G_n \sim Bernoulli\left(\beta_n F\left(\tau\right)\right)$ and Z_n is the noise at slot n. Since Y_n is defined in the range $\{0, 1, 2, \cdots, n\}$ and noise in the range $\{0, 1, 2, \cdots, n-1\}$, they can be described as *Poisson-Binomial* random variables with probability mass function given as

$$p_i = \sum_{A \epsilon S_i} \prod_{k \epsilon A} \lambda_{nk} \prod_{j \epsilon A^c} \left(1 - \lambda_{nj}\right) \tag{3.14}$$

$$q_i = \sum_{B \epsilon T_i} \prod_{l \epsilon B} \lambda_{nl} \prod_{m \epsilon B^c} \left(1 - \lambda_{nm}\right) \tag{3.15}$$

where S_i and T_i define the sets that includes all subsets of i integers that can be selected from $\{1, 2, \cdots n\}$ and $\{1, 2, \cdots n-1\}$, respectively. A and B refer to the elements of S_i and T_i. A^c and B^c refer to the complements of A and B defined as $A^c = \{1, 2, \cdots n\} \setminus A$ and $B^c = \{1, 2, \cdots n-1\} \setminus B$.

The channel capacity is the maximum achievable information rate that is transmitted in the medium and is defined as

$$C = max I\left(X_n, Y_n\right) \tag{3.16}$$

where $I\left(X_n, Y_n\right)$ is the mutual information between channel input and output. The mutual information of the channel input and output is defined as

$$I\left(X_n, Y_n\right) = H\left(Y_n\right) - H\left(Y_n \mid X_n\right) \tag{3.17}$$

Since channel input i.e., X_n and noise i.e., Z_n is independent, the mutual information can be written as

$$I\left(X_n, Y_n\right) = H\left(Y_n\right) - H\left(Z_n\right) \tag{3.18}$$

$$= -\sum_{i=0}^{n} p_i log p_i + \sum_{i=0}^{n-1} q_i log q_i \tag{3.19}$$

The maximum achievable MC rate can be obtained by an optimal transmission probability. In (Source: Atakan, 2013), the optimal transmission probability that maximizes the mutual information is derived as

$$\widehat{\beta_n} \approx \frac{-\delta + F\left(\tau\right)\sqrt{\left[\delta - F\left(\tau\right)^2\right] - 4\left(1 - q_0\right)\left[-\delta F\left(\tau\right) + F\left(\tau\right)q_0 + F\left(\tau\right)^2 q_0\right]}}{2\left[-\delta F\left(\tau\right)F\left(\tau\right)q_0 + F\left(\tau\right)^2 q_0\right]} \tag{3.20}$$

The probability of bit 1 transmitted at the slot successfully reaching the receiver in the slot duration is defined as $\beta_n F(\tau)$. Since $F(\tau)$ is a constant probability, optimizing β_n is sufficient to find the optimal transmission probability. However, the probability of time delay experienced by molecules, i.e., $F(\tau)$, depends on the molecule's diffusion coefficient. Therefore, the effect of CGMF on the diffusion coefficient of magnetically susceptible molecules changes the diffusion coefficient and the propagation of molecules in the medium. Therefore, the maximum information rate of MC is altered under EMF due to the concentration gradient magnetic force.

3.5. Conclusion

This chapter focuses on MC systems under EMF. Mainly, MC systems under MF are studied to determine the effect of magnetic forces' effects on MC rate. In this thesis, the information is transmitted with magnetically susceptible molecules in the proposed MC system. The change in information rate is studied by considering the applied magnetic forces. MF's configuration and distribution are significant in determining the direction and magnitude of the applied magnetic force. Since a parallel MF only introduces convection to the medium, a perpendicular MF is considered to analyze the effects of magnetic forces on molecular diffusion. Magnetic properties of molecules present the possibility of control over the system. Therefore, a non-uniform EMF distribution is considered to obtain MFG in the medium.

The strength of a heterogeneous EMF varies across the field and results in MFG. The effect of applied magnetic forces changes with respect to MF's strength. Therefore, the effect of MFG force varies according to the molecule's type and MF's strength. Paramagnetic molecules are attracted, and diamagnetic molecules are repelled by high MFG. If the concentration and MF gradient are in the same direction, the MFG force is in the same direction with diffusion for paramagnetic molecules. However, the direction of the MFG force opposes the diffusion direction for diamagnetic molecules. The effect of MFG on the concentration gradient of paramagnetic and diamagnetic molecules alters the system's magnetic energy.

System's magnetic energy is defined by the net magnetic moment and MF's strength. A non-uniform MF and magnetically susceptible molecules affect the net magnetic moment. Hence, the magnetic energy of the system changes depending on the magnetization and interaction of molecules. Therefore, the conservation of the system's magnetic energy is achieved by a flux of magnetically susceptible molecules. A concentration gradient magnetic force is introduced to the system to obtain a magnetically driven molecular flux.

Molecular movement under CGMF is modeled as diffusion with drift. Therefore, CGMF affects the molecule's velocity. The solution of diffusion with drift by considering the effect of CGMF on the molecule's velocity yield a change in the molecule's diffusion coefficient. The effect of CGMF on the molecule's diffusion coefficient is proportional to the molecule's magnetic susceptibility and MF's strength. Therefore, the diffusion

coefficient of paramagnetic molecules decreases, and diamagnetic molecules' diffusion coefficient increases under CGMF. Paramagnetic molecules' concentration decreases, and the concentration of diamagnetic molecules is expected to increase with respect to the diffusion coefficient of molecules. Though a decrease in the concentration of paramagnetic molecules is observed, diamagnetic molecules' concentration does not increase as expected. However, the decrease in the concentration of diamagnetic molecules is lower than in paramagnetic molecules. The change in the diffusion coefficient of molecules also affects the time delay experienced by molecules in the medium. The probability of successful information transmission is altered due to the CGMF. Hence, the maximum achievable information rate changes according to MF's strength, distribution, and the type of information-carrying molecules.

CHAPTER 4

MOLECULAR COMMUNICATION SYSTEMS UNDER ELECTROMAGNETIC FIELDS

Molecular communication is a process that information molecules are sent from one or multiple transmitters to receiver nanomachines. The physical and chemical properties of information-carrying molecules are significant for the performance of MC. The transmitter and receiver design and characteristics may change according to these properties. For instance, a protein's folding mechanism affects the molecule's active region. Protein's three-dimensional structure affects the reception and propagation processes. Hence, the reaction dynamics at the receiver nanomachine changes (Source: McCammon, 1984; Enomoto et al., 2011). Moreover, the concentration of molecules can be employed as a modulation scheme (Source: McGuiness et al., 2019; Kuran et al., 2011; Mahfuz et al., 2016).

