# Distance Estimation in Concentration-Based Molecular Communications

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Abstract—The advance in nanotechnology has enabled the fabrication of nanomachines for health applications. Recently, molecular communication has become a promising communication paradigm that allows nanomachines to exchange information by using messenger molecules in fluid environments. To enable molecular communications, the knowledge of distance between nanomachines is critical since the distance affects both the performance and the efficiency of molecular communication. However, works on molecular communication either assume the distance is known or the distance estimation is based on the assumption of clock synchronization between nanomachines. In this paper, we propose novel methods for distance estimation using only one-way transmission and requiring no clock synchronization between nanomachines. The noise of diffusion channel due to random walk of molecules is investigated and methods to effectively improve the estimation accuracy are proposed.

Index Terms—Molecular communications, nanomachine, distance estimation, diffusion, Brownian motion.

## I. INTRODUCTION

The thriving nanotechnology enables the fabrication of nanomachines in a scale ranging from one to hundreds nanometers for health applications such as drug delivery and cancer treatment [1]–[3]. A nanomachine is a nanoscale device which has the ability to execute specific tasks such as sensing, signal processing, data storage, actuation and so on [4]. Owing to the limited power supply and computational capability of one single nanomachine, systems consisting of multiple nanomachines are designed to achieve more complex functionality [5]. As a consequence, communication between nanomachines plays an essential role [6].

Due to limitations of nanomachines such as antenna size and computational capability, existing technologies in electromagnetic communication are not feasible in nanonetworks. Several approaches for communicating at nanoscale have been proposed recently, and among these schemes, molecular communication is expected to be an effective and promising method for transporting information in nanonetworks formed by nanomachines [4], [7], [8]. In molecular communication, message molecules are used to encode, transmit, and receive information. Among different approaches in molecular communication, the diffusion-based method is a popular one in fluid medium [9]–[11]. The random moving of diffusing molecules in the fluid medium is the so-called Brownian

motion. Through the macro perspective, the collective motion of Brownian particles forms the variation of concentration which is governed by the Fick's law [12]. The information can then be embedded in the waveform of molecule concentration and transferred to the destination following the diffusion law [13].

Distance between nanomachines is one of the critical parameters in a diffusion process. Different distances between nanomachines cause different arrival probability of the message molecules at the receiver [14], significantly impacting the performance of the diffusion-based molecular communication. With the knowledge of the distance, a transmitter can adjust the number of transmitting molecules to achieve desired information rate. Therefore, the distance estimation should be a preparatory step for any diffusion-based molecular communication systems, and developing a mechanism to estimate the distance between two nanomachines is of great importance.

Existing works on distance estimation mainly adopt the round-trip approach [15], [16]: a nanomachine measures distance by comparing the signal it transmits and the feedback signal it receives from the target. Nevertheless, this approach is time consuming. We show in this paper that a nanomachine is able to obtain the distance information from the received signal alone, and thus not requiring a round-trip treatment. We call such methods the "one-way" approach in contrast to the round-trip one. Another issue of the existing distance estimation methods is the synchronization assumption. In traditional electromagnetic wave communications, the clock synchronization problem has been studied for decades and many solutions have been proposed, e.g., phase lock loops (PLL). It is thus reasonable to assume the transmitter and the receiver are synchronized. However, in the field of molecule communications, synchronization remains an open problem due to the complexity of achieving synchronization (if possible). Different from the existing distance estimation works in molecular communications, our approach does not require synchronization between nanomachines, and is thus more practical in realization.

The remainder of this paper is organized as follows. In Sec. II, we introduce the system model and the environment. Our proposed methods for distance estimation are presented in Sec. III. In Sec. IV, numerical results and the performance

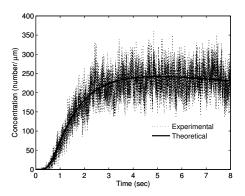


Fig. 1: Noise induced by random walk of diffusing molecules.  $N=10000,\ D=10\ \mu\mathrm{m}^2/\mathrm{sec},\ \Delta t=0.001\ \mathrm{sec},\ \mathrm{and}$  the concentration is measured at  $x=10\ \mu\mathrm{m}.$ 

evaluation of the proposed methods are discussed. Finally, conclusions are given in Sec. V.

### II. SYSTEM MODEL

In this section, we first elaborate the diffusion environment considered in this work. Then, we introduce an end-to-end model of nanomachines.

