Analysis of Molecular Nano Communication Channels with Relays

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ABSTRACT

A nanomachine is a device whose components are in nanoscale, and can perform only simple tasks. However, nanomachines can cooperate with each other and form up a nanonetwork to achieve more complex tasks. Free diffusion based molecular communication is one of the information transport methods that are employed among these nanomachines. In contrast with the traditional communication techniques where electromagnetic waves are employed as information carriers for the communications, here the molecules are used as information carriers. As a general scenario, a sender nanomachine encodes the information into the information molecules and then releases them in a fluidic medium. These information molecules propagate in the medium according to Fick's laws of diffusion, and then are received by the receiver nanomachine where their information will be decoded. The main disadvantage of using free diffusion is the fact that the number of information molecules that can reach to the destination falls down drastically as the distance between the sender and receiver nanomachines increases. In this thesis, a repeater nanomachine (i.e., relay node) is introduced to the scenario discussed above, which is positioned between the sender and receiver nanomachines, and its responsibility is to get the weakened molecular signal sent by the sender, and repeat it by releasing the same molecular signal in the medium. According to the numerical analysis and the results, employing a relay node can increase the signal strength and increase the number of molecules that can reach to the receiver, while the total number of molecules available for communication is held constant.

Keywords: Diffusion, Molecular Communication, Nanonetworks, Relay Node

ÖZ

Bir nanomakine, parçaları nano ölçekte olan ve sadece basit işler yapabilen bir cihazdır. Ancak, nanomakineler işbirliği yapıp daha karmaşık işler yapmak için bir nano ağ oluşturabilirler. Nanomakineler arasında iletişim için kullanılan metodlardan biri moleküllerin serbest difüzyonudur. Bu teknikte, elektromagnetik dalgaların kullanıldığı alışılmış iletişim tekniklerinin aksine, bilgi taşıyıcı olarak moleküller kullanılmaktadır. Genel olarak, gönderici bir nanomakine bilgiyi moleküllere kodlayıp molekülleri sıvı bir ortama bırakır. Moleküller Fick kanununa göre yayılıp bir alıcı nanomakine tarafından alınır. Serbest difüzyonun en büyük dezavantajı hedefe ulaşabilen bilgi moleküllerinin sayısının hedefin uzaklığının artmasıyla çok fazla azalmasıdır. Bu tezde, kaynak ve hedef arasında tekrarlayıcı (aktarıcı) bir nanomakine kullanılması araştırılmıştır. Bu makinenin görevi, zayıflayan moleküler sinyalin tekrar moleküller bırakmak suretiyle güçlendirmektir. Numerik analizlere göre terkrarlayıcı bir nanomakine kullanılması sinyal gücünü, toplam molekül bütçesi de gözönünde bulundurulduğunda, hedefte arttırmaktadır.

Anahtar Kelimeler: Difüzyon, Moleküller İletişim, Nano Ağlar, Aktarıcı Cihazlar

To my family,
for their unconditional love

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At first, I have to thank God who has always paid attention to my needs and never left me alone throughout my life. He has always been there for me and I hope that in return I could be a better person each day and make him happy.

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In the third place, I would like to dedicate this thesis to my beloved grandfather who passed away during the time of writing this thesis. He used to encourage me to broaden the horizons of my imagination as a child, and he has a nonnegotiable role in whoever I am and wherever I am now.

In the fourth place, I would like to thank my family who have supported me through my education, and I hope that dedicating this thesis to them, even though it is not much, could return a tiny part of their favor.

Last but not least, I want to extend my love to my dear Nakisa, whose love and thought have always kept me going through all hardships of life in Cyprus.

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Chapter 1

INTRODUCTION

The very idea of nanotechnology originates from Richard Feynman's lecture: "There's plenty of room at the bottom" [1]. He had a vision in which miniaturization of machines even to atomic level could be plausible. However, nobody in those days would have thought that his vision would become the foundation of one of the most ground-breaking areas of technology of this day, nanotechnology.

1.1 Nanotechnology

According to Taniguchi [2], nanotechnology mainly discusses the processing, separation, and deformation procedures of materials. Moreover, these procedures can be done using one atom or one molecule. A nanometer is equal to 10^{-9} meters and nanotechnology is about devices that at least one of their dimensions is in nanoscale. Moreover, one of the most amazing characteristics of this realm is that Isaac Newton's physics is no longer valid here. The chemical and physical properties of particles change compared to macroscopic systems and bulk materials, and several phenomena can become pronounced as the size of the system reduces to nanoscale. For instance, opaque substances become transparent (copper); stable materials become combustible (aluminum); solids turn into liquids at room temperature (gold). The goal of nanotechnology could be described as manufacturing machines in nanoscale and using

them as building bricks to build millions of tiny factories to achieve numerous applications in biology, chemistry, physics, and engineering [2] [3].

1.2 Manufacturing Nanomachines

As depicted in Figure 1.1, there are mainly three different approaches for creating nanomachines, namely: top-down, bottom-up, and bio-hybrid [4] [5].

Top-down approach: The main goal here is to manufacture nanoscale devices by merely downscaling the existing microscale components. Unfortunately, to this day only simple mechanical structures have been created using this approach since it is still at an early stage. For instance, the components of nano-electromechanical systems (NEMS) are being produced [6] [7]. Using this method, simple mechanical structures like nanogears can be created [8].

Bottom-up approach: Here, the nanomachines are made using a method called molecular manufacturing. As the name implies, the molecules are used as building bricks to assemble nanomachines. Although this approach possesses a great deal of accuracy, the required technology does not exist yet [9].

Bio-hybrid approach: Biological structures such as nano-biosensors and nano-actuators, which could be found in living organisms like cells, can be considered as nanomachines. Interestingly, the expected characteristics of prospective nanomachines such as self-replicating property are already present in cells [10] [11].

In Figure 1.1, different systems are drawn based on their origin which could be categorized in two groups, namely: nature and man-made. Among all of them the biological approach has caught a great deal of attention, due to existing nanomachines in nature with desired attributes such as low power consumption. Thus, they could be chosen as building blocks for later developments.

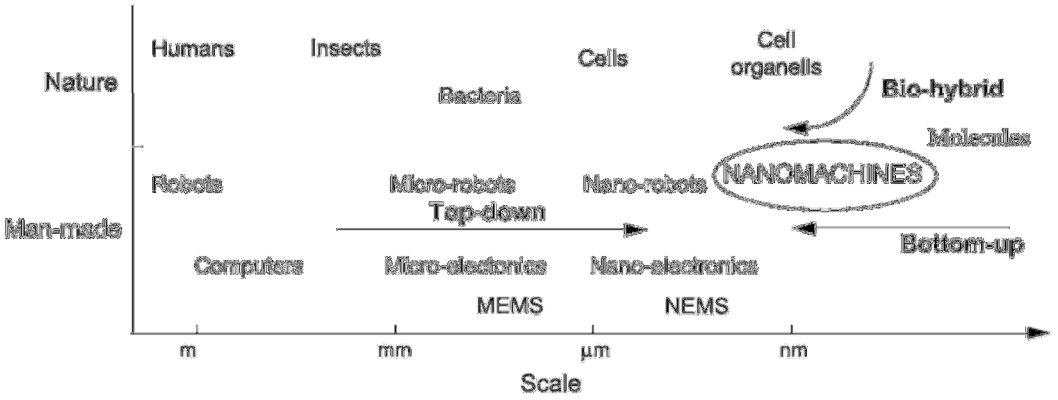

Figure 1.1: Different Approaches in Developing Nanomachines (Reproduced from [4])

1.3 Nanomachine Architecture

Depending on the complexity, a nanomachine could consist of a number of components. However, the most complete nanomachine is made of the following components [4]:

1) *Control unit:* This unit is responsible for controlling and coordinating other components of the nanomachine so that the desired task could be done.

2) *Communication unit:* It has a transceiver which is capable of both sending and receiving information at nanoscale (e.g., molecules).

3) *Reproduction unit:* The main task of this component is to create every part of the nanomachine using exterior sources and to put them together to make a nanomachine.

4) *Power unit:* It powers all the units in a nanomachine. Moreover, it is capable of absorbing energy from the exterior sources like light, and temperature in order to keep it for future needs.

5) *Sensors and Actuators:* They could be seen as an interface between nanomachine and surrounding environment. There could be a number of both of them in one nanomachine (e.g., light and temperature sensors, motors, and pumps).

Unfortunately, with the state-of-the-art technology it is not possible to build such complex nanomachines, however, there are equivalents in nature, such as living cells, which not only possess all the aforementioned units but also can perform complicated tasks, which are assumed to be feasible by a sophisticated nanomachine. The following shows the mapping between a living cell and a generic nanomachine [4]:

1) *Control unit:* The control unit of the cell is Nucleus. Moreover, it possesses all the instructions needed to understand the functions of the cell.

2) *Communication unit:* The gap junctions, and pheromonal and hormonal receptors, which are located on the membrane of the cell, can be considered as transceivers for sending / receiving information between cells.

3) *Reproduction unit*: Several nanomachines like centrosome and molecular motors are involved in reproduction process.

4) *Power unit:* A large fraction of substances, which are employed as the source of energy for the processes of the cell, are produced by mitochondrion.

5) *Sensors and actuators:* There could be a number of sensors and different actuators on a particular cell. For instance, different conduits for tastes and also the flagellum for the movement of bacteria.

An interested reader is encouraged to refer to [4], [12], and [13] and the references therein for more detailed information about biological structures. In Figure 1.2 a mapping is shown between a nanomachine and a cell.