An MC system has five fundamental steps: encoder, transmitter, channel, receiver, and decoder. In the encoder part, messages are translated into information molecules. Information can be encoded in various characteristics of molecules, such as a specific DNA sequence (Source: Gregori et al., 2011) or concentration of neurotransmitters (Source: Balevi and Akan, 2013; Veletić et al., 2016; Khan et al., 2017). Furthermore, the release time of molecules can also be employed in encoding (Source: Murin et al., 2017a). The transmitter is a bio-nanomachine that emits information molecules to the communication medium. There are various modulation methods to encode and transmit information through the medium. These methods are analogous to the modulation schemes in traditional communication. The molecular emission could be instantly and continuously. Furthermore, the number and type of molecules vary in different modulation schemes. The on-off shift keying (OOK) is applied to the molecular communication by emitting a certain number of molecules while sending bit 1 and no molecular emission when sending bit 0 (Source: Mahfuz et al., 2010). The information could be modulated by employing the concentration of molecules. Concentration shift keying (CSK) is a modulation method that the information is encoded and transmitted by the instant emission of molecules.

Furthermore, different types of molecules can also be employed in transmission. In molecular shift keying (MoSK), the type of information-carrying molecules changes. In a binary communication scheme, information is transmitted by the modulation of molecule type A for bit 1. The transmission of bit 0 is done through the modulation of molecule type B (Source: Kuran et al., 2012). The release time shift keying is employed in timing channels where the information is encoded to the emission time of molecules (Source: Srinivas et al., 2012).

In the communication channel, molecules propagate through the medium by diffusion, i.e., passive MC (Source: Atakan, 2016), or actively transported by another molecule, i.e., active MC (Source: Moore et al., 2006; Farsad et al., 2011). The channel characteristics are significant in the design of the communication system. The transmitter and receiver need to compensate for the noise and inter-symbol interference (ISI) in the channel (Source: Pierobon and Akyildiz, 2012; Mahfuz et al., 2011). Receivers are bio-nanomachines that capture information molecules in the medium. The reception process can be carried out through permeable surfaces, i.e., passive receivers. Receptors for specific molecules may also react with the information molecules in the medium, i.e., active receivers (Source: Noel et al., 2016, 2014a; Kilinc and Akan, 2013). Decoders are the part where captured molecules react with the receiver nanomachine. This reaction may lead to the production of new molecules or physical and chemical changes in the receiver nanomachine. Many detection designs and algorithms are proposed to deal with the effects of transmission, channel, and reception processes (Source: Noel et al., 2014b; Meng et al., 2014; Murin et al., 2017b). Each part needs to be designed considering the stochastic nature of molecules (Source: Nakano et al., 2013).

An interdisciplinary approach that includes communication engineering, bioengineering, and natural sciences enhances the design and analysis of MC and benefits various research areas. The research in targeted drug delivery systems is escalated in recent years. These systems are designed to focus the drug delivery process on a targeted region. In this way, the side effects of the drugs are reduced. An MC model is derived for a targeted drug delivery system in (Source: Chahibi and Akyildiz, 2014). In this model, a computer-controlled syringe is employed as a transmitter nanomachine. The cardiovascular system is the propagation channel which emitted drug molecules diffuse through. The cell in the targeted area is employed as a receiver. The noise in all stages

in the MC system is analyzed to present an optimized, targeted drug delivery system. An MC model is presented for an endocrine nanonetwork in (Source: Malak and Akan, 2012). The MC system includes glands as a transmitter, the bloodstream as a channel, and the targeted cell as a receiver. These types of systems could be utilized in hormone regulation processes.

MC can be utilized in wound healing applications as well. Wound healing is a process of repairing the damaged skin and the tissues beneath the wound site. It is a sequential biochemical event that leads to tissue regeneration. An MC model can be designed where two cells in the wound site act as a transmitter and receiver. The extracellular medium is the communication channel, and specific proteins produced in the wounded site can be information-carrying molecules (Source: Levin, 2012). Another significant part of wound healing is the appropriate distribution and development of cells in the three-dimensional tissue structure. An MC nanonetwork between cells can affect cell assembly and control tissue regeneration (Source: Levin, 2007). In addition to biological and medical applications, MC can improve the reliability and applicability of various environmental applications to detect contamination and pollution (Source: Giné and Akyildiz, 2009).

EMFs have a wide range of applications in medical devices and therapeutic applications. Magnetic resonance imaging (MRI), microwave imaging, radar monitoring, magnetotherapy, and therapeutic ultrasound are EMF applications in medicine. The developments in medicine have increased the use of medical devices. Therefore, understanding the effects of EMF on the human body and biological structures has become a significant research interest. In addition to the external EMF, biological structures also have an internal biofield. Endogenous fields play an essential role in inter and intra-cellular communication, cell migration, and orientation (Source: Hammerschlag et al., 2015). These studies suggest that EMF affects molecular structures and movement. Furthermore, any change in the temperature may change the molecular or environmental properties.

Electromagnetic fields affect and interfere with various processes and materials' physical, chemical, and biological properties. The interaction between EMF and materials is based on electric and magnetic forces. These forces cause an energy transfer. The transferred energy causes a temperature increase in the exposed area. Due to the increased temperature, the diffusion coefficient and the kinetic energy of molecules change.

The number of collisions between molecules increases and alters molecular movement's direction. Hence, molecules behave differently under an EMF.

In an MC system, molecular movement and communication medium is significant for communication performance. The increase in the temperature affects the molecules' energy and binding kinetics. Therefore, the transmission and reception rate of molecules changes. The directional effect of EMF affects the velocity and displacement of molecules. Furthermore, the thermal and directional changes also affect the type of diffusion. In this chapter, the effect of EMF on molecular communication is studied by considering the temperature change in the environment and the directional effects of EMF on molecular movement. Furthermore, EMF's effect on the type and characteristics of diffusion is also considered. In section 4.1.1, molecular communication systems are studied as reaction-diffusion systems to evaluate the temperature effect on chemical reaction rate. Section 4.2 focuses on the molecular movement under EMF by considering molecules' velocity, displacement, and mean-squared displacement. In section 4.3, we conclude the EMF effect on molecular movement and binding kinetics.

4.1. Energy Transfer under Electromagnetic Field

The interaction between EMF and particles is the result of applied electromagnetic forces. Furthermore, some energy is transferred through the charges. This energy transfer happens in the form of heat energy in molecular interactions. The movement of molecules caused by thermal fluctuations is defined as diffusion. A change in temperature affects the thermal fluctuations experienced by molecules. As a result, the number of molecules diffusing through the medium also changes. The diffusion coefficient specifies the amount of diffusing molecules through a unit area in time and is directly proportional to temperature. Therefore, EMF affects the diffusion coefficient and flow of molecules. Furthermore, the mean position of the molecules changes more rapidly. The probability of collision between molecules increases. As the number of collisions increases, the torque applied to the molecule also increases (Source: Kaviany, 2014). A simple example to explain the relation between heat and molecular movement is represented in Figure 4.1. Heat source increases the temperature of the system. Due to the change in the molecule's kinetic energy, thermal fluctuations experienced by molecules increase. The molecular

bonds and structure is altered, and the state of the system changes.

