DISTANCE ESTIMATION IN TABLETOP MOLECULAR COMMUNICATION

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ABSTRACT

DISTANCE ESTIMATION IN TABLETOP MOLECULAR COMMUNICATION

Although existing communication technologies based on electrical and electromagnetic signals are applicable for a variety of applications, these technologies are insufficient in some applications. Especially, developments in nanotechnology and biotechnology require an alternative communication paradigm. Molecular communication (MC) paradigm is a promising solution needed to fill the gap in both nano- and macro-scale. It is one of the oldest communication paradigm in which molecules are used as information carrier. Its mechanism provides a basis for all living organisms from unicellular bacteria to humankind to continue their existence. For instance, the information transfer among nerve cells is accomplished via MC. These kind of biological activities inspire a base for communication between nanomachines. The realization of MC occurs by sending and receiving molecules between nanomachines. The information about distance between transmitter (Tx) and receiver (Rx) is one of the critical points to enable an efficient performance in terms of clock synchronization, transmission rate, etc. in the design of MC system. However, most of the existing works on MC are based on the assumption distance is pre-known. In addition, the proposed theoretical methods are validated using an ideal simulation environment. Furthermore, there is a limited number of studies about macroscale practical applications.

In this thesis, an end-to-end tabletop MC testbed is established to transmit chemical signals from a Tx to Rx. This testbed allows us to provide an estimate about the distance using molecular information received by the Rx. In the development of the estimation algorithms, the principles of molecular random walk are used. We propose three novel approaches that are called as peak time, correlation based and relative entropy based approaches to estimate the distance between Tx and Rx for a practical MC system. The performance of the proposed estimation methods is evaluated in the tabletop MC testbed. The experimental results shows that our proposed methods present a satisfactory performance in terms of estimation error and the methods can be used to develop new potential macro-scale MC applications.

ÖZET

MASAÜSTÜ MOLEKÜLER HABERLEŞME SİSTEMİNDE MESAFE TAHMİNİ

Mevcut elektriksel ve elektromanyetiksel sinyallere dayanan iletişim teknolojileri çeşitli uygulamalar için uygulanabilir olmasına rağmen, bu teknolojiler bazı uygulamalarda yetersizdir. Özellikle nanoteknoloji ve biyoteknolojideki gelişmeler alternatif bir haberleşme paradigmasına ihtiyaç duymaktadır. Moleküler haberleşme (MH) paradigması hem nano hem de makro ölçekte bu boşluğu doldurmak için gereken umut verici bir çözümdür. Moleküllerin bilgi taşıyıcı olarak kullanıldığı en eski haberleşme paradigmalarından biridir. Bu paradigmanın mekanizması tekhücrelilerden insanoğluna kadar tüm canlı organizmalara varlıklarını sürdürebilmek için temel oluşturmaktadır. Örneğin, MH'ın en iyi anlaşılabilir durumu beynimizdeki sinir hücreleri arasında binlerce kez meydana gelmektedir. Bu tür biyolojik aktiviteler nanomakineler arasındaki haberleşme için temel oluşturur. MH'nin gerçeklenmesi nanomakineler arasında moleküllerin gönderilmesi ve alınmasıyla gerçekleşir. Verici ve alıcı arasındaki mesafe bilgisi, MH sisteminin tasarımında zamansal senkronizasyon, iletim hızı vb. açıdan verimli bir performans sağlamak için kritik bir parametrelerden biridir. Fakat, MH üzerinde var olan çalışmaların çoğu, mesafenin önceden bilindiği varsayımına dayanmaktadır. Ek olarak, önerilen teorik metotlar ideal simülasyon ortamında doğrulanmaktadır. Ayrıca makro ölçekli pratik uygulamalar hakkında sınırlı sayıda çalışma var.

Bu tezde, uçtan uca bir masa üstü MH sınama ortamı oluşturularak kimyasal sinyaller göndericiden alıcıya iletilir. Bu sınama ortamı alıcının tespit ettiği moleküler bilgileri kullanarak mesafeyi tahmin etmemizi sağlar. Tahmin algoritmalarının gelişim sürecinde moleküler rastgele hareket ilkeleri kullanıldı. Alıcı ve verici arasındaki mesafeyi tahmin etmek için tepe zamanı, korelasyon esaslı ve izafi entropi esaslı olarak adlandırılan üç farklı yaklaşım sunuyoruz. Önerilen tahmin yöntemlerinin performansı masa üstü MH sınama ortamında değerlendirilir. Önerdiğimiz yöntemlerin deneysel sonuçları tahmin hatası ve yöntemler açısından yeni potansiyel makro ölçekli MC uygulamaları geliştirmek için kullanılabilir olduğunu göstermektedir.

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LIST OF ABBREVIATIONS

MC	Molecular Communication
Tx	Transmitter
Rx	Receiver
LOS	Line of Sight
DBMC	Diffusion Based Molecular Communication
PMC	Passive Molecular Communication
AMC	Active Molecular Communication
DE	Distance Estimation
RE	Relative Entropy
PMF	Probability Mass Function
RTT	Round Trip Time
RTT-T	Round Trip Time Threshold Concentration
RTT-P	Round Trip Time Peak Concentration
GUI	Graphical User Interface
SA-P	Signal Attenuation Peak Concentration
SA-T	Signal Attenuation Time Elapses
MLE	Maximum Likelihood Estimation
ISI	Inter Symbol Interference
CRLB	Cramer – Rao lower Bound
MIMO	Multi Input Multi Output

CHAPTER 1

INTRODUCTION

Recently, the developments in nanotechnology provide an oppurtunity to manufacture nanomachine with a size in the nano- to macro-scale range [1,2]. The system of nanomachines initiate a resource to enable applications such as drug-delivery, health monitoring and tracking of cancer cells [3-6]. A single nanomachine has only ability to accomplish simple tasks such as sensing and data storage by itself [4]. The limitations can be exceeded with a couple of nanomachines to perform more complex tasks. Therefore, a communication paradigm among nanomachines is needed for the realization of nanonetworks. Molecular Communication (MC) paradigm that uses chemical signals as carriers of information is a promising solution to enable communication among nanomachines in both nano- and macro-scale. MC is carried out by simply transmitting and receiving molecules between the Tx and Rx. MC is classified into two classes in terms of the energy that is required for the propagation of chemical signals. These classes are called as passive MC (PMC) and active MC (AMC) [8]. In PMC, diffusion occurs by the random movements of molecules through thermal energy and it is known as free diffusion in the literature [7, 9-11]. However, AMC uses intermediate transporting mechanisms for the propagation of molecules. There are several types of AMC such as bacterial assisted propagation and molecular motor based propagation [12-15]. In this research, our experiments are performed according to the principle of PMC. The spatial and temporal distribution of the molecules based on random movement is called as Brownian motion and is governed by the Fick's law [16]. In Section 2.3, the solution of the diffusion equation can be followed with detailed explanations. The distance between the Tx and Rx is one of the critical parameters in diffusion based MC (DBMC). The different distances between the Tx and Rx cause a change in the arrival probability of messenger molecules at the Rx [17]. The knowledge of distance parameter affects the performance of the DBMC in terms of transmission rate, clock synchronization [18-20, 37]. For instance, the Tx can adjust the the number of the transmitted molecules to avoid excessive or insufficient transmission rate to optimise channel capacity. Therefore, the distance estimation (DE) is so important for

reliable DBMC. In the literature, there are few studies to estimate distance parameter between the Tx and the Rx. In [3], peak concentration and double spikes methods are proposed. In peak concentration method, the distance between the Tx and the Rx is estimated by detecting peak concentration of molecules at the Rx. Double spike method measures the time difference between spikes at the Rx to estimate the distance without requiring synchronization between the Tx and the Rx. In [22,23], the authors propose two different methods which are called as round trip time (RTT) and signal attenuation. In RTT, the transmitted signal and feedback signal is compared with each other to estimate distance between the Tx and the Rx. Signal attenuation method detects decrease of the molecular concentration after the propagation of signal from the Tx to the Rx and from the Rx to the Tx, respectively. In [24,25], DE methods are realized by using maximum likelihood estimation to prevent computational complexity. In [26], the two methods are proposed to estimate the distance. One of them is peak time method which has similar with the proposed method in [21]. The other method uses the energy term which is defined as the sum of the molecular concentration at Rx. In addition to that, the authors propose an algorithmic DE scheme for synchronized and unsynchronized conditions by using the similar methods proposed in [26].

In this thesis, a macroscale MC system similar to the setup in [27] is used to examine experimental molecular information. In the literature, all of the existing studies about DE are realized in simulation environment. The propagation guide of the system is based on line-of-sight (LOS) approach. Besides, it is assumed that the arrival time of molecules is perfectly known by the Rx in order to provide synchronization between the Tx and Rx. Furthermore, it is assumed that there is no molecule in the medium before the experiments. In the experiments, alcohol molecules are released into medium with initial drift but without any continuous flow. The Tx is controlled by a board which includes a microcontroller. In the experiments, each puff has constant emission time to keep the number of molecules constant. However, we are unable to know the number of released molecules with our experimental setup. The chemical signals are detected by using an MQ3 alcohol sensor at the Rx. A circuit board is used to control and adjust the capability of the MQ3 sensor. Test scenarios are built on changing distance between the Tx and Rx. Based on these criteria, a tabletop MC system is designed to examine experimental molecular information. In this thesis, we propose three novel methods that are peak time, correlation and relative entropy (RE) based methods for DE. The peak

time method follows a similar idea as given in [21,26]. It is based on detecting the time instant when the Rx reaches the peak concentration. Correlation based method detects how the measurements from the different distances differ from each other. Lastly, the RE based method is proposed to measure the distance among two different distances. Briefly, the main aim of this research is to develop estimation methods to evaluate the distance parameter in a practical macroscale MC system.

1.1. Motivation

In this section, the motivation of this thesis is presented by considering the DE challenges of the experimental tabletop DBMC system. In recent years, there is a growing demand for nano and micro scale communication systems. MC is the most preferred paradigm to meet this demand in nano-scale communication systems. Thereby, a tabletop MC system is designed to examine experimental molecular information. This practical testbed is relatively cheap and easily modifiable for different applications requirements. In the propagation, chemical signals use the advantage of diffusion process to reach the Rx. The proposed DE techniques are developed by considering the principles of free diffusing carrier molecules. Besides, the proposed DE methods might be employed for the development of DE methods in nano-scale MC applications. The existing DE techniques in the literature are executed in simulation environment with simplified cases. Hence, there are many studies in the theoretical perspectives of MC without any physical implementation. Therefore, most of the previous studies that are performed in simulation environment are inadequate in practical scenarios. The determination of diffusion coefficient is a challenging part because theoretical knowledge does not fully fit into the experimental environment as applied in the simulation environment. For the experiments in this study the released number of molecules, emission time, temperature parameters are kept constant while the distance is varied.

1.2. Research Objectives

In this thesis, our objective is to estimate distance parameter in the DBMC system. The distance between the Tx and Rx is an important channel parameter which can be

used to appropriately determine the communication parameters such as number of emitted molecules and symbol time. Furthermore, the localization of a molecular source may be very important to pave the way of sophisticated medical and environmental applications. In the literature of DBMC, the distance is generally assumed to be known by the Tx and Rx. Furthermore, the studies about DE are based on the data which are obtained through the simulations. In these approaches, molecule movements are characterized according to ideal conditions where random walks of molecules aer taken into account. However, in a practical scenario, many other effects such as time-varying drift and absorber and reflector boundary conditions have to be also considered and it is important to examine how such effects disturb the ideal conditions. Therefore, a tabletop MC system similar to the setup in [27] is used to examine experimental molecular information. Within the scope of this thesis, the DE methods have been developed for this experimental MC system.

Additionally, one of our objectives is to determine the diffusion coeffficient that should be known in order to realize some of the DE methods.

1.3. Thesis Outline

The rest of this thesis is organized as follows :

Chapter 2 describes the overall background information about MC, tabletop testbed, diffusion process and related works, respectively. In Section 2.1, the brief history of MC is presented. In Section 2.2, tabletop testbed is presented by dividing it into major parts. In Section 2.3, the underlying principles of diffusion process and its mathematical expressions with sample solutions are introduced. In Section 2.4, The literature survey on related works are given.