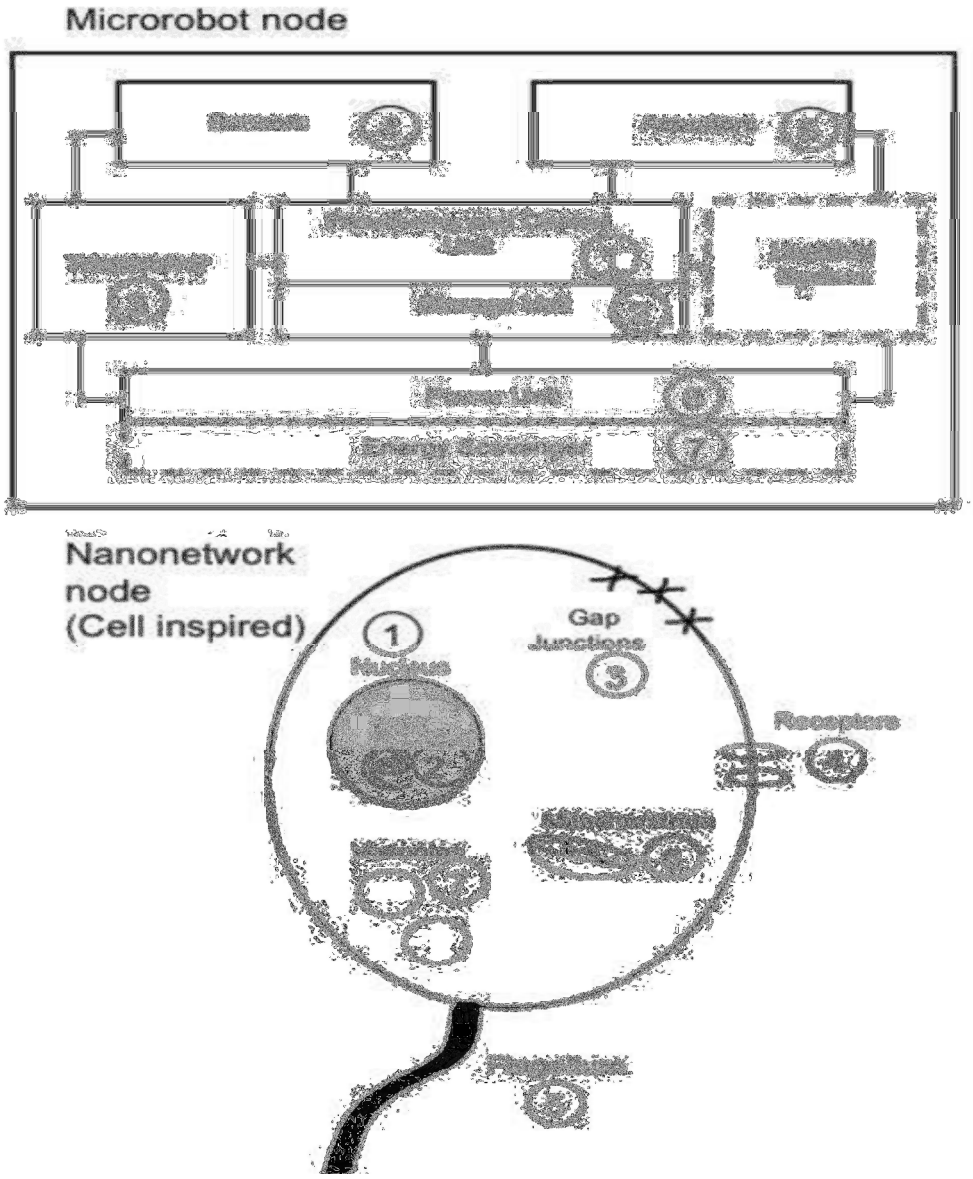

Figure 1.2: Mapping Between a Nanomachine and a Cell (Reproduced from [4])

1.4 Nanonetworks

Even though nanomachines are capable of performing tasks at nanoscale, their functions are limited to simple sensing and actuating tasks. However, In order to handle more complex tasks, one can benefit from the cooperation between multiple nanomachines in the form of a nanonetwork. Using nanonetworks, the capabilities of a nanomachine is magnified in terms of complexity and range of operation due to their interconnection and capability of sharing data [4] [5].

1.5 Applications of Nanonetworks

Although the potential applications of nanonetworks are unlimited, in [4] they have been classified into four main groups, as follows:

- *Biomedical Applications*

Due to the infinitesimal size and biocompatible nature of nanomachines, this area seems to be a great fit for nanonetworks' applications. A few examples in this area are immune system support, biohybrid implants, drug delivery systems, health monitoring, and genetic engineering or tissue engineering [14] [15] [16].

- *Industrial and Consumer Good Applications*

Nanonetworks could be employed to create new materials, manufacturing processes and quality control mechanisms. For example, in the case of quality control mechanisms, nanonetworks could help us detect the matter of interest (e.g., bacteria, toxic

components) with a high accuracy, which are not possible using traditional sensing technologies [17] [18].

- *Military Applications*

Nanonetworks play a contributing role in this area [19] [20]. Additionally, monitoring soldiers' performance, and battlefield surveillance are two examples. In the case of the latter, nanosensors could be deployed all over the battle field to detect the presence of chemical agents in the environment, and also coordinate a defensive response.

- *Environmental Applications*

In this area, nanonetworks could be used to overcome some previously unachievable applications, such as biodegradation purposes and air pollution control. For instance, in the case of air pollution control, nanonetworks can be used for monitoring air. In addition, nano-filters can remove toxic and harmful substances from the air, thus improving air quality [21].

1.6 Problem Statement

According to [22], there are two ways in which nanosensors can communicate with each other. First is through nanoelectromagnetic waves where nanosensors utilize electromagnetic radiation. Moreover, the main issue about this communication paradigm is that it uses the tera-hertz frequency band (0.1-10.0 THz). However, there is also another choice for communication which is called molecular communication where the information carriers are molecules. Molecular communication is a biocompatible

alternative to nanoelectromagnetic communication. Here, the sender encodes the information to molecules and sends them through the medium, and the receiver also decodes the information from the sent information molecules. However, using molecular communication to achieve node-to-node and network connectivity [5] is challenging. The strength of "molecular signal" decays rapidly as the distance between the source and destination increases. To this end, in this thesis, use of a relay node to repeat the molecular signals will be considered and analyzed. In the analysis, total no. of molecules available for communication will also be taken into account.

The rest of the thesis is arranged as follows. In Chapter 2, the main focus will be on describing molecular communication. In Chapter 3, related work and the mathematics of diffusion will be studied, in Chapter 4, modeling the molecular channel with relay node is discussed, in Chapter 5, the numerical results are discussed, and finally Chapter 6 is for the conclusion.

Chapter 2

MOLECULAR COMMUNICATION

2.1 A New Communication Paradigm

Molecular communication is still at its early stage considering the fact that the first research on it was started in 2005 [13]. Moreover, molecular communication is a new paradigm used in communication between nanomachines over a short range e.g., nano or microscale ranges. In contrast with traditional communication paradigms where information was encoded to and decoded from electromagnetic waves, here information molecules (e.g., protein, DNA molecules) are used as information carriers. The big picture of this communication paradigm is like this: the sender encodes its information into information molecules and sends them into a fluidic medium; the molecules propagate into the medium until the receiver receives them and starts to decode the information. Additionally, the decoding process could result into triggering an action like drug release [13]. An interested reader is encouraged to refer to [4] and [13] and the references therein for more detailed information.

2.2 Molecular Communication vs. Telecommunication

In traditional communication paradigms, the information (e.g., text, voice, and video) carriers are electromagnetic waves traveling through space or electron/optical signals travelling through cables. The main characteristics of this paradigm are high speed, long

transmission range, high level of accuracy and reliability, which are achieved by consuming electrical power.

On the other hand, in molecular communication, the information molecules are used as information carriers, and they propagate through a fluidic medium in the form of a chemical signal. Compared to telecommunication paradigm, here the signal speed and range are both limited. The communication is a stochastic and unreliable process, which stems from noise effects in the environment. However, molecular communication is bio-compatible and also energy efficient as opposed to telecommunication paradigm. In Table 2-1 there is a summary comparison between the two paradigms.

Table 2.1: Telecommunication vs. Molecular Communication (reproduced from [13])

	Telecommunication	Molecular communication
Information carrier	Electromagnetic waves, electrical/optical signals	Chemical signals
Media	Space, cables	Aqueous
Speed	Speed of light (3×10^8 m/s)	Extremely slow (nm ~ μm/s)
Range	Long distance (~km)	Short distance (nm ~ m)
Information	Texts, audio, videos	Chemical reactions, states
Other features	Reliable, high energy consumption	Unreliable, biocompatible energy efficient

2.3 Molecular Communication in Biological Systems

Biological nanomachines employ molecular communication for inter/intra cell communication. Here, two ways by which this communication takes place are described [5] [13].

2.3.1 Passive Transport vs. Active Transport

In the passive transport, the released molecules randomly diffuse into the medium. This could be beneficial where we are facing a dynamic environment, and also where having an infrastructure for communication is not possible. Although there is no energy consumption for this type of communication, it is not flawless. For example, a large number of molecules are needed in the source to increase the probability of them reaching to the destination since the molecules move randomly at all possible directions. Also, this method is not appropriate for large signal molecules due to their size [13] [23].

On the other hand, in active transport the information molecules are directed by force towards a specific destination, which makes larger distances possible (e.g., up to meters). This force is produced by chemical energy. Not only this method provides reliability, but also it requires less number of molecules. However, there are three main disadvantages related to this type of transport. First, it requires a communication infrastructure on which the transport could take place. Second, it uses interface molecules such as molecular motors, microtubules filaments, and vesicles, in order to direct the information molecules. Third, there is some sort of chemical interaction between the information molecules and the molecules in the environment, and of course to reduce this interaction a supply of energy is needed [13].

2.4 Molecular Communication Process

The following general phases happen in molecular communication [4] [24]:

- Encoding

- Sending
- Propagating
- Receiving
- Decoding

Encoding: At first stage of molecular communication, the sender starts by translating its information into the information molecules. Moreover, there are different ways by which this encoding could be done. The first way is to encode the information onto the type of the information molecules (e.g., protein). For instance, if molecule type A is released by the sender this means bit 1, and if type B is released then this corresponds to bit 0. Also, encoding could take place on characteristics of information molecules such as concentration (i.e., number of molecules per unit of volume) of information molecules (e.g., calcium concentration). For example, if the concentration of the released information molecules into the medium by the sender were higher or lower than some predefined threshold, then this would correspond to bit 1 or 0, respectively. Moreover, encoding using sequence information is also possible (e.g., DNA). Last but not least, modulation schemes like Frequency Modulation (FM) and Amplitude Modulation (AM), which are used in calcium signaling [25] can be adopted. Here, the sender encodes the information in amplitude and frequency of the function that describes the concentration of the information molecules [13].

Sending: After encoding stage, the sender starts to release the information molecules into the medium. It is important to mention that using only one sender would impose limitations onto the communication capability. This stems from the fact that, a sender

nanomachine has limited energy and finite number of information molecules. As a conclusion, if multiple senders would send the same signal, the signal power would increase on the receiver side. Alternatively, there could be also a repeater nanomachine placed between the sender and receiver, which could amplify the signal sent by the sender, thus increasing the signal power.

Propagating: After information molecules have been released into the fluidic medium, they propagate using either active or passive transport methods. During propagation, the information molecules are exposed to the noise present in the medium. Additionally, to cancel out this noise effect an interface molecule could be used such as vesicle-based interface molecules. In this method, the information molecules are placed into the vesicle to prevent them from any possible chemical reaction with the molecules in the environment.

Receiving/Decoding: The surface of the receiver is covered with receptors, which have a high level of affinity with the information molecules, and this makes receiving operation possible. Moreover, upon receiving the information molecules, the receiver translates them into a chemical reaction. The chemical reaction could be a simple task like producing new molecules or creating a new signal using another information molecule.

2.5 Characteristics of Molecular Communication

Molecular communication has several key characteristics which arise from employing biological mechanisms for communication in a fluidic medium [4] [13].

2.5.1 Stochastic Communication

There is a high level of uncertainty in the speed and direction of information molecules' movement due to incalculable movement of the environmental molecules. As a result, in order to achieve reliability, the sender increases the signal to noise ratio by releasing a large number of information molecules into the medium. Using this approach, the effect of the noise of environmental molecules will be negligible.

2.5.2 Large Communication Delay

Due to the environmental noise, the information signal would experience some reduction in its speed, both in active and passive transport methods. This could result in high delay and high loss rate and could cause problems. For example, if the information molecules stay in the environment for a long time, then the sender is obligated to delay its next communication attempt until the previously sent molecules degrade and vanish. This is mainly because of preventing any possible interference between the old and new communication. This delay could grow drastically based on the information carrier that is used. For example, DNA molecules can survive in the environment for months.

2.5.3 Molecule Based Coding

As mentioned earlier, unlike traditional networks, in molecular communication, the information carriers are molecules. The information can be encoded in the information molecules using different methods. For instance, type of the information molecules, concentration level (i.e., number of information molecules per unit of volume) and sequence information (e.g., DNA) [26]. Moreover, the amount of information that can be encoded in the information molecules is dependent on the decoding ability of the

receiver nanomachine. This is due to the limited number of configurations that a receiver nanomachine could possibly have. For example, when a receiver nanomachine receives an information molecule, only the fraction of information corresponding to the number of possible configurations in the receiver nanomachine, can be received by the receiver nanomachine.