#### A. Environment

A one-dimensional (1-D), flow-free, diffusion channel is assumed. (Note that the proposed methods can be applied to a two- or three-dimensional environment as long as the environment is isotropic [17]). The expected concentration of diffusing molecules as a function of spatial coordinate x and time t is predicted by Fick's second law. In an unbounded 1-D space, the expected concentration satisfies the diffusion equation with some initial condition (I.C.) g(x):

$$\left\{ \begin{array}{l} \displaystyle \frac{\partial C(x,t)}{\partial t} = D \frac{\partial^2 C(x,t)}{\partial x^2}, & -\infty < x < \infty, 0 < t < \infty, \\ C(x,0) = g(x), & \text{I.C.,} \end{array} \right.$$

where D is the diffusion coefficient of the molecule in the environment. The impulse response of a diffusion channel

$$C^*(x,t) = \begin{cases} \frac{1}{\sqrt{4\pi Dt}} e^{\frac{-x^2}{4Dt}}, & t \in (0,\infty), \\ 0, & t = 0 \end{cases}$$
 (2)

is obtained by letting  $g(x) = \delta(x)^{-1}$  and solving the partial differential equation (1). If there are N molecules in an impulse spike, the concentration would be N times the impulse response, that is,

$$C(x,t) = NC^*(x,t). \tag{3}$$

The context above describes the behavior of a huge collection of diffusing molecules in terms of concentration. Nevertheless, on the microscopic level, the motion of a single diffusing

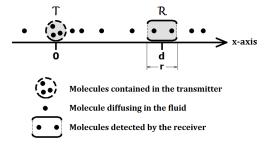


Fig. 2: 1-D diffusion-based system model

particle is described as Brownian motion, which can be modeled by a random walk in the form of successive random displacements [18]. The displacements are assumed to be independent, identically distributed Gaussian random variables with zero mean and variance  $\sqrt{2D\Delta t}$ , where  $\Delta t$  is the duration of an infinitesimal time step [19]. One can find that it is consistent to (2) by substituting  $\Delta t$  to t.

Let us see how the microscopic random walk affects the behavior of the macroscopic concentration. Fig. 1 illustrates the experimental results from a transmission of a spike signal in a diffusion channel. From this figure, we see that the random walk of molecules causes rapid variations in the concentration with respect to the theoretical expected value. In general, when dealing with a concentration-based problem, only the expected value is considered as the signal. As a result, we call such unwanted perturbation the noise induced by random walk in a diffusion channel.

### B. End-to-end Model

Let us now focus on the communication between a pair of nanomachines—a transmitter T, which releases information molecules into the environment, and a receiver R, which is responsible for measuring the concentration of molecules in the medium. In this paper, we model the transmitter as a point and the receiver a ball with diameter r. The coordinate is chosen such that the transmitter is located at the origin x=0 and the receiver lies in the positive axis. The distance between transmitter and receiver is defined to be the absolute distance of their center, denoted by d. Fig. 2 illustrates the system model.

At the beginning of a measurement t=0, the transmitter is set to release N molecules. These molecules propagate in the environment by diffusion as described in Sec. II-A. After the transmitter releases molecules, the receiver measures concentration over time in order to estimate d.

## III. DESIGN AND ANALYSIS

In this section, two methods for distance estimation are proposed, namely, peak concentration-based and the double spikes approach.

### A. Method I: Peak Concentration

According to (3), the concentration of molecules at the receiver is C(d,t). A typical curve of such function is shown

 $<sup>^{1}</sup>$ The notation  $\delta(x)$  is the Dirac delta function, which is zero everywhere except at the origin.

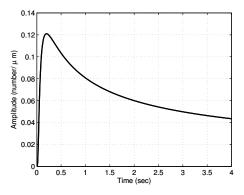


Fig. 3: Impulse response of 1-D diffusion channel

in Fig. 3 with  $D=10~\mu\text{m}^2/\text{sec}$  and  $d=2~\mu\text{m}$ . Since C(d,t) is a positive continuous function defined on  $[0,\infty)$  and tends to 0 as t goes to infinity, there must exist a global maximum of C(d,t) in  $[0,\infty)$ . Furthermore, the only solution of

$$\frac{\partial C(d,t)}{\partial t} = \left(\frac{-1}{2t} + \frac{d^2}{4Dt^2}\right) \frac{N}{\sqrt{4\pi Dt}} e^{\frac{-d^2}{4Dt}} = 0 \qquad (4)$$

is  $t=\frac{d^2}{2^D}$ . It follows that C(d,t) attains its maximum at  $t_p=\frac{d^2}{2^D}$  (the subscript p means peak). If the receiver is able to measure the concentration accurately, we can estimate d directly from the value of the peak concentration. By substituting  $t_p$  into (3), we obtain the value of the peak concentration

$$C_p := \sup_{t \in [0,\infty)} C(d,t) = C(d,t_p) = \frac{N}{d\sqrt{2\pi e}}, \quad (5)$$

where e is the natural exponential base. The distance d can then be estimated as

$$d = \frac{N}{C_p \sqrt{2\pi e}}. (6)$$

This method is termed *peak detection*. Note that the peak concentration is measured by the receiver directly, requiring no synchronization to the transmitter.

