İSTANBUL TECHNICAL UNIVERSITY ★ GRADUATE SCHOOL OF SCIENCE ENGINEERING AND TECHNOLOGY

A TRANSMISSION MODEL FOR DIFFUSION BASED MOLECULAR COMMUNICATION NANO NETWORKS

M.Sc. THESIS

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İSTANBUL TEKNİK ÜNİVERSİTESİ ★ FEN BİLİMLERİ ENSTİTÜSÜ

YAYILIM TABANLI MOLEKÜLER HABERLEŞME NANO AĞLARI İÇİN BİR AKTARIM MODELİ

YÜKSEK LİSANS TEZİ

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Bilgisayar Mühendisliği Anabilim Dalı

Bilgisayar Mühendisliği Programı

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MAYIS 2016

Daniel Nzinga KINSUMUNA (504111537), a M.Sc.student of İTUGraduate School of Science Engineering and Technology, successfully defended the thesis entitled "**A TRANSMISSION MODEL FOR DIFFUSION BASED MOLECULAR COMMUNICATION NANO NETWORKS**", which he prepared after fulfilling the requirements specified in the associated legislations, before the jury whose signatures are below.

Thesis Advisor : **Assoc. Prof. Dr. D.Turgay ALTILAR** .....

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Jury Members : **Prof. Dr. Sema OKTUĞ** .....

Asst. Prof. Dr. Müjdat SOYTÜRK .....

Date of Submission : 21 April 2016

Date of Defense : 9 May 2016

To my family for their endless love, support and courage...

FOREWORD

I would like to express my heartiest thanks to Dr. Deniz Turgay Altılar, who has been not only my MSc. advisor, but also a special person for me, from the very moment I came to Istanbul Technical University with my heart full of hopelessness, he gave me hope to go far eventually completing my MSc. He truly shaped my will and my strength, he showed me the right path, he taught me how to focus, concentrate, believe in my potential, and he made me achieve what I would have never thought. Now I am changed, I feel stronger, more confident of who I am, what I want, and where I am going, and this is primarily thanks to Dr. Deniz Turgay Altılar, to whom I owe a lot.

My sincere and warm thanks go also to the whole computer engineering faculty family of Istanbul Technical University, to past and currentmembers, from whom I learnedmany subjects in computer engineering field. Amazing personalities, open hearts and willing to teach knowledge, were thetrue gifts I received from them. People I will never forget in my entire life.

I would like to extend my sincere thanks to Deniz Demiray,who accepted to serve as co-advisorduring my entire work, and whose constrictive criticismhelped me take the final leap towards the completion of this lifechangingexperience.

I dedicate this work to my wife, for her endless care and love for our happiness, and for her continuous moral support over many difficulties, where she exercised great and endless encouragement; and to my lovely son and daughter Daniel NZINGA KINSUMUNA and Davina NYUMBA KINSUMUNA, for the happiness they have brought in to my life. I will always remember the greatest love, support, and courage from my family which is more than expected by all means.

May 2016 Daniel Nzinga KINSUMUNA

(Computer Engineer)

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ABBREVIATIONS

MC **:** Molecular Communication

SYMBOLS

β **:** The harvester rate

τ **:** The time step

δ **:** The spatial step

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A TRANSMISSION MODEL FOR DIFFUSION BASED MOLECULAR COMMUNICATION NANO NETWORKS

SUMMARY

Molecular communication has been an attractive topic for researchers afterthe introduction of the nanoscale communications. Numerous potential applications of nanonetworks make molecular communication even more appealing.These potential applications range from biomedical applications, such as intelligent drug delivery and health monitoring systems, to military and environmentalapplications such as air pollution monitoring. Nanonetworks is a communication between nanodevices, called nanomachines or molecular machine. A nanomachine can be definedas an artificial device that relies on nanometer-scale components.Molecular communication is one of the types of nanonetworks in which nanomachines are able to sense, calculate, actuate and intercommunicate. Transmission, propagation and reception are the three main stages to provide information exchange between sender and receiver in molecular communication. Diffusion based molecular communication that is an essential type of molecular communication, relies on propagation of molecules between sender and receiver nodes through free diffusion. There are three different phases in diffusion based molecular communication. The first phase is named emission process. In this phase, the transmitter nanomachine or the sender node emits particles into the medium. The second phase is composed of diffusion process. In this part, emitted particles by the transmitter node are subject to Brownian motion. Finally, the last phase, the reception process in which the receiver nanomachine or receiving node absorb or capture all particles within its range. Throughout this thesis, the harvester and receiver nodes have been considered as absorbers that capture particles which are in contact with their range. For the working operating environment is a bounded confined one, no particle escapes from it. Furthermore, particles released by the transmitter node during transmission process, circulate in the bounded operating environment and when a particle reaches the edge or boundary of the working environment, it is bounced back into the

working environment. Therefore, the total number of particles within the bounded operating environment remains unchanged along the time. The amount of particles to be released by the transmitter node at a certain time t represents the input or the signal of the model. Afterwards, the signal of the model propagates in the bounded fluidic space via diffusion. In this work, the diffusion of particles is achieved via random walk. Therefore, the propagation of particles between transmitter and receiver nodes is uniquely accomplished via Brownian motion. Harvester nodes have been assigned a limited harvesting capacity that cannot exceed a certain amount of particles in order to investigate their impact upon the signal reception at the receiving node. For example, if the harvesting node reservoir capacity is full, a new particle reaching its range will result to hitting one particle from the harvester reservoir. A particle has a kinetic energy along each axis, which is the half of the product of the absolute temperature and Boltzmann's constant. And also it has a mass and speed or velocity that has been assumed to be unchanged and independent of time. The model is to investigate the impact of the harvester nodes on signal reception at the receiver node. The receiver node measures the concentration within its range, which is subject to the signal strength. This thesis investigates how harvesting nodes can degrade the signal strength of the receiver node in a confined space. The analytic expression of the received signal at the receiver node has been drawn; the effects of the increasing number of harvesting nodes and the harvesting rate have been discussed in this work.Scientists in diffusion based molecular communication may use that analytic expression proposed in this current paper when dealing with nanonetworks composed of more than two receiving nodes. The signal received in terms of concentrations at the receiver node has been approximated using finite difference methods and the accuracy of each numerical scheme (Explicit, Implicit and Crank Nicolson) has been computed and compared to the analytic solutions. The rest of the thesis is organized as follows. The introduction is given in section I. The model description is presented in section II. In section III, the analytic expression that computes the concentration of receiver node in a scenario of multiple harvesters is proposed. The results are discussed in section IV. The section V provides the approximations on the signal received at the receiver nanomachine. Finally, a conclusion has been drawn based on the results obtained at sections IV and V in section VI.

YAYILIM TABANLI MOLEKÜLER HABERLEŞME NANO AĞLARI İÇİN BİR AKTARIM MODELİ

ÖZET

Nano ölçekli haberleşmenin tanıtımından sonra moleküler haberleşme, bilim adamları için cazip bir araştırma konusu haline çevrilmiştir. Nanoağların çok sayıda olası uygulamaları günümüzde moleküler haberleşmeyi daha da çekici kılmıştır. Bu olası uygulamalar biyomedikal alanında akıllı ilaç dağıtımı ve sağlık izleme sistemlerinden başlayıp, askeri ve çevresel alanlarda uygulanan hava kirliliğini izleme gibi uygulamalarla değişe bilir.Nanoağ, nanomakine veya moleküler makine gibi adlandırılan nanocihazlar arasında haberleşme veya iletişim biçimidir. Nanomakine, nanometre ölçekli bileşenlere dayanan yapay cihaz olarak düşünüle bilir. Moleküler haberleşme, nanomakinelerin algılaya, hesaplaya ve haberleşe bildiği iletişim türlerinden biridir. Transmisyon veya aktarma, yayılma/üreme ve resepsiyon - moleküler haberleşmede gönderici ve alıcı arasında bilgi değişimini sağlamak için üç ana aşamadır. Moleküler haberleşmenin önemli bir türü olan difüzyon tipli moleküler iletişim, serbest difüzyon yolu ile gönderici ve alıcı düğümleri arasında moleküllerin yayılmasına esaslanıyor. Difüzyon tipli moleküler iletişimde üç farklı aşama vardır. İlk aşama emisyon aşamasıdır. Bu aşamada, verici veya geçirici nanomakine veya gönderen düğüm çalışma ortamına parçacıklar yayar. İkinci faz veya aşama ise difüzyon sürecini oluşturmaktadır. Bu fazda vericiden yayılan hissecikler Brown hareketine tabidir. Son olarak, sonuncu aşama olan resepsiyon fazında alıcı nanomakine veya alıcı düğümler tüm parçacıkları yakalıyorlar.

Bu tez boyunca, verici ve alıcı düğümler bir-biriyle temas halinde olan ve parçacıkları yakalayan düğümler olarak görülmüştür. Çalışma ortamı ise hiç bir molekülün veya başka bir parçacığın kaçıp kurtulamadığı sınırlı bir sistemdir. Ayrıca, transmisyon veya aktarma sürecinde verici düğümden ayrılan ve etrafa yayılan molekül ve parçacıklar, sınırlı çalışma ortamında dolaşıyor ve eğer bir parçacık çalışma ortamının sınırına ulaştığında, duvara değerek sisteme geri dönüyor. Bu nedenle, sınırlı çalışma ortamında parçacıkların sayısı zaman boyunca

değişmezkalıyor. Belirli t zamanında verici düğüm tarafından serbest bırakılan parçacıkların toplam sayısı mdoeliin girdisini veya sinyalini göstermektedir.Daha sonra, model sinyali difüzyon yoluyla sınırlı akışkan alanda ilerler. Bu çalışmada, molekül ve tüm parçacıkların difüzyonu rastegele yürüyüşle elde edilmiştir.Bu nedenle, verici ve alıcı düğümler arasındakı parçacıkların ilerlemesi ve yayılımı benzersiz Brown hareketi ile gerçekleştirilmektedir. Verici düğümün kapasitesi, alıcı düğümün sinyal alımı üzerine yaptığı etkileri incelemek amacıyla sınırlandırılmış ve belli bir miktarın üzerinde olamaz hale getirilmiştir. Örneğin, eğer verici düğümün rezervuar kapasitesi doluysa, yeni gelen parçacık verici düğümden çıkan diğer parçacıklara çarpa bilir. Her parçacık, her bir eksen boyunca mutlak sıcaklık ve Boltzman sabitinin çarpımının yarısına eşit olan kinetik enerjiye sahiptir. Ve aynı zamanda, her parçacık, zamandan bağımsız olduğu kabul edilen kitle ve hıza da sahiptir. Modelin esas amaçlarından biri, verici düğümün alıcı düğüm üzerinde olan sinyal resepsiyon etkisini araştırmaktır. Alıcı düğüm, kendi aralığı dahilinde sinyal gücüne tabi olan konsantrasyonu ölçer. Bu tez çalışması,alıcı düğümlerin sinyal gücünün verici düğümler tarafındansınırlı bir çalışma alanında nasıl zayıflatıla-bilindiklerini araştırıp göz önüne sergiliyor. Alıcı düğümde gerçekleşen alıcı sinyalin analitik ifadesi grafiksel olarak gösterilmiştir; verici düğümlerinin ve onların vericilik performanslarının artan sonuçlarının etkileri bu çalışmada söz konusu olmuştur. Bilim adamları iki veya daha fazla verici düğümlerinden ibaret nanoağlar üzerinde çalışırken bu makale ve çalışmada ireli sürülen analitik ifadeni difüzyon sürece dayanan moleküler haberleşme ve iletişimlerde bu makaleyi referans olarak gösterip kolaylıkla kullana bilirler.