2.5.4 Biocompatibility

Since the communication method among nanomachines and biological systems are identical, they can directly communicate with biological systems. This could result in numerous medical applications. For instance, nanomachines can be inserted into biological systems (e.g., human body) for drug-delivery, cancer treatment, and other possible applications.

2.5.5 Energy Efficiency

Molecular communication in biological systems is absolutely efficient. For instance, Myosin (i.e., a molecular motor) can convert chemical energy (i.e., ATP) to mechanical movement with the efficiency of 90%. Moreover, energy could also come from external sources. For example, in human body, nanomachines can gain energy from energy sources (e.g., glucose) [4].

2.5.6 Molecular Communication based Nanonetworking

In this thesis, the main focus is on passive molecular transport using free diffusion, and it is due to the fact that not only this type of transmission requires no external force for the information molecules to propagate through the medium but also it can be used in

highly dynamic environments and also in scenarios where it is not feasible to have a communication infrastructure. Models and methods employed in this thesis for analyzing diffusion based molecular communication are described next.

Chapter 3

MODELS AND METHODS

3.1 Related Work

As mentioned earlier, molecular communication using free diffusion has considerable advantages, however, it is not absolutely flawless. Moreover, when a source nanomachine releases an instantaneous spike of information molecules in the fluidic medium, each one of these molecules move randomly in all possible directions. As a result, only a fraction of them would reach to the destination in a given time. This phenomenon is known as attenuation of signal strength. In addition, the distance between the source and destination nanomachines has a considerable effect on the fraction of successfully delivered molecules to the destination. Thus, as the distance increases the number of successfully delivered molecules in a given time drops down according to a power law and this makes long-distance communication practically impossible.

One possible solution is to have a very large number of molecules stored in sender nanomachine, in order to neutralize the effect of distance over the transmission. However, in practical scenarios, there are only a limited number of molecules in hand which we call the molecule budget. The other solution is to put an intermediate node between the sender and the receiver, which is responsible for amplifying the signal sent

by the sender. This node is similar to hubs (i.e., repeaters) in traditional communication systems, and is called the relay node. In this chapter, previous work on the subject will be discussed. The studies deal with having one or more repeaters between the sender and receiver nanomachines in order to amplify the attenuated signal.

In [27], the main focus is on molecular communication networks, which are based on biological cells and the design of repeater cells, as signal amplifier, has been investigated. Moreover, the non-excitable cells and intercellular calcium (Ca^{2+}) signaling mechanisms are used as biological material and mechanism, respectively. In [27], a mathematical model of calcium signaling in non-excitable cells is proposed which studies the conditions under which these cells turn into efficient repeaters of calcium signals. Here, after a cell increases the intra-cellular concentration of Ca^{2+}, these ions start to diffuse through gap junction channels to the neighboring cells, which respond by increasing their own intra-cell Ca^{2+} concentration. Similarly, the generated Ca^{2+} would diffuse to the neighboring cells, thus amplifying the very first sent calcium signal. As a result, the designed cells efficiently play the role of repeaters by amplifying the received signal and propagating it over longer distances. However, there are some issues that have not been covered in this work. For example, in this paper it is assumed that the repeater cells have filled the gap between the sender and receiver completely, and are standing by each other back to back. As a result, this paper has not covered the more fundamental scenario of positioning only one repeater since they have assumed that we can use as many repeaters as possible to fill the whole distance between the sender and the receiver. Moreover, they have not taken the limited molecule budget into account.

However, the main advantage of the paper is the biological perspective of molecular communication which is the natural application area of nanomachines.

In [28], the channel capacity of three main communication channels is investigated: multiple-access, broadcast, and relay channels. In the last one, which is related to this thesis, it is assumed that there is only one nanomachine between sender and receiver, which is capable of both molecular signal reception and emission. Using numerical and theoretical results, it is revealed that relay nanomachines can increase the communication capacity between a source nanomachine and destination nanomachine, under certain conditions. No attempt has been made for analysis of signal attenuation and the signal strength improvement associated with using the relay.

Overall, some critical questions are still unanswered by previous studies: where should the relay node be positioned so that the maximum concentration in the destination is obtained? Moreover, when exactly should the relay node get activated and generate its own signal to amplify the sender's signal? Based on the limited molecule budget condition is there an optimum position for the relay node to be placed and an optimum activation time for it so that the highest possible concentration in the destination nanomachine is achieved? What is the minimum number of molecules that should be stored in sender to make sure that sender's signal could be strong enough to activate the relay node? These questions have been studied and investigated in this thesis.

3.2 Mathematics of Diffusion

In this work, we are interested in diffusion-based molecular communication since unlike active transport method, no energy consumption is needed as the information molecules propagate freely through the medium. If a drop of water soluble dye is placed in a glass of water, it will start to spread out while its color becoming weaker as time goes by until the water inside the glass has a uniform color. Moreover, the process by which the dye particles propagate from areas with higher concentration to the areas with less concentration is called *diffusion* [29]. According to Fick's first law of diffusion, there is a relationship between the concentration and flux of molecules in the environment. For one dimensional case, Fick's first formula states that the flux of particles in positive x-direction is proportional to the spatial gradient of particle concentration, as follows:

$$\emptyset(\boldsymbol{x},\boldsymbol{t}) = -\boldsymbol{D}\frac{\boldsymbol{\partial C}(\boldsymbol{x},\boldsymbol{t})}{\boldsymbol{\partial x}} \tag{3.1}$$

Where $\phi(x,t)$ denotes the flux of particles in direction of x in units of [mole/(length^2.time)], that is the net number of particles which pass through a unit area perpendicular to the x-axis and located at x. D is called the diffusion coefficient or diffusivity with a unit of [length^2/time], t is the time, and x is the distance between the source and destination. Moreover, the value of D represents the velocity of diffusing particles through the fluidic medium, and as a result it depends on the temperature of the environment, viscosity of the fluid, and of course the size of the diffusing particles and in the case of biological molecules D ranges from 10^{-11} to 10^{-10} m^2/s.

Moreover, Fick's second law of diffusion predicts the way concentration varies with respect to time:

$$\frac{\partial C(x,t)}{\partial t} = D\frac{\partial^2 C(x,t)}{\partial x^2} \tag{3.2}$$

Last but not the least, Fick's laws of diffusion are easily extendable to 2 and 3 dimensional cases, where in addition to x-axis and time, there will be also *y* and *z* directions, as well.

$$\vec{\phi}(x,y,z,t) = -D\nabla C(x,y,z,t) \tag{3.3}$$

and:

$$\frac{\partial C(x,y,z,t)}{\partial t} = D\nabla^2 C(x,y,z,t) \tag{3.4}$$

where in 3 dimensional case:

$$\nabla = \left(\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z}\right) \text{ and } \nabla^2 = \left(\frac{\partial^2}{\partial x^2}, \frac{\partial^2}{\partial y^2}, \frac{\partial^2}{\partial z^2}\right) \quad (3.5)$$

In the next chapter, modeling the molecular channel using a relay node is studied. This model is based on free diffusion as the communication method between nanomachines follows the assumptions listed below:

1- The diffusing information molecules move randomly in any possible direction in the medium, forever.

2- There is no molecule absorption neither by the medium nor by the nanomachines.

3- There is no chemical reaction between the information molecules and the molecules of the medium.

Chapter 4

MODELING THE MOLECULAR CHANNEL WITH RELAY NODE

The nanonetwork topology considered in this study is depicted in Figure 4.1:

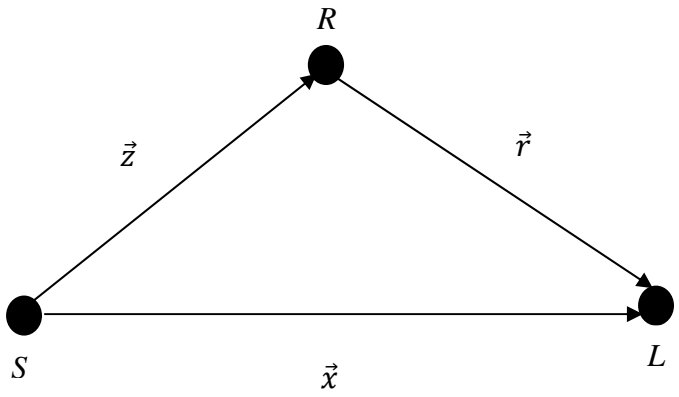

Figure 4.1: The Nanonetwork Topology

In this thesis the following assumptions are made:

- There is one Sender (*S*), one Relay Node (*R*), and one destination Receiver (*L*).

- The Euclidean distance from *S* to *R*, *R* to *L*, and *S* to *L* are defined as:$\|\vec{z}\|$, $\|\vec{r}\|$, and $\|\vec{x}\|$, respectively, where the summation of two sides of the triangle is always greater than or equal to the third side. The maximum value of $\|\vec{r}\|$ is equal to$\|\vec{x}\|$.

- There are a total number of m molecules (i.e., molecule budget), which has to be divided between S and R in a way that there are m_1 molecules for S and m_2 molecules for R (i.e., $m=m_1+m_2$). Moreover, it is important to mention that we are facing with a limited molecule budget and we cannot just allocate as many molecules as we want, to S and R.

- The idea is, the Sender (S) would start diffusing m_1 molecules into the medium all at once, and the relay node upon sensing an amount of concentration of the diffused molecules, would start to diffuse its own m_2 molecules into the medium all at once, which would result in the amplification of the molecular signal previously sent by the Sender (S). R could be seen as a repeater in traditional communication networks, where it is used to amplify the attenuated electrical/electromagnetic signals, thus making communication over long distances possible. In general, one expects that m_2 is much less than m_1 since relay is envisioned as a low-capability device. Note also that due to the molecule budget, one cannot store an arbitrary number of molecules on R.

- The minimum amount of concentration that R needs to sense in order for it to trigger its own diffusion, is called detection threshold and is denoted by θ which is dependent on the sensitivity of the Relay node nanomachine (R). As an example for 3 dimensional environment, in Figure 4.2, R samples the number of information molecules per unit of volume (i.e., molecular concentration) in its vicinity, which is a sphere with radius δ and centered at R. This procedure is

called concentration detection. Moreover, if the result is less than θ, R remains inactive but if it is equal or more than θ then R is activated and starts its own diffusion. Figure 4.2 illustrates the idea of concentration detection in 3 dimensional environment.

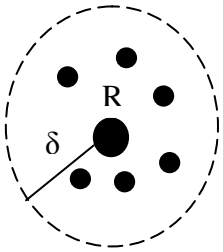

Figure 4.2: R Samples the Number of Information Molecules (Little Black Points) in the Reception Volume and Divides it by the Volume of its Spherical Vicinity (i.e., $\frac{4}{3}\pi\delta^3$)

It is important to mention that δ is much less than the distance between S and L (i.e., $\|\vec{x}\|$).

- It is critical to compute the minimum number of molecules that have to be placed in S, so that the θ concentration in R is surpassed.

- The main goal here is to achieve the maximum possible concentration in the Destination (L), by finding a proper division of the molecule budget between S and R (i.e, m_1 and m_2), and the exact time t_2 by which R has to start emitting its own signal upon the one sent by S.

- R is not activated unless the threshold θ is surpassed. Now could t_2 be any time, or there has to be some optimum t_2 so that if θ is surpassed exactly at that time, the total molecular concentration at L could reach its highest value?