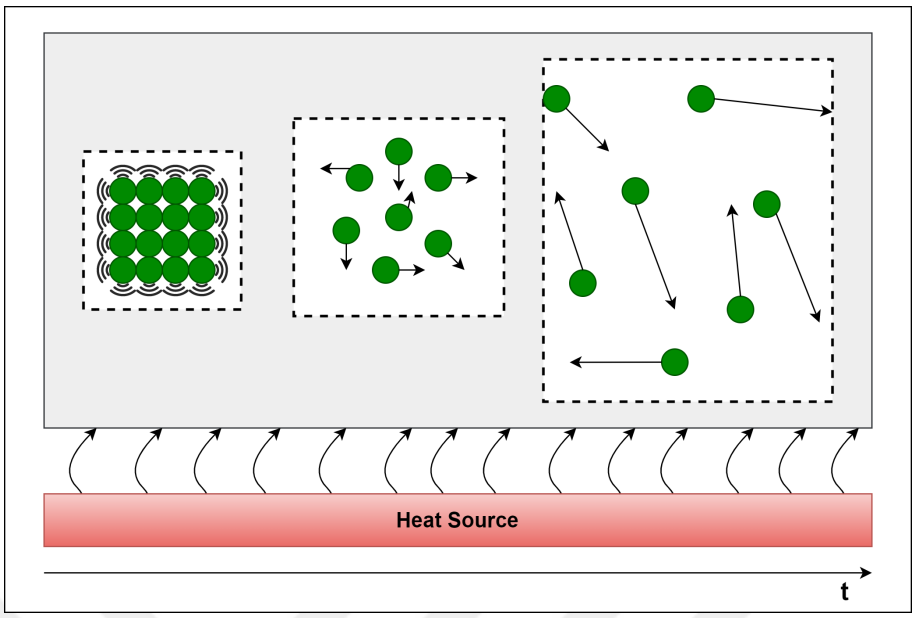

Figure 4.1. The effect of heat transfer on molecules (Source: Kaviany, 2014)

The distribution of transferred energy differs for different types of tissues and EMFs. The geometry, density, conductivity, and homogeneity of tissues are important to assess the temperature increase caused by the EMF. Specific absorption rate (SAR) is employed as a measure for temperature increase in tissues (Source: Furse et al., 2009). It defines the energy absorbed by unit EMF exposed mass. SAR is defined by

$$SAR = \frac{\sigma |E|^2}{\rho} \tag{4.1}$$

where σ is the tissue conductivity, E is the electric field, and ρ is the tissue density. The SI unit for SAR is watt per kilogram (W/kg). There are universal guidelines and limits for suitable SAR values (Source: Lin, 2003).

The strength, frequency, and exposure time of the EMF affect the temperature distribution in the exposed area. Heat transfer in tissues is a heat conduction process that includes blood circulation, metabolic heat generation, and heat dissipation. Any temperature change may affect the blood flow and change the thermoregulation of the tissue. The temperature distribution in the tissue is governed by the bio-heat transfer equation (Source: Pennes, 1948). The bio-heat transfer equation is based on the thermal

energy balance and derived as

$$\rho c \frac{\partial T}{\partial t} = \nabla \left(k \nabla T \right) + q_s + q_p + q_m \tag{4.2}$$

where ρ is the tissue density, c is the tissue's specific heat capacity, and k is the heat conduction coefficient of the tissue. The variables q_s, q_p, q_m differ for each analysis depending on the source and exposed body area. They represent heat loss by absorption, i.e., q_s, blood perfusion, i.e., q_p, and metabolic heating, i.e., q_m. The effect of EMF in tissues is studied by considering the SAR value and the resulting temperature increase. In (Source: Bernardi et al., 2003), the SAR value induced by an EMF in the 10-900 MHz frequency range is calculated with the finite difference time domain method. As a result, $0.7°C$ temperature increase is observed in the muscle tissue. The temperature increase caused by EMF exposure to the human head is studied in (Source: Bernardi et al., 2000). The exposure region is limited to the brain and ear. A regular cell phone is employed for EMF exposure. The effect of EMF is maximum in the external part of the brain with a SAR value of 1 W/kg and temperature increase in the range of 0.10 to 0.16 $°C$. These studies indicate that EMF causes a temperature increase in the tissues. However, the amount of transferred energy and temperature increase depends on several parameters of the tissues and EMF.

Every process in the human body can be modeled as an MC system. The neural system employs neurotransmitters as information carriers. Hormones are emitted from glands to the bloodstream in the endocrine system for various communication and regulation mechanisms in the body. The temperature distribution and transferred energy are significant for the performance of MC. The molecular movement and binding kinetics affect the transmission and reception of molecules. Therefore, any temperature change in the medium may affect the information rate of MC.

4.1.1. Temperature Change Under Electromagnetic Fields

The random fluctuations of molecules present a dynamic behavior that is discrete and stochastic. Since molecules interact, the molecular systems can be modeled

as reaction-diffusion systems. Generally, the system is assumed to be well-stirred and in a state of thermal equilibrium. This assumption allows specifying the state of the system rapidly. If this assumption is invalid, molecular dynamics and positions must be considered to define the system's state. Initially, deterministic reaction rate equations (RRE) are employed to analyze reaction-diffusion systems (Source: Gillespie, 1977, 1976). However, RRE is suitable for large molecular populations. Later, stochastic differential equations are employed to model particle-based molecular systems' chemical kinetics mathematically. The basis for stochastic chemical kinetics is established by the chemical master equation (CME) defined in (Source: Gillespie, 1992). CME provides the time-evolution and state changes of the molecules in a reaction-diffusion system. CME can be solved for the systems in the simplest form only. A degradation i.e., Eq 4.3, or a simple transformation reaction i.e., Eq 4.4, are examples of such simple system.

$$S \rightarrow \varnothing \tag{4.3}$$

$$S_a \rightarrow S_b \tag{4.4}$$

For more complex systems, CME does not have any closed-form solution. CME can be solved numerically for higher order systems that are given as

$$S_a + S_b + S_c \rightarrow S_d + \cdots \tag{4.5}$$

CME forms the basis for many simulation algorithms of molecular dynamics. Furthermore, sample trajectories of the stochastic process in state space can be computed numerically by employing a Monte Carlo simulation of CME. The time-evolution and probabilistic behavior of the molecules are defined by CME, is given as

$$\frac{\partial}{\partial x} P\left(\boldsymbol{n}, t \mid \mathbf{n}_0, t_0\right) = \sum_{\mu=1}^{M} \left[c_\mu h_\mu\left(\mathbf{n} - \mathbf{v}_\mu\right) P\left(\mathbf{n} - \mathbf{v}_\mu, t \mid \mathbf{n}_0, t_0\right) - c_\mu h_\mu\left(\mathbf{n}\right) P\left(\mathbf{n}, t \mid \mathbf{n}_0, t_0\right)\right] \tag{4.6}$$

where $\mathbf{n} \equiv (n_1, n_2 \cdots, n_N)$ is the vector notation for the molecular population of N molecule species before reaction, $h_\mu\left(\mathbf{n}\right)$ is the number of reactant molecule combinations,