Tezin geri kalanı ise şu şekilde düzenlenmiştir: I. bölümde giriş kısmı belirlenmiştir. II. bölümde ise tüm detaylı açıklamalarıyla model tasvirinden bahsedilmiştir. III.bölümde ise, iki veya daha fazla verici düğümün olduğu her durum için verici düğümün konsantrasyonunu veya yoğunluğunu hesaplayan analitik ifade gösterilmiştir. Simulasyon sonuçlari IV. bölümde açıklanmış ve detaylı şekilde anlatılmıştır. V. bölümde, difüzyon denklemi için sayısal bir çözüm üretmede kullanılansayısal yaklaşım denklemleri ile elde edilen kesin sonlu yöntemler anlatıldı. Bu bölümde alıcı düğümün sinyal gücünü ölçmek icin açık sayısal, kapalı sayısal ve Crank Nicolson şablonları kullanılmıstır. Açık sayısal ve Crank Nicolson şablonları ile elde edilen sonuçlar, kapalı sayısal şablon ile elde edilen sonuçlar ile

karşılaştırıldığında daha iyi sonuçlar ürettiği görülmüstür. Son olarak, VI. bölümdeki sonuç kısmında ise IV. ve V. bölümdeki hesaplama sonuçlarını da kullanarak tüm sonuçlar grafiksel olarak çizilmiştir.

1. INTRODUCTION

Molecular Communication is a bio-inspired paradigm where the exchange of informationis realized through the transmission, propagation, and reception of molecules [1]. MC has been both inspired by biological communication systems and performed by biological cells [2]. Therefore, biological cell based communication has to be investigated at biological cell level.Molecular communication is mostly used by biological systems in nature. For instance, many bacteria respond to signaling molecules which are secreted by theirneighbors.This process, known as quorum sensing, enables bacteria to coordinate theirbehaviour, including their motility, antibiotic production, spore formation, and sexualconjugation.Signaling molecules, for example pheromone, are also extensively used by agreat variety of animal species ranging from insects to higher primates to transmitand receive information. For example, pheromonesmay be secreted by an individual for directing others to targeted food places. Furthermore, cells communicate using signaling molecules to makea multicellular organism, human. In endocrine system,endocrine cells release hormone molecules, known as signaling molecules, into the bloodstream to communicate with distant target cells. Besides these fascinating molecular communication mechanisms in nature, developments in nanotechnology and biotechnology have recently revealed that molecular communication is also a promising alternative for the interconnection of very tinymachines commonly known as nanomachines such as engineeredcells and bionanorobots.The interconnection of these nanomachines which is named nanonetwork [3],is expected to enable sophisticated medical, industrial, and environmentalapplications [3]. In [4], an extensive survey on molecular nanonetworking paradigms has been introduced. In [5], the concept of molecular communication is introduced and the design of a molecular communication system has been sketched. In [6], diffusion-based molecular communications, which is the most widely used molecular communication technique, resources propagate by means of diffusion in a fluid medium, according to Fick’s laws of diffusion [7], has been investigated. Distance effect of molecular harvesting over signal reception and harvesting performance in DIRECT, which

results are based on one harvesting node, and also focuses on the effect of the harvester node location , is discussed in [8].In molecular communication, particles are physicallytransferred from sender to receiver nodes. The transmissionprocess can be accomplished in several ways, including the usage of molecular motors [9], bacteria [10], through gap junction channels [11] or by means of diffusion [12]. For instance, indiffusion-based molecular communications, which is the mostwidely used molecular communication technique to date [13],resources propagate by means of diffusion in a fluid medium,according to Fick's laws of diffusion [14]. In DIRECT, which is arecent networking scheme [15], focused to the analysis of molecular communication techniques operating in a confined operating environment. In this scheme, if particles are properly harvested, they can be theoretically reused an infinite number of times. The main objectives of this research presented in this thesis are as follows: first, the effect of harvester nodes (Harvesting nanomachines) on signal strength at the receiving nodehas to be investigated. Furthermore, the harvesting rate over signal deterioration has been studied. Secondly, an analytic expression on the signal reception at the receiving node has been proposed, which takes into account a number of harvesting nodes. Thirdly the signal strength in terms of density at the receiver node has been investigated using finite difference methods. While excluding the harvesting scenario, the concentration at the receiver node has been approximated using derivatives evaluated at the receiver node location by applying backward, forward or central difference methods to come up with the Explicit, Implicit and Crank Nicolson Numerical Schemes.

1.1 General Concepts

Currently, a great research effortis spent in the attempt to realize nanoscale machines, also called molecular machines ornanomachines, defined by E. Drexel as mechanical devices that perform useful functionsusing components of nanometer-scale and defined molecular structure [16]. More specifically, nanomachines [17] are expected to have the ability to sense, compute, actuate,manage their energy, and interconnect into networks, termed nanonetworks, to overcometheir individual limitations and benefit from collaborative efforts [18]. The communication between transmitter node and receiver node may be affected by the environment in which the communication is taking place. For example, in a confined operating environment,

particles are kept in the environment and no particle escapes from it [19]. In this environment, no particle is lost. As a result, particles are 100 percent reusable. However, in unconfined operating environment, particles under diffusion are not constrained by any boundary conditions [20], therefore, particles under diffusion spread in an infinite working space, without any restriction. In this thesis, a confined operating environment has been considered. Figure 1.1 illustrates such an environment which particles move in according to Brownian motion, in a fluidic medium. The confined working space may be defined as an ensemble of five essential components: boundaries, particles, sender node, receiver node and harvesting nodes [21]. The space is characterized by two measures, its width and length.

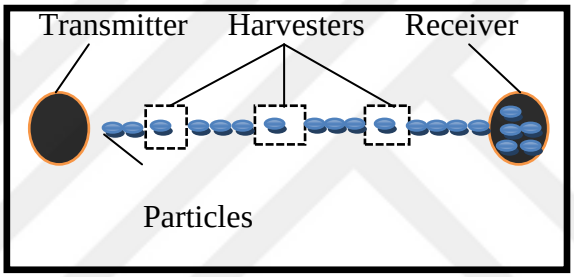


Figure 1.1: 1D Confined Working Space [22].

The 1D confined operating environment has two boundaries: the left and right boundaries. The distance from left boundary to the right boundary defines the length of the operating environment. Particles reaching boundaries are bounced back into the working space. A particle is an essential active entity that moves in the space. A particle has two properties: its position and the space in which it moves. Therefore, it has three different instance variables: its abscissa, ordinate and space. In case of one dimensional space, the ordinate is considerate as zero. Therefore, the particle has two possibilities, it randomly moves either to the East or to the West. However, in two dimensional working space, each particle has four possibilities; it may move either to the East, West, North or South. Figure 1.2 depicts a single particle trajectory in 1D confined working environment. Figure 1.3 illustrates multiple particles trajectory in three dimensional space.

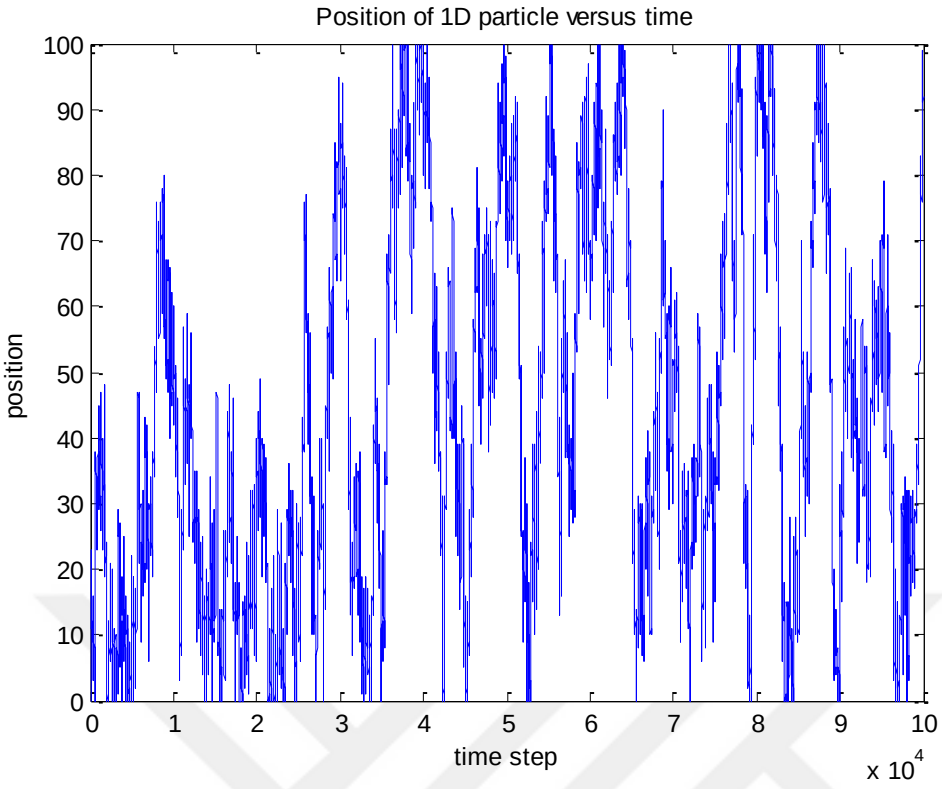


Figure 1.2: Single particle trajectory in 1D confined space.