Last but not least, this thesis addresses the following crucial questions:

1- What is the minimum number of molecules (i.e., m_1), required in S?
(This depends on $\|\vec{z}\|$, $\|\vec{r}\|$, and θ)

2- How is that possible to achieve the maximum concentration in L?
(This depends on the starting time of signal amplification in R (i.e., t_2))

4.1 Problem Formulation

When the source instantaneously emits m particles, the molecular concentration in $\|\vec{x}\|$ units of distance away from the signal emitter, at time t is calculated using the solution of Eq.(3.2) (here there is just one emitter):

$$C(\vec{x}, t) = \frac{m_1}{(4\pi D t)^{d/2}} e^{\frac{-\|\vec{x}\|^2}{4Dt}} \tag{4.1}$$

where d is the dimension (i.e., 1,2, or 3), m_1 is the number of released molecules, $\|\vec{x}\|$ is the magnitude of the distance vector originating from the sender and ending to the point of interest, and t shows the time at which we are interested in, to measure the concentration.

In our case we have two signal emitters, where one of them is the Source (*S*) and the other is the Relay node (*R*). In this case, due to the linearity property of the Fick's second law of diffusion [30], we can simply add the concentration of molecules sent by *S* and *R*, to get the total concentration at *L*. As a result, the molecular concentration at *L* is calculated by the following formula:

$$C(\vec{x},t) = \underbrace{\frac{m_1}{(4\pi D(t-t_1))^{d/2}}\, e^{\frac{-\|\vec{x}\|^2}{4D(t-t_1)}}\, U(t-t_1)}_{C_1} + \underbrace{\frac{m_2}{(4\pi D(t-t_2))^{d/2}}\, e^{\frac{-\|\vec{r}\|^2}{4D(t-t_2)}}\, U(t-t_2)}_{C_2} \qquad (4.2)$$

where t_1 and t_2 are the activation times of *S* and *R*, and C_1 and C_2 refer to the molecular concentration at the destination (*L*) caused by the source (*S*) and the relay node (*R*), respectively. $U(t)$ is the unit-step function: $U(t-t_i)$ is equal to 1 only if $t \geq t_i$, otherwise it is equal to zero.

In order to determine the time at which *C* could reach its maximum value at the destination (*L*), first it is required to calculate the times at which C_1 and C_2 are maximized, and then by equating them or coinciding the two peaks at *L*, we obtain the optimum time for *R* at which it must start diffusing the signal, so that the summation of the two signal would be the maximum at *L*.

As a result if we take the derivative of C_1 and C_2 with respect to *t* and equate them to zero, the time by which the concentration of the molecules sent by *S*, reaches to its maximum (i.e., concentration peak) in *L* is equal to:

$$S(t_{opt}) = \frac{\|\vec{x}\|^2}{2dD} + t_1 \tag{4.3}$$

and the time by which the concentration of the molecules sent by *R*, reaches to its maximum in *L* is equal to:

$$R(t_{opt}) = \frac{\|\vec{r}\|^2}{2dD} + t_2 \tag{4.4}$$

where t_1 and t_2, are the starting time of diffusion process in *S* and *R*, respectively.

However, in order to achieve the maximum concentration in *L*, the two peaks need to occur at the same time, or in other words, have to coincide. Thus, we have to equate the peak times related to *S* and *R*, and by equating Eq. (4.3) and Eq. (4.4), we get the following:

$$t_2 = \frac{\|\vec{x}\|^2 - \|\vec{r}\|^2}{2dD} + t_1 \tag{4.5}$$

This relates the activation time of *R* to $\|\vec{x}\|$, $\|\vec{r}\|$ and t_1. So, this means that if the Relay node (*R*) starts diffusing its molecules in to the environment, exactly $\frac{\|\vec{x}\|^2 - \|\vec{r}\|^2}{2dD}$ units of time after the source (*S*) started its signal, we could have the maximum concentration (*C*) at the destination (*L*), which could be calculated by plugging in the optimum times in Eq. (4.3) and Eq. (4.4), with variable *t* in C_1 and C_2, respectively. As a result, the maximum value of C_1 is:

$$C_{1max} = \frac{m_1}{\|\vec{x}\|^d (\frac{2\pi e}{d})^{\frac{d}{2}}} \tag{4.6}$$

and the maximum value of C_2 is:

$$C_{2max} = \frac{m_2}{\|\vec{r}\|^d (\frac{2\pi e}{d})^{\frac{d}{2}}} \tag{4.7}$$

This is the case when t_1=0. Thus, the maximum concentration (C) at L, is calculated by summing Eq. (4.6) and Eq. (4.7) together:

$$C_{max} = \frac{\|\vec{r}\|^d m_1 + \|\vec{x}\|^d m_2}{(\|\vec{r}\|\|\vec{x}\|)^d (\frac{2\pi e}{d})^{\frac{d}{2}}} \tag{4.8}$$

However, it is important to remember that there is a condition for Relay node (R) to be able to start sending its molecules into the environment at time equal to $\frac{\|\vec{x}\|^2 - \|\vec{r}\|^2}{2dD} + t_1$, which implies that exactly at this time, the concentration of the molecules sent by S must surpass a certain threshold Θ at R, so that the diffusion process in R would get triggered, that is:

$$C_1(t_2) > \Theta \tag{4.9}$$

By replacing variable t in C_1 with t_2 in Eq.(4.2) , we get the following condition for activation of the repeater (we assume that t_1=0, without loss of generality):

$$\frac{m_1}{(4\pi D t_2)^{\frac{d}{2}}}\, e^{\frac{-\|\vec{z}\|^2}{4Dt_2}} > \Theta \tag{4.10}$$

And if we replace t_2 with its equivalent in Eq. (4.5), we get the following inequality:

$$m_1 > \Theta\left(\frac{2\pi(\|\vec{x}\|^2 - \|\vec{r}\|^2)}{d}\right)^{\frac{d}{2}} e^{\frac{d\|\vec{z}\|^2}{2(\|\vec{x}\|^2 - \|\vec{r}\|^2)}} \tag{4.11}$$

So, this implies that in order to trigger the action in Relay node at time t_2, the minimum number of molecules in the Source (*S*) nanomachine is equal to the lower bound for m_1. Since the total number of molecules is equal to *m*, the value of m_2 is calculated easily by subtracting m_1 from *m*.

As mentioned earlier, our nanonetwork topology can be in 1,2 and 3 dimensions. If the nanonetwork is being implemented in a very thin environment like a capillary, the model for 1 dimensional model should be used (i.e., d=1). However, if the nanonetwork is established on a surface like a membrane or a dish then the 2 dimensional model is appropriate (i.e., d=2). Last but not least, if the nanonetwork is used in a 3 dimensional environment like communications between cells then the 3 dimensional model must be used (i.e., d=3).

Chapter 5

NUMERICAL RESULTS

This chapter will exhibit some numerical results for the derivations presented in the previous chapter.

5.1 Molecular Concentration at Single Source-Single Destination Scenario, in 1, 2, and 3 Dimensions:

As the number of delivered information molecules decreases, consequently, the concentration of those molecules will also decrease exponentially as $\|\vec{x}\|$ grows. Here, the effect of $\|\vec{x}\|$ on molecular signal attenuation is studied. In the most basic scenario, it is assumed that there is one sender nanomachine (*S*) and one destination nanomachine (*L*) whose distance from each other is denoted with $\|\vec{x}\|$. Using Eq.(4.1), the spike of molecules that are released by *S* instantaneously is analyzed for 1, 2, and 3 dimensions.

According to [31], the size of a typical animal cell is 10 μm, and as a result the value of $\|\vec{x}\|$ under consideration ranges from 0 to 100 μm. Moreover, the typical number of particles that can be released in a puff by a cell is 10^5 particles [31]. In Figure 5.1, Figure 5.2, and Figure 5.3 the effect of distance over the concentration of information molecules at the destination for 1, 2, and 3 dimensional cases is shown. The value of diffusion coefficient (*D*) is considered as $10^{-9}\ \frac{m^2}{s}$.

The initial distance between *S* and *L* is set to 25µm and then increased to 50µm and 100µm. Finally, *S* starts signal emission at time equal to 0, and the behavior is analyzed up to time 10 *s*, which is the typical time for diffusion for a distance of 100µm when D=10^{-9} $\frac{m^2}{s}$. In the figures, the unit for number of particles is mole, where 1mole=6.02×10^{23} particles.

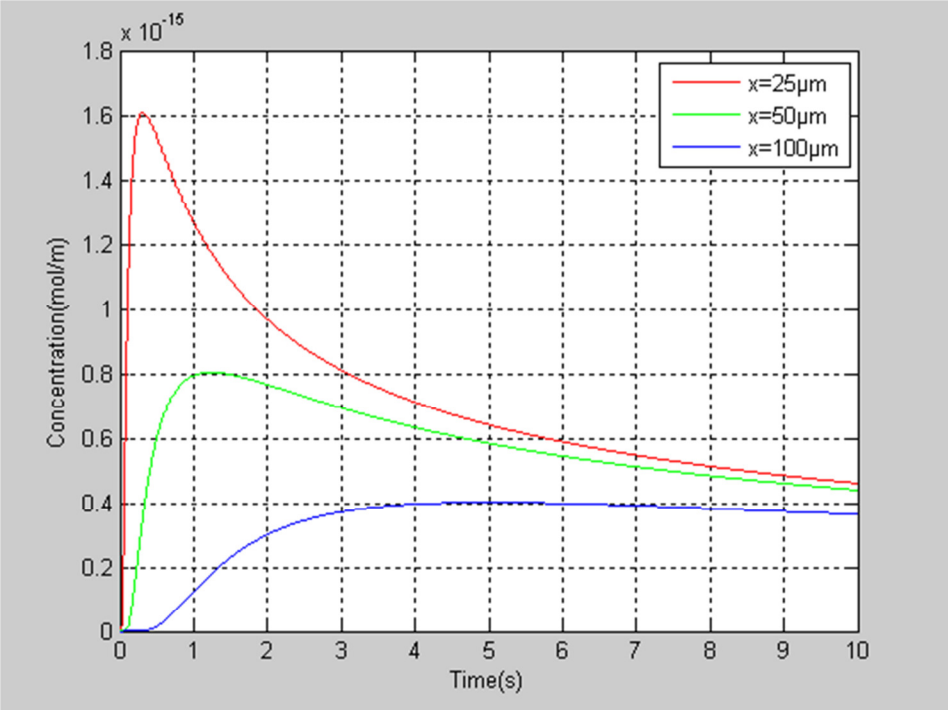

Figure 5.1: Molecular Concentration at Destination Nanomachine with Respect to Time in *1D* Environment