Chapter 3 introduces the proposed estimation techniques including the peak time estimation, correlation based estimation and relative entropy based approach.

In Chapter 4, the results of proposed methods are evaluated. In addition, their performances are compared.

Finally, Chapter 5 concludes all the objectives and key results appeared in previous chapters. Also, the future works are included.

CHAPTER 2

BACKGROUND

In the first section, a brief history of MC paradigm is presented. In the second section, the details of our practical tabletop MC system is reviewed. In the third section, the diffusion process is explained from random walk to Fick's law. Finally, the existing studies which focus on the DE and the experimental studies are reviewed in the MC literature.

2.1. Brief History of Molecular Communication Paradigm

The root of miniaturization of devices are traced to speech of physicist Richard Feynmann, ''There's Plenty of Room at the Bottom.''(1959). In the years to come , this idea has shed light on the fundamentals of nanotechnology. Nanotechnology provides a facility to fabrication of devices from 100 down to 1 nanometer. A single nano-machine is only capable of performing simple tasks. Therefore, a large number of nano-machines has to be interconnected coopereatively to overcome more complex tasks. The interconnected nano-machines constitute a network is known as nanonetwork.

In the perspective of communication engineering, a nanonetwork can be designed with the MC paradigm. MC paradigm uses molecules as carrier of information between the Tx and Rx. The usage of molecules as carrier in MC provides a promising basis for nanonetworks. In comparison to the traditional communication paradigms, MC presents the following advantages such as; feasibility, scability, bio-compability and energy efficiency [2]. Because the widespread use of nano-machines has not yet reached to desired levels to operate molecular structures in a precise way, the detection and evaluation of molecular information is evaluated by the MC system in different scales. Therefore, MC is categorized into macro, micro and nano-scale MC.

2.2. Tabletop Molecular Communication Testbed

In this thesis, the practical MC system is designed with a single Tx and Rx. The Tx and Rx are positioned in the coordinate system at the origin $(0, 0, 0)$ and $(x, 0, 0)$, respectively. In each scenario, while the Tx is fixed at the origin, Rx is fixed at different points on the x-axis. Although MC literature is a rapidly developing literature, there are few studies about experimental MC in macro scale. The main motivation of this thesis is to propose DE methods via a tabletop MC system. Our tabletop MC system is similar to the system proposed in [27], but it differs at some points such as the use of fan. As in each communication system, it basically includes three main parts that are transmitter, tranmission guide and receiver. The block diagram of a basic communication system is represented in the Figure 2.1.

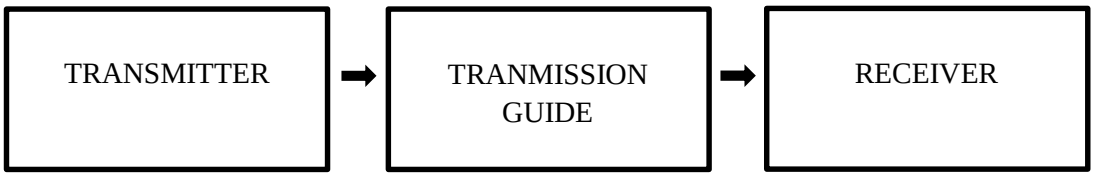

Figure 2.1 Block diagram of a characteristic communication system

- Transmitter Part : The task of the Tx is to release the chemical signals for propagation in the environment. A custom electrical circuit board and microcontroller are needed to perform the tasks of the Tx part. Firstly, the chemical carrier signal which is in the liquid form is stored in an sprayer. Then, the container is integrated into the electrical circuit board. The sprayer is controlled by microcontroller. The microcontroller is capable of managing configuration settings such as spray duration. Moreover, these configuration settings can be adjustable through graphical user interface (GUI). The released molecules start their movement with an initial drift provided by the sprayer. By using the same spray duration, the number of released molecules is kept constant in each test trial. In addition, our system does not use any external fan device to increase the flow rate of the propagation medium contrary to the setup used in [27].

- Transmission Guide: The propagation scheme that is known as free diffusion is considered in our system. The released molecules reach to the receiver by diffusing in the air. The diffusion based propagation scenario does not require external energy. The distribution of molecular concentration in the environment is defined by Fick's second law as a function of the coordinate (x, y, z) and the time (t). The detail discussion about diffusion process is given in the section 2.3.

- Receiver Part : The Rx is responsible for detecting the transmitted molecular signal. Therefore, a MQ-3 alcohol sensor is used as a receiver in the system. The sensitivity of the sensor limits the performance of the MC system [28-31]. The sampling frequency of the sensor is defined as $125\,Hz$. The molecular concentration information detected by the sensor is transferred to personal computer via RS-232 serial port connection from the microcontroller. The molecular density is converted to digitized values in the range of [0, 1024]. These values can be displayed over GUI in real time and recorded to a text file. The GUI is given in the Figure 2.3.

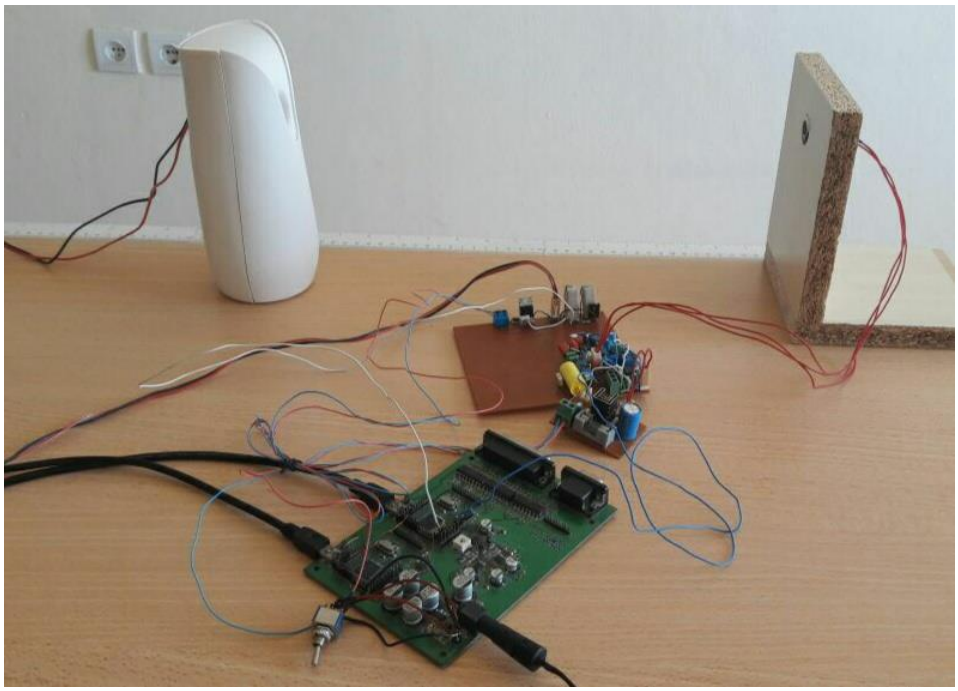

Figure 2.2 Tabletop MC System

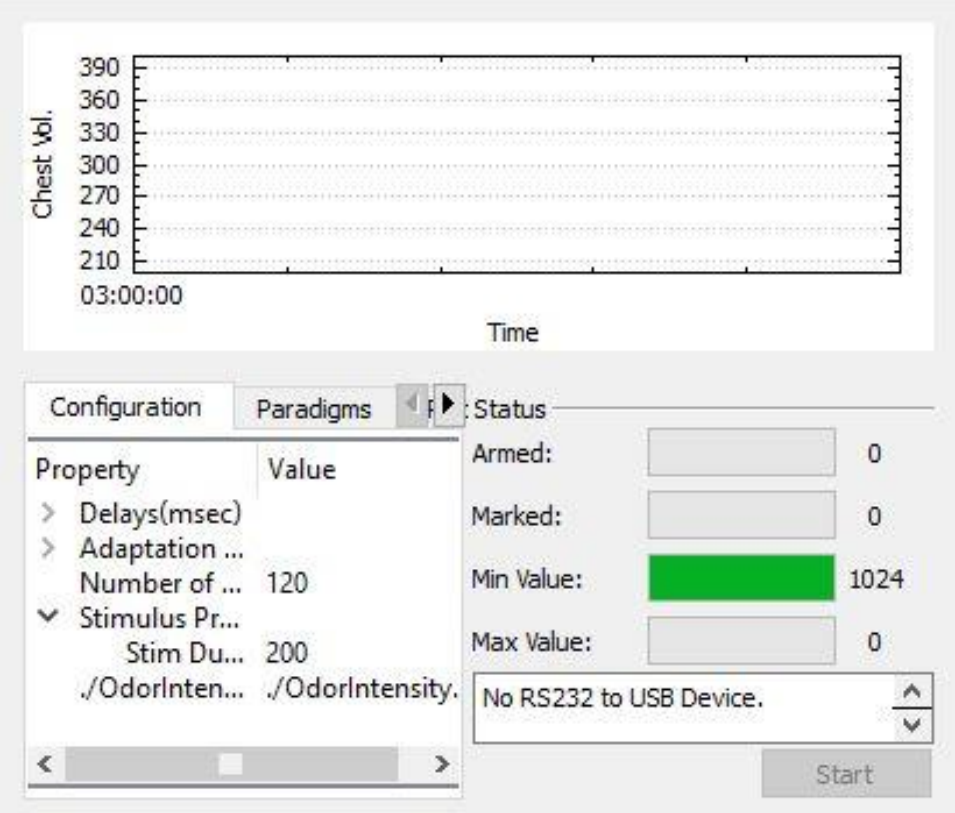

Figure 2.3 Graphical User Interface (GUI)

As seen in Figure 2.2, the Tx and Rx are positioned to the coordinates $(0, 0, 0)$ and $(x, 0, 0)$, respectively. The tests are carried out in the following order. All parameters of the system are configured according to the requirements of the system. The tabletop MC system can then be activated by turning the power control button on. The RS-232 ports of the microcontroller are connected to the USB ports of the computer. The setup can be triggered by clicking the start button on GUI. It is assumed that the Tx and the Rx are synchronized in time. In each trial, the Tx is triggered only once to avoid interference between succesive sprays. Thus, the impulse response is detected more clearly for different distances.

2.3. Diffusion Process

The molecules diffuse in the medium according to the concentration gradient. Diffusion process is the random movements of molecules in the medium and its characteristics are basically defined with random walk. In principle, random walk is covered under three rules. Firstly, the particle is considered in one-dimensional random walk at time $t = 0$ and at position $x = 0$. Then, in one time step τ, a particle can step δ to right or left with respective probabilities $p = \frac{1}{2}$, $q = \frac{1}{2}$. Secondly, in a time period, the successive steps of the molecules are statistically independent from each other. Lastly, it is assumed that molecules do not interact with each other in the propagation since their movements are independent. These basic principles provide a basis for the Fick's equations.

The Fick's first equation is given as

$$J_x = -D\frac{dC}{dx} \tag{1}$$

where $D\left(\frac{cm^2}{s}\right)$ is the diffusion coefficient, J_x is the flux and C represents the concentration of the molecules.