Figure 1.2 shows the trajectory of a single particle in 1D confined working space. The particle randomly moves to the left or right at each time step. The particle bounces into the working space in case that it is in contact with one of the boundaries (i.e. left or right boundary). In the Figure 1.2 above, both left and right boundaries have been set to -1 and 101 respectively. The particle starts its journey at position $x = 0$ and at time $t = 0$. The maximum simulation time and length of the space have been set to 10^5ns and 100nm respectively.

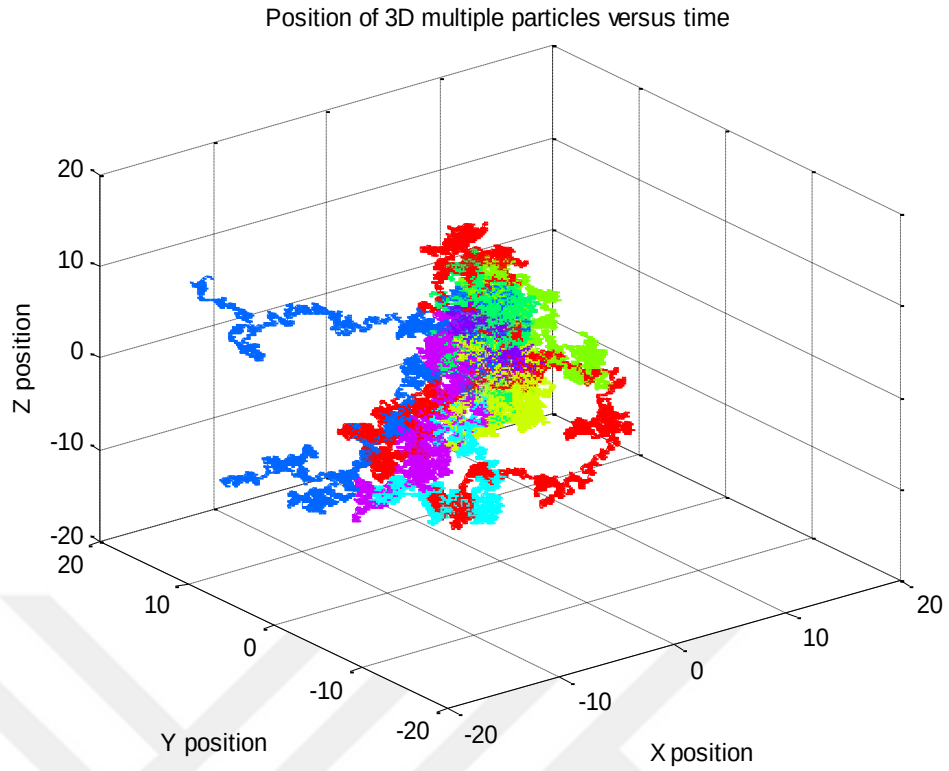


Figure 1.3: Normally distributed multiple particles trajectory in 3D space.

- A node that has the property of releasing particles at a specific time is named as transmitter node or sender node. However, released particles are subject to Brownian motion through a
- fluidic medium, eventually reaching to the receiver node. Therefore, the emission process is realised by the transmitter node at time t = 0.
- The receiver node has a range which is the size in nanometres of the region it occupies. Particles randomly move within the confined environment. Whenever a particle reaches the receiver range, it is absorbed. Therefore, the receiver node counts all particles within its range, which is subject to signal strength.
- Harvesting node is also a receiving node which has the ability to retransmit received particles in its range or to keep them in its reservoir until future reuse. As it has been stated in the above paragraph, each particle reaching the harvesting node range will be absorbed by it. All absorbed particles within harvester range are reusable for a specific purpose, in occurrence, in the case of a low signal reception at the receiver node, particles kept at harvester node

may be released to reinforce or improve the signal strength at the receiving node.

2. MODEL DESCRIPTION

The bounded operating environment has been used such that particles released by the transmitter node circulate in it and when a particle reaches boundaries, it is bounced back in to the working environment. The total amount of particles within the environment does not change along the time. The transmitter node sends a signal, which is the input of the model, by releasing a number (Q) particles. It is assumed that released particles are subject to only a random movement, called Brownian motion, in one dimensional bounded fluidic space. Therefore, the propagation of particles between transmitter and receiver nodes is uniquely accomplished by the Brownian motion. In order to analyse the impact of harvesters a discrete time system is defined. Within this model it is assumed that an harvester would keep only a percent of particles available in its range. The model is to investigate the impact of harvesters on signal reception at the receiving node. The receiver node measures the concentration within its location, which is subject to the signal strength in its range.

2.1 Communication Architecture for a Diffusion Based Molecular Communication

The first step that has been taken to modelling diffusion based molecular communication systems is to give an overview on communication architecture that can reflect the main functionalities of a diffusion based molecular communication as shown in Figure 2.1 for an unconfined operating environment and in Figure 2.2 for the confined working environment with harvester nodes as it has been shown in Figure 1.1. Throughout the rest of this thesis, the confined operating environment has been used to serve as our experimental working space. As it is shown in Figure 2.1, there are three main phases in diffusion based molecular communication. Primo, emission of particles. In this phase, the transmitter node instantaneously emits particles into the fluidic medium. The emitted particles are the input of the model. Secondo, diffusion of particles emitted by the transmitter node. The input of the model is subject to a random walk which eventually will produce the result of the

model. The last phase is composed of the reception of particles at the receiver node.Received particles at the receiving node are interpreted as the result produced by the model and are subject to the signal strength of the model. Particles that are in contact with the range of the receiving node are totally absorbed in the receiving node reservoir. Similarly, particles which are in the range of the harvesting node are absorbed in the harvester node reservoir unless its capacity is not yet full. In the next pages, the three phases will be presented.

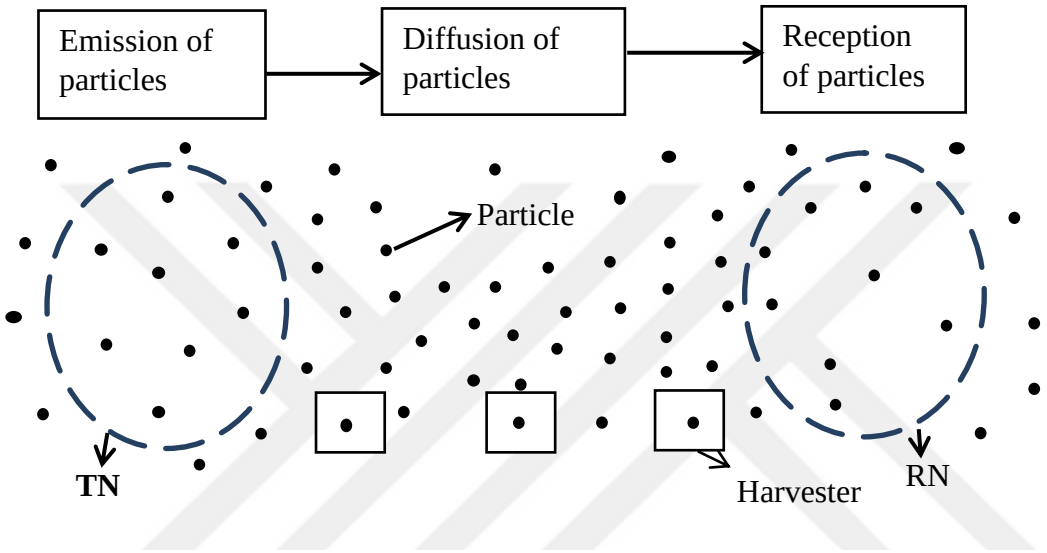


Figure 2.1:Diffusion based molecular communication architecture in unconfined working space [23].

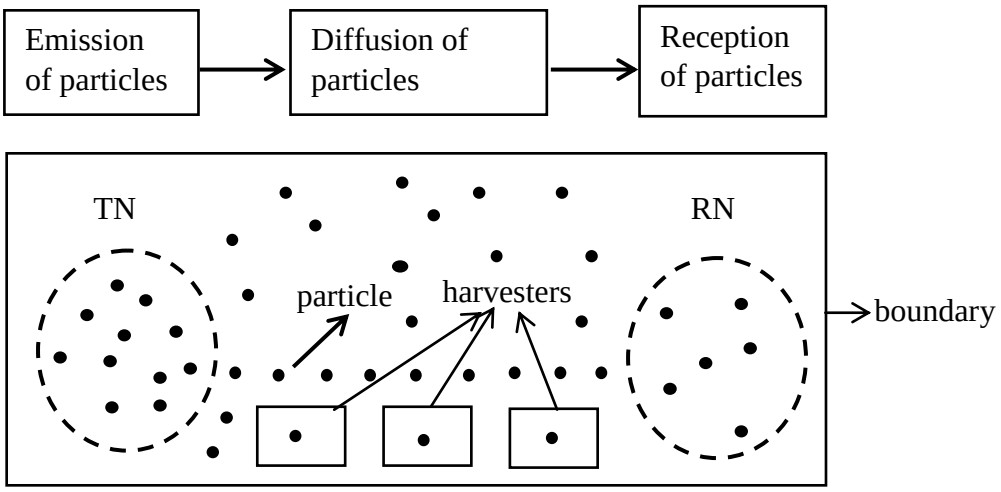


Figure 2.2: Diffusion based molecular communication architecture in confined space.

2.2 Emission of Particles

In diffusion based molecular communication, the transmitter node is responsible for the emission of particles. The emitted particles propagate in the bounded space from the transmitter node to receiver node. It has been assumed that the transmitter node emits a number of Q particles at time t=0 into the medium. We have also taken into account the fact that the transmitter node emits particles into the fluidic medium with a certain rate, let say α. In this case, at a certain time t, some number of particles will already transmitted into the fluidic medium while another number will be still waiting to be transmitted. Let's represent by Q' the number of particles waiting to be transmitted into the working space and Q the number of particles already under diffusion in the working environment as shown in Figure2.3. Therefore, the emission of particles from transmitter node can be characterized by a transition from Q' to Q as follows.

$$Q{:}Q' \xrightarrow{\alpha} Q \tag{2.1}$$

Q is a constant function that is the number of particle to be transmitted by the transmitter node. The emission phase is a two state transition, let's note n_1 and n_2 the substitutes of those two states, states Q and Q' respectively. Initially, at time t=0 in the second state n_2 no particle is supposed to reach that state. On the other hand, at the same instant time t=0, all particles are supposed to be in state n_1. Since there are Q particles to be released into the working operating environment, the following equation describes well the emission process as described above.

$$n_1(t) + n_2(t) = Q \tag{2.2}$$

where

$n_1(0) = Q$ and

$n_2(0) = 0$ based on the emission rate α.