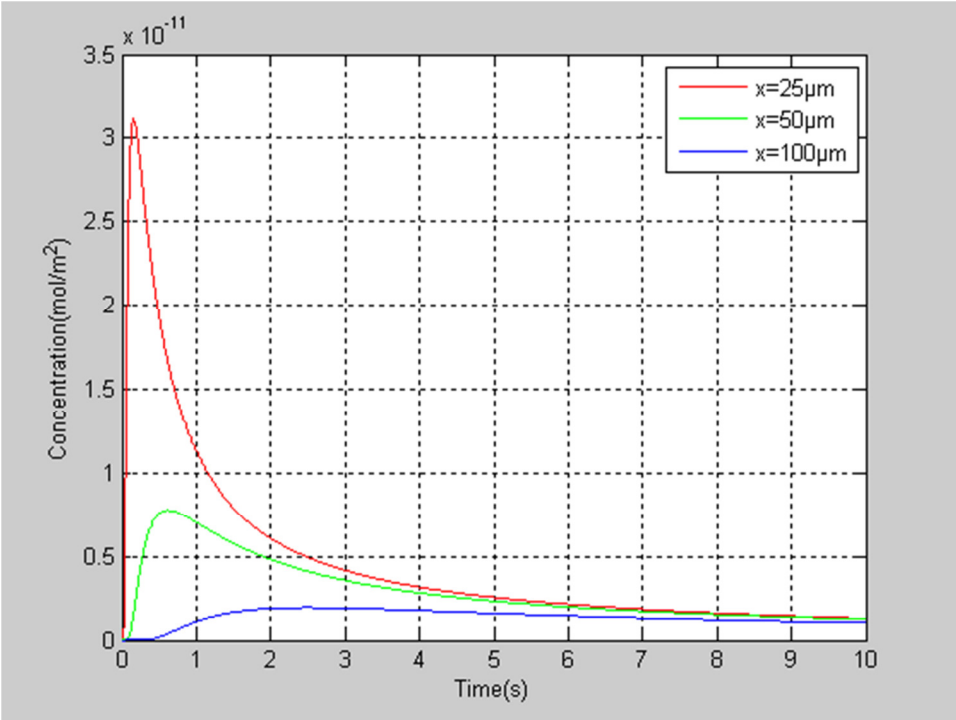

Figure 5.2: Molecular Concentration at Destination Nanomachine with Respect to Time in *2D* Environment

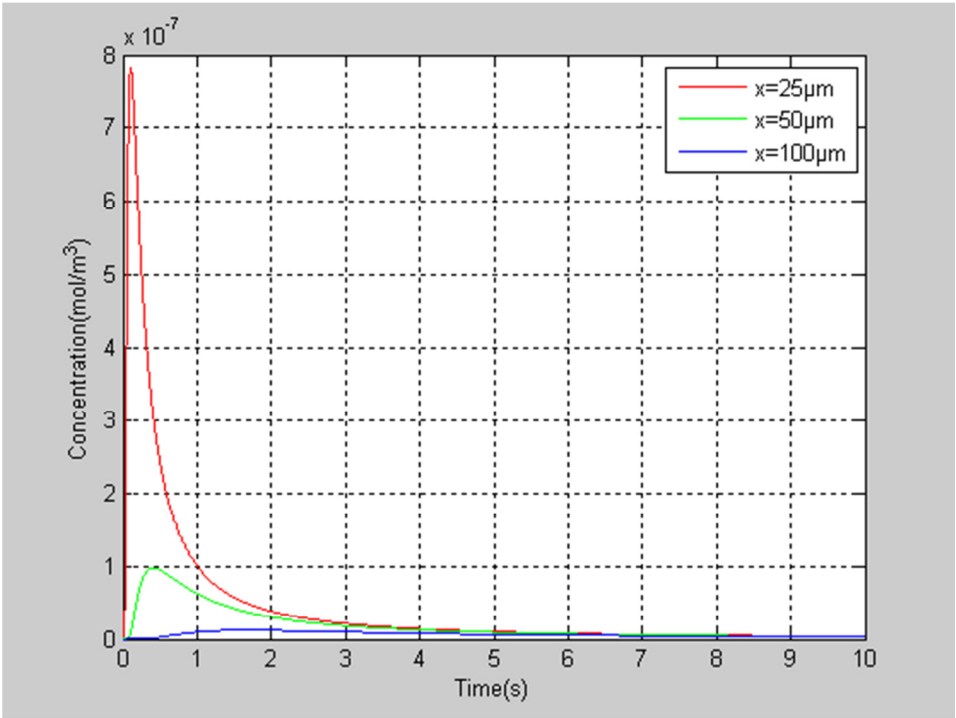

Figure 5.3: Molecular Concentration at Destination Nanomachine with Respect to Time in *3D* Environment

If we consider each figure separately, it is understood that as *x* grows not only we have a sudden drop in the maximum concentration level at *L* but also the time at which this maximum occurs is delayed, which means that regardless of the dimensions, as the distance between the sender and the receiver increases, the peak at which the maximum concentration at the destination occurs will be delayed. For instance, in Figure 5.3 when $\|\vec{x}\| = 25\mu m$ the peak occurs sooner compared to when $\|\vec{x}\| = 50\mu m$ or $\|\vec{x}\| = 100\mu m$, and this applies to Figure 5.1 and Figure 5.2, as well.

As seen in all three results, the distance between the two nanomachine, has a crucial effect on the concentration of the information molecules at *L*. As a result, in this thesis, by using a relay nanomachine (i.e., *R*) between the S and *L*, it is shown that with the same number of molecules (i.e., *m*) and by simply dividing them between *S* (i.e.,m_1)and R (i.e., m_2), higher concentration at *L* is achievable compared to a scenario where all *m* molecules are placed in *S*.

5.2 Introducing the Relay Node to the Scenario

In our second scenario, we are dealing with one sender(*S*), one receiver(*L*) and one relay node(*R*). By using Eq. (4.2), the main goal is to investigate the effect of different divisions of m molecules between *S* and *R*, plus the effect of the distance between *R* and *L*, and different activation times of *R* on the maximum molecular concentration at *L*. The topology of the network is according to Figure 4.1. The results are shown in the figures 5-4 to 5-6 below, where m=10^5 particles, D=$10^{-9}\ \frac{m^2}{s}$, and $\|\vec{x}\|$=$100\mu m$:

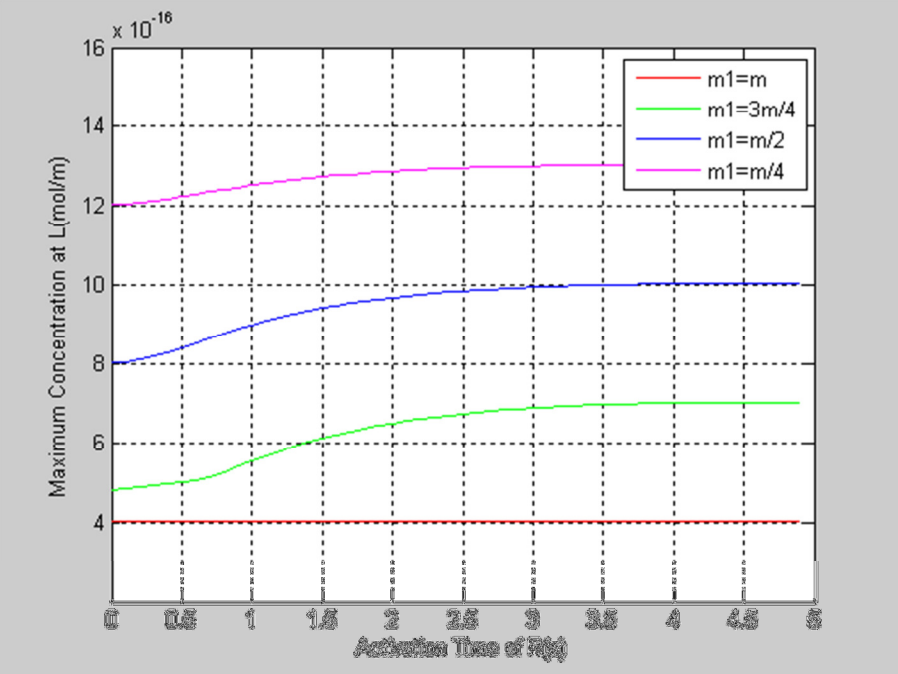

Figure 5.4: The Effect of Different Divisions of Molecule Budget (i.e., *m*), and Different Activation Times of *R* on the Maximum Concentration in Destination Nanomachine (*L*), when $\|\vec{r}\| = \frac{\|\vec{x}\|}{4}$ (for *1D* Environment)

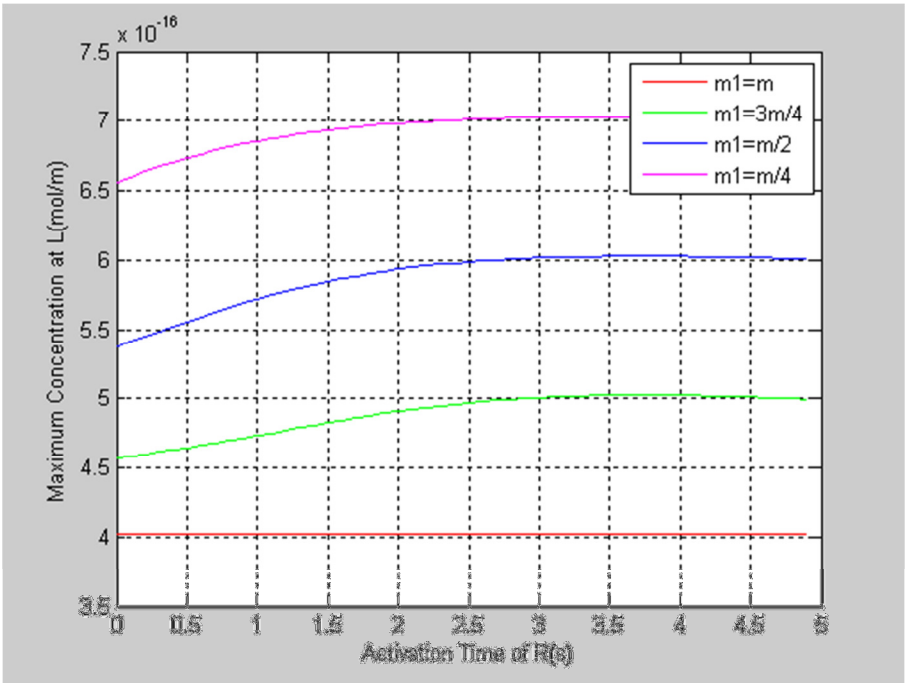

Figure 5.5: The Effect of Different Divisions of Molecule Budget (i.e., *m*), and Different Activation Times of *R* on the Maximum Concentration in Destination Nanomachine (*L*), when $\|\vec{r}\| = \frac{\|\vec{x}\|}{2}$ (for *1D* Environment)

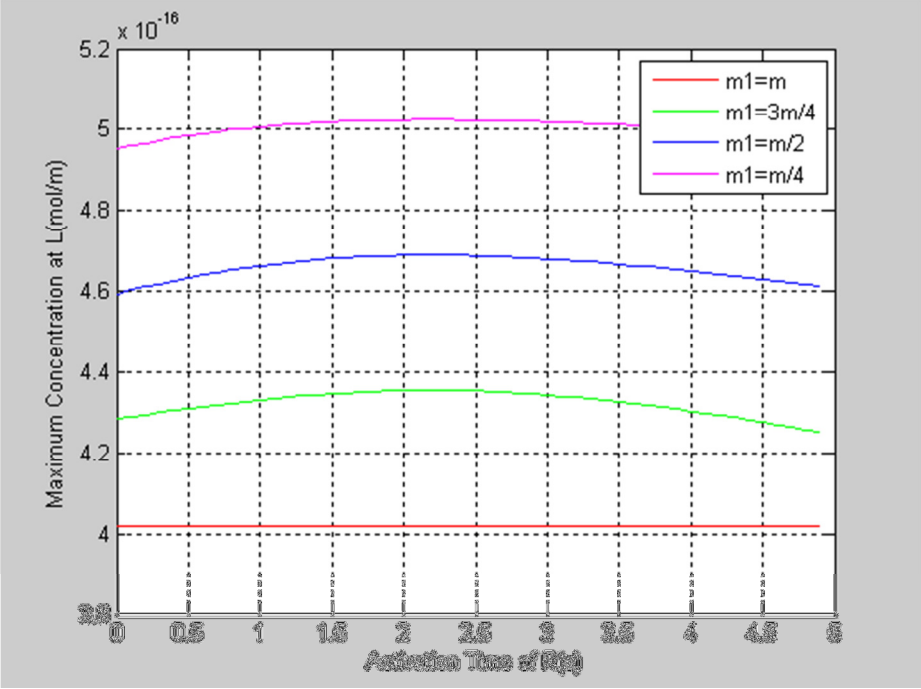

Figure 5.6: The Effect of Different Divisions of Molecule Budget (i.e., m), and Different Activation Times of R on the Maximum Concentration in Destination Nanomachine (L), when $\|\vec{r}\| = \frac{3\|\vec{x}\|}{4}$ (for *1D* Environment)

For instance, in Figure5.4, as we decrease m_1, number of molecules that are put in S, m_2, number of molecules that are put in R, increases, and as a result we can see that when we put $\frac{1}{4}$ of molecule budget in S (i.e., $m_1=\frac{m}{4}$ and $m_2=\frac{3m}{4}$) the maximum concentration is always higher than other divisions of m between S and R, specially a great deal more than the case where we put all the molecules in S (i.e., $m_1=m$ and $m_2=0$), which shows the benefit of using a relay node, and this applies to Figure 5.5 and Figure 5.6, as well.