The Fick's second equation or diffusion equation can be derived based on conservation of the number of molecules and given by

$$\frac{dC}{dt} = D\frac{d^2C}{dx^2} \tag{2}$$

where, $-\infty < \mathrm{x} < \infty,\ 0 < \mathrm{t} < \infty$.

$$C = \frac{K}{\sqrt{t}}e^{-\frac{x^2}{4Dt}} \tag{3}$$

Let us assume the released number of molecules from the origin at $t = 0$ is M then,

$$M = \int_{-\infty}^{\infty} C dx \tag{4}$$

$$M = \int_{-\infty}^{\infty} \frac{K}{\sqrt{t}} e^{\frac{x^2}{4Dt}} dx \tag{5}$$

By means of the following parameter change, M can be expressed as

$$\frac{x^2}{4Dt} = a^2,\ dx = 2\sqrt{Dt}da \tag{6}$$

$$M = 2K\sqrt{D}\int_{-\infty}^{\infty} e^{-a^2} \tag{7}$$

$$\mathrm{M}= 2K\sqrt{\pi D} \tag{8}$$

Then, C can be written by writing K into the equation (3) as follows:

$$C = \frac{M}{\sqrt{4\pi Dt}} e^{-\frac{x^2}{4Dt}} \tag{9}$$

The similar approach is valid for two and three dimensional diffusion equations, respectively, as follows:

$$C = \frac{M}{4\pi Dt} e^{-\frac{x^2+y^2}{4Dt}},\quad C = \frac{M}{(4\pi Dt)^{\frac{3}{2}}} e^{\frac{-(x^2+y^2+z^2)}{4Dt}} \tag{10}$$

2.4. Related Works

In this section, some of the previous works on the distance estimation methods, which can be related to this thesis, are introduced. In [21], the authors present the peak concentration and double-spikes methods to estimate the distance parameter. In these methods, it is described that distance is estimated using only one-way transmission and requiring no clock synchronization. The Rx has ability to estimate distance by itself according to received molecular signal. The methodology of the peak concentration-based methods is based on detecting the time instant when the maximum concentration is observed at the Rx. The double-spikes method allow to the Tx to transmit two spikes at the same measurement time interval. Then, the DE is done by using the time difference between peak time of the spikes. The performance analyses of those methods are performed in a simulation environment at micro scale. Finally, the authors are compared their methods according to criteria such as accuracy, precision and time delay. The results represent that peak concentration-based method presents a better accuracy for smaller distance. However, double spikes-based method perform better

when the distance is larger. As a result, the performances of proposed methods vary for different distance ranges. In [26], the authors present the peak concentration-based and energy-based methods to estimate distance parameter. The peak concentration-based method has a similar idea proposed in [21]. However, in energy-based method, the distance between the Tx and the Rx is estimated by using energy of the received signal. The energy of the signal is defined as the sum of the sensed molecular concentration at the Rx. The energy-based method has better performance on the accuracy compared to peak concentration-based method. However, it is stated that it has a higher requirement of the complexity in the system. Furthermore, the results indicate that when distance between the Tx and Rx increases, the accuracy of estimations reduces for both proposed methods. In [32], the authors present a distance estimation method which is called as Round Trip Time (RTT). In this method, the RTT is defined as the time which is necessary for the signal to propagate from transmitter to receiver and then back from receiver to transmitter. In this research, the proposed methods are performed for different design choices in each step of MC system. In the Tx part, the options are stated as the release of molecules in a spike or gradually. The propagation options are defined based on the presence or absence of repeater in the environment. In the Rx part, the design options are increased by defining a threshold to the receiver or by filtering for some specific molecules. As a result, the authors state that these options have impact on the accuracy of the distance estimation. Besides, it is concluded that the RTT produces a higher delay compared to proposed one-way transmission methods in [21]. In [22,23], the authors present the RTT and signal attenuation (SA) methods to estimate distance. The RTT method follows the similar idea of [32]. However, the RTT method is examined in two different processes which are called as peak concentration (RTT-P) and threshold concentration (RTT-T). Besides, they introduce a new approach called the SA method. The SA method use the attenuation information of molecular concentration after signal propagating from the Tx to Rx and from the Rx to Tx. Moreover, the authors apply the SA method according to the processes that are called as peak concentration (SA-P) and concentraiton when time elapses (SA-T). Finally, the authors compare the results of proposed methods in terms of accuracy and delay. It is observed that RTT-T method has the lowest error and delay compared to other methods. In [25], the authors use multiple symbols to get more accurate results. The DE is done by using the maximum likelihood estimation (MLE) protocol. Besides, they use Newton-Raphson method to estimate the distance in the derivation of closed-from expressions.

Moreover, the effect of the inter-symbol interference (ISI) is considered in the model. The experiments are performed according to the a point-to-point MC model in an unbounded 3-D simulation environment. As a result, it is stated that the addition of ISI into the model improves the accuracy of the DE compared to previous studies. In [33], the authors design a MC system between two nanomachines in the simulation environment. The DE method is based on counting the number of molecules at the Rx. The authors examine the algorithmic DE schemes which are classified as synchronous and asynchronous. The synchronization refers to setting a the clock of the Tx and RX the same. Besides, they propose parameter optimization methods to achieve more accurate DE. This paper concludes that proposed DE schemes and optimisation methods should be adjusted according to the specific requirements of the design to obtain more accurate results. In [35], the Cramer - Rao lower bound (CRLB) on the variance of the distance estimation error is derived. In addition, the authors derive the MLE method to compare the with CRLB in terms of accuracy. Moreover, the SA-T and the RT-T methods are compared with CRLB. As a result, it states that derived MLE and CRLB methods achieve more accurate results to the exisitng DE methods. In [27], the authors describe the first macroscopic MC platform for transmitting a message using chemical signals as a carrier. This platform is designed to be a bridge between theoretical and practical applications. For instance, the equipments such as the sensor and the transmitter are choosen as inexpensive and widely available in the design. In addition, the authors generate different types of flows in the propagation of chemical signals. Then, the effects of different types of flows are examined on the system response. Furthermore, the authors achieve to transmit a text message by using tabletop MC system. In [34], the authors design a novel multiple-input multiple-output (MIMO) practical MC system to enhance the data rate. In the design, multiple molecular transmitters and multiple molecular receivers are used similar to antennas in radio frequency communication. Therefore, this study also takes into account inter-symbol and inter-link interference effects. Furthermore, this study is the first practical molecular MIMO application in the literature. The studies given above show that there is a limited number of studies about the DE at macroscale practical applications. In this thesis, our aim is to develop new DE methods by using experimental setup at macro scale.

CHAPTER 3

PROPOSED METHODS AND EXPERIMENTAL RESULTS

In this thesis, our main goal is to estimate the distance parameter between the Tx and Rx at the macro scale MC system. The test scenarios are based on evaluating the differences in the system impulse responses when the distance between the Tx and Rx changes.

3.1. The Data Collection

In each experiment, the state of the physical environment is kept constant to accurately define the effect of the distance parameter on the system response. Therefore, the inter-emission time of the sprayer is set to be approximately one hour to ensure that the molecular concentration in the environment is the same before each experiment. The performance of the proposed DE algorithms are tested for the incremental distance values from 10 cm to 200 cm with the step length 10 cm. In addition, each experiment is performed five times for the same distance to obtain more accurate distance estimations. The experiment results for 10 cm distance show that the sensor reachs to a saturation level. Therefore, the experimental results for 10 cm distance are not evaluated as input in the proposed methods. The experimental data is shown in the following Figures 3.2 - 3.6.

The detection time of the sensor is shown in the Figure 3.1 for each distance. The results show that the maximum concentration decreases with the distance. On the contrary, as the distance increases, the detection time of the sensor increases.