The time derivative of $n_1(t)$ and $n_2(t)$ can be given as

$$\frac{dn(t)}{dt} = Cn(t) \tag{2.3}$$

where

$$n(t) = \begin{bmatrix} n_1(t) \\ n_2(t) \end{bmatrix},\ C = \begin{bmatrix} -\alpha & 0 \\ \alpha & 0 \end{bmatrix} \tag{2.4}$$

For initial condition $n_1(0) = Q$, the solution of equation (2.3) can be given by

$$n_1(t) = Qe^{-\alpha t} \text{ and } n_2(t) = Q(1 - e^{-\alpha t}) \tag{2.5}$$

If we assume that Q' and Q denote state 1 and state 2 respectively, the emission of particles can be also viewed as a state transition from state 1 to state 2. In this case, a number of particles may be either in state 1 or state 2. However, the total number of particles that are in state 1 and state 2 are equal to Q. It has been assumed that if a particle has not yet been emitted, then it is in state 1. In the case that the particle has been already emitted, then it is no longer in state 1, instead it is in state 2. Therefore, the diffusion takes place in state 2. In the next paragraphs, we will discuss the diffusion of particles in the confined environment.

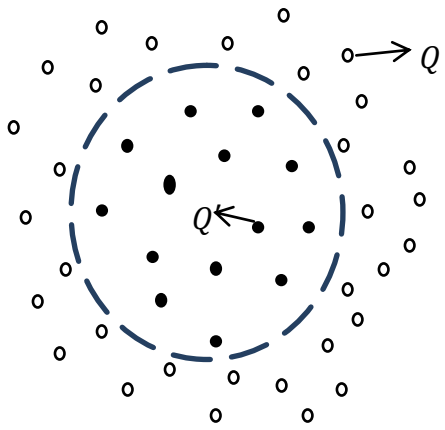


Figure 2.3: Emission of particles [23].

2.3 Diffusion of Particles

Later the emission of particles into the fluidic medium by the transmitter, particles start diffusing. Diffusion is the random movement also known as Brownian motion

of particles due to the thermal energy. A particle has the average kinetic energy [24], for one dimension is given by equation (2.6).

$$\frac{1}{2}m\langle v\rangle^2 = \frac{kT}{2} \tag{2.6}$$

where

m stands for particle mass,

v represents the particle velocity,

k is the Boltzmann's constant,

T denotes the absolute temperature and,

$\langle . \rangle$ is the average over time or over a set of similar particles.

Using equation (2.6), the root mean square velocity can be also given by equation (2.7).

$$\langle v\rangle = \sqrt{\frac{kT}{m}} \tag{2.7}$$

The approximation of the root mean square velocity in equation (2.7) can be used to estimate the instantaneous velocity of a particle [25]. In order to understand the main principles of diffusion of particles, the random walk has been discussed.

2.3.1 Random walk

The motion of particle undergoing diffusion has been assumed to be described as a random walk. Suppose that particles start diffusing at time *t = 0* at position *x= 0* and execute one dimensional random walk. The random walk of a particle among these particles is illustrated in Figure 2.6. The random walk of particles are governed by the following rules [25]:

1. Each particle steps to the right or to the left once every τ seconds with the velocity $\Delta x = \pm v$ and the step length $\delta = \pm v\tau$.

2. The probabilities of going to the right or the left at each step are equal to each other and $1/2$ in one dimension. Note that the successive steps are statistically independent and the walk is not biased.
3. Each particle moves independently of the other particles. The particles do not interact with each other.

Considering the fact that there are *N* particles and $x_i(n)$ be the position of the *i*th particleafter the *n*th step. Based on rule 1 defined above, the position of the *i*th particle at time step *n* can be written as

$$x_i(n) = x_i(n-1) \pm \delta \tag{2.8}$$

Let us consider all of the *N* particles. Then, using rules 2 and 3, the + sign in equation (2.8) can be applied to the half of the particles and the – sign can be applied to the other half. Hence, the mean displacement of the particles after *n*th step i.e $\langle x(n) \rangle$, can be computed by

$$\langle x(n) \rangle = \frac{1}{N} \sum_{i=1}^{N} x_i\,(n)$$

$$\langle x(n) \rangle = \tfrac{1}{N} \textstyle\sum_{i=1}^{N} [x_i(n-1) \pm \delta] \tag{2.9}$$

Since the signs + and – are applied to the two half of the total amount of particles, the term $\pm\delta$ can be approximated as 0 and $\langle x(n) \rangle$ can be given by

$$\langle x(n) \rangle = \frac{1}{N} \sum_{i=1}^{N} [x_i(n-1)]$$

$$\langle x(n) \rangle = \langle x(n-1) \rangle \tag{2.10}$$

The physical interpretation of equation (2.10) is that the mean position of particles does not change from step to step. However, it is possible to determine how particles spread. To this end, the average mean square displacement $\langle x(n) \rangle$ of the particles, which is expressed as,

$$\langle x^2(n) \rangle = \tfrac{1}{N} \textstyle\sum_{i=1}^{N} {x_i}^2\,(n) \tag{2.11}$$

can be used to measure the spreading. Using equation (2.8), $x_i{}^2(n)$ can be given by

$$x_i{}^2(n) = x_i{}^2(n-1) \pm 2\delta x_i(n-1) + \delta^2 \tag{2.12}$$

By substituting $x_i{}^2(n)$ in equation (2.11),

$$\langle x^2(n)\rangle = \frac{1}{N}\sum_{i=1}^{N}[x_i{}^2(n-1) \pm 2\delta x_i(n-1) + \delta^2]$$

$$\langle x^2(n)\rangle = \langle x^2(n-1)\rangle + \delta^2 \tag{2.13}$$

Since all the particles are assumed to be in origin, at time *0*, i.e $x_i(0) = 0 \ \forall i$, the mean square displacement of the particles at step 0 or time 0, i.e $\langle x^2(0)\rangle$, is equal to zero. Thus, based on on the result in equation (2.13), it can be inferred that $\langle x^2(1)\rangle = \delta^2$, $\langle x^2(2)\rangle = 2\delta^2$, … , $\langle x^2(n)\rangle = n\delta^2$. The physical interpretation of this result reveals that the mean square displacement increases with the step number *n* and the root mean square displacement increases with the square root of *n*. Since each time step lasts for τ second, the step number *n* can be expressed as $n = t/\tau$ and using this result, the time varying function of the mean square displacement can be given by

$$\langle x^2(t)\rangle = \frac{t}{\tau}\delta^2 = \left(\frac{\delta^2}{\tau}\right)t \tag{2.14}$$

By setting $\delta^2/2\tau$ as the diffusion coefficient of the particles, i.e $D = \delta^2/2\tau$, the mean square displacement in equation (2.14) and the square root of this displacement can be expressed as

$$\langle x^2\rangle = 2Dt, \langle x\rangle = \sqrt{2Dt} \tag{2.15}$$

Note that *t* in $\langle x^2(t)\rangle$ is drooped for ease of illustration and thus, $\langle x^2\rangle$ denotes $\langle x^2(t)\rangle$. The diffusion coefficient *D* reflects how a particle migrates at a given temperature. The diffusion coefficient mostly depends on the size of the particle, the structure of the medium and the absolute temperature.

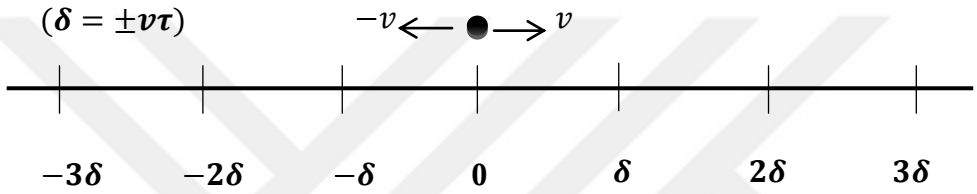
Similar to the one dimensional random walk of particle i.e. along x-axis, the two and three dimensional random walks can be analysedby following the similar way given

above. First of all, rules 1 and 3 can be directly applied to each axis i.e. x,y and z. Furthermore, the motion of the particles in the negative *x*, *y*, and *z* directions is statiscally independent. Then similar to $\langle x^2 \rangle = 2Dt$ as introduced in equation (2.15), $\langle y^2 \rangle = 2Dt$ and $\langle z^2 \rangle = 2Dt$. More specifically, in two dimensions, the square of the distance from the origin to the point *(x,y)* is $r^2 = x^2 + y^2$. Thus, for two dimensions,

$$\langle r^2 \rangle = 4Dt \tag{2.16}$$

and similarly, for three dimensions where $r^2 = x^2 + y^2 + z^2$

$$\langle r^2 \rangle = 6Dt. \tag{2.17}$$



step to the left with probability $1/2$ for each time step τ.

step to the right with probability $1/2$ for each time step τ.

Figure 2.4: Illustration of a one dimensional random walk of a particle which starts at the origin and steps to the right or to the left with probability $1/2$ and the time step τ and the step length$\delta = \pm v\tau$.

In the following section, the statistical characterization of the particle random walk is presented based on the deterministic characterization introduced above.

2.3.2 Statistical characterisation of random walk

The statistical characterization of one dimensional random walk along the x-axis has been considered. It has been assumed that the particle steps to the right with a probability *p* and to the left with a probability *q*. Since the movement of the particle is one dimensional, $q = 1 - p$. Given that there are a total amount of *n* steps, the probability that the particle steps exactly *k* times to the right is given by the following binomial distribution:

$$P(k; n, p) = \frac{n!}{k!(n-k)!} p^k q^{(n-k)} \tag{2.18}$$

The total displacement of the particle at the end of *n* steps, i.e. *x(n)*, can be found by extracting the number of left steps from the number of right steps as follows:

$$x(n) = [k - (n - k)]\delta = (2k - n)\delta \tag{2.19}$$

where δ is the step length of the particle as introduced in the previous subsection.