Moreover, if we compare the three figures above, it can be understood that as the distance between R and L (i.e., r), decreases the maximum concentration at L would also get higher. According to all the figures, as m_2 increases and r decreases, the maximum possible concentration at L increases, drastically, where in our analysis the highest

maximum concentrations happen when $m_1 = \frac{m}{4}$ (i.e., $m_2 = \frac{3m}{4}$) and $\|\vec{r}\| = \frac{\|\vec{x}\|}{4}$. Moreover, the same rule applies to *2D* and *3D* environments according to the Figures 5.7 through 5.12 below:

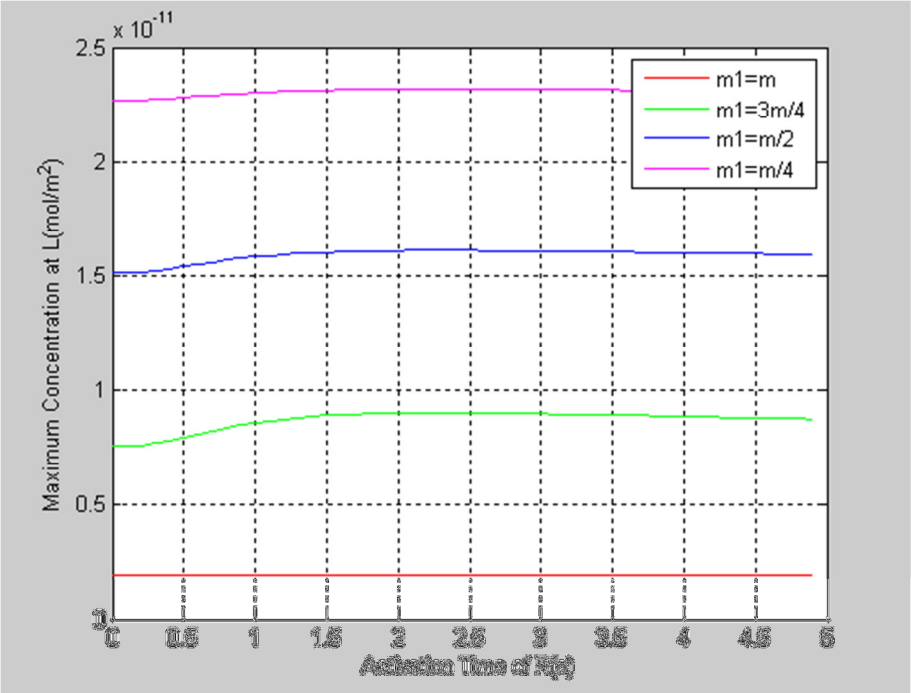

Figure 5.7: The Effect of Different Divisions of Molecule Budget (i.e., *m*), and Different Activation Times of *R* on the Maximum Concentration in Destination Nanomachine (*L*), when $\|\vec{r}\| = \frac{\|\vec{x}\|}{4}$ (for *2D* Environment)

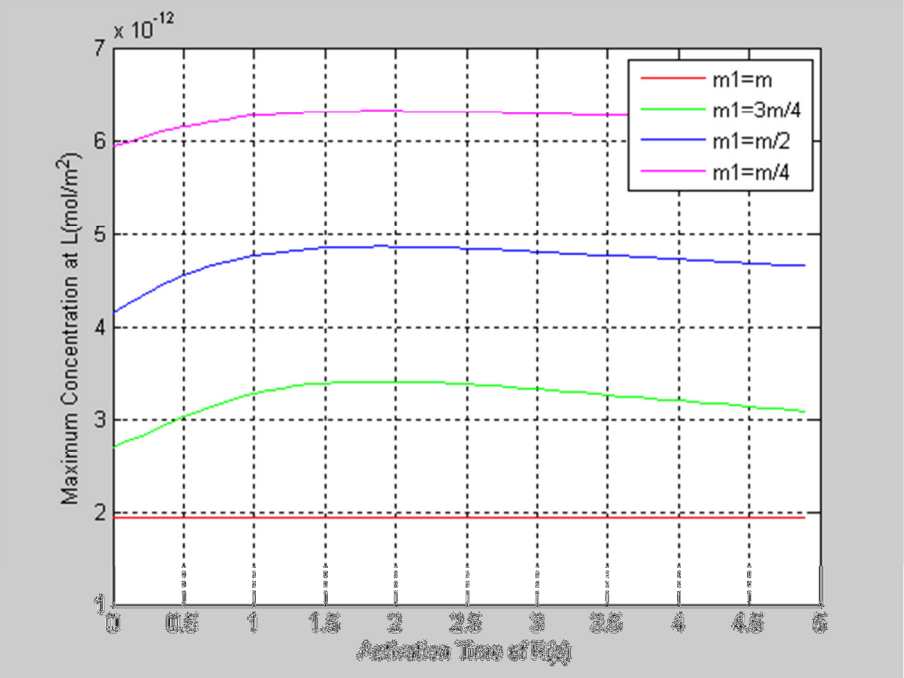

Figure 5.8: The Effect of Different Divisions of Molecule Budget (i.e., m), and Different Activation Times of R on the Maximum Concentration in Destination Nanomachine (L), when $\|\vec{r}\| = \frac{\|\vec{x}\|}{2}$ (for *2D* Environment)

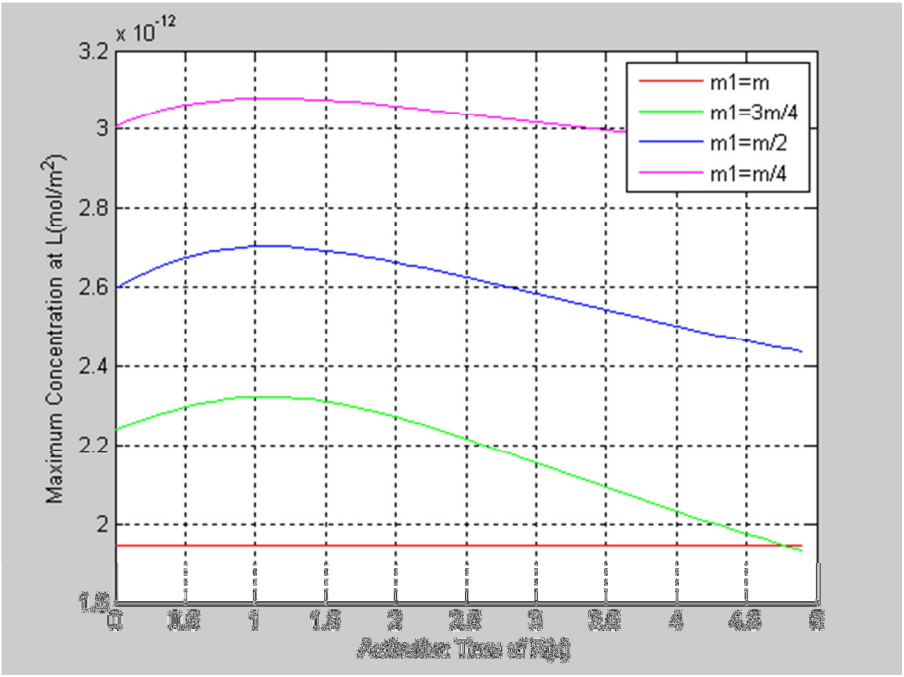

Figure 5.9: The Effect of Different Divisions of Molecule Budget (i.e., m), and Different Activation Times of R on the Maximum Concentration in Destination Nanomachine (L), when $\|\vec{r}\| = \frac{3\|\vec{x}\|}{4}$ (for *2D* Environment)

As we can see, the highest maximum concentrations happen when $m_1 = \frac{m}{4}$ (i.e., $m_2 = \frac{3m}{4}$) and $\|\vec{r}\| = \frac{\|\vec{x}\|}{4}$. This is also the case in *3D* environment.

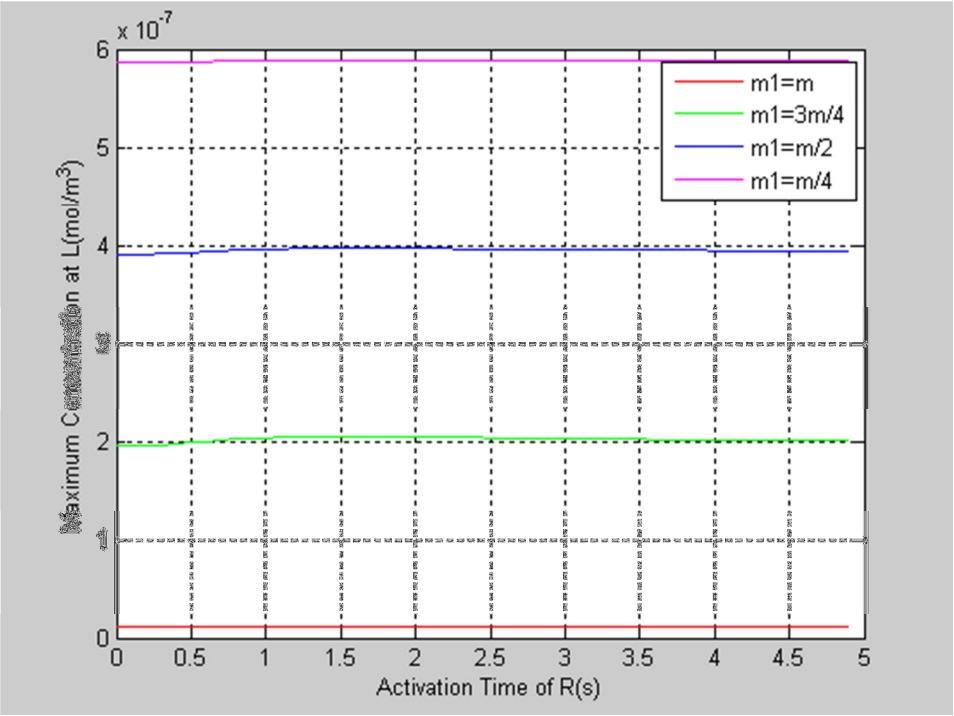

Figure 5.10: The Effect of Different Divisions of Molecule Budget (i.e., *m*), and Different Activation Times of *R* on the Maximum Concentration in Destination Nanomachine (*L*), when $\|\vec{r}\| = \frac{\|\vec{x}\|}{4}$ (for *3D* Environment)