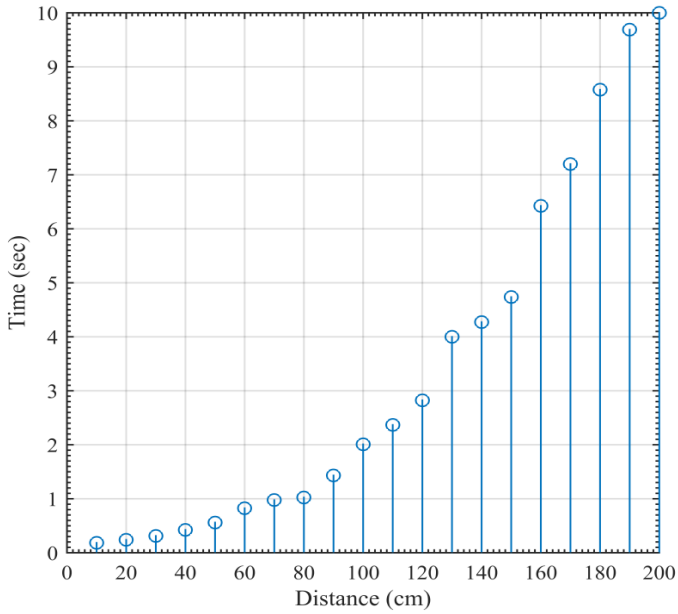

Figure 3.1 The time of the detection as the distance increases

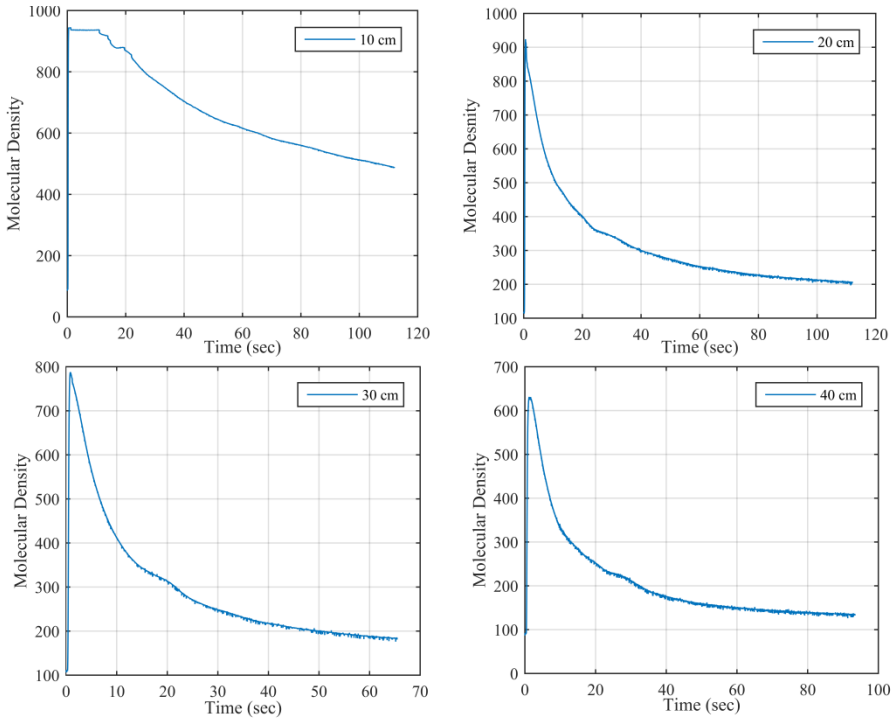

Figure 3.2 Experimental results between 10 cm and 40 cm

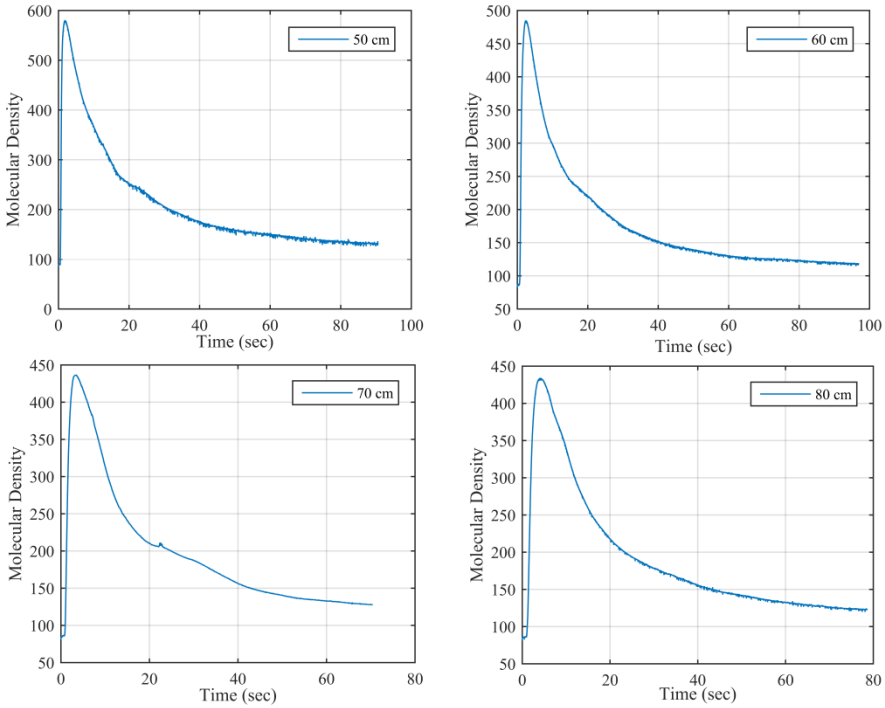

Figure 3.3 Experimental results between 50 cm and 80 cm

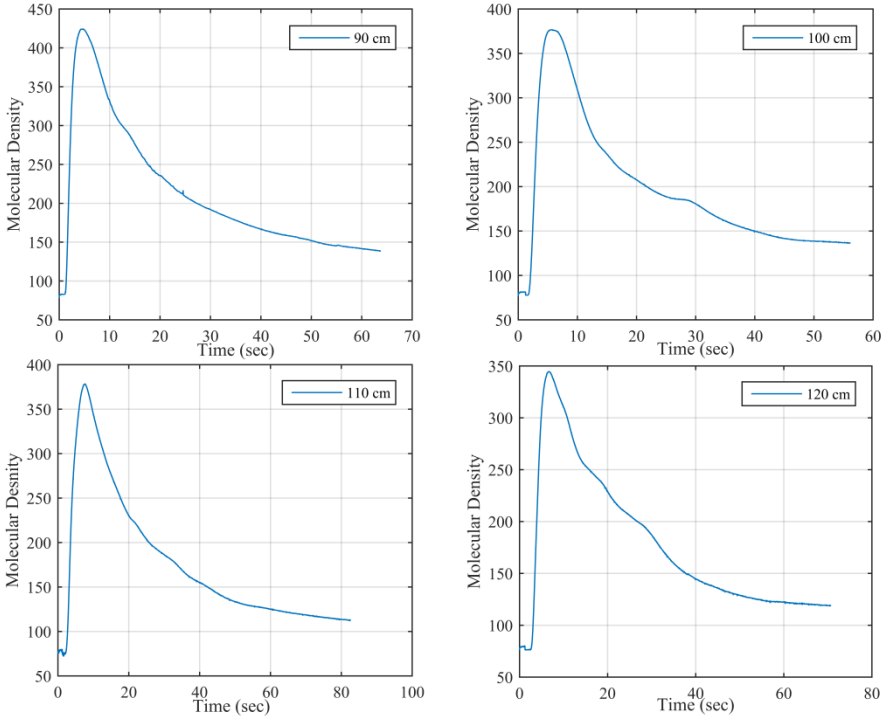

Figure 3.4 Experimental results between 90 cm and 120 cm

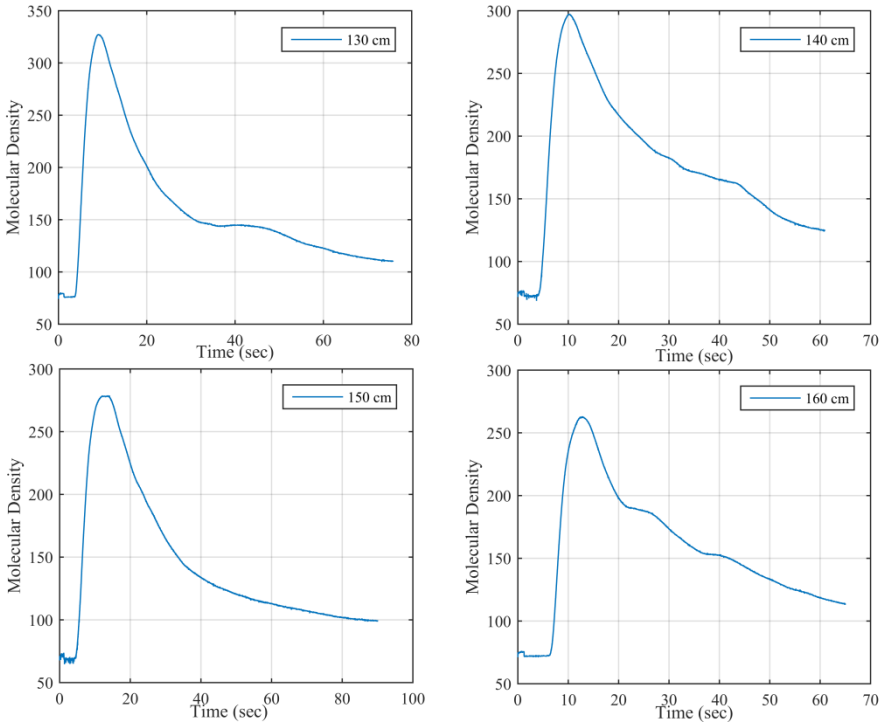

Figure 3.5 Experimental results between 130 cm and 160 cm

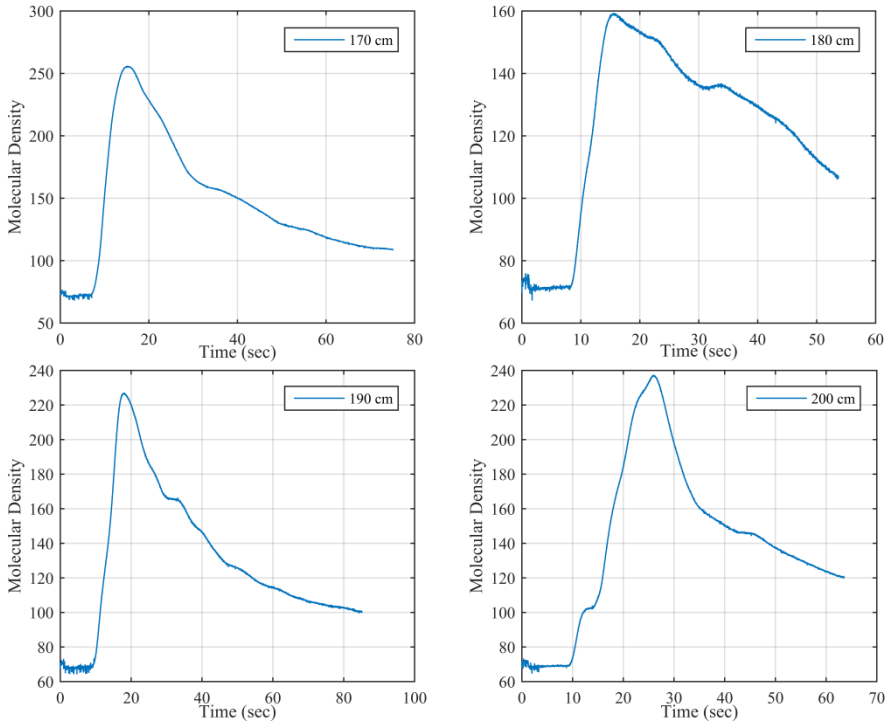

Figure 3.6 Experimental results between 170 cm and 200 cm

3.2. The Estimation of Diffusion Coefficient

In the system, all parameters affecting the impulse response must be clearly defined to make an accurate estimation on the distance. The diffusion of molecules in the medium is an important parameter for the MC system. The diffusivity of the environment is defined by the diffusion coefficient. In diciplines such as thermodynamic, the diffusion coefficient is calculated by the equation (11). However, the values of the input variables in the equation (11) are not known by our MC system.

$$\mathrm{D} = \frac{\mathrm{kT}}{6\pi\eta\mathrm{r}} \tag{11}$$

where k is Boltzmann constant, T is temperature, η is dynamic viscosity and r is the particle radius. Therefore, alternative methods for the determination of diffusion coefficient is needed. In [36], the authors present a method for the case of instantaneous emission in still air. This method records the time when the molecules are detected at the distances r_1 and r_2, as t_1 and t_2, respectively. These pairs (r_1, t_1) and (r_2, t_2) are taken into calculation in the equation (14). In the derivation of (15), the system response function $C(r,t)$ is equalized to constant value $\frac{Q}{k}$ for both measurement. Then, the diffusion coefficient can be calculated by the equation (14). In (14), the measurement (r_1, t_1) is specified as reference pair. The specified reference measurement is choosen as 20 cm in our case. It is seperately processed with all other measurement pairs. Then, the arithmetic mean of each pair is defined as the diffusion coefficient for our MC system and shown in the Figure 3.7. However, the diffusion coefficient results of measurements up to 50 centimeter have negative values. A similar situation is observed in [36] and the author states that these negative values have to be ignored. The authors assume that these results do not fit their model. These negative values are not taken into account in our study by following the same approach. Besides, it seen that the theoretically presented method does not fully coincide with the practical setup since the setup includes a sensor and sprayer which are not considered in the theoretical model. Therefore, some estimated values of diffusion coefficient become neative as shown in Figure 3.7. Those unrealistic values are discarded in the given numerical analyses. It should be noted that the unit of the diffusion constant is in square meters per second. The flowchart of estimating the diffusion coefficient is given below in the Figure 3.8.

Diffusion coefficient is determined for the (r_1, t_1) and (r_2, t_2) as follows:

$$\mathrm{k} = \frac{2\mathrm{Q}}{(4\pi \mathrm{D t_1})^{3/2}} \mathrm{e}^{-\frac{{r_1}^2}{4\mathrm{D t_1}}} \tag{12}$$

where, k is a reference concentration measured at the distance r_1 and r_2 and Q is the number of emitted molecules at the origin of a coordinate system at time $t = 0$. In the analysis of such particular systems, D, Q and k might be unknown. However, the ratio of the Q and k, not the absolute values of Q and k, describes the diffusion of emitted molecules. Therefore, D can be computed by equalizing to the ratio for each measurement such as (r_1, t_1) and (r_2, t_2).

$$\left(\frac{\mathrm{Q}}{\mathrm{k}}\right) = \frac{1}{2}(4\pi D t_1)^{3/2} \mathrm{e}^{-\frac{{r_1}^2}{4\mathrm{D t_1}}} = \frac{1}{2}(4\pi \mathrm{D t_2})^{3/2} \mathrm{e}^{-\frac{{r_2}^2}{4\mathrm{D t_2}}} \tag{13}$$

$$\mathrm{D} = \frac{\frac{{r_1}^2}{t_1} - \frac{{r_2}^2}{t_2}}{6\log {}^{t_2}/_{t_1}} \tag{14}$$

The value of D can be taken as the average of the values obtained for each pairs of measurements according to the reference measurement. The mean calculation of the diffusion coefficient is the last step to determine our diffusion coefficient as illustrated in the Figure 3.8.

$$D = \frac{D_{60-20} + D_{70-20} + \cdots + D_{190-20} + D_{200-20}}{\mathrm{n{=}15}} = 0.0294 \ \mathrm{m^2/sec} \tag{15}$$