$\mathbf{v}_\mu$ is the difference in the molecular population after reaction and c_μ is a constant that defines the occurrence probability for the chemical reaction. Complete modeling of the chemical reaction and molecular behavior in the reaction channel can be described by CME. The specific probability rate constant i.e., c_μ is significant for the reaction channel and defined by

$$c_\mu = \Omega^{-1} \left(\frac{8 k_b T}{\pi m^*} \right)^{1/2} \pi \left(r_a + r_b \right)^2 p_\mu \tag{4.7}$$

where Ω is the volume of the reaction channel, k_b is the Boltzmann constant, T is the absolute temperature, m^* is the reduced mass of two reactants, r_a and r_b is the radius of reactant molecules. The probability that a randomly selected two colliding molecules will react is defined as p_μ and defined by

$$p_\mu = \frac{\omega_a \omega_b}{(4\pi)^2} \tag{4.8}$$

The CME and specific probability rate constant express that molecular reactions highly depend on the temperature and spatial distribution of the reactant molecules and can be disturbed by any change in these parameters. Furthermore, the active regions of molecules also affect the collision probability of molecules. The active regions of two reactant molecules, A and B, are represented in Figure 4.2.

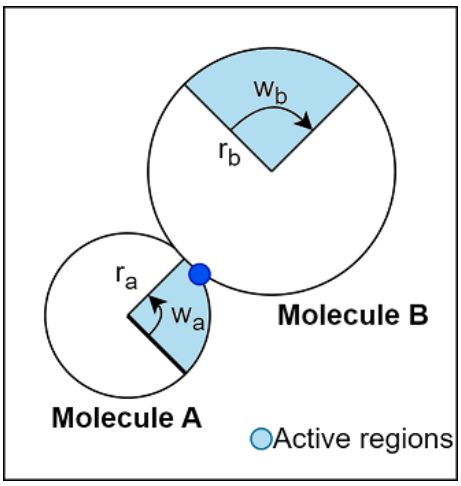

Figure 4.2. Active regions of reactant molecules A and B (Source: Gillespie, 1992)

A bimolecular reaction is considered to see the effect of temperature change on the specific rate constant. Simulation parameters are represented in Table 4.1.

Table 4.1. Simulation parameters for specific reaction constant

Volume of reaction channel (Ω)	$2 \times 10^{-3}(m^3)$
Boltzmann's constant (k_b)	1.38×10^{-23} (J/K)
Temperature (T)	$[273, 500]$ (K)
Mass of reactant A (m_a)	$0.04(kg/mol)$
Mass of reactant B (m_b)	$0.002(kg/mol)$
Radius of reactant A (r_a)	0.139×10^{-9} (m)
Radius of reactant B (r_b)	0.12×10^{-9} (m)
Active region angles of reactants A and B	$\pi/2$

Figure 4.3. represents the change of specific reaction rate constant for a range of temperature values. The simulation results indicate that a substantial temperature increase is required for a considerable change in the specific reaction rate constant.

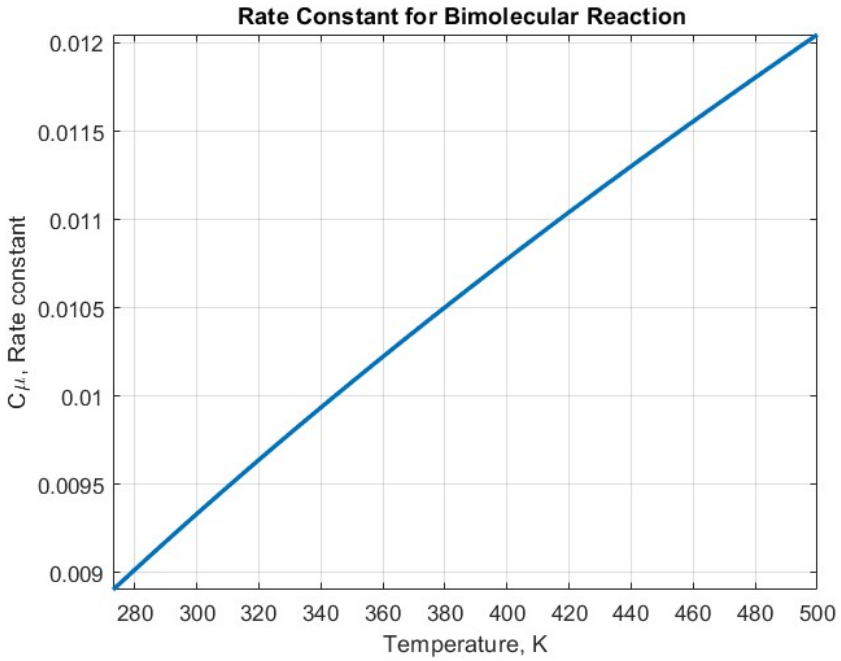

Figure 4.3. Specific reaction rate constant c_μ (mol/s) versus temperature T (K)

Since molecules react in proportion to their active regions, the specific reaction rate constant is analyzed for different active region angles. The effect of active region angles on specific reaction rate constant is represented in Figure 4.4. As the angle of the active reaction region increases, the specific reaction rate constant also increases.

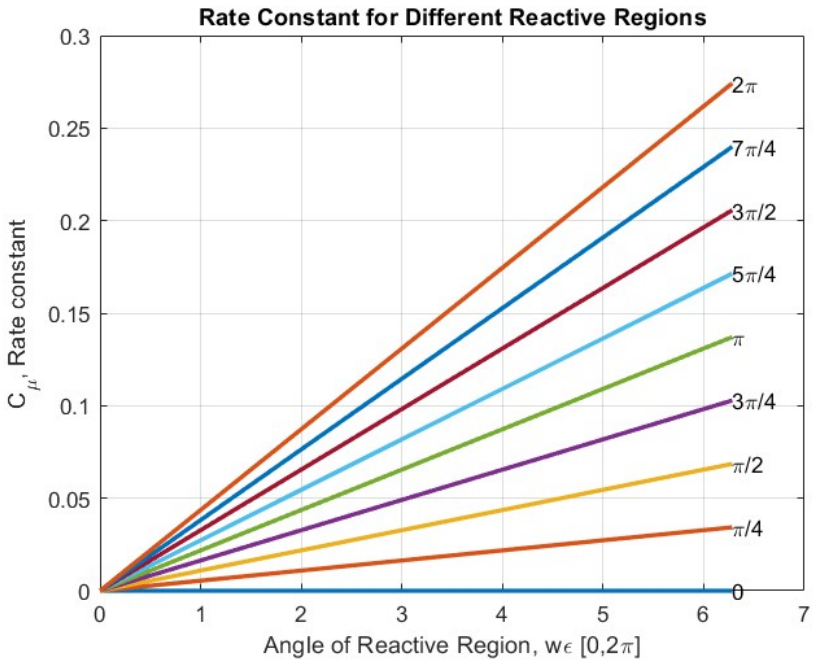

Figure 4.4. Specific reaction rate constant c_μ (mol/s) versus active region angles (rad/s) at T=300 K

The electromagnetic forces applied by the EMF affect the kinetic energy of molecules. The change in the energy increases the temperature. Therefore, the molecular movement and reaction energetics is altered. The transferred energy affects the molecule's displacement and velocity. Furthermore, the dependency of the diffusion coefficient on the temperature indicates that diffusion changes proportionally. As a result, the probability of molecular reactions increases. Therefore, the specific rate constant is studied to understand the effect of temperature change on molecular reactions.