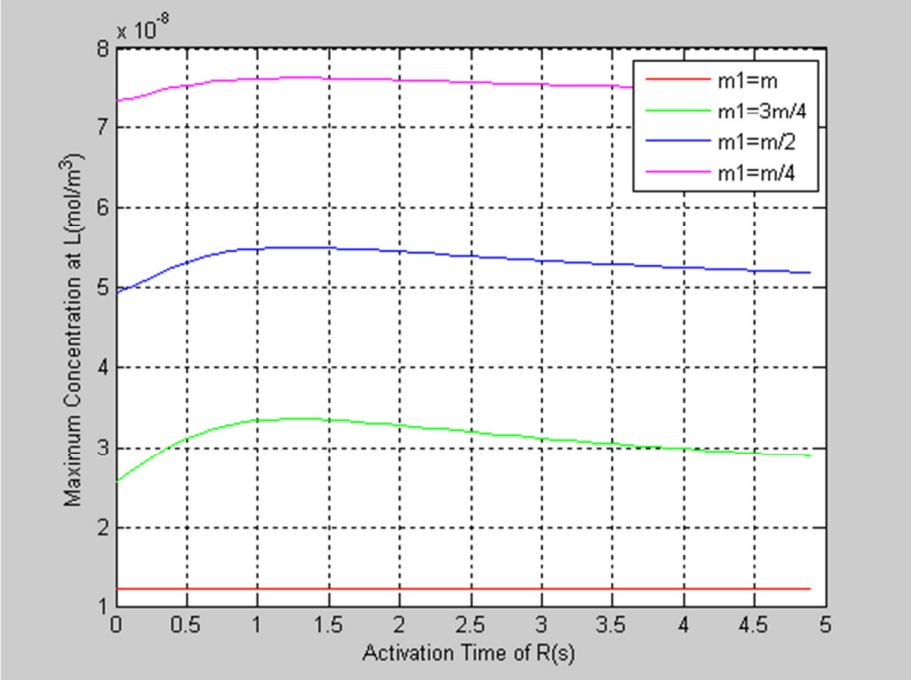

Figure 5.11: The Effect of Different Divisions of Molecule Budget (i.e., *m*), and Different Activation Times of *R* on the Maximum Concentration in Destination Nanomachine (*L*), when $\|\vec{r}\|=\frac{\|\vec{x}\|}{2}$ (for *3D* Environment)

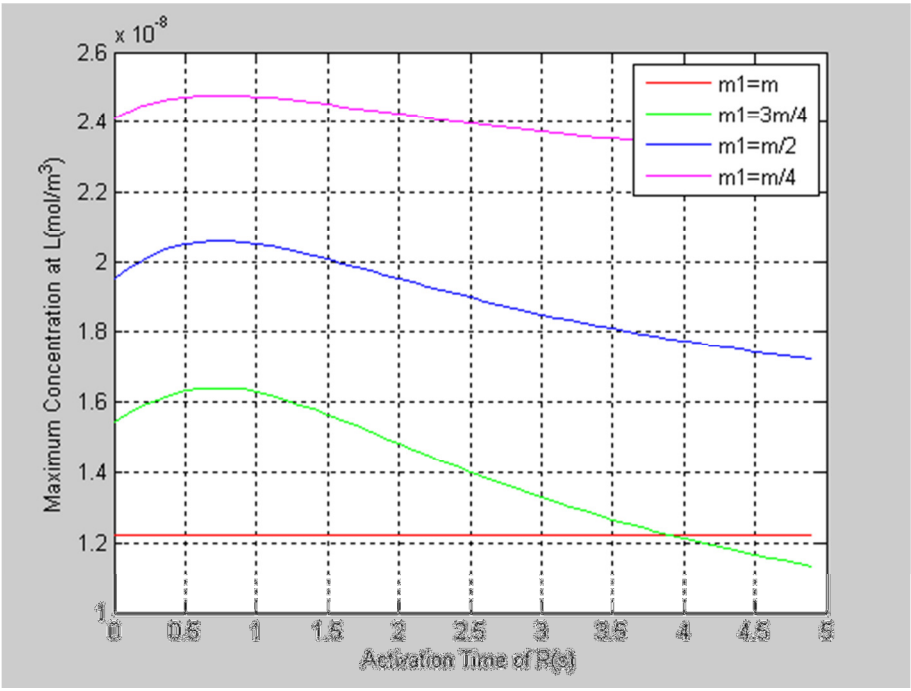

Figure 5.12: The Effect of Different Divisions of Molecule Budget (i.e., *m*), and Different Activation Times of *R* on the Maximum Concentration in Destination Nanomachine (*L*), when $\|\vec{r}\| =\frac{3\|\vec{x}\|}{4}$ (for *3D* Environment)

According to the results, a relay node could help us achieve much higher concentrations with the same molecule budget compared to the scenario in which all *m* molecules are stored in *S* and there is no relay node to amplify the attenuated signal. One other important issue in the results is the fact that for all cases, the plots are concave and have a maximum. This means that there is an optimum activation time for the relay node which results in the maximum concentration at *L*. As mentioned before, this optimum time is calculated using Eq. (4.5). For example, consider Figure 5.12:

Using Eq. (4.5), and by replacing corresponding values with the variables we can calculate the optimum t_2 for the relay node *R*. In this figure, t_1=$10^{-9}\ s$, $\|\vec{x}\|$=100μm, $\|\vec{r}\|$=75μm, d=3 and D=$10^{-9}\ \frac{m^2}{s}$, thus the optimum t_2 is equal to:

$$t_2 = \frac{(10^{-4})^2 - (75\times10^{-6})^2}{2\times3\times10^{-9}} + 10^{-9} = 0.7291$$

As it is obvious from the figures, this is independent of m_1. So far, it was assumed that the relay node (*R*) starts to emit at a certain time (i.e., t_2). However, in the real life applications, *R* would not start emission unless it senses some predefined concentration of information molecules at its vicinity (i.e., threshold or θ), as discussed in previous chapter. Therefore, one must carefully allocate enough number of molecules from the molecule budget on *S*. Now, let's say we are given a particular position to place a relay node, and we are asked to determine the minimum number of molecules that should be placed in *S*. This can be easily achieved by using the inequality (4.11). According to [31], since the typical number of particles released by a cell in a puff is 10^5 , then the

value of detection threshold could be for example 100 particles. Moreover, according to [31] since the size of an animal cell is 10µm then, for the vicinity size of R (i.e., δ) the size of the cell itself (i.e. 10 micrometer) is considered. In Figure 5.13, using the inequality. (4.11), the effect of r over m_1 is investigated for 1, 2 and 3 dimensions.

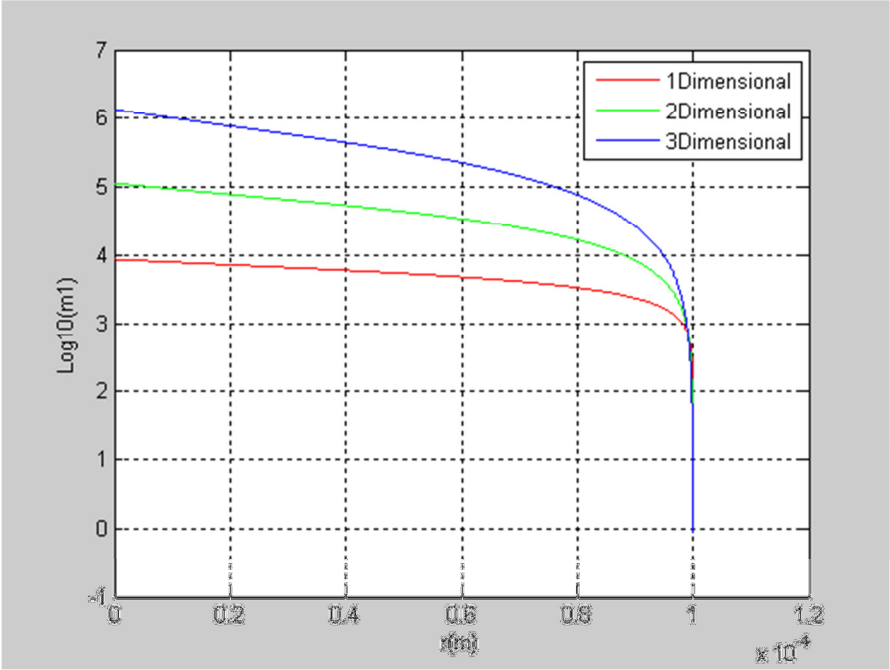

Figure 5.13: The Effect of r on the Number of Molecules in S (i.e., m_1)

As it can be seen, as r leans to x, which means R gets closer to S, we need a less number of molecules in S, and naturally, when r is equal to x, m_1 drops to zero. The main important issue is to compare this behavior in 1, 2 and 3 dimensions. As depicted in Figure 5.13, the minimum required m_1 in S for a 3 dimensional environment is approximately 10 times and 100 times greater than 2, and 1 dimensional environments, respectively. This means that for a specific r, the minimum number of particles that we have to put in S will be m_1, $10m_1$, and $100m_1$, for 1, 2 and 3 dimensions, respectively.

The last issue to be discussed is a scenario where we are given the threshold Θ, and m_1 and we are asked to find an appropriate r for positioning the R. In this thesis, this scenario is specialized to 1 dimensional environment, where by using Matlab, we solve the transcendental Eq. (5.1) numerically for r:

$$\frac{m_1}{\sqrt{2\pi(\|\vec{x}\|^2 - \|\vec{r}\|^2)}}\, e^{\frac{-(\|\vec{x}\| - \|\vec{r}\|)}{2(\|\vec{x}\| + \|\vec{r}\|)}} - \Theta = 0 \qquad (5.1)$$

Assuming that S releases 10^5 particles in the medium, Table 5-1 depicts the computed values of r according to different values of Θ in R. For easy comparison, values of Θ are written in terms of number of particles per meter instead of moles per meter. As expected, as R becomes more sensitive (i.e., Θ becomes smaller) the value of r decreases accordingly, which means that R can be placed further from S and yet it can get triggered by the molecules sent by S.

Table 5.1: The effect of Θ on the position of R when m_1=$\mathbf{10^5}$ particles and x=100µm

Θ (No.of particles/m)	20000	17500	15000	12500	10000	7500	5000
$r(\mu m)$	92.049	89.621	85.892	79.748	68.655	46.395	3.3158

Chapter 6

CONCLUSION

In this thesis molecular communication, which is a new communication paradigm, has been studied. Moreover, it has been shown that using a relay node in our scenario between the sender and the receiver nanomachines in 1,2, and 3 dimensional environments is actually quite beneficial in terms of maximizing the molecular concentration at the destination nanomachine for signal detection. According to the numerical analysis, assuming that we have a molecule budget restriction called *m*, in order to get the maximum possible concentration we can divide *m* between the sender and nanomachines and get much more concentration at the destination compared to the scenario where all *m* molecules are put in the sender nanomachine. The main contribution of this thesis is to answer some critical questions such as:

- How should *m* be divided between the sender nanomachine and the relay node.

- What is the optimal time at which the relay node should be activated in order to maximize the molecular concentration at the receiver nanomachine.

-

- In case we are given the position of the relay node what is the minimum number of molecules that should be put in the sender nanomachine in order to guarantee the maximum concentration at the destination nanomachine.