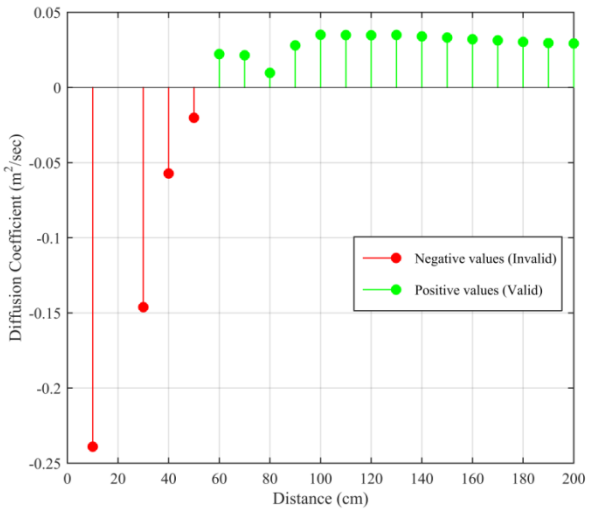

Figure 3.7 Estimation of Diffusion Coefficient

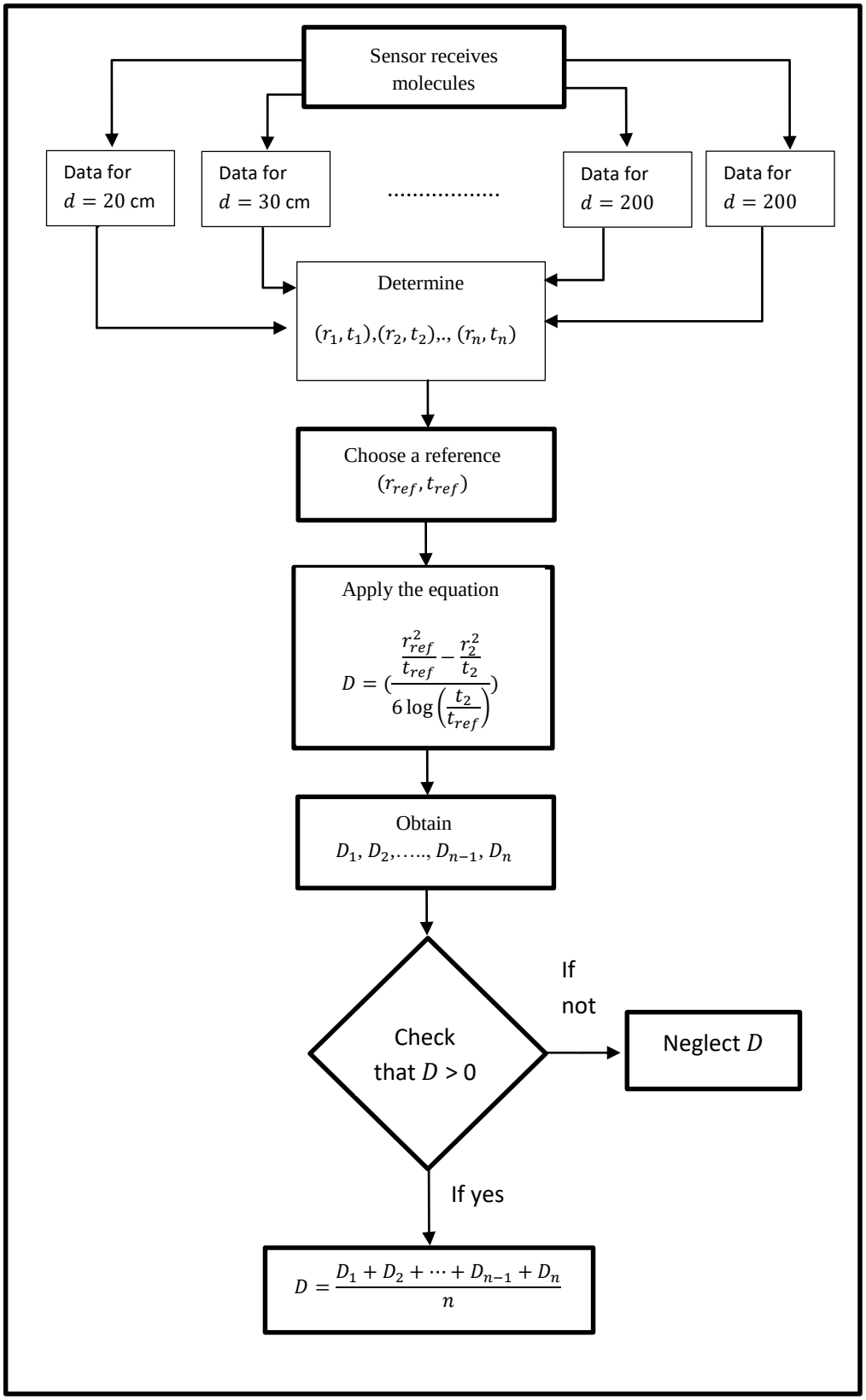

Figure 3.8 Flowchart to determine diffusion coefficient

3.3. Peak Time-Based Estimation

The curve shape of the received signal has the same typical shape for each different distance between the Tx and the Rx. However, as the distance between the Tx and the Rx increases, the peak point of the curve shifts right and becomes wider. Besides, after the concentration reaches to the peak rapidly, it drops down slowly. Therefore, when the time goes to infinity, the system response seems like a long-tailed curve. This curve form is similar to the response of diffusion channel in the equation (2.3) as $C(d,t)$. Thus, $C(d,t)$ is defined in the range of $[0,\infty)$ as a positive continuous function. Therefore, the impulse response of the system must include a global maximum point at the interval $[0,\infty)$. Briefly, the time instance of the peak concentration is used to estimate distance. The derivative of the impulse system response is taken to detect the time instance for the maximum concentration. Then, the derived equation (17) is equalized to zero to determine the peak time instance.

$$C(d,t) = \begin{Bmatrix} \frac{M}{\sqrt{4\pi Dt}} e^{-\frac{d^2}{4Dt}} & ,t \in (0,\infty) \\ 0 & ,t = 0 \end{Bmatrix} \tag{16}$$

$$\frac{d}{dt} C(d,t) = \frac{d}{dt}\left(\frac{M e^{-\frac{d^2}{4Dt}}}{(4\pi Dt)^3} \right) = 0 \tag{17}$$

$$d = \sqrt{6Dt_{peak}} \tag{18}$$

The results of the experiments are recorded for each distance. The peak time is determined by the data received from the sensor. The experiments are performed up to 200 cm. Because the molecular concentration is too low for detection of peak time at distances greater than 200 cm in our system. The distance range can be extended by using fan apparatus as same as in [27]. However, a fan apparatus is not used in our MC system to prevent effects such as turbulent. The diffusion of the molecules can be applied to each axis in a similar way. However, our experimental test results belongs to the movement of molecules in the x direction.

The estimation results show that the error rate ismostly low. However, it is clearly observed that the error rate is relatively higher for the distance interval up to 50 centimeter. The error rate is %10 or less for other distances up to 200 cm. These results can be explained by the fact that the initial drift effect has great impact on the released molecules up to 50 cm. The estimation results and flowchart of the peak time-based method are given in the Figure 3.10 and Figure 3.11, respectively.

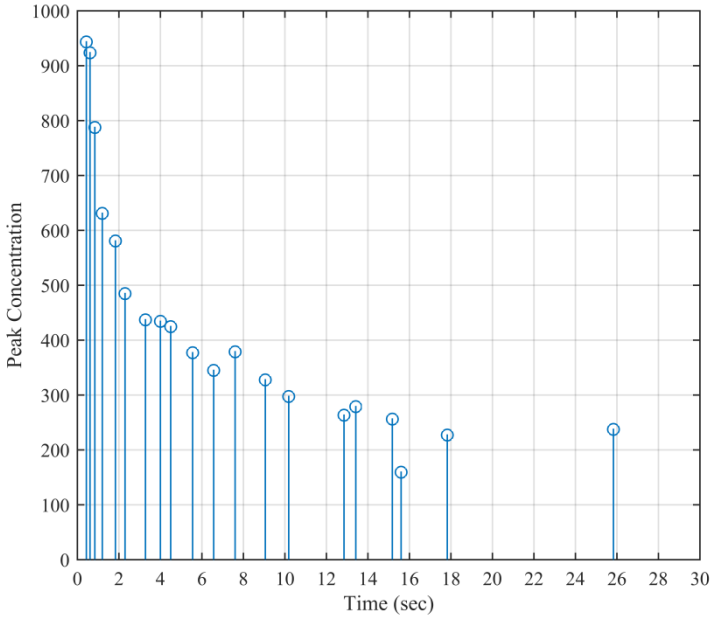

Figure 3.9 Peak time of experimental results

In the Figure 3.9, each bar shows the peak concentrations for the distances from 10 cm to 200 cm, respectively. As shown in the Figure 3.9, the peak concentration decreases with the distance. However, the time at which the peak concentration is detected increases as the distance increases.

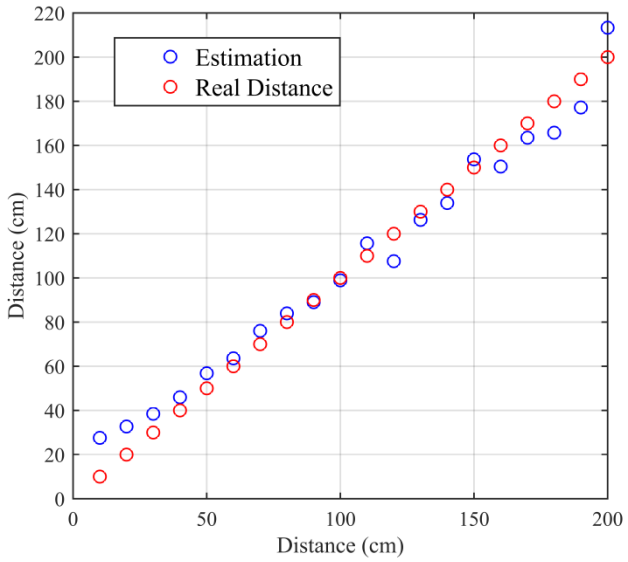

Figure 3.10 Distance estimation by using peak time-based method

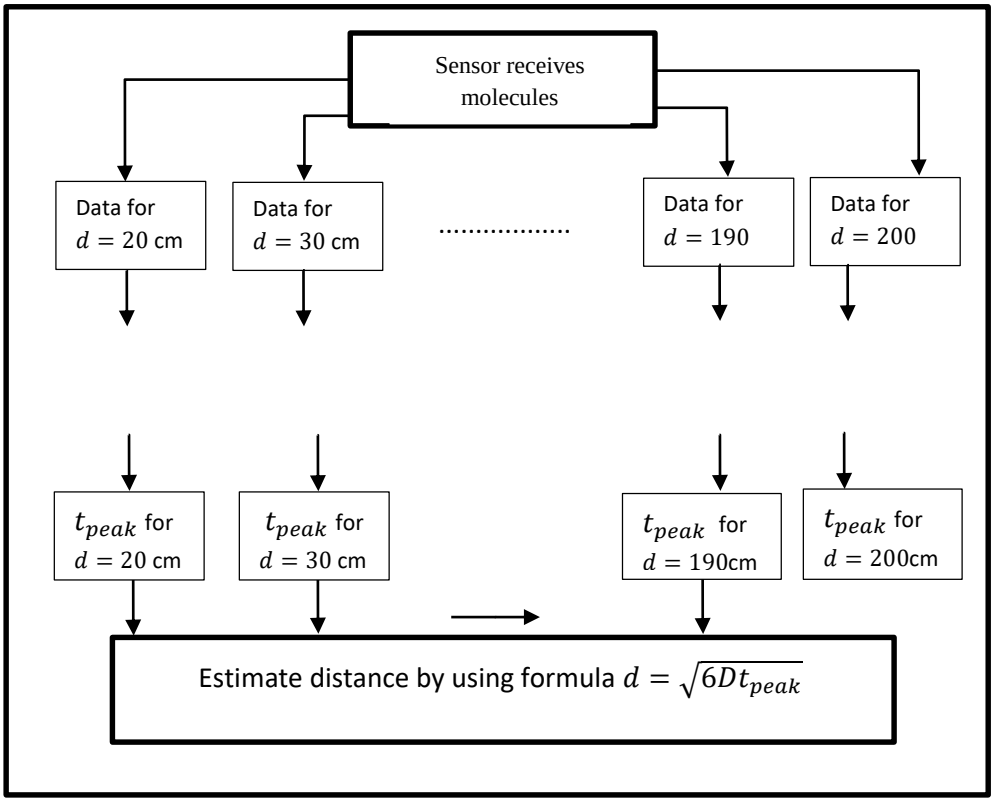

Figure 3.11 Flowchart of peak time estimation method

3.4. Correlation Based Estimation

In our system, the measurements are performed up to 200 cm. As we mentioned before, it is known that as the distance between the Tx and Rx increases, the maximum concentration shifts to right on the time axis. In other words, the curve shape of different distances are in the form of shifted versions of each other. The similarity between the curve shapes for two different distances can be determined by using the correlation method. In this method, the received signal from the detection to the peak concentration is just considered. Firstly, the concentration distribution is partially divided from initial point to peak point. This segment is flipped according to y-axis and combined with itself. A symmetric distribution curve is obtained as a result of this manipulation. Secondly, one of the measured distances which is choosen as 20 cm in our case is selected as a reference. The reference symmetric curve distribution is convolved with another curve distribution of different distance. The peak point of the curve resulting from convolution is the sum of the peak points of the two curves used as input. Since the peak time of the reference curve is known, the peak time of the curve which is processed with the reference can be found. In addition, any distance up to 200 cm can be estimated by using experimental data. The correlation method has better performance in terms of accuracy in short distances. In detail, the estimation results indicate that the error rate is lower for distances up to 80 centimeter. The error rate is %10 or less for the range of distances up to 80 centimeter. In the Figures 3.12 - 3.15, the convolution process of the distributions are given in order. In all the tests given below, the curve of 20 cm is fixed and it is convolved with the distributions at different distances. In this method, the diffusion constant which is an external parameter is used in the last step. The results of correlation method and the flowchart of the method are given in the Figure 3.16 and Figure 3.17, respectively. In addition, the numerical results are listed in the Table 3.1.