Then, the mean displacement of the particle, $\langle x(n)\rangle$, can be given as

$$\langle x(n)\rangle = (2k - n)\delta \tag{2.20}$$

Since *k* follows a binomial distribution in equation (2.18), the mean displacement of the particle moving exactly to the right can be given as $\langle x\rangle = np$. Furthermore, the mean square displacement of the particle can be expressed as

$$\langle x^2(n)\rangle = \langle[(2k - n)\delta]^2\rangle$$

$$\langle x^2(n)\rangle = (4\langle k^2\rangle - 4\langle k\rangle n + n^2)\delta^2 \tag{2.21}$$

where

$$\langle k^2\rangle = (np)^2 + npq.$$

For the case that *p=q=1/2*, $\langle x(n)\rangle = 0$ and $\langle x^2(n)\rangle = n\delta^2$ and this the expected result as it has been already obtained in the previous section. The number of steps taken by each particle is enormously high. In the following section, by taking into account the microscopic essentials of the random walk phenomenon, Fick's equations also called diffusion equations are derived.

2.3.3 Fick's equation

Fick's equations [26] characterize the spatial and temporal distributions of diffusing particles. The derivation of Fick's equations is possible to follow the basic principles of random walk. Let *N(x)* and *N(x+δ)* be the number of particles at points *x* and *x+ δ*along the x-axis at time *t*, respectively, as shown in Figure 2.5. In order to understand the spatial and temporal distributions of the particles at points *x*and *x+ δ*, there are two essentials issues needed to be addressed [26]:

- How many particles will traverse unit area from point *x* to the point *x*+ δ in unit time?
- What is the next flux in the *x* direction i.e. J_x ?

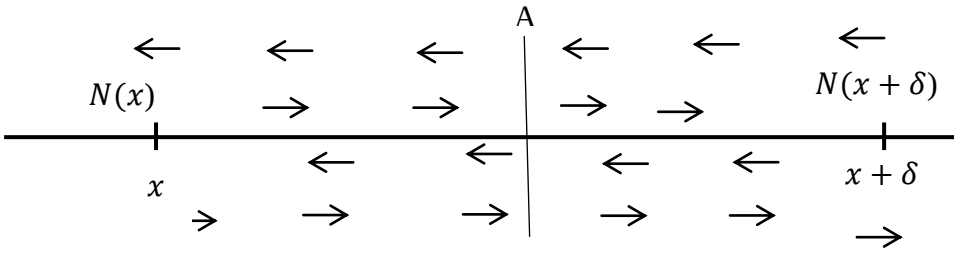


Figure 2.5: At time *t*, there are $N(x)$ and $N(x+\delta)$ particles at position *x* and *x*+δ, respectively. At time *t*+τ, half of *N(x)* and *N(x*+δ*)* steps to the right while the other half of them steps to the left at time *t*+τ [27].

At time *t*+τ, half of the particles at point *x* steps across the dashed line from left to right and half of the particles at point *x*+ δ steps across the dashed line from right to left. Hence the number of crossing to right can be given as $-1/2[N(x+\ \delta) - N(x)]$. Dividing this expression by unit area normal to the x-axis i.e. A, and by the time interval τ, the net flux J_x can be given by

$$J_x = -\frac{1}{2}\frac{[N(x+\delta)-N(x)]}{A\tau} \tag{2.22}$$

As introduced previously, the diffusion coefficient *D* can be given by $D = \delta^2/2\tau$. Then by substituting $\tau = \delta^2/2D$, $J_x$can be rewritten as

$$J_x = -\frac{D}{\delta}\frac{[N(x+\delta)-N(x)]}{A\delta} \tag{2.23}$$

Since $A\delta$ is a unit volume, $N(x)/A\delta$ and $N(x+\delta)/A\delta$ in equation (2.23) are the concentration of the particles at points *x* and $+\delta$, respectively. Let *C(x)* and $C(x+\delta)$ denote these concentrations, respectively. Then, equation (2.23) becomes

$$J_x = -\frac{D}{\delta}[C(x+\delta) - C(x)] \tag{2.24}$$

Finally, for $\delta \to 0$, the second term of J_x becomes the derivatives of *C(x)* and this yields

$$J_x = -D\frac{\partial C}{\partial x} \tag{2.25}$$

Equation (2.25) is called Fick's first equation and it can be interpreted as follows. If the particles are uniformly distributed, $\partial C/\partial x = 0$ and $J_x = 0$. In this case, the distribution does not change with time and the system is at equilibrium. If the concentration C is a linear function of x, $\partial C/\partial x$ and J_x are constant. Based on the conservation of total number of the particle, Fick' second equation can be also derived by following the first equation in equation (2.25). Let us consider a box with the area of A as shown in Figure 2.6. During the time period τ, the number of particles entering from the left of the box is $J_x(x,t)A\tau$ while the number of particles leaving from the right is $J_x(x+\delta,t)A\tau$. Since the particles are neither creatednor destroyed, the difference of the entering and leaving particles concentration in the volume of the box, i.e $A\delta$, must satisfy

$$[C(t+\tau) - C(t)] = -\frac{[J_x(x+\delta) - J_x(x)]A\tau}{A\delta} \tag{2.26}$$

Multiplying equation (2.26) by $1/\tau$, it can be expressed as

$$\frac{1}{\tau}[C(t+\tau) - C(t)] = -\frac{1}{\tau}\frac{[J_x(x+\delta) - J_x(x)]A\tau}{A\delta}$$

$$\frac{1}{\tau}[C(t+\tau) - C(t)] = -\frac{1}{\delta}[J_x(x+\delta) - J_x(x)] \tag{2.27}$$

As $\tau \to 0$ and $\delta \to 0$, and since the right hand side of the equation (2.27) indicates the derivative of J wrt. x we may conclude as follows

$$\frac{\partial C}{\partial t} = -\frac{\partial J_x}{\partial x} \tag{2.28}$$

$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2} \tag{2.29}$$

Note that equation (2.29) is obtained by substituting equation (2.25) into equation (2.28). The final expression in equation (2.29) is known as Fick's second equation or diffusion equation. It has been assumed that particles freely diffuse in the fluidic medium. In the next section, the solution to equation (2.29) is discussed.

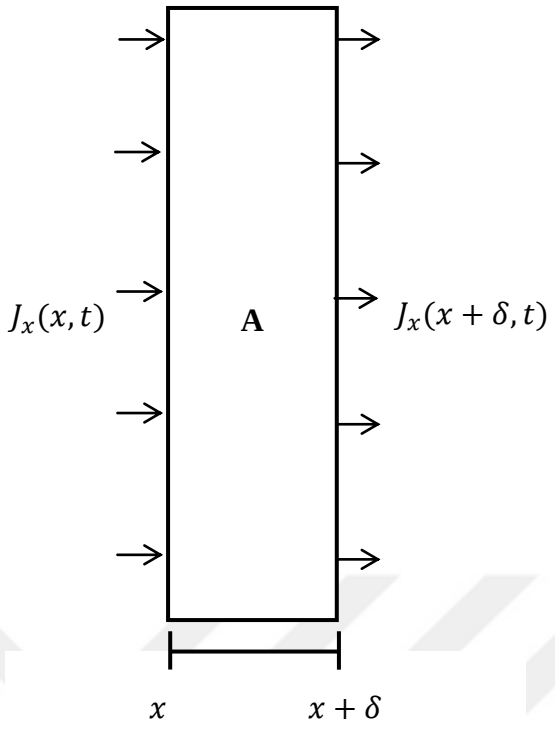


Figure 2.6: The flux $J_x(x,t)$ enters from the left side of the box with the area A and the flux and the flux $J_x(x+\delta,t)$ leaves from the right side of the box [23].

2.3.4 A solution for one dimentional diffusion equation

The solution of diffusion equation can be obtained for different initial andboundary conditions. As these conditions vary, many different solutions can beobtained. In general, the solutions are either in the form of a series of error functionsor in the form of a trigonometric series. The trigonometric series can be replacedby a series of Bessel functions for the case in which the diffusion takes place ina cylinder [28]. In the literature, there are many textbooks and research papersdealing with the solution of Fick's equations (or diffusion equations). For example,[28] is an important textbook discussing the solution approaches to Fick's equationsextensively. Furthermore, the heat equation has the same form with Fick's equations.Therefore, the textbooks on the heat equation can be also used to understandhow diffusion equations are solved. For example, [29] is a prominent book whichprovides many important solutions of diffusion equations with respect to manydifferent initial and boundary conditions. Some of the examples solutions can begiven as follows.Let us consider the one-dimensional diffusion equation in (2.29):

$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2} \tag{2.30}$$

It can be proven that

$$M = \frac{K}{\sqrt{t}} e^{\frac{-x^2}{4Dt}} \tag{2.31}$$

is a solution of equation (2.30) for an arbitrary constant *K* [29].

Let us assume that *M* particles are instantaneously released at the origin of a cartesian coordinate system at *t=0*. Then using equation (2.31), *M* can be expressed as

$$M = \int_{-\infty}^{\infty} C dx$$

$$M = \int_{-\infty}^{\infty} \frac{K}{\sqrt{t}} e^{\frac{-x^2}{4Dt}} dx \tag{2.32}$$

By changing variable *x* as

$$\frac{x^2}{4Dt} = a^2, \quad dx = 2\sqrt{Dt} da \tag{2.33}$$

M can be re-written as

$$M = 2K\sqrt{D}\int_{-\infty}^{\infty} e^{-a^2} da$$

$$M = 2K\sqrt{\pi D} \tag{2.34}$$

Hence, $K = \frac{M}{\sqrt{4\pi D}}$ and by substituting *K* into equation (2.31), *C* can be given by

$$C = \frac{M}{\sqrt{4\pi Dt}} e^{\frac{-x^2}{4Dt}} \tag{2.35}$$

It is worth to note that for *M = 1*, the solution in equation (2.31) is equal to the probability density function of particle position given as follows.

$$P(x,t) = \frac{1}{\sqrt{4\pi Dt}} e^{\frac{-x^2}{4Dt}} \tag{2.36}$$

This means that the diffusion equation is satisfied by the probability density function of particles position in one dimension. Using this distribution, the probability distribution of the delay required by a particle to travel the distance *d* can be given as

$$f(t) = \frac{d}{\sqrt{4\pi D t^3}} e^{\frac{-d^2}{4Dt}} \tag{2.37}$$

If a particle moves in a random manner in space that means it continually changes its directions and velocities in a random manner, then the resultant of these random motions as a whole is called drift velocity. Hence, if there is a drift velocity *v* in the medium [30, 31, 32, 33], equations (2.36) and (2.37) become

$$P(x,t) = \frac{1}{\sqrt{4\pi D t}} e^{\frac{-(x-vt)^2}{4Dt}} \tag{2.38}$$

$$f(t) = \frac{d}{\sqrt{4\pi D t^3}} e^{\frac{-(vt-d)^2}{4Dt}} \tag{2.39}$$

Figure 2.7 shows that as *t* increases, the concentration value approaches zero and the curve's peak value decreases. This is because particles continuously diffuse and scatter in the medium as time proceeds.