The dissipation of heat energy varies depending on the molecular structure's chemical, physical and biological characteristics. Therefore, the literature on temperature distribution caused by heat transfer consists of studies for specific tissues. Mainly, muscle, fat, bone, and skin tissues are studied to improve the utilization of EMF in medicine. Temperature distribution in tissues is affected by several external factors. The EMF source and the physical and chemical properties of the exposed area are essential to determine the temperature distribution. Furthermore, blood circulation and metabolic heating need to be considered to evaluate the thermal regulation in tissues. The theoretical and experimental studies with different EMF sources indicate that EMF exposure causes a small increase in the temperature of the exposed area. Moreover, the temperature change caused by

the EMF does not significantly affect the specific reaction rate constant and the collision probability of molecules.

4.2. Molecular Diffusion under Electromagnetic Field

The Fickian theory of diffusion describes the molecular behavior on the macroscale. An improved theory of diffusion that analyzes the probabilistic behavior of each molecule is introduced by Einstein (Source: Einstein, 1956). The random movement of molecules is modeled as Brownian motion. Molecules experience random collisions with solvent molecules. These collisions occur in a time interval that is infinitesimally small for a macro scale system. On the other hand, the time interval is large enough for molecules to collide in a micro-scale system (Source: Gillespie and Seitaridou, 2013). However, Einstein's theory of diffusion is not valid for small timescales. Langevin's theory of diffusion enhances Einstein's theory for all time scales (Source: Langevin, 1908). The effect of the environment on the molecule is modeled by considering the viscous friction force and the fluctuating force. The viscous friction force is defined by the dynamic friction coefficient β. The fluctuating force models the effect of collisions between molecules and surrounding fluid. It is characterized as a stationary random process.

In this section, the diffusion of molecules under EMF is modeled in all time scales with regard to Langevin's theorem. The molecule's velocity and displacement are studied to model the molecular behavior comprehensively. Furthermore, the effect of EMF on the diffusion type is investigated.

Langevin's diffusion theory presents a proper analysis of molecular behavior for all time scales (Source: Gillespie and Seitaridou, 2013). In small-time scales, the state of the molecular system is highly affected by thermal fluctuations. These effects are compensated over time, and the molecular system reaches a steady state. Naturally, this is not the case for every molecular system. In (Source: Gillespie and Seitaridou, 2013), these types of systems that are unsteady in the beginning and reach a steady state over time are defined as overdamped systems. In an overdamped system, the friction is high, and the inertia is low. In other words, the friction coefficient ($\beta = \frac{\gamma}{m}$) is much larger than the molecule's mass. And the condition that examines this property of the system is given

as

$$\left| m\frac{\partial u(t)}{\partial t} \right| \ll |\gamma u(t)| \tag{4.9}$$

where γ is the drag coefficient of the system and defined by Stokes' law as

$$\gamma = 6\pi r\eta \tag{4.10}$$

where r is molecule's radius and η is viscosity of the fluid. A comparison between the friction coefficient of the medium and the molecule's mass is performed to understand the state of the molecular system. For a molecular bead with radius $r = 0.145\mu m$ in a viscous fluid with viscosity $\eta = 10^{-3}$ kg/m.s, β is much larger than the molecule's mass. Therefore, a system that involves a micron-sized molecular bead in a viscous environment is overdamped. Furthermore, the time limit, i.e., τ, that the system changes its behavior is determined by calculating $1/\beta$ (Source: Chandrasekhar, 1943). The time limit for the overdamped molecular system is equal to 4.9×10^{-9} s.

In (Source: Chandrasekhar, 1943), the Brownian motion of a molecule is studied in free space and under a force field. Langevin's equation given in Eq. 4.11 is considered the definition of a free molecule's motion. Langevin's equation describes the relationship between the rate of change in the molecule's velocity, dynamic friction, and fluctuation caused by the Brownian motion.

$$\frac{\mathrm{d}u}{\mathrm{d}t} = -\beta u + A\left(t\right) \tag{4.11}$$

where u is the velocity of the molecule, $A(t)$ is the fluctuating force, and β is the dynamic friction coefficient. $A(t)$ describes the fluctuating friction of the molecule in the system due to the characteristic behavior of Brownian motion. Furthermore, it is specific to the molecule.

A new acceleration term is introduced to Langevin's equation to consider the effect of a force field on a molecule, and Eq. 4.11 is rewritten as

$$\frac{\mathrm{d}u}{\mathrm{d}t} = -\beta u + A\left(t\right) + K\left(r,t\right) \tag{4.12}$$

where $K(r,t)$ represents the acceleration effect caused by the force field. The solution of Eq. 4.11 and Eq. 4.12 leads to the probability distribution functions for the molecule's velocity and displacement. The behavior of a free molecule and a molecule under a force field can be modeled with these probability distribution functions. The probability of occurrence of molecule's velocity is specified by

$$W\left(u,t;u_0\right)=\left(\frac{m}{2\pi kT\left(1-e^{-2\beta t}\right)}\right)^{\frac{3}{2}}exp\left(\frac{-m|u-u_0e^{-\beta t}|^2}{2kT\left(1-e^{-2\beta t}\right)}\right) \tag{4.13}$$

where u is the molecule's velocity, m is the mass of the molecule, k is the Boltzmann's constant, T is the temperature in Kelvin, β is the dynamic friction coefficient and u_0 is molecule's initial velocity. As $t >> \frac{1}{\beta}$ i.e., the system is at a steady state, $W(u,t;u_0)$ becomes

$$W\left(u,t;u_0\right)\rightarrow\left(\frac{m}{2\pi kT}\right)^{\frac{3}{2}}exp\left(\frac{-m|u|^2}{2kT}\right) \tag{4.14}$$

The probability distribution function of molecule's displacement is obtained as

$$W\left(r,t;r_0,u_0\right)=\left(\frac{m\beta^2}{\left(2\pi kT\left[2\beta t-3+4e^{-\beta t}-e^{-2\beta t}\right]\right)}\right)^{\frac{3}{2}}exp\left(-\frac{m\beta^2|r-r_0-u_0\left(1-e^{-\beta t}\right)/\beta|^2}{2kT\left[2\beta t-3+4e^{-\beta t}-e^{-2\beta t}\right]}\right) \tag{4.15}$$

where r_0 is the molecule's initial position. As $t >> \frac{1}{\beta}$, $W(r,t;r_0,u_0)$ becomes

$$W\left(r,t;r_0,u_0\right)\simeq\frac{1}{\left(4\pi Dt\right)^{\frac{3}{2}}}exp\left(\frac{-|r-r_0|^2}{4Dt}\right) \tag{4.16}$$

where r is the displacement of molecule and *D* is the diffusion coefficient and defined by Eq. 2.14. As the system reaches a steady state, i.e., large timescales, the probability distribution function of the molecule's velocity and displacement does not depend on its initial velocity, i.e., Eqs. 4.14 and 4.16.