Although this peak detection method is simple, the performance is affected by the random walk described in Sec. II-A. From Fig. 1, we observe two properties of the noise resulting from random walk:

- the expected concentration is approximately the average of the upper and lower envelopes of the noisy received signal, and
- (ii) locally the number of time instants when the measured concentration is greater than the expected value approximately equals to the number of its counterpart.

The second observation can be explained in a macro point of view. The noise is regarded as a perturbation in the concentration. A positive perturbation causes the second derivative of concentration in the spatial coordinate to be more negative than in the unperturbed case. Therefore, the concentration would

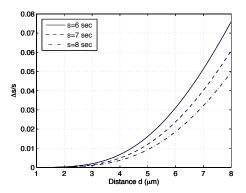


Fig. 4: Relation between  $\Delta s/s$  and d

drop more rapidly than expected, which may cause a negative perturbation at the next time instant.

In order to reduce the effect of noise at the receiver and improve the accuracy in distance estimation, three improvements are proposed. Suggested by observation (i), the first method is envelope detection. The receiver detects the upper and lower envelopes of the received signal, and then takes the average of them. The second method, resulted from observation (ii) as well as the continuity of C(d,t), is named moving average, which calculates the mean of the data points in a sampling window. The third method, named weighted moving average, gives different weights to each data point in a sampling window. To obtain information of the concentration at time t from the locally measured concentrations in a sampling window, we use least-squared method to approximate the slope of the cumulative measured concentration curve. This is simply implemented by assigning specific weights to the data points in a sampling window. In our numerical results, the window size is chosen to be 5, and the weights are chosen as:

$$\hat{C}_t = \frac{1}{35} (5C_{t-2\Delta t} + 8C_{t-\Delta t} + 9C_t + 8C_{t+\Delta t} + 5C_{t+2\Delta t}).$$
 (7)

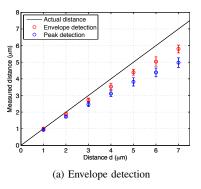
## B. Method II: Double Spikes

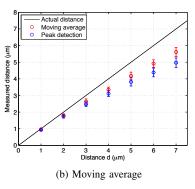
A noticeable characteristic of the waveform of impulse response is that the curve is always positive but tends to zero as t goes to infinity (see Fig. 3). We call such waveform having a residual tail. In most cases of concentration-based molecular communication, the residual tail is undesirable since it is the leading factor of inter-symbol interference [20]. However, if we allow the transmitter T to transmit n > 1 spikes during the same measurement, the residual tail of the impulse response of diffusion channel can be exploited for distance estimation. In this work, we consider the case n = 2.

Let s denote the duration of the time interval between the spikes that T releases. Then the initial condition in (1) becomes  $N(\delta(x) + \delta(x-s))$  and the solution is given by

$$\tilde{C}(x,t) = \begin{cases} C(x,t), & 0 < t < s, \\ C(x,t) + C(x,t-s), & s < t < \infty. \end{cases}$$
 (8)

By solving  $\partial \tilde{C}(d,t)/\partial t = 0$ , we look for two distinct solutions





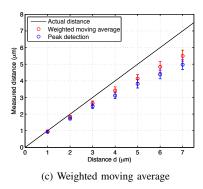


Fig. 5: Performance of the peak concentration-based methods

 $t_{p_1}$  and  $t_{p_2}$ . This happens when  $s > t_p$ . To estimate the distance, we are interested in the difference  $s' \coloneqq |t_{p_1} - t_{p_2}|$ . Due to the existence of the residual tail of the impulse response, by (8) we see that  $t_p = t_{p_1} < t_{p_2} < 2t_p$ . Intuitively, the residual tail pulls the second peak closer to the first. In fact, fixing s and D, the difference  $\Delta s \coloneqq s - s'$  is a bijective function of d. Fig. 4 illustrates the relation between  $\Delta s/s$  and d with s = 6, 7, and 8 seconds. Note that the time difference can be measured by the receiver directly, without requiring the synchronization between nanomachines.

As shown in Fig. 4, a larger s means the two peaks are more separated from each other such that the second peak is less influenced by the residual tail. On the other hand, a larger d implies a slower decay in the residual tail, thus pulling the peaks much closer. In practical realization, s is predetermined and known by the receiver. The receiver detects  $\Delta s$  and estimates d by referring to the curve of d- $\Delta s/s$ , which is known by the receiver in advance.

#### IV. PERFORMANCE EVALUATION

In this section, we demonstrate the performance of the proposed distance estimation methods via Monte Carlo simulations.