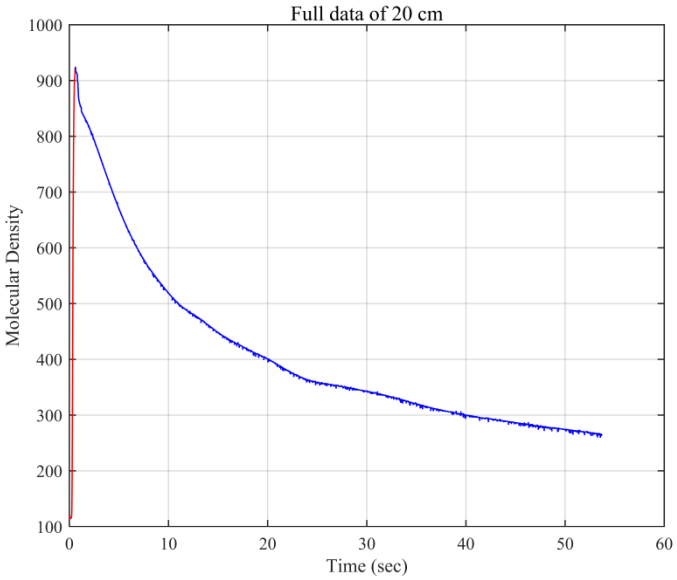

Figure 3.12 The data belongs to 20 cm

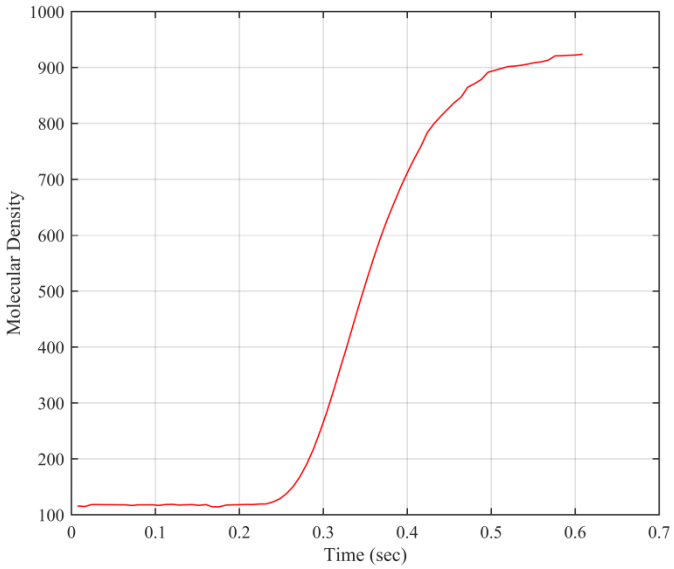

Figure 3.13 Interrupted version of data 20 cm up to peak concentration

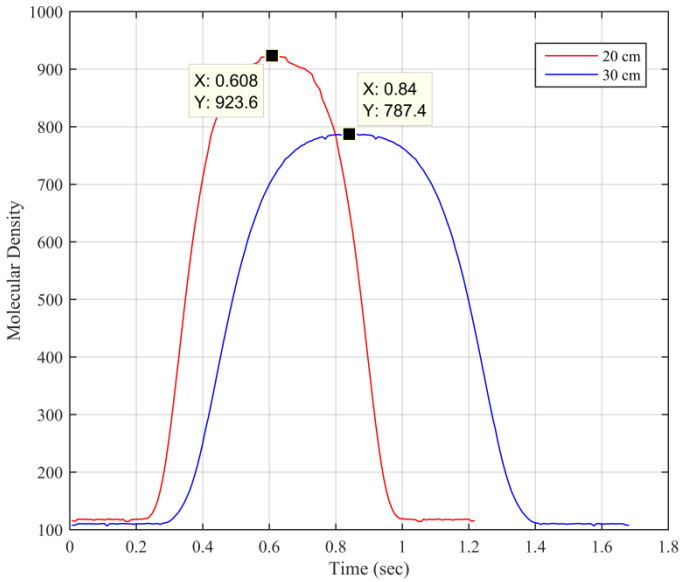

Figure 3.14 A sample for symmetrical form of data cut to peak concentration values

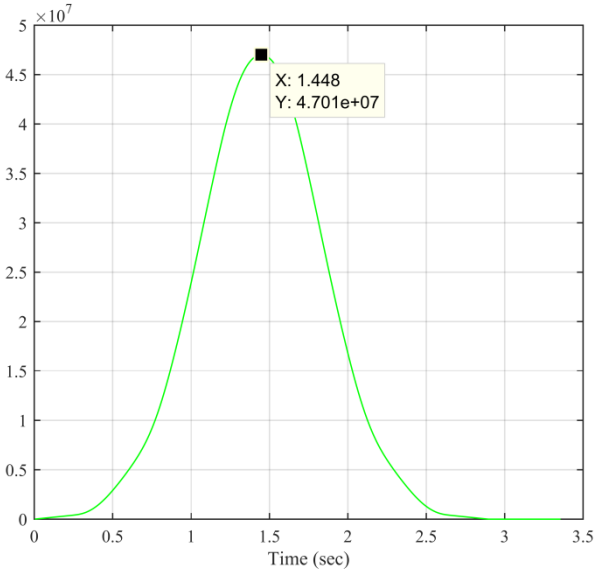

Figure 3.15 The relevant result of convolution

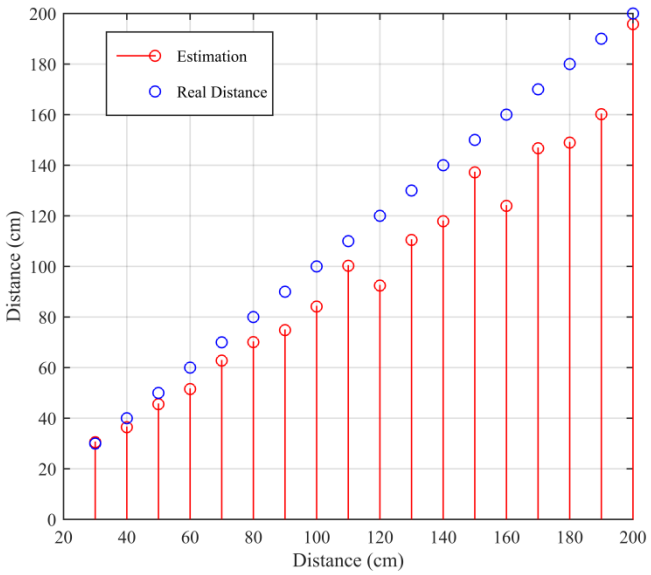

Figure 3.16 Estimation results compared with real result

Table 3.1 Correlation approach results and relevant error value

$d_{estimation}$(cm)	d_{real}(cm)	Error (cm)
30.5	30	+0.5
36.43	40	-3.57
45.56	50	-4.44
51.52	60	-8.48
62.75	70	-7.25
70.09	80	-9.91
74.82	90	-15.18
84.16	100	-15.84
100.24	110	-9.76
92.43	120	-27.57
110.47	130	-19.53
117.87	140	-22.13
137.17	150	-12.83
123.95	160	-36.05
146.74	170	-23.26
148.96	180	-31.04
160.18	190	-29.82
195.8	200	-4.2

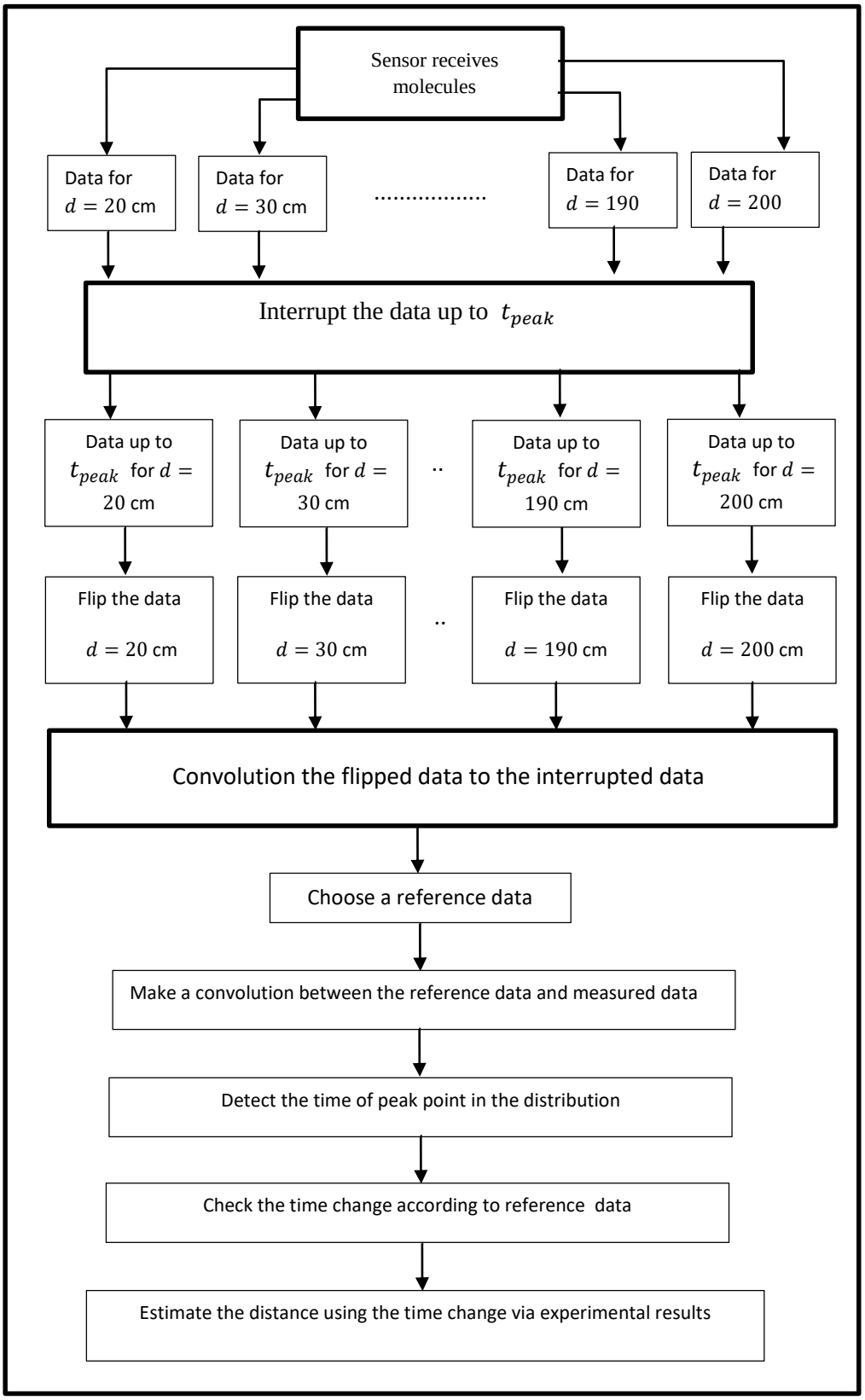

Figure 3.17 Flowchart of correlation based method

3.5. Relative Entropy Based Estimation

Relative entropy (RE) approach is the last proposed method to estimate distance parameter. It is also known as Kullback–Leibler Divergence in the literature. In our system, the experiments can be carried out for a distance between the Tx and Rx in the range of 0 to 200 cm. However, the measurements could not be made for each distance. Therefore, there is a lack of information to estimate the non-measured distances. The RE based method supplies ability to handle this issue. RE is a measure of distance between two probability distributions that are defined over the same alphabet. The two discrete probability mass functions (pmf) $p(x)$ and $q(x)$ are compared to measure similarity between them.