- In case we are given the threshold of the relay node where should it be placed between the sender and the receiver nanomachines in order to maximize the molecular concentration at the destination nanomachine.

REFERENCES

[1] E. Drexler, 29 12 2009. [Online]. Available: http://www.metamodern.com.

[2] N. Taniguchi, "On the Basic Concept of 'Nano-Technology'," in *Proc. Intl. Conf. Prod.Eng*, Tokyo: Japan Society of Precision Engineering, 1974.

[3] S. Cavalle, "Cooperative Signal Amplification for Molecular Communication in Nanonetworks," Thesis, Barcelona, 2011.

[4] l. F. Akyildiz, F. Brunetti and C. Blázquez, "Nanonetworks: A new communication paradigm," *Computer Networks,* vol. 52, no. 12, pp. 2260-2279, 2008.

[5] A. Fereidouni, "Analysis of Connectivity in Diffusion-Based Molecular Nano Communication Networks," M.Sc. thesis, Gazimagusa, North Cyprus, 2013.

[6] H. Goldstein, "The race to the bottom," vol. 42, no. 3, pp. 32-39, 2005.

[7] M. Meyyappan, J. Li, J. Li and A. Casselle, "Nanotechnology: An overview and integration with MEMS," in *Proceedings of the 19th IEEE International*

Conference on Micro Electro Mechanical Systems, 2006.

[8] C.-Y. Chang, "The highlights in the nano world," in *Proceedings of the IEEE 91*, 2003.

[9] C. Peterson, "Taking technology to the molecular level," *IEEE Computer 33,* vol. 33, no. 1, pp. 46-53, 2000.

[10] E. Drexler, C. Peterson and G. Pergami, "Unbounding the future: The nanotechnology revolution," Foresight Institute, Technical Report, 1991.

[11] G. Whitesides, "The once and future nanomachine," *Scientific American,* pp. 77-83, 2001.

[12] T. Nakano, M. Moore, F. Wei, A. Vasilakos and J. Shuai, "Molecular Communication and Networking: Opportunities and Challenges," *NanoBioscience, IEEE Transactions,* vol. 11, no. 2, 2012.

[13] T. Nakano, M. Moore, A. Enomoto and T. Suda, "Molecular Communication Technology as a Biological ICT," *Biological Functions for Information and Communication Technologies,* pp. 49-86, 2011.

[14] C. Chen, Y. Haik and J. Chatterjee, "Development of nanotechnology for biomedical applications," in *Proceedings of the Emerging Information Technology Conference*, 2005.

[15] R. Freitas, "What is nanomedicine?," *Nanomedicine: Nanotechnology, Biology and Medicine,* vol. 1, no. 1, pp. 2-9, 2004.

[16] R. Freitas, "Nanotechnology, nanomedicine and nanosurgery," *International Journal of Surgery 3,* p. 243–246, 2005.

[17] I. F. Akyildiz, F. Fekri, R. Sivakumar, C. Forest and B. Hammer, "MoNaco: Fundamentals of Molecular Nano-Communication Networks," *IEEE Wireless Communication,* vol. 19, no. 5, pp. 12-18, 2012.

[18] J. Aylott, "Optical nanosensors – an enabling technology for intracelular measurements," *Analyst 128,* p. 309–312, 2003.

[19] M. Endo, T. Hayashi, Y. Kim and H. Muramatsu, "Development and applications of carbon nanotubes," *Japanese Journal of Applied Physics 46,* p. 4883–4892, 2006.

[20] M. S. Dresselhaus, G. Dresselhaus, P. Avouris and R. E. Smalley, Carbon

Nanotubes: Synthesis, Structure, Properties and Applications, Springer, 2001.

[21] J. F. R. S. J. Han, "Molecular sieving using nanofilters: past, present and future," *Lab on a Chip 8,* pp. 23-33, 2008.

[22] I. F. Akyildiz and J. M. Jornet, "Electromagnetic wireless nanosensor networks," *Nano Communication Networks (Elsevier),* pp. 3-19, 2010.

[23] B. I. T.R. de Kievit, "Bacterial quorum sensing in pathogenic relationships.," *Infect.Immun.,* p. 4839–4849, 2000.

[24] S. Hiyama, Y. Moritani, T. Suda, R. Egashira, R. Enomoto, M. Moore and T.Nakano, "Molecular Communication," *Nanotechnology Conference,* pp. 391-394, 2005.

[25] M. Berridge, "The AM and FM of calcium signalling," *Nature 386,* pp. 759-760, 1997.

[26] J. Smith, "The concept of information in biology.," *Philos. Sci.,* p. 177–194, 2000.

[27] T. Nakano and J. Shuai, "Repeater Design and Modeling for Molecular Communication Networks," *IEEE Conference on Computer Communications*

Workshops, pp. 501-506, 2011.

[28] B. Atakan and O. B. Akan, "On Molecular Multiple-Access, Broadcast, and Relay Channels in Nanonetworks," in *3rd International Conference on Bio-Inspired Models of Network, Information and Computing Sytems*, Brussels, Belbium, 2008.

[29] J. Crank, The mathematics of diffusion, New York: Oxford University Press Inc., 1975.

[30] S. Farlow, "Partial Differential Equations for Scientists and Engineers," in *Partial Differential Equations for Scientists and Engineers*, Dover, 1982, pp. 6-7.

[31] R. A. Freitas Jr., Nanomedicine, Volume I: Basic Capabilities, Georgetown, TX: Landes Bioscience, 1999.

APPENDIX

Appendix: Source Codes

The Effect of Distance between Sender and Receiver Nanomachines on Molecular Concentration at the Receiver Nanomachine for 25, 50, and 100µm:

```
a=6.02*10^23;
m=10^5/a;
D=10^-9;
x=[25e-6,50e-6,100e-6]; % Distance between Sender and Receiver
t=0:10^-6:5;
c=zeros(length(x),length(t));
d=1;                    % The Dimension of the Environment (Could be 1, 2 or 3)

for i=1:length(x)
   for j=1:length(t)
   c(i,j)=m/((4*pi*t(j)*D)^(d/2))*exp((-x(i)^2)/(4*t(j)*D));
   end
end

plot(t,c(1,:),'r',t,c(2,:),'g',t,c(3,:),'b')
legend('x=25µm','x=50µm','x=100µm');
xlabel('Time(s)');
ylabel('Concentration(mol/m)');
grid on;
```

The Effect of the Relay Node's Activation Time, Different Divisions of Molecular Budget between Sender and Relay Node, and Relay Node's Position on the Maximum Molecular Concentration at Receiver:

```
a=6.02*10^23;
m=(10^5)/a;
x=100e-6;
D=10^-9;
d=3;  % The Dimension of the Environment (Could be 1, 2 or 3)
tk1=10^-9;
tk2=10^-9:10^-1:5;
t=10^-9:10^-1:10;
c=zeros(1,length(t));
a=zeros(1,length(t));
```

```
b=zeros(1,length(t));
x1=0;
m_fraction=[1,3/4,1/2,1/4];
x_fraction=[1/4,1/2,3/4];
         maxx=zeros(length(m_fraction),length(x_fraction),length(tk2));
        for j=1:length(m_fraction)
        m1=m*m_fraction(j);
        m2=m-m1;
        for dist=1:length(x_fraction)
        x2=x*x_fraction(dist);
        for k=1:length(tk2)
        for i=1:length(t)
        if (t(i)-tk1)<0
        flag1=0;
        else
        flag1=1;
        end
        if (t(i)-tk2(k))<0
        flag2=0;
        else
        flag2=1;
        end
   a(i)=((m1/((4*pi*(t(i)-tk1)*D)^(d/2))*exp((-(x-x1)^2)/(4*(t(i)-tk1)*D))))*flag1;
   b(i)=((m2/((4*pi*(t(i)-tk2(k))*D)^(d/2))*exp((-(x2)^2)/(4*(t(i)-tk2(k))*D))))*flag2;
        end
       a(isnan(a))=0;
       b(isnan(b))=0;
        c=a+b;
        maxx(j,dist,k)=max(c);
        end
        end
        end
        grid on;
plot(tk2,reshape(maxx(1,1,:),1,50),'r', tk2,reshape(maxx(2,1,:),1,50),'g',
tk2,reshape(maxx(3,1,:),1,50),'b', tk2,reshape(maxx(4,1,:),1,50),'m')
legend('m1=m','m1=3m/4','m1=m/2','m1=m/4')
title('Relay Distance from L is x/4')
xlabel('Activation Time of R(s)');
ylabel('Maximum Concentration at L(mol/m^3)');
grid on;
figure
plot(tk2,reshape(maxx(1,2,:),1,50),'r', tk2,reshape(maxx(2,2,:),1,50),'g',
tk2,reshape(maxx(3,2,:),1,50),'b', tk2,reshape(maxx(4,2,:),1,50),'m')
legend('m1=m','m1=3m/4','m1=m/2','m1=m/4')
title('Relay Distance from L is x/2')
xlabel('Activation Time of R(s)');
```

```
ylabel('Maximum Concentration at L(mol/m^3)');
grid on;
figure
plot(tk2,reshape(maxx(1,3,:),1,50),'r', tk2,reshape(maxx(2,3,:),1,50),'g',
tk2,reshape(maxx(3,3,:),1,50),'b', tk2,reshape(maxx(4,3,:),1,50),'m')
legend('m1=m','m1=3m/4','m1=m/2','m1=m/4')
title('Relay Distance from L is x/2')
xlabel('Activation Time of R(s)');
ylabel('Maximum Concentration at L(mol/m^3)');
grid on;
```

The effect of Relay Node's Position on the Value of m_1 for 1,2, and 3 Dimensions:

```
a=6.02*10^23;
m=10^5;
x=100e-6;
delta=10e-6; %Detection vicinity in destination
area=pi*(delta^2);
volume=(4*pi*(delta^3))/3;
max_c=m/(x^3); %maximum available concentration in 3D at distance x
particles=max_c*volume;
thresh=[particles/(2*delta) particles/area particles/volume];
r=0:1e-8:x;
z=x-r;
m1=zeros(3,length(r));
for d=1:3
   for i=1:length(r)
         m1(d,i)=log10(thresh(d)*((2*pi*(x^2-
        ((r(i))^2))/d)^(d/2))*exp(d*(z(i)^2)/(2*(x^2-((r(i))^2)))));
   end
end
plot(r,m1(1,:),'r',r,m1(2,:),'g',r,m1(3,:),'b')
legend('1Dimensional','2Dimensional','3Dimensional')
xlabel('r(m)');
ylabel('Log10(m1)');
grid on;
hold on
```

Determining the Position of the Relay Node based on Θ and m_1 (Specialized to 1D):

```
a=6.02*10^23;
m=10^5/a;
delta=10e-6; %Detection vicinity in destination
x=100e-6;
area=pi*(delta^2);
volume=(4*pi*(delta^3))/3;
max_c=(m/x); %maximum available concentration in 1D at distance x
particles=max_c*2*delta;
th=particles/(2*delta);
r=0:1e-8:x;
yplot=m./(2*pi*(x.^2-r.^2)).^(1/2).*exp(-(x-r)./(2*(x+r)))-th;
plot(r,yplot)
y=@(r) m/(2*pi*(x^2-r^2))^(0.5)*exp(-(x-r)/(2*(x+r)))-th;
number_of_released_particles_by_S=m*a
threshold_of_R=particles*a
the_value_of_r=fzero(y,[0,99.9e-6])
```