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# Parameter Estimation of Diffusive Molecular Communication With Drift

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**ABSTRACT** Molecular communication is a novel communication paradigm, which has prospective potential applications in many fields. Obtaining knowledge of the diffusive molecular channel is important for the design of the molecular communication systems as well as proper working of many application systems. In this paper, we focus on a kind of molecular communication system with flow drift, which is modeled as an inverse Gaussian distributed channel. The maximum likelihood estimation method is applied to obtain the estimator of parameters such as medium velocity, propagation distance, and diffusion coefficient. This paper also derives the closed-form expressions of the Cramer-Rao lower bounds. The performances of our channel parameter estimators are validated in MATLAB and the results confirm its effectiveness.

**INDEX TERMS** Molecular communication, drift, channel parameter estimation, maximum likelihood estimation, Cramer Rao lower bound.

## I. INTRODUCTION

Molecular communication is envisioned to realize information transmission between nanomachines at the micro- to nano- scale [2], [3]. In molecular communication, the information can be modulated by the properties of molecules. The transmitter nanomachine releases these signal molecules and they spread in the diffusive medium before finally reaching the receiver. The receiver recovers the original information based on the received or sensed signal molecules [4]. Molecular communication can achieve a variety of promising applications, such as the drug delivery system in the field of biomedicine [5], advanced manufacturing, environmental monitoring [6], and complex heterogeneous networks [7].

Molecular communication can be simply divided into free diffusion and flow assisted diffusion: 1) *Free diffusion*. In the free diffusion channel, information molecules move randomly driven by Brownian motion. From a macroscopic perspective, the molecules propagate from regions of high concentration to regions of low concentration [8]–[10]. 2) *Flow Assisted diffusion*. The molecule propagation is based on flow drift [11]–[14]. The information-bearing molecules propagate by Brownian motion to the receiver nanomachine at the flow velocity in the fluid medium.

Studies about channel parameter estimation for molecular communication systems have been investigated in the literature [15]–[21]. In terms of distance estimation, there are usually two categories of schemes: A) one-way message exchange. In the case of implementing this information exchange method, the receiver nanomachine estimates the distance by observing and analyzing the releasing molecules. B) two-way message exchange. While in this scheme, the transmitter estimates the distance using the feedback which is sent by the receiver nanomachine. In [15], the round-trip time was obtained by applying the two-way message exchange scheme. Furthermore, the propagation delay was determined, which indicates the transmission time of information molecules takes to the destination node. When the concentration modulation is implemented, the relationship between the propagation delay and the distance can be determined. So the distance can be estimated by calculating the transmission time. In [16] for example, the receiver determines the propagation time by detecting the concentration peak and calculates the distance in such modulation mode. In [17], the authors used a similar system model as in [16], whereas the distance between the transmitter and the receiver

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is calculated by using the peak molecular concentration at the receiver side. Further, as the dominant factor of ISI at the receiver, the residual tail of the concentration can also be utilized as another method for distance estimation. In other words, one can analyze the time interval between two consecutive peaks received by the receiver to estimate the distance. Neither of these distance estimation methods requires the synchronization between the transmitting and receiving nodes. In [18], the maximum likelihood estimation method was used to determine channel parameters. In fact, more than one channel parameters are jointly estimated in [18] at the receiver side, such as the releasing time of molecules, the number of released molecules, the diffusion coefficient, etc.. In [21], the blood viscosity is estimated as a channel parameter using molecular communication system. It is based on the release of a burst of small molecules in the blood stream, and subsequent measurement of their downstream absorption by the vessel wall.

In this paper we focus on the estimation of the channel parameter in a flow assisted channel. The inverse Gaussian channel is a channel with positive drift in which an individual molecule moves by Brownian motion. The time duration for a single molecule by Brownian motion to reach a fixed positive level in a positive drift can be considered as the inverse Gaussian random variable. Blood vessels can be approximated as examples of inverse Gaussian channels [11]–[14]. In this paper, the channel parameters we focused on include the distance from the transmitter nanomachines to the receiver nanomachines, the diffusion coefficient of the medium, and the fluid flow velocity. Obtaining knowledge of these parameters is important for the design of molecular communication systems as well as practical applications in the nano biomedical field. The main contributions of this paper are as follows:

1) Based on the inverse Gaussian molecular communication channel, the parameters including diffusion coefficient, propagation distance, and drift velocity are estimated by different maximum likelihood estimation methods. The closed-form estimators are derived.