## A. Parameter Setting

The diameter r of the receiver is set to be  $0.2~\mu\mathrm{m}$ . Each signal spike the transmitter releases contains N=10000 molecules. Molecules perform random walk with a diffusion coefficient of  $D=10~\mu\mathrm{m}^2/\mathrm{sec}$  (roughly the scenario of a protein in the water). The time step  $\Delta t$  is  $0.001~\mathrm{sec}$ . The concentration at the receiver at a time instant is calculated by dividing the number of molecules in the interval  $\left[d-\frac{r}{2},d+\frac{r}{2}\right]$  by r.

Simulated distance d between the transmitter and the receiver ranges from 1 to 7  $\mu$ m, about tens times of the diameter of the receiver. Total simulation time of a single experiment is 15 seconds (15000 time steps).

### B. Numerical Results

Fig. 5 presents the statistics of the performance of peak detection (using (6) directly), envelope detection, moving

average, and weighted moving average. Each point represents the averaged result over 100 simulations with a confidence interval  $[\mu - 2\sigma, \mu + 2\sigma]$ , where  $\mu$  represents the mean, and  $\sigma$  represents the standard deviation. We see that the estimated distance is always less than the true value. This is because the maximum value detected from the noisy signal is always greater than the expected value. The error (the difference between the estimated distance and the actual distance) and the standard deviation become larger when the receiver becomes farther away from the transmitter. The reason is that when d is large, the curve C(d,t) changes more gently and thus the variation in actual concentration induced by random walk becomes relatively severe. The proposed envelope detection, moving average, and weighted moving average methods all improve the estimation precision of simple peak detection. Among these three methods, envelop detection performs best, followed by moving average, although the weighted moving average has smaller variance.

The performance of the double spikes method is shown in Fig. 6. Envelope detection is employed since it performs best in the peak concentration method. Unlike the results from the peak concentration method, Fig. 6 shows that the double spikes method results in positive mean error and the farther the receiver is, the more accurate the estimation would be. It can be explained through Fig. 4 that  $\Delta s/s$  becomes smaller with smaller d. Therefore, a smaller error of  $\Delta s/s$  contributes to a larger error of estimated distance when the actual distance is smaller. Nevertheless, as discussed in Sec. III-B, there is an upper limit of the allowed value of d for one to use the double spikes method to estimate distance with a designed s. Therefore, to assure that the double spikes method is applicable, a larger s has to be used.

## C. Comparison of Proposed Approaches

We compare both the peak concentration and double spikes methods by their accuracy, precision, and time delay.

For distance ranging from 1 to 7  $\mu$ m, the method of peak concentration is of better accuracy for measuring smaller distance while the double spikes method gets better when the distance is larger. This is because the influence of variation on

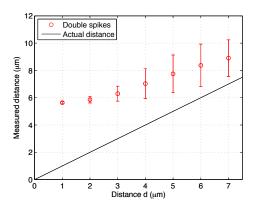


Fig. 6: Performance of the double spikes method

the curve C(d,t) is positively related to the distance, which results in larger error resulted from the larger distance in the peak concentration method. On the contrary, the influence of error of  $\Delta s/s$  is negatively related with the distance, which affects accuracy more when estimating smaller distance. As to the precision, for distance ranging from 1 to 7  $\mu$ m, the peak concentration method has better precision than the double spikes method. Now let us discuss the time delay. Since in the peak concentration method the receiver only detects the peak concentration, the transmission time is about  $t_p$  seconds. Analysis in Sec. III-B points out that the theoretical transmission time for the double spikes method is about 2s seconds. In other words, the peak concentration method has shorter delay.

Besides the comparison mentioned above, it is worth noticing that the double spikes method can be extended to the scenario that multiple data points are obtained in a single transmission. For example, the transmitter may be allowed to transmit multiple signal spikes spaced by the same time period. The advantage of this approach is the saving of time: the receiver is able to estimate the distance in a single transmission. As to the peak concentration method, one possible extension is using a receiver with multiple detectors. That is, after a spike is transmitted, each detector uses the peak concentration method to estimate the distance. The distance between any pairs of detectors is known and the distance is not affected by the channel effect. With the known distances, the number of detections can thus be lowered down.

## V. CONCLUSIONS

In this work, we investigate the peak concentration and double spikes approaches to estimate distance via one-way molecular communication in a 1-D diffusion-based channel. The impractical requirement of clock synchronization is avoided in our proposal. We find that the noise effect induced by random walk of molecules has great impact on the distance estimation, and the methods of envelope detection, moving average, and weighted moving average have been proposed to circumvent this problem. Monte Carlo simulations confirm the effectiveness of the proposed methods.

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