The RE is defined as follows:

$$D(p||q) = \sum_{x \in X} p(x) log(\frac{p(x)}{q(x)}) \quad (19)$$

The experimental molecular data is divided into equal width sections on the molecular density axis as shown in Figure 3.18 and 19. Firstly, the measurement time of the data is set equally for all measurements. Besides, it is important to decide how the signal amplitude should be divided into equal intervals in order to derive the probability mass function of the received signal. The adjustment of the interval setting has an affeect on the performance in terms of accuracy. In the Figures 3.18 and 3.19, the width of the intervals is selected as 100. When the interval width is selected as larger than 100, it causes to the similarity of pmfs for different distances. On the other hand, if the width is smaller then 100, it causes to overlap between pmf's of different distances. In the Figure 3.20 and Figure 3.21, the number of samples falling into each interval is counted and converted to the probabilistic ratios for 60 cm and 70 cm, respectively. The pmfs are obtained as a vector for each distance distribution. The elements of the vectors that have the same index number are processed with each other and then the summation of the processing results is defined as the RE of the related distributions. The pmf belonging to the distance 60 cm is assigned to marginal pmf $q(x)$ and considered as a reference pmf for the calculation of RE by using the pmfs generated for other distance values. The RE results are given in the Figure 3.22.

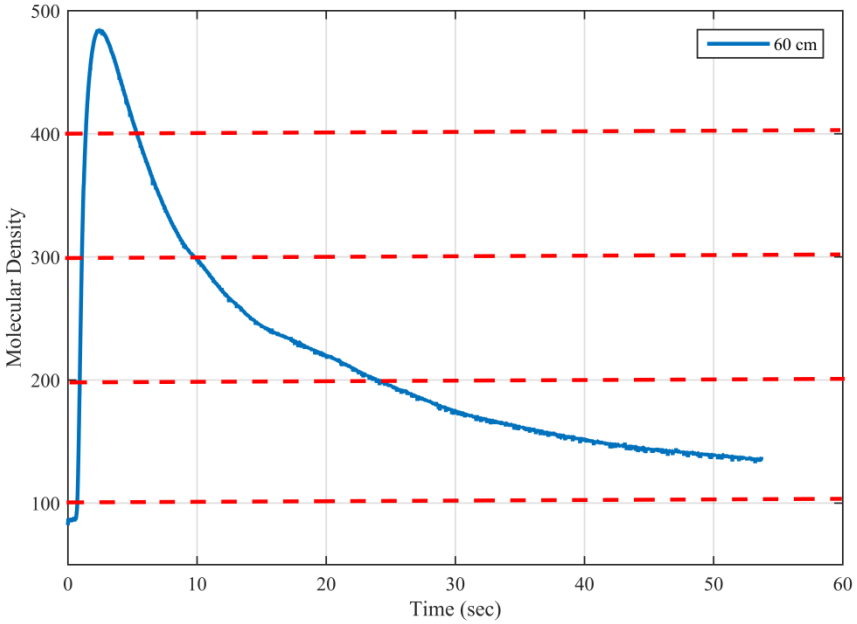

Figure 3.18 The data belongs to 60 cm

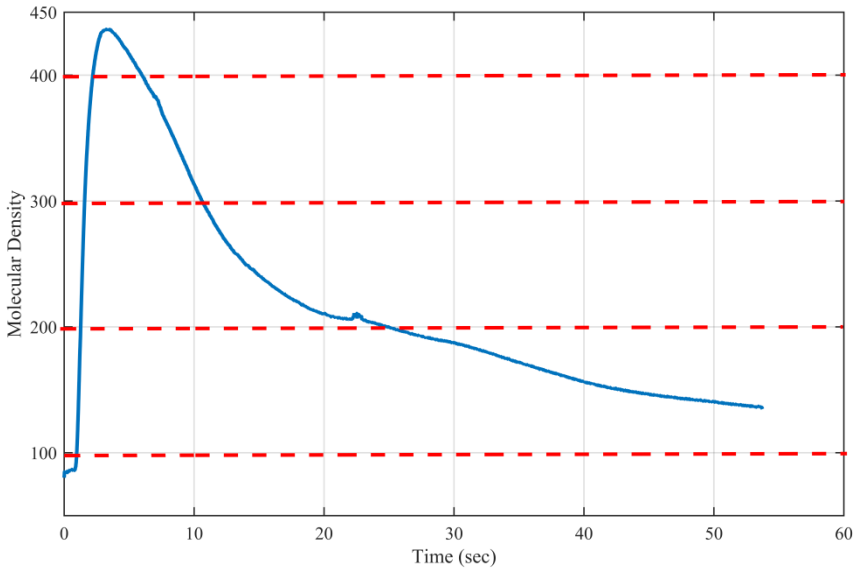

Figure 3.19 The data belongs to 70 cm

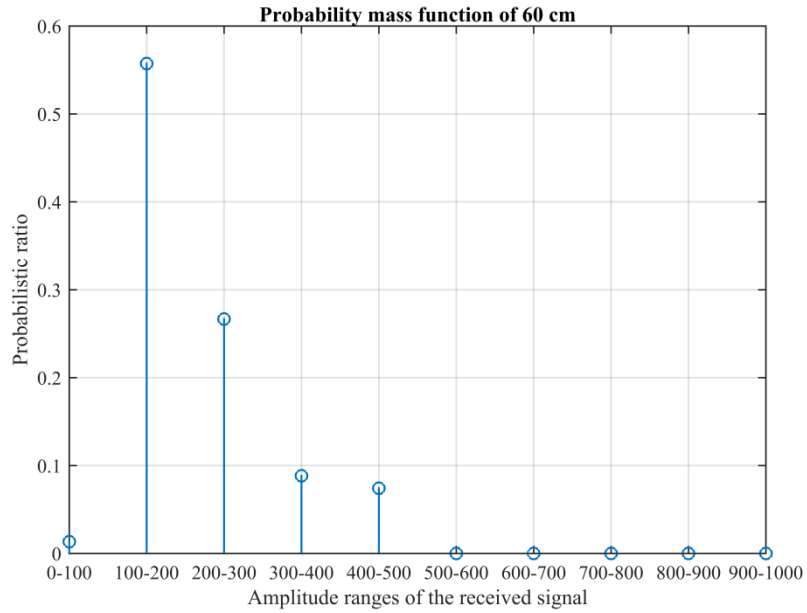

Figure 3.20 Probability mass function ratios for each interval when the distance between the Tx and Rx is 60 cm

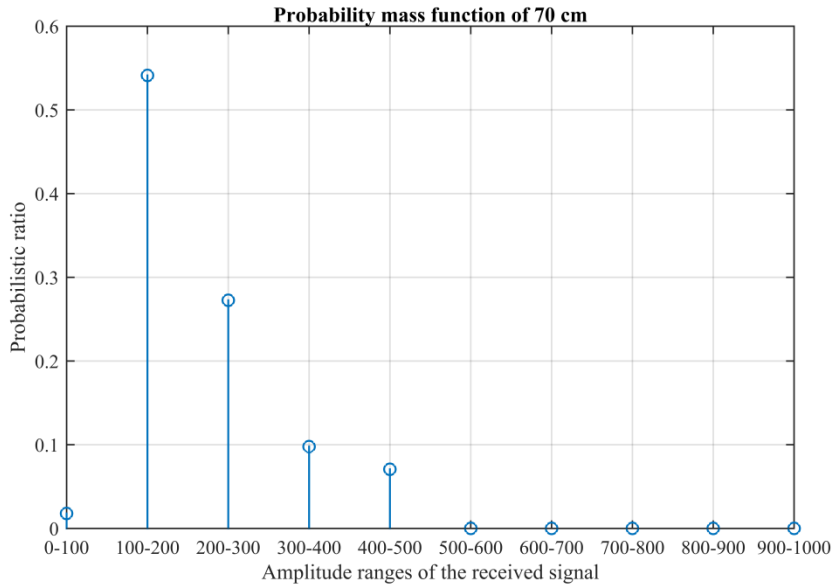

Figure 3.21 Probability mass function ratios for each interval when the distance between the Tx and Rx is 70 cm

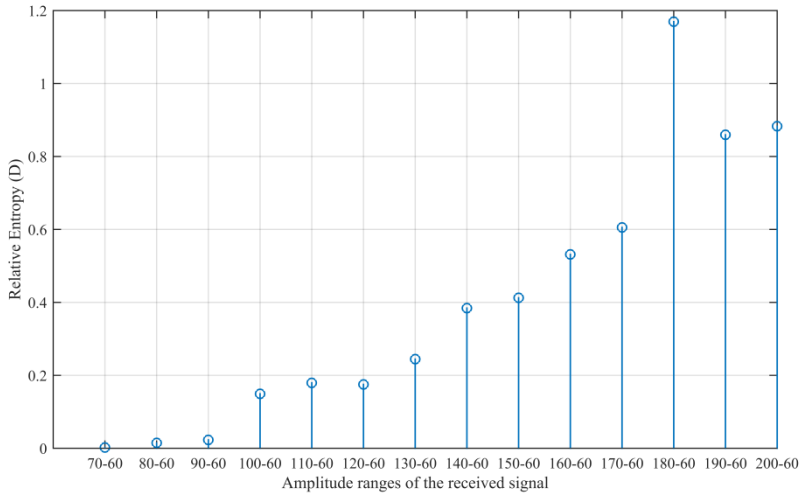

Figure 3.22 The results obtained from relative entropy method

As mentioned earlier, the measurements are obtained for a 20 different distances between 0 to 200 cm. However, there is also need to estimate the RE values for untested distances. Therefore, curve fitting operation is applied to existing RE values to obtain a mathematical function expressing in the range we are working on. Thus, the distance parameter of the data can be estimated via pmf by applying some kind of reverse operation.

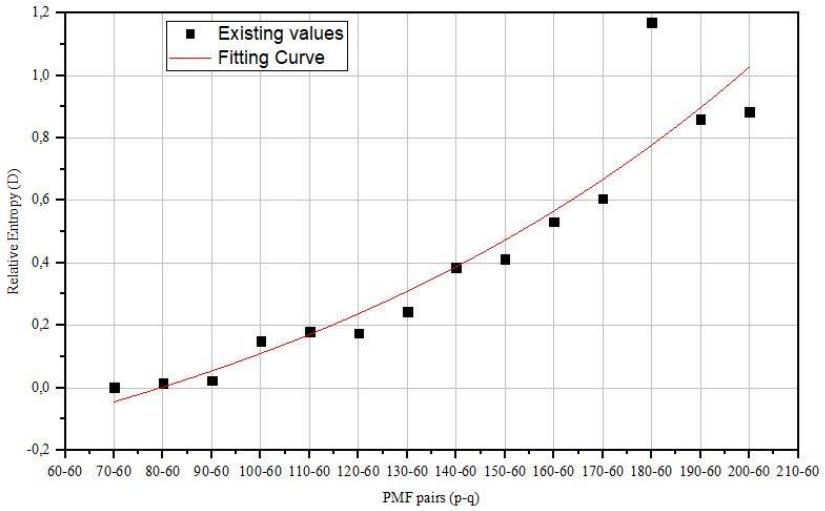

Figure 3.23 Curve fitting of the relative entropy results

The resulting curve fitting function that is given in the Figure 3.23 has an independent variable x and a dependent variable y, it has also constant parameters such as y_0, A and k. The numerical values of the parameters are given in the Table 3.2.

The curve fitting process is performed by using Levenberg Marquardt Iteration algorithm. The curve fitting equation model and its related stastistics are represented below.

$$y = y_0 + A.e^{x/k} \tag{20}$$

Table 3.2 Fit results for relative entropy

Parameters	Value	Standart Error	Dependency
y_0	-0,43613	0,71821	0,99751
A	0,35817	0,62928	0,99927
k	99,0563	87,40521	0,9973

In the equation (20), the x refers to the distance difference according to the reference distance. The equation (20) is arranged to leave the x parameter alone on the right side of the equation as follows.

$$k * \ln\left(\frac{y-y_0}{A}\right) = x \tag{21}$$

The relative entropy values which are obtained from experiments are placed into the place of y in the equation (21).