2) The special case that all the channel parameters are unknown is analyzed and discussed.

3) The Cramer-Rao lower bound is derived for evaluation.

The organization of the rest of the paper is as follows. In Section II, the system model is presented. In section III, the maximum likelihood estimation for the channel parameters of the inverse Gaussian channel is described in detail. The simulation results are described in Section V. Finally, Section VI draws the conclusion.

## II. SYSTEM MODEL

### A. THE PHYSICAL DESCRIPTION

Molecular communication is a bio-inspired method for establishing communication from a transmitter nanomachine to a receiver nanomachine over fluidic environments using molecules as the information carriers (Fig. 1). The entire communication process can be divided into three steps: a transmission process, a propagation process, and a receiving process. The one-way message exchange is a propagation mechanism that information molecules diffuse in a single direction from the transmitter nanomachine to the receiver nanomachine in a molecular communication system. In a one-way message exchange, there are five processes: modulation, transmission, propagation, reception, and demodulation.

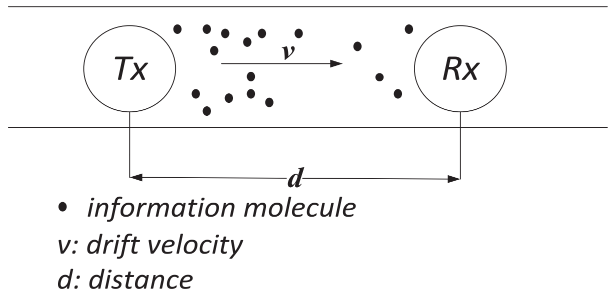


FIGURE 1. Flow assisted diffusive communication model.

Modulation is the process of conveying message or information based on biological molecules. The transmitter nanomachine translates information source into molecules that the receiver nanomachine can detect. Information can be modulated based on the type of molecules [17], the structure of molecules [22], the concentration of molecules [23], the concentration rate of molecules [24], the releasing time of molecules [25] and the sequence of molecules. In this paper, we assume that each molecule can carry multiple bits, such as n-ary MoSK [26].

Transmission is the process that a transmitter nanomachine releases information molecules into the environment. When the transmitter nanomachine senses an information source, it opens a gate that allows the information molecules to diffusive into the channel. It sends a specific number of messenger molecules at the beginning of a symbol and waits for the next release of molecules until the inter-symbol interference (ISI) becomes less significant.

Propagation is a process that information-bearing particles move from the transmitter nanomachine to the receiver nanomachine in a diffusive channel. These messenger molecules randomly move following the Brownian motion random process without chemical reactions including generation and degradation spontaneously, and it has no influence on other information molecules other than elastic collision [27].

Reception is the process that receiver nodes capture information particles moving in a diffusive channel. One scheme for capturing them is to use the theory of ligand-receptor binding [34]. Another option to capture them is to have them enter into the receiver through channels (e.g., gap-junction channels) without using a receptor.

Demodulation is the process of decoding information molecules. Once the receiver nanomachine captures these molecules, it can decode the received molecules and then attain the transmitted information. Demodulation at the receiver node may cause multiple consequences. For example, they may produce new molecules at the receiver or produce another signal by sending other molecules. Here we do not discuss too much.

As the complexity of the molecular communication system including layered architecture [28], we just consider a point-to-point molecular communication system that the fluid medium is homogeneous [9], all the molecules are considered as mono-atomic with negligible spatial dimension [29]. No matter which process they are in among the transmission, propagation or reception, they have the same characteristics with regard to their shapes and sides. They have a very low speed and move based on Fick's law [30]. The transmitter and the receiver are assumed to be synchronized [31], [32].