As described in the previous sections, after the diffusion of particles, in the phase of reception, the transmitted particles that are eventually able to reach the close proximity of the receiver node are received by the receiver node. In the following section, the reception of particles is introduced.

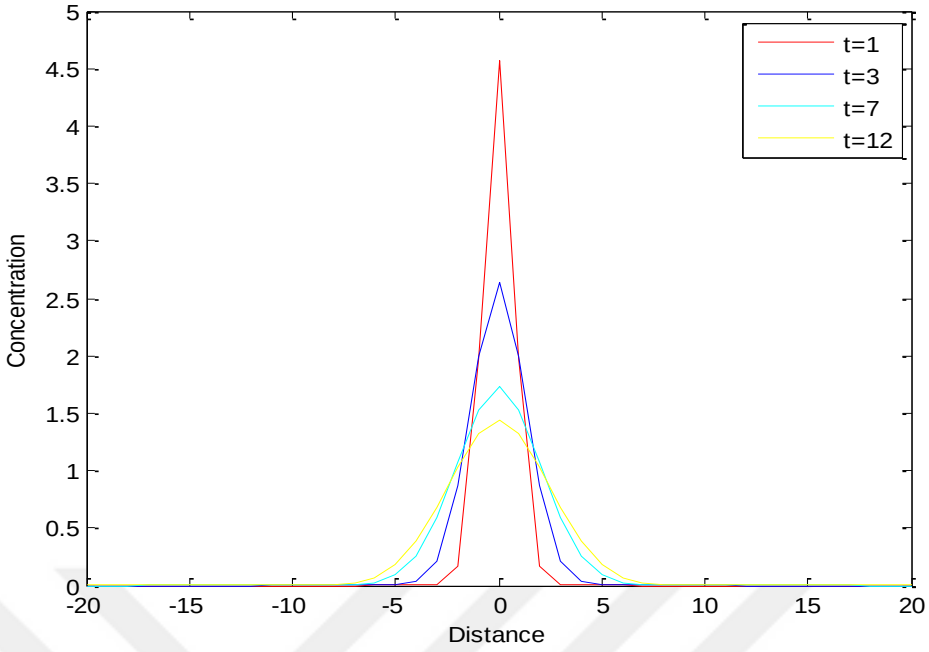


Figure 2.7: Distance versus Concentration using equation (2.35) for *M=5* and *D=0.3*.

2.4 Reception of Particles

After the particles are released by the transmitter node, they diffuse in the fluidic mediumby following the physical rules introduced in the previous section. The particles that are able to reach the close proximity of the receiver node are received by the receiver node. Hence, the receiver node can be viewed as a particle reducer i.e if there are *p* particles in the medium under diffusion such that one particle reaches the receiver node's range, and then there will remain *p-1* particles under diffusion. This means that the receiver node has reduced by one the number of particles under diffusion. Therefore, the receiver node has the following properties:

- It has a range defined by its radius *r*.As shown in Figure 2.8. The range that has been set to *2r* in one dimension since it is not spherical.
- Particles within the receiver node's range i.e *2r* are totally received and the total number of particles under diffusion will be reduced by the number of particles in the range of the receiver node. Thus, the receiver node has been assumed as a reducer.

- The receiver node increases the signal strength as long as it receives many particles.

In the next section, the analysis of the described model in the previous sections, which takes into account the presence of harvester nodes is discussed.

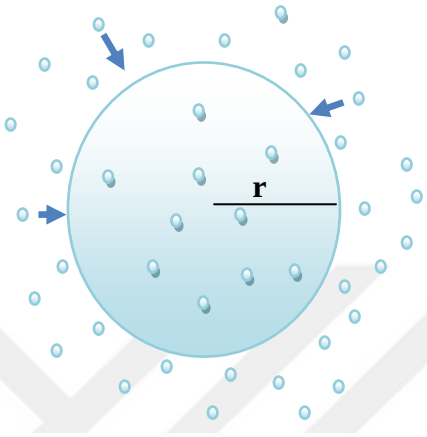


Figure 2.8: Receiver node receives particles which freely roam in close proximity of it. All surrounding particles are captured by absorption by the receiver nod [23]

3. ANALYSIS OF THE MODEL WITH HARVESTING NODES

After describing the three phases of the model in diffusion based molecular communication, the emission of particles by the transmitter node, the diffusion of particles with certain physical rules and the reception of particles by the receiver node. It has been assumed that the receiver node can be viewed as a reducer of particles. Thus, the signal strength at the receiver node is subject to the number of the reduced particles by the receiving node. In the next section, harvester nodes between sender and receiver nodes have been considered and the model investigates the impact of harvester nodes on the signal reception at the receiving node. Ultimately the impact of increasing number of harvested particles on signal reception at the receiver node has been observed. In this thesis, the analysis for different number of harvester nodes has been considered. Each harvesting node has granted with the ability of harvesting a limited number of particles in its range. Once the capacity of a harvesting node is fully used, a new particle reaching its range will not be reduced or absorbed. Ultimately the impact of harvested particles on signal reception at the receiver node is analysed. In the next section, harvesting nodes with finite capacity has been discussed.

3.1 Harvesting Node with Finite Capacity

The harvesting operations have an important role on the persistence of the resource recirculation [34]. As we will see next, the location of an harvesting node has a significant impact over its harvesting performance, as well as over the signal reception performance of a receiving node. In this work, first we have investigated the role of the harvesting node capacity over signal reception at the receiver node. A series of experiments have been performed, considering diffusionbased molecular communicationusing the instantaneous emission of particles, physical rules presented in the previous sections for diffusion of particles and capture of particles by the receiver node that is viewed as a reducer of particles which captures all particles in contact with its proximity. To modulate a single bit of information,the sender node instantaneously emits a pulse consisting of Q resources. The emitted pulse

propagates over the operating environment according to equation (3.1), eventually reaching the receiver node.

$$C(x,t,Q) = \frac{Q}{\sqrt{4\pi Dt}} e^{\frac{-x^2}{4Dt}} \tag{3.1}$$

where

Q is the amount of particles emitted by sender node, also called pulse amplitude,

x represents the distance between sender and receiver,

t stands for the time elapsed since emission of the signal,

C is the concentration of particles at location x and time t,

D represents the diffusion coefficient of the working environment.

Assume that harvesting nodes are located between sender and receiver nodes, and that harvesters have a finite capacity of H particles. Although all received particles will be used later in the course of operation. The receiver would not have the chance of receiving the harvested particles. Since particles are kept in the harvester temporary the number of particles has been reduced to R. Therefore, the receiver would be under the diffusion of that many particles which yields to a new equation for diffusion equation (3.2).

$$c(x,t,Q) = \frac{R}{(\sqrt{4D\pi t})^{\sigma/2}} e^{-x^2/4Dt} \quad . \tag{3.2}$$

where:

$$R = Q - \mathrm{H}. \tag{3.3}$$

where

$$H = \sum_{i=1}^{n} H_i\,(x_i, t) \tag{3.4}$$

where

n stands for the total number of harvesting nodes,

H_i represents the concentration held at harvesting node i at position x_i and time$t$. Note that H_i also stands for harvester capacity i

x_i is the distance from the sender node to the harvesting node i such that $x_1 < x_2 < x_3 \ldots < x_{n-1} < x_n$.

If harvesting nodes are located at the transmitter node location, the harvesters will absorb H resources at timet = 0. This scenario is similar to emitting$Q - H$ resourcesat time t = 0. In this case, the concentration of resourcesreaching the receiver node is given by:

$$c(x,t,Q) = \frac{Q-H}{(\sqrt{4D\pi t})^{\sigma/2}} e^{-x^2/4Dt} \quad (3.5)$$

where H is the total capacity of harvesting nodes.

If we have harvesting nodesare located at the same location withthe receiver node, the harvesting nodes will absorb H resourcesinstantaneously. If H >Q, all particles reaching the receivernode would be absorbed by the harvester nodes. For H < Q, thereceiver would receive $Q - H$ particles. In this case, Q represents the number of particles assumed to be received by the receiver node. Harvesting nodes receive more particles as there are located closer to the transmitter node, whereas the midpointbetween sender and receiver nodes is the optimum location interms of signal strength at receiver node. In the next section, harvesting nodes with rational harvesting is presented.

3.2 Harvester Nodes with Rational Harvesting

In the case that the harvesting nodes are placed at the same location with sender node, it is more likely that all particles from sender node will be absorbed by harvesters at instant time $t = 0$. In this case, no resource will reach the receiving node if the total capacity of harvester nodes is greater or equal to the total amount of particles that is the input of the model, noted by Q. On the other hand, if harvesters are placed at the same location with the receiver node,unless harvesters' total capacity be lesser than the number of received particles by the receiving node, otherwise, all particles supposed to be received by the receiver node will be absorbed by the harvester nodes.Therefore, one should take these cases with more care when dealing with model in diffusion based molecular communication composed of

sender, harvester and receiver nodes. To recapitulate, placing harvester nodes at the same location with sender and receiver nodes is referred as irrational harvesting.

In rational harvesting, each Harvesting node has a wise limited capacity such that each harvester may only harvest up to $\beta\%$ of the particles within its range. This prevents negative impact on the signal strength at the receiving node. At each instant time t, each harvester cannot exceed to harvest more than $\beta\%$ of the received particles. This has a significant positive impact on the signal strength at the receiving node. Therefore, instead of reducing the number of particles to R as it has been considered in equation (3.2), the number of particles will be wisely reduced by $\frac{\beta H}{100}$. Hence, equation (3.2) becomes

$$c(x,t,Q) = \frac{Q - H(\frac{\beta}{100})}{(\sqrt{4D\pi t})^{\sigma/2}} e^{-x^2/4Dt} . \quad (3.6)$$

where:

$\beta$is harvesting parameterwhich depends on the nature of the harvester

H stands for the total number of particles received by the harvester node.