Probability distribution functions for the molecule's velocity and displacement under a force field are obtained by solving Eq. 4.12. The force field is defined as a one-dimensional harmonic oscillator. Hence, the Langevin equation given in Eq.4.12 is rewritten as

$$\frac{\mathrm{d}\mathbf{u}}{\mathrm{d}t}=-\beta\mathbf{u}+A\left(t\right)-\omega^2x \tag{4.17}$$

where ω defines the circular frequency of the oscillator. The solution of Eq. 4.17 gives the probability distribution for the molecule's displacement and velocity under a force field.

The probability distribution of displacement under the force field is given as

$$W\left(x,t;x_0,u_0\right)=\left[\frac{m}{4\pi\beta kT\int_0^t\psi^2\left(\xi\right)d\xi}\right]^{\frac{3}{2}} exp\left(-\frac{\left(x-x_0e^{\frac{-\beta t}{2}}\left[\cosh\frac{1}{2}\beta_1t+\frac{\beta}{\beta_1}\sinh\frac{1}{2}\beta_1t\right]-\frac{2u_0}{\beta_1}e^{\frac{-\beta t}{2}}\sinh\frac{1}{2}\beta_1t\right)^2}{\frac{2kT}{m\omega^2}\left\{1-e^{-\beta t}\left(\frac{2\beta^2}{\beta_1^2}\sinh^2\frac{1}{2}\beta_1t+\frac{\beta}{\beta_1}\sinh\beta_1t+1\right)\right\}}\right) \tag{4.18}$$

where $\psi\left(\xi\right)$ is defined by

$$\psi\left(\xi\right)=\frac{1}{\sqrt{\beta^2-4\omega^2}}\left[exp\left[\mu_1\left(t-\xi\right)\right]-exp\left[\mu_2\left(t-\xi\right)\right]\right] \tag{4.19}$$

where $\mu_1=\frac{-\beta}{2}+\sqrt{\frac{\beta^2}{4}-\omega^2}$ and $\mu_2=\frac{-\beta}{2}-\sqrt{\frac{\beta^2}{4}-\omega^2}$. The $\psi^2\left(\xi\right)$ is defined by

$$\int_0^t\psi^2d\xi=\frac{1}{2\omega^2\beta}-\frac{e^{-\beta t}}{2\omega^2\beta_1^2\beta}\left(2\beta^2sinh^2\left(\frac{1}{2}\beta_1t\right)+\beta\beta_1\sinh\left(\beta_1t\right)+\beta_1^2\right) \tag{4.20}$$

where $\beta_1=\sqrt{\beta^2-4\omega^2}$. In addition to the friction of the system, the acceleration introduced by EMF, i.e., $K(r,t)$, affects the molecule's velocity and displacement. Though the effect of friction decreases over time, the electromagnetic force can still change the molecule's velocity and displacement at large timescales.

A probability distribution function can be described by various properties. The moment of a probability distribution function measures the distributions' scale, shape, and location properties. The scale of a distribution refers to the extension or compression of it along the x-axis. The shape of the distribution relates to its geometry. According to their shape, probability distributions can be classified as bimodal, uniform, symmetric and asymmetric. The geometric center of the distribution yields the location of the distribution. The first moment of a probability distribution function defines the location, i.e., the mean. The second moment gives the scale of the distribution. Variance is defined as the second central moment of a probability distribution function. The accumulation

of moments specifies the distribution (Source: Hsu, 1996; Shynk, 2012). Therefore, the first and second moments of the probability distribution function of the molecule's displacement are studied to understand the molecular behavior under EMF.

The first and second moments of the probability distribution of the molecule's displacement are analyzed to model the molecular behavior under an EMF at all time scales. The first moment of a probability distribution is the mean, and the second moment is the variance about the mean. They can provide a complete understanding of the molecular distribution under EMF. The first moment of the probability distribution of the molecule's displacement is derived in (Source: Chandrasekhar, 1943) for a molecule under a force field. The mean of the distribution is given as

$$\langle x \rangle_{Av} = x_0 e^{\left(\frac{-\beta t}{2}\right)} \left(\cosh\left(\frac{1}{2}\beta_1 t\right) + \frac{\beta}{\beta_1} \sinh\left(\frac{1}{2}\beta_1 t\right) \right) + \frac{2u_0}{\beta_1} e^{\frac{-\beta t}{2}} \sinh\left(\frac{1}{2}\beta_1 t\right) \tag{4.21}$$

In addition to the EMF's frequency, the molecule's initial position and velocity also affect the mean. As $t \rightarrow \infty$, the mean is expected to go to zero. The mean displacement of a molecular bead moving in a viscous fluid under an EMF is simulated for all time scales to understand the molecular distribution. In order to understand the behavior of the system, the time intervals are adjusted as $[0, \tau \times 10^{-4}]$ and $[0, \tau \times 10^{4}]$ for times that are much smaller and larger than the time limit. Furthermore, the frequency of the EMF is set to $1GHz$ and $1PHz$ to understand the effect of EMF with different frequencies. The rest of the simulation parameters are given in Table 4.2.

Table 4.2. Simulation parameters for a bead moving in a viscous fluid under a force field

Mass (m)	$1.37 \times 10^{-17}(kg)$
Radius (r)	$0.145(\mu m)$
Viscosity (η)	$10^{-3}(kg/m\dot{s})$
Temperature (T)	$300(K)$
Initial displacement (x_0)	0
Initial velocity (u_0)	$0.0176(m/s)$
Boltzmann's constant (k_b)	$1.38 \times 10^{-23}(J/K)$

Figure 4.5 represents the change in the molecule's mean position for small and large time scales. As seen in Figure 4.5.(A), the molecule's mean position changes linearly with time when $t << \tau$. Figure 4.5.(B) represents the mean value at a steady state. As the frequency of the oscillator and time increases, the mean displacement reaches its steady state value. Hence, the system becomes more stable, and molecules perform normal diffusion under an EMF.