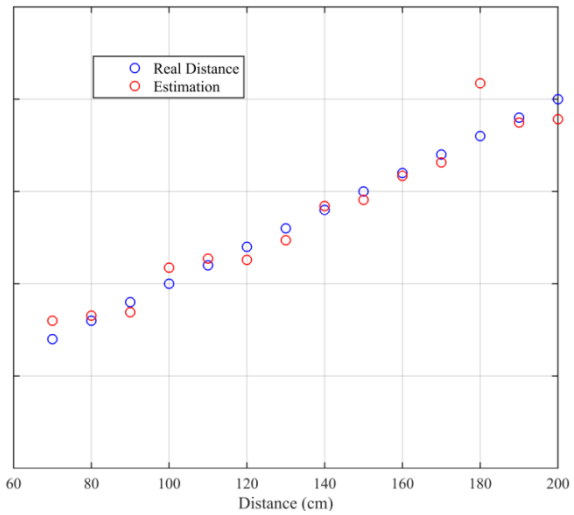

Figure 3.24 Estimation results of Relative Entropy Method

The estimation results of the RE-based distance estimation are given in the Figure 3.24. The estimation results have an error rate which varies between 1% and 16% values. The reasons of error rates can be basically explained in two ways. One of them is the deviations caused by the curve fitting operation. The second reason can be specified as

the value of the range that is defined in the step of creating pmf. The RE based method does not require to use the diffusion constant as in the correlation method since the RE method uses statistical similarity approach between the experimental results. The process of the RE method are summarized in the Figure 3.25.

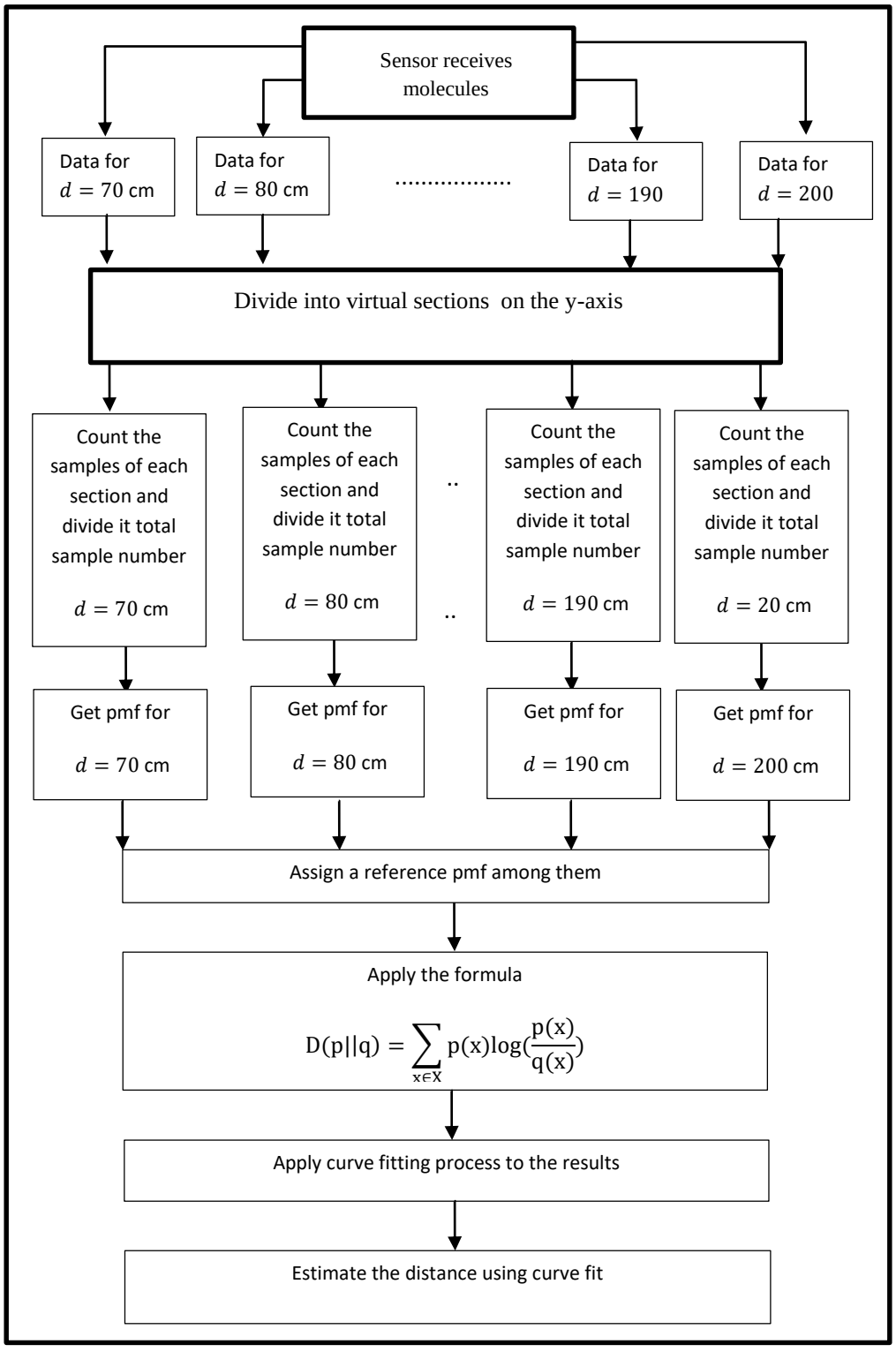

Figure 3.25 Flowchart of relative entropy based method

CHAPTER 4

COMPARISON OF METHODS

In this thesis, three different distance estimation methods are proposed. The performance evaluations of all methods rely on the accuracy of the distance estimation through the estimation error. The proposed methods that are the peak time, correlation based and relative entropy based are compared in terms of their average percentage errors. The experimental results mainly show that the proposed methods present a close performance to each other. Firstly, the performance analysis of each proposed method is interpreted for all distances. Then, the performance analysis of proposed methods is then examined and compared with each other for each distance. Besides, the proposed methods are compared with each other in terms of computational complexity. Peak estimation method performs poorly up to 60 cm with error rates higher than 13%. However, it performs very well with the maximum error rate 10% in the range of 60 to 200 cm. The reason of difference at the error rate can be explained by the initial drift effect since the initial drift shifts the peak concentration. In the correlation method, the maximum error rate is observed as 16% up to 120 cm. It seems that correlation based method has poor performance as distance between the Tx and the Rx increases. Relative entropy method performs well specifically in the range of 110 to 200 cm. The error rates of RE vary between 1% and %16. The high error rates can be explained by curve fitting process.

The proposed methods are compared according to the their error rates for each distance. The best performance is obtained by correlation method to estimate distance between the Tx and Rx up to 50 cm. When the distance between the Tx and Rx is increased to 60 cm and above, it seems that the peak-based and relative entropy based methods provide the close and successful performance. In addition, the performance of correlation method is very close to the peak estimation method at 70 cm and 110 cm and even performs better at 200 cm.

The RE method has satisfactory performance when compared to other proposed methods in the range from 110 cm to 200 cm. Besides, the RE method does not need to know the value of the diffusion coefficient. Therefore, we might say that it is more easy to implement in comparison with the other methods. The estimated distance and the values of the aforementioned error values can be seen in detail in Table 4.1.

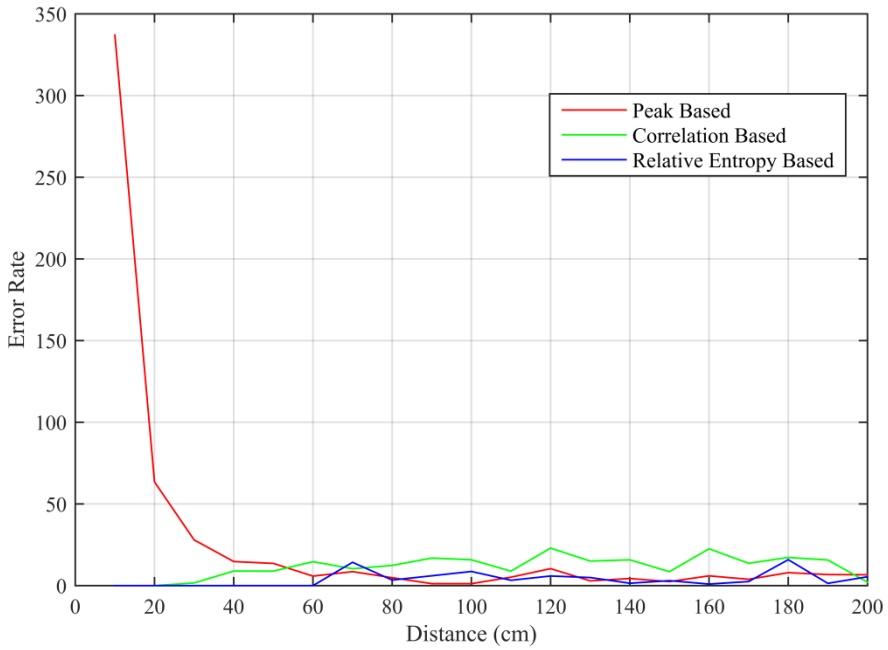

Figure 4.1 The error rates of corresponding methods

Table 4.1 Error results of proposed methods

Real Distance (cm)	Peak Estimation (cm)	Error of the Peak Estimation	Correlation Based Estimation (cm)	Error of the Correlation Based	Relative Entropy Estimation (cm)	Error of the Relative Entropy
10	43,7	%337	*	*	*	*
20	32,7	%63.5	*	*	*	*
30	38,4	%28	30,5	%1,66	*	*
40	45,9	%14.75	36.43	%8.92	*	*
50	56,8	%13.6	45.56	%8.88	*	*

Table 4.1 Error results of proposed methods (cont.)

60	63,5	%5.83	51.52	%14.66	*	*
70	76,0	%8.57	62.75	%10.35	80	%14.28
80	83,9	%4.87	70.09	%12.38	82,74	%3.42
90	88,9	%1.22	74.82	%16.86	84,57	%6.03
100	98,8	%1.2	84.16	%15.84	108,67	%8.67
110	115,7	%5.18	100.24	%8.87	113,62	%3.29
120	107,5	%10.41	92.43	%22.97	112,92	%5.9
130	126,2	%2.92	110.47	%15.02	123,56	%4.95
140	133,9	%4.35	117.87	%15.80	142,08	%1.48
150	153,7	%2.46	137.17	%8.55	145,43	%3.04
160	150,4	%6	123.95	%22.53	158,44	%0.97
170	163,4	%3.88	146.74	%13.68	165,74	%2.5
180	165,7	%7.94	148.96	%17.24	208,61	%15.89
190	177,1	%6.78	160.18	%15.69	187,34	%1.4
200	213,3	%6.65	195.8	%2.1	189,13	%5.43

Note that, the star sign (*) indicates that there is no estimation for the signed values in the table since those distance values are either the values in which the sensor saturates or the reference distances.

CHAPTER 5

CONCLUSION AND FUTURE WORKS

5.1. Conclusion

In this thesis, three DE methods and a procedure for the determination of the diffusion coefficient are introduced for a practical tabletop MC system. In addition, the performance analyses of the proposed methods are evaluated in terms of error rate. The distance between the Tx and the Rx is a crucial parameter in the definition of channel response. Besides, this study provides an opportunity to the researchers to implement new macro-scale MC applications.

Firstly, the peak concentration of the experimental data is examined to estimate distance. The main contribution of this metholodgy is to test and enhance the theoretically proposed peak estimation method with a practical macro scale MC system. Secondly, the correlation based method is presented to evaluate the experimental data according to one reference measurement. In other words, when a measurement at a random distance is carried out, its distance will be estimated by using the experimental data. Lastly, the relative entropy is examined and it is based on the same procedure as the correlation approach. Besides, the diffusion coefficient is calculated to define the characteristic of the propagation environment. Our proposed methods have ability to detect the system impulse response by estimating the distance parameter. The experimental results show that the error rates of all methods are reasonable values for a practical testbed.

Consequently, the proposed DE methods provide a reasonable performance in terms of the error rate. Besides, it can be concluded that macro scale tabletop MC system is a solution to experiment the desired applications with simple and cost efficient design.

5.2. Future Works

The DE methods can provide an enhanced communication mechanism between the Tx and the Rx. Moreover, the distance knowledge provides a basis to design a network. Our study can be extended in different ways to realize such a network. In addition, the number of the experiments can be increased to enhance the results. Furthermore, the proposed methods can be combined in one method to enhance accuracy.

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