If β is too small, then there will be nosignificant negative impact on the signal reception at the receiving node.The higher values for βmay yield a negative impact on the signal strength at the receiving node.

In the next section, results from simulations for different values of β and number of harvesting nodes are presented.

4. SIMULATION RESULTS AND DISCUSSION

In order to better understand the analysis of different theories discussed in the previous sections, MATLAB R2013a has been used as a tool to validate the proposed analytic expressions and visualize the impact of harvesting parameter as well as number of harvesting nodes on the signal reception at the receiving node. For the given parameters in Table 1 and values A and B, the results have shown that the signal strength deteriorates, becomes worse in quality when the number of harvester nodes $Nh = 187$ (labeled as 187HN in Figure 4.1). As shown in Figure 4.1 for $Nh = 3$, there is no much change in signal strength at the receiving node. It can be seen that as the number of harvesting nodes increases, the received signal decreases. This rule is valid for all locations where harvesting nodes may be placed at.

Table 4.1: Parameters and parameters' values used in simulations

Parameters	Values A	Values B
Q	500000 particles	500000 particles
x	1500 nm	1500 nm
x_i	[10,600,1190]	[10,600,1190]; [10:30:1480]; [10:8:1498]
t	From 1 to $4 * 10^5 ns$	From 1 to $4 * 10^5 ns$
D	1	1
β	-	-
Nh	3	3,50,187

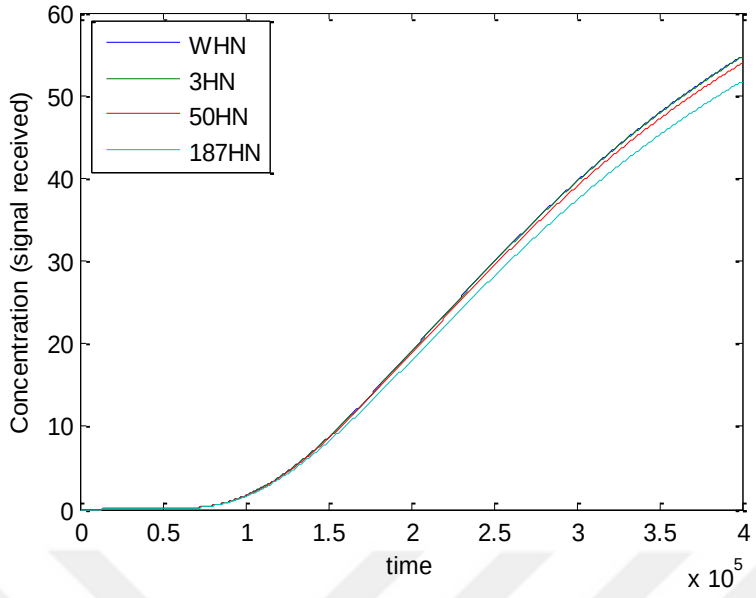


Figure 4.1: Signal received by the receiver node versus time with different number of harvesters between the sender and the receiver nodes.

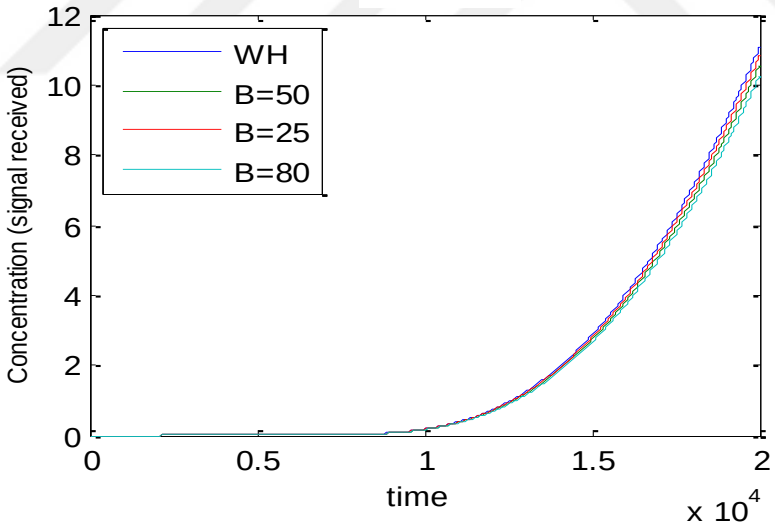


Figure 4.2: Signal received by the receiver node versus time with different values of the harvesting parameter.

The time axis is the time direction and the ordonate axis represents the received signal that is concentration actually. The legend indicates the signal strength for different number of Harvester Nodes (HN) and harvesting parameter (β) in both Figure 4.1 and Figure 4.2 respectively. Parameters' values in Figure 4.2 show that the harvesting parameter is very important to preserve the signal strength at the receiving point. The red line is closer to the blue line, which is the expected signal (concentration) without harvesting. This is due to the fact that the lesser harvesting rate is used, the better signal strength is received.

In Figure 4.1 the simulations have been ran for four hundred thousands nano seconds. If the simulations have been expanded to up one million nano seconds, the signal received in terms of concentrations would have been increased and probably reached at least seventy. Since Harvester nodes have to absorb no more than twenty percents of the particles, the expected signal eventually reaching the receiver node range would be eghty percents. However, it is not obvious that the receiver node will receive eighty percents of the emitted signal by the transmitter node because there would still be some particles wandering within the confined operating environment. The random walk performed by a particle within the working environment does not ensure that the next successsive steps will follow exactly to the right direction. Thus, by increasing the the simulations time may not necessarily ensure that the receiver node will exactly increase the concentrations within its range to hundred percents of the expected signal it is supposed to receive.

5. SIGNAL APPROXIMATIONS IN DIFFUSION BASED MOLECULAR COMMUNICATION NANONETWORKS

In this Chapter, finite diffence methods are utilised to define an numerical approximation models.

The diffusion equation for a concentration$c(x,t)$ of some resource (given by number of particles per unit length), is given by

$$\frac{\partial c}{\partial t} - D\frac{\partial^2 \beta}{\partial x^2} = 0 \tag{5.1}$$

Our intention in signal strength of a molecular communication nanonetwork is to define a molecular communication scheme based on discrete approximation and compare its signal strength to the analytical one dimensional diffusion equation.

5.1 Finite Difference Method

Finite Difference Method [35] is used to obtain a numerical solution to an analytic function by replacing continuous partial differential equation by discrete approximation. Our physical domain $\Omega = [0, M]$, which is the working operating environment, will be subdivided in to M_x discrete points and discrete approximations are found at each discrete point. The distance between two consecutive discrete points in space is known as space step, and that in time is said to be time step, denoted Δx and Δt respectively. As the basic idea is to replace spatial and time derivatives by suitable approximations, then to numerically solve the resulting difference equations. Specifically, instead of solving for$c(x,t)$, with x and t continuous, we solve for $c(x_i, t_j)$, where $x_i = i\Delta x$ and $t_j = j\Delta t$define the grid shown in figure 5.1.

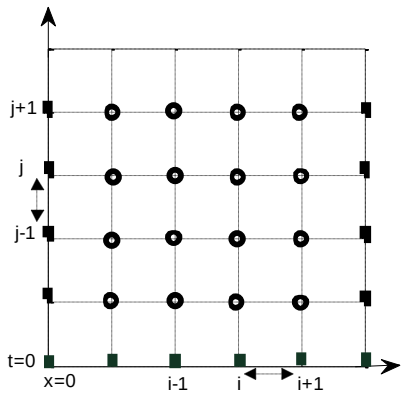


Figure 3

Figure 5.1: Discretized space (grid)

As defined above, $0 \leq x_i \leq M$ and $0 \leq t_j \leq T$ such that

$$x_i = i\Delta x\ ,\ \ i = 0,1,2,\dots M_x$$

$$t_j = j\Delta t\ ,\ \ j = 0,1,2,\dots T_j$$

where M_x and T_j are the total number of spatial nodes including those on the boundaries and the number of time steps.

The space and time steps are computed as follows.

$$\Delta x = \frac{M}{M_x - 1} \text{ and } \Delta t = \frac{T}{T_j - 1}$$

The discrete points on the columns $x = 0$ and $x = M_x$ are boundary values. The solid circles are nodes where finite difference approximation is calculated with respect to the following Dirichlet boundary conditions:

$$c(x_i = 0, t_j) = c(x_i = M, t_j) = 0 \tag{5.2}$$

where $0 \leq x_i \leq M$ and $0 \leq t_j \leq T$.

In the rest of this paper, we will use the notation $c(i,j)$ at the place of $c(x_i, t_j)$ without any loss of generality in the outcome.

The Taylor series expansion for $c(i, j + \Delta t)$, $c(i + \Delta x, j)$ and $c(i - \Delta x, j)$ are given below with respect to time and space respectively.

$$c(i,j+\Delta t) = c(i,j) + \Delta t\, c'(i,j) + \Delta t^2 \frac{c''(i,j)}{2!} + \Delta t^3 \frac{c'''(i,j)}{3!}$$

$$+\Delta t^4 \frac{c'^v(i,j)}{4!} + \Delta t^5 \frac{c^v(i,j)}{5!} + \cdots \quad (5.3)$$

$$c(i+\Delta x,j) = c(i,j) + \Delta x\, c'(i,j) + \Delta x^2 \frac{c''(i,j)}{2!} + \Delta x^3 \frac{c'''(i,j)}{3!}$$

$$+\Delta x^4 \frac{c^{iv}(i,j)}{4!} + \Delta x^5 \frac{c^v(i,j)}{5!} + \cdots \quad (5.4)$$

$$c(i-\Delta x,j) = c(i,j) - \Delta x\, c'(i,j) + \Delta x^2 \frac{c''(i,j)}{2!} - \Delta x^3 \frac{c'''(i,j)}{3!}$$

$$+\Delta x^4 \frac{c'^v(i,j)}{4!} - \Delta x^5 \frac{c^v(i,j)}{5!} + \cdots \quad (5.5)$$

From equation (5.3), the first derivative of $c(i,j)$ with respect to time t is:

$$c'(i,j) = \frac{c(i,j+\Delta t) - c(i,j)}{\Delta t} - \Delta t \frac{c''(i,j)}{2!} - \Delta t^2 \frac{c'''(i,j)}{3!}$$

$$-\Delta t^3 \frac{c'^v(i,j)}{4!} - \Delta t^4 \frac{c^v(i,j)}{5!} + \cdots \quad (5.6)$$