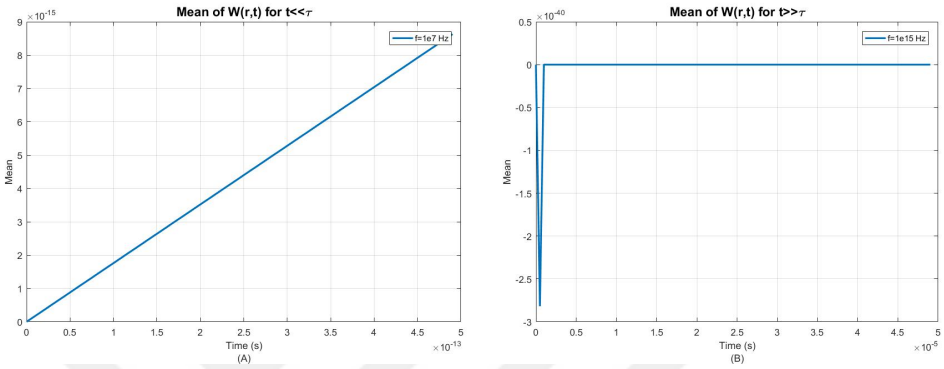

Figure 4.5. Mean of molecular displacement, Eq.4.18, when $t << \tau$ (A) and $t >> \tau$ (B)

The second moment of a probability distribution function gives its variance about the mean. The scale of the molecular distribution is characterized by its variance. The variance of molecule's displacement is derived in (Source: Chandrasekhar, 1943) and given as

$$\left\langle x^2 \right\rangle_{Av} = \langle x \rangle_{Av}^2 + \frac{kT}{mw^2} \left\{ 1 - e^{-\beta t} \left(2\frac{\beta^2}{\beta_1^2} \sinh^2 \left(\frac{1}{2}\beta_1 t \right) + \frac{\beta}{\beta_1} \sinh\left(\beta_1 t\right) + 1 \right) \right\} \tag{4.22}$$

The steady-state value of the variance is calculated as

$$\left\langle x^2 \right\rangle_{Av} = \frac{kT}{m\omega^2} \tag{4.23}$$

The mean displacement of the molecule and EMF's frequency are significant parameters for the variance of molecular distribution at all time scales. The second moment of the probability distribution function given in Eq. 4.18 is simulated to see

the variance of molecules about the mean defined in Eq. 4.21. The parameters given in Table 4.2 are also employed in the simulation of the variance of the molecular distribution. Figure 4.6 represents the variance in molecular movement due to the thermal fluctuations. As seen in Figure 4.6.(A), the variance changes quadratically when $t << \tau$. Eq. 4.23 indicates that the variance changes in reverse proportion to the frequency of EMF as $t \to \infty$. The change in the variance is represented by Figure 4.6.(B) for large time scales, i.e., $t >> \tau$. The variance converges to a value calculated by Eq. 4.23 as expected. Moreover, molecules approach the steady state as time and the frequency of the EMF increase.

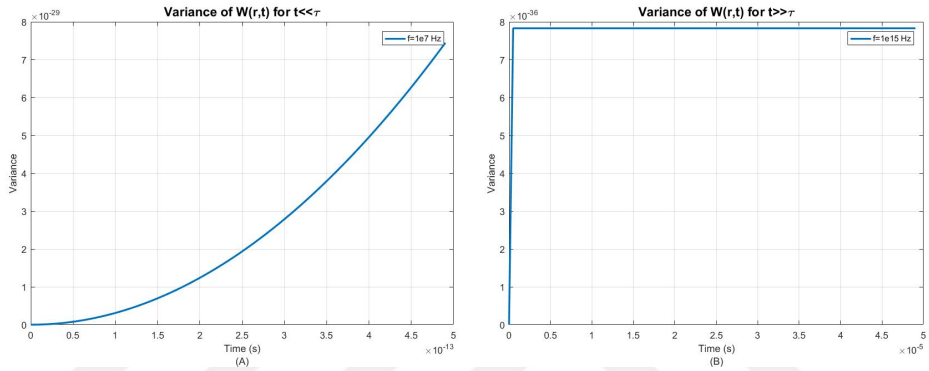

Figure 4.6. Variance of molecular displacement, Eq.4.18, when $t << \tau$ (A) and $t >> \tau$ (B)

Nonetheless, molecular behavior can be examined by other measures as well. The mean squared displacement (MSD) is a measure to understand the characteristics of molecular motion. The ensemble average of the fluctuations experienced by a molecule gives the MSD. Furthermore, the diffusion type of the molecule is defined by the relation between MSD and time. The relation given in Eq. 4.24 determines the type of diffusion depending on the value of $2\mu/\alpha$. If $2\mu/\alpha = 1$, molecules perform normal diffusion through the medium. If $2\mu/\alpha < 1$ or > 1, molecules perform anomalous diffusion (Source: Cao et al., 2015).

$$\left\langle \Delta x^2 \right\rangle \sim t^{\frac{2\mu}{\alpha}} \tag{4.24}$$

The coefficients μ and α are related to the waiting time and jump length divergence. If the waiting time is large and the jump length is small, molecules perform subdiffusion. A short waiting time and a large jump length result in superdiffusion. The MSD of a molecule under EMF is studied to see the effect of EMF on the type of diffusion.

The molecule's MSD is calculated as

$$MSD_f = x_0^2 e^{-\beta t}\left(\cosh\left(\frac{1}{2}\beta_1 t\right) + \frac{\beta}{\beta_1}\sinh\left(\frac{1}{2}\beta_1 t\right)\right)^2 + \frac{4u_0^2}{\beta_1^2}e^{-\beta t}\sinh^2\left(\frac{1}{2}\beta_1 t\right) + \frac{kT}{m\omega^2}\left(1 - e^{-\beta t}\left(\frac{2\beta^2}{\beta_1^2}\sinh^2\left(\frac{1}{2}\beta_1 t\right) + \frac{\beta}{\beta_1}\sinh\left(\beta_1 t\right) + 1\right)\right) \quad (4.25)$$

where k_B is the Boltzmann constant, T is the temperature, m is the mass of the molecule, ω is the frequency of the harmonic oscillator that models the EMF, $\beta_1 = \sqrt{\beta^2 - 4\omega^2}$, x_0 is the initial displacement of the molecule and u_0 is the initial velocity of the molecule. As $t \to \infty$, MSD goes to

$$MSD_f = \frac{kT}{m\omega^2} + x_0^2 \quad (4.26)$$

Eqs. 4.25 and 4.26 indicate that the initial position of a molecule, the frequency of the EMF, and the temperature of the medium affect the MSD of a molecule at all time scales. The effect of EMF on a molecule's diffusion type is studied by analyzing the MSD of a molecule under an EMF. Figure 4.7 represents the MSD of a molecule when EMF's frequency is equal to 1GHz. The MSD of a molecule has a nonlinear relationship with time when $t << \tau$. As represented in Figure 4.7.(A), molecules perform superdiffusion i.e. $2\mu/\alpha > 1$. The MSD of the molecule is represented in Figure 4.7.(B) when $t >> \tau$ and the frequency of the EMF is equal to 10^{15}. The MSD changes linearly, and molecules perform normal diffusion at a steady state.