Using mean value theorem in equation (5.6) considering that $j \le \epsilon \le j + \Delta t$, we get

$$\Delta t \frac{c''(i,j)}{2!}\Big|_\epsilon = \Delta t \frac{c''(i,j)}{2!} + \Delta t^2 \frac{c'''(i,j)}{3!} + \Delta t^3 \frac{c'^v(i,j)}{4!} + \Delta t^4 \frac{c^v(i,j)}{5!} + \cdots \quad (5.7)$$

Substituting equation (5.7) in to (5.6), we get

$$c'(i,j) = \frac{c(i,j+\Delta t) - c(i,j)}{\Delta t} + \Delta t \frac{c''(i,j)}{2!}\Big|_\epsilon \quad (5.8)$$

The term $\Delta t \frac{c''(i,j)}{2!}\Big|_\epsilon$ is called the truncation error of the finite difference approximation. It comes from truncating the series in equation (5.6). The parameter ϵ is not known and $c(i,j)$ is also unknown. As a result, $c''(i,j)$ with respect to j cannot be calculated. Since the second right term of equation (5.8) is not known, $\frac{c''(i,j)}{2!}\Big|_\epsilon$ will be substituted by O to represent an unknown value. Then equation (5.8) becomes

$$c'(i,j) = \frac{c(i,j+\Delta t) - c(i,j)}{\Delta t} + O(\Delta t) \quad (5.9)$$

We may control the error to be very negligible by choosing Δt as small as possible. The equation (5.9) is named forward difference approximation with respect to time. Similarly we get the backward difference approximation equation with respect to time by carefully substituting $c(i, j + \Delta t)$ by $c(i, j - \Delta t)$ in equation (5.3) and then follow all steps realized to obtain equation (5.9) , that produce

$$c'(i,j) = \frac{c(i,j)-c(i,j-\Delta t)}{\Delta t} + O(\Delta t) \tag{5.10}$$

The central difference approximation with respect to space is obtained by adding equation (5.4) and (5.5), along with using both mean value theorem and big O notation we get

$$c''(i,j) = \frac{c(i+\Delta x,j)+c(i-\Delta x,j)-2c(i,j)}{\Delta x^2} + O(\Delta x^2) \tag{5.11}$$

The Explicit Numerical Scheme (**ENS**) is obtained by replacing equations (5.9) and (5.11) in to equation (5.1) , after rearranging and discarding the truncation error terms, we get

$$c(i, j + 1) = (1 - 2\alpha)c(i, j) + \alpha c(i + 1, j) + \alpha c(i - 1, j) \tag{5.12}$$

where $\alpha = \frac{D\Delta t}{\Delta x^2}$, $j + 1 \approx j + \Delta t$, $i - 1 \approx i - \Delta x$, $i + 1 \approx i + \Delta x$ and $c(i, j + 1)$ represents the concentration c at time $j + 1$ at location i .

The computation of c at time $j + 1$ is completely determined by the computation of c at time j .The **ENS** is not always stable. The parameter α must be lesser than $\frac{1}{2}$ to make **ENS** stable.

The Implicit Numerical Scheme (**INS**) is obtained by substituting equations (5.10) and (5.11) in to (5.1), after rearranging and dropping the truncation error terms, we obtain

$$c(i, j - 1) = (2\alpha + 1)c(i, j) - \alpha c(i + 1, j) - \alpha c(i - 1, j) \tag{5.13}$$

where $\alpha = \frac{D\Delta t}{\Delta x^2}$, $j - 1 \approx j - \Delta t$, $i - 1 \approx i - \Delta x$ and $i + 1 \approx i + \Delta x$.

Equation (5.13) is a one equation in a system of equations for the values of c because $c(i, j)$ depends on $c(i - 1, j)$ and $(i + 1, j)$. At each time step, the **INS** requires solving simultaneous linear equations. This renders the **INS** computational time greater than **ENS**. Fortunately, the system is tridiagonal, this makes the

problemsimple. The solution is given in [36]. The great advantage of the **INS**, it is unconditionally stable.

The Crank Nicolson Scheme (**CNS**) is the average of **ENS** and **INS**. The first derivatives with respect to time on the left hand side in equation (5.1) is replaced by equation (5.10) and the second derivatives with respect to space on the right hand side of equation (5.1) is substituted by the mean of the central difference approximation evaluated at current and precedent time step, j and $j-1$ respectively. Discarding the error terms and rearranging values of c at time j on the left hand side and those at time $j-1$ on the right hand side, gives

$$(1+\alpha)c(i,j) - \frac{\alpha}{2}c(i+1,j) - \frac{\alpha}{2}c(i-1,j) =$$

$$(1-\alpha)c(i,j-1) + \frac{\alpha}{2}c(i+1,j-1) + \frac{\alpha}{2}c(i-1,j-1) \qquad (5.14)$$

where $\alpha = \frac{D\Delta t}{\Delta x^2}$, $j-1 \approx j-\Delta t$, $i-1 \approx i-\Delta x$ and $i+1 \approx i+\Delta x$.

The **CNS** is unconditionally stable and second order both in time and space. It is implicit, and as a result a system of linear equations must be solved for each time step.

5.2 Evaluation and Comparison of Methods

All three schemes presented in this paper are evaluated based on parameters used at Table 1 and are compared to the analytic one dimensional diffusion equation given below:

$$c(x,t) = \frac{Q}{\sqrt{4\pi Dt}}\exp\left[\frac{-x^2}{4Dt}\right] \qquad (5.15)$$

with boundary conditions $c(0,t) = c(M,t) = 0$ and initial condition $c(x,0) = \frac{Q}{\sqrt{4\pi Dt}}$

where

Q represents the amplitude emitted by the sending node,

D stands for diffusion coefficient and $c(x,t)$ is the concentration at location x at time t.

Table 5.1: Parameters used

Parameters	Values
Q	500
D	0.5
$x = M$	5 nm
$t = T$	30 ns
M_x	100
T_j	1000

We have assumed that the receiver node range is six times the spatial step, i.e, the receiver node occupies locations $X_r = X(M_x - \omega)$where $\omega = 1,2,\ldots 7$

X_r is the receiver node ranges and all concentrations within the receiver node ranges are considered as the signal output of the model that will be compared to the output of the model produced by the analytic expression given in equation (5.15).

Xstands for an array containing M_x different locations that result from the discretization of the working environment into M_x discrete spots or points. We observed the results at time $t = T$.

The average signal received has been compared to both numerical solutions and analytic solution. The table below shows the results produced by the analytic expression, Explicit, Implicit and Crank Nicolson schemes. Simulations have been performed using Matlab R2013a as a tool.

Table 5.2: Results produced by the three schemes

Ranges	Crank Nicolson scheme	Implicit Num. Scheme	Explicit Numerical Scheme	Analytic Solution
9,3939	10,96	10,957	0,131	6,838
9,4949	9,15	9,1477	0,109	6,846
9,5960	7,32	7,3292	0,0878	6,854
9,6970	5,50	5,5034	0,0878	6,862
9,7980	3,67	3,672	0,0659	6,870
9,8990	1,84	1,836	0,0439	6,878
Average	6,42	6,40	0.184	6.85
Accuracy	93,7%	93,4%	2,7%	

For a threshold $\beta = 80$, which means that a signal strength reaching at least 80 percents of the analytic solution is considered as received. Based on this assumption, our experiments have revealed that both Crank Nicolson and Implicit numerical schemes have over performed compared to Explicit numerical scheme. Therefore, **CNS** and INS are more reliable compared to **ENS**. As it can be seen on the above *Table 5.2* that the accuracy of both **CNS** and INS is 90 percents higher than the one of **ENS**.

6. CONCLUSION

Molecular communication is one of the most appealing research areas. Transmission, propagation and reception are the three main stages to provide information exchange between sender and receiver in molecular communication. Diffusion based molecular communication that is an essential type of molecular communication, relies on propagation of molecules between sender and receiver nodes through free diffusion. There are three different phases in diffusion based molecular communication. The first phase is named emission process. In this phase, the transmitter nanomachine or the sender node emits particles into the medium. The second phase is composed of diffusion process. In this part, emitted particles by the transmitter node are subject to Brownian motion. Finally, the last phase, the reception process in which the receiver nanomachine or receiving node absorb or capture all particles within its range. The current work provides an analysis of diffusion based molecular communication nanonetwork which takes into account the effects of the number of harvesting nodes over signal reception at the receiving node. In addition, this thesis has examined the harvesting parameter at which harvesters harvest particles without affecting the signal strength. Furthermore, The signal strength in terms of the concentration at the receiving node has been approximated using the Explicit, Implicit and Crank Nicolson schemes. The three schemes, Explicit, Implicit and Crank Nicolson, produced numerical solutions, which in return have been compared to the analytic solution. Our research has found out that the received signal strength deteriorates progressively as the number of harvesting nodes increases. The results have also found that a significant number of particles may be harvested without much affecting the received signal strength at the receiving node if the harvesting rate is lesser than twenty five percent of the received particles. Choosing a limited number of harvesting nodes and adopting for a small harvesting rate are the key for wiser harvesting without affecting negativelythe signal strength at the receiving node. However, the current work has not covered the optimum number of harvester nodes needed for wiser particles harvesting without deteriorating the signal strength at the receiving node. The Signal approximations obtained using both Crank Nicolson and

Implicit Numerical Schemes are more reliable compared to the Explicit Numerical Scheme.The accuracy of both CNS and INS is better than the one produced by the ENS. A new research in the future may be undertaken to design and implement a Discrete Simulator for Diffusion Based Molecular Communication Nanonetworks.

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PUBLICATIONS / PRESENTATIONS ON THE THESIS

- Daniel Nzinga KINSUMUNA, D. Turgay ALTILAR, Deniz DEMİRAY, "A Signal Transmission Model for Diffusion Based Molecular Communication Nanonetworks", Joint International Mechanical, Electronic and Information Technology Conference (JIMET 2015), *ATLANTIS PRESS*, pp. 1008-1011, December 20, Chongqing, China, 2015.
- Daniel Nzinga KINSUMUNA, D. Turgay ALTILAR, "Signal Approximations in Diffusion Based Molecular Communication Nanonetworks", submitted for publication to ACSIT (International Conference of Advanced Computer Science and Information Technology) 2016, Zurich, Zwitzerland.