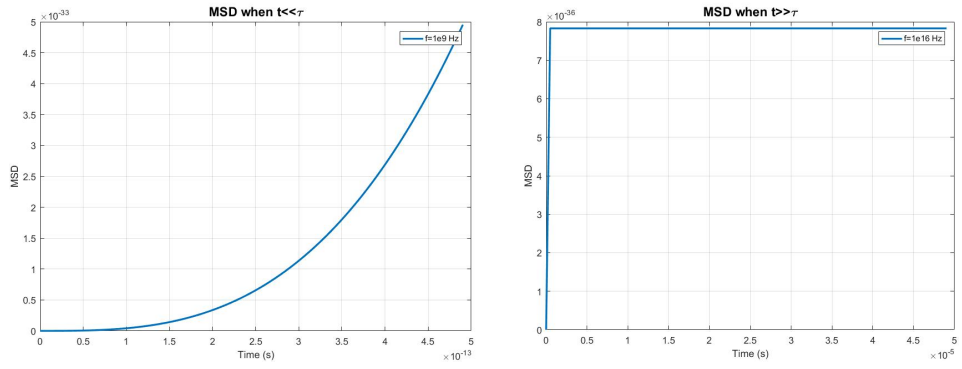

Figure 4.7. Mean-squared displacement of a molecule

Molecules start with superdiffusion, whether or not an EMF is present. The MSD of a molecule for times shorter than the time limit is nonlinear under an EMF. On the other

hand, the MSD converges to a value for times that are greater than the time limit. The behavior of molecules differs if the frequency of the field increases. The mean displacement of molecules decreases for all timescales. The analysis of molecular behavior under EMF indicates that molecules perform normal diffusion at large time scales. Furthermore, the molecular system stabilizes more quicker as the EMF's frequency increases.

4.3. Conclusion

The performance of an MC system depends on the properties of the transmitter, receiver, and communication medium. The transmitter and receiver are designed to compensate for the channel effects and optimize the performance of MC. The design of the transmitter is significant for the emission rate of information-carrying molecules. A proper encoding and modulation scheme improves the information rate. The receiver's design depends on the molecules' properties and the channel. Various decoding schemes are developed to increase the reception rate and the performance of MC. The physical and chemical properties of the communication medium affect molecular movement. For instance, molecules experience a greater drag force in a more viscous fluid. Furthermore, the temperature of the environment affects the thermal fluctuations experienced by molecules. Therefore, an external factor that affects the channel may alter the molecular behavior. The change in the molecular behavior may introduce noise to the system and require a different transmitter and receiver designs.

The performance of MC under EMF changes due to the effect of electromagnetic forces. Molecular movement is altered under EMF. An energy transfer between EMF and the communication medium causes an increase in the temperature. Furthermore, the change in temperature affects the kinetic energy and diffusion coefficient of molecules. As a result, the velocity and the diffusion rate of molecules increase. In addition to this, the direction of molecular movement changes due to the torque applied by electromagnetic forces. The change in the molecule's kinetic energy increases the occurrence probability of molecular interactions. The alterations in the diffusion rate and molecular interactions affect MC's transmission and reception rate. Hence, the performance of MC changes under an EMF.

The effect of temperature change on molecular movement is examined by model-

ing MC systems as reaction-diffusion systems. Molecular interactions are an important part of the reception process. The receiver can be passive, i.e., absorber, or reactive, i.e., reaction-diffusion model. In the case of a reactive receiver, the reception rate of molecules is affected due to the change in the reaction rate. Therefore, a bimolecular reaction's specific reaction rate constant is studied to understand the effect of temperature change on molecular interactions. The analysis indicates that a significant amount of temperature increase is needed to see any considerable change in the reaction rate. However, EMF causes a small amount of temperature increase. Hence, the effect of temperature increase caused by EMF on molecular interactions is negligible.

The EMF alters the molecular movement because of the electromagnetic forces. Langevin's diffusion theorem provides a comprehensive model for molecular behavior. Therefore, Langevin's equation is employed to model the molecules' movement for all timescales. The mean-squared displacement of molecules is studied to understand the probabilistic behavior of molecules under an EMF. Furthermore, the diffusion type is determined by the linearity of mean-squares displacement. The EMF is modeled with a harmonic oscillator in Langevin's equation. The oscillator's frequency, the system's dynamic friction coefficient, and the molecule's mass determine the system's state. If the friction coefficient is much greater than the molecule's mass and the frequency of the harmonic oscillator is smaller than 10^{14}, the system is in an overdamped state. In an overdamped state, the external forces cannot overcome the thermal fluctuations experienced by molecules. Therefore, molecules perform super diffusion. However, the state of the system changes over time. Furthermore, increasing the harmonic oscillator frequency also affects the system's state. Under a high-frequency EMF, the system is not overdamped, and molecules perform normal diffusion. Hence, EMF does not affect the diffusion type of molecules. Nonetheless, the range of molecules' displacement is affected by EMF. The angular frequency of the harmonic oscillator affects the variance of molecules' displacement. The mean-squared displacement of molecules also changes. The increase in the frequency of the EMF suppresses diffusion and decreases the range of molecular movement.

CHAPTER 5

CONCLUSION

The concluding remarks are presented in this chapter. The thesis begins with the analysis of forces applied to particles under EMF. The electrical and magnetic attributes of particles are significant in determining the total effective forces on particles. EMF's type, strength, and configuration also affect the impact of electromagnetic forces. The thermal effects of EMF are caused by the energy transfer that occurs between EMF and particles. The molecule's velocity and displacement are altered by the change in temperature. In Chapter 2, a comprehensive analysis of applied forces is presented for molecules under EMF. The effect of applied forces on paramagnetic and diamagnetic molecules is studied particularly. The total effect of applied forces results in the change of the diffusion rate of magnetically susceptible molecules. The information rate of an MC is affected by the decrease or increase in the diffusion rate of molecules. In Chapter 3, the performance of an MC system is analyzed that transmits information with magnetically susceptible molecules. The proposed system is under an EMF that is configured perpendicularly. Furthermore, the EMF's distribution is non-uniform. Hence, magnetic field gradient and concentration gradient magnetic forces change the magnetic energy of the system. A magnetically driven molecular flux introduces drift to the medium. The magnetically induced drift alters the molecule's velocity, diffusion coefficient, and concentration. The effects of magnetic susceptibility and MF's strength are represented with an effective diffusion coefficient. The propagation of molecules in the medium is altered because of the changes in the molecule's velocity and diffusion coefficient. Furthermore, the probability function of time delay is also altered due to the diffusion coefficient. Therefore, the successful transmission probability of bit 1 and bit 0 changes for paramagnetic and diamagnetic molecules. Hence, the information rate of MC is altered under EMF due to magnetic field gradient and concentration gradient magnetic forces.

The molecular behavior under EMF is discussed in the final chapter of the thesis. EMF's effect on molecular systems is studied from two perspectives. Firstly, molecular systems are modeled as reaction-diffusion systems to assess the effects of thermal

changes on molecular reaction and binding kinetics. The model indicates that the temperature increase required to introduce a significant change in the molecular reaction rate is very high. Therefore, the temperature change caused by the EMF is negligible, considering the SAR evaluations and temperature distribution models on various tissue types. The remaining part of the chapter focuses on Langevin's theory of molecular movement under EMF. The mean, variance, and mean-square displacement of molecules are obtained from the probability distributions of the molecule's velocity and displacement. The analysis of mean and variance under various timescales and EMF frequencies indicates that molecules move with super diffusion for small timescales. Moreover, molecules start to diffuse normally as timescales and EMF's frequency increases. However, molecular movement range decreases as EMF's frequency increases. The mean-square displacement of molecules is studied to determine the effect of EMF on diffusion type. The analysis does not indicate any anomalous diffusion characteristics under EMF.

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