### B. THE RANDOM DELAY MODEL

In one-way message exchange, there exist many unknown parameters including the medium velocity, the propagation distance and the diffusion coefficient we mentioned earlier. The propagation delay can be caused by Brownian motion since the propagation of molecules is affected by Brownian motion at a medium velocity. In [12], an inverse Gaussian distribution has been used to describe the propagation delay in the diffusive channel and the probability density function (PDF) $f(t;\mu,\lambda)$ is

$$f(t;\mu,\lambda)=\left(\frac{\lambda}{2\pi t^3}\right)^{\frac{1}{2}}\exp\left(\frac{-\lambda(t-\mu)^2}{2\mu^2 t}\right), \qquad (1)$$

where $\lambda$ denotes the shape parameter, $t$ denotes the propagation time between the transmitter and the receiver for the molecule, $\mu$ represents the mean of the propagation time.

Reference [13] shows that the parameter $\mu$ and $\lambda$ can be represented by communication channel parameters. Accordingly, the expressions of $\mu$ and $\lambda$ are written as

$$\mu=\frac{d}{v}, \qquad (2)$$

$$\lambda=\frac{d^2}{2D}, \qquad (3)$$

where $d$ is the propagation distance, $v$ represents the medium velocity and $D$ is the diffusion coefficient.

Whether diffusion or advection is dominant in the molecule propagation depends on the relationship of $\mu$ and $\lambda$. Similar to the discussions in [33] and [34], in this paper it can be considered that if $\mu$ is smaller than $\lambda$, then advection is dominant in the propagation. An extreme case can be that it is an advection only transport if $\mu$ is much smaller than $\lambda$. On the contrary, if $\mu$ is larger than $\lambda$, then diffusion is dominant in the propagation. An extreme case is when $v$ approaches zero, i.e., $\mu=\infty$, it is a diffusion only scenario.

Channel parameter estimation usually refers to estimating distance $d$, the diffusion coefficient $D$ and the velocity $v$. In our scenario, the transmitter sends $N$ messages totally. Once a message is going to be sent, the transmitter will record the current transmission time instant $T_{1,i}$, and then embed this value into the message to be sent. These information molecules traverse across the aqueous channel to the receiver nanomachines. On reaching the receiver, the arriving time $T_{2,i}$ is recorded. After $N$ information message exchanges, a set of samples $\left\{T_{1,i},T_{2,i}\right\}_{i=1}^{N}$ can be recorded, from which the channel parameters such as $d$, $v$, and $D$ can be estimated.

It should be noted that $\left\{T_{1,i},T_{2,i}\right\}_{i=1}^{N}$ are the whole observations used for channel parameter estimation, therefore, the precision and accuracy of acquiring these samples are very important and will influence the estimation accuracy. It is assumed that the molecule embedding and releasing time is ignored at the transmitter side [14]. It is also assumed that the time duration for which the receiver sensor senses the molecule arrival and records the corresponding time instant is ignored [18]. Based on these assumptions, the paper would focus on the influence of the random delay of the molecule, which is the result of Brownian motion and flow drift as shown in (1), on the estimation accuracy of the channel parameters.

## III. MAXIMUM LIKELIHOOD ESTIMATION

When the probability density function (PDF) of the random variables is known, we can implement maximum likelihood estimation (MLE) for any parameter estimation problem [35]. As the number of observations approaches infinity, that is, $N\rightarrow\infty$, the estimator can be considered unbiased. The channel parameters(i.e. $d$, $v$ and $D$)are estimated by implementing MLE. The observations are the set $\left\{T_{1,i},T_{2,i}\right\}_{i=1}^{N}$ mentioned in Section II. For the $i$th message exchange, the propagation time, $T_i$ is formulated as:

$$T_i=T_{2,i}-T_{1,i}, \qquad (4)$$

where $\{T_i\}_{i=1}^{N}$ is a set of inverse Gaussian variables random variables that can be characterized as i.i.d. variables with the parameters $\mu$ and $\lambda$.

Our objective is to estimate the channel parameters $d$, $v$, and $D$ based on the observations of the receiver. In this paper, two schemes will be implemented: A) directly estimate the parameters $d$, $v$, and $D$ with the MLE method, and B) estimate the parameters $\{\mu,\lambda\}$ by applying MLE. Then $d$, $v$, and $D$ are calculated by (2) and (3). Both of these two schemes are discussed below.

In Section II, we have described the diffusive channel which is modeled by the inverse Gaussian distribution. Substituting (2), (3) and (4) into (1), the PDF represented by $d$, $v$ and $D$ can be written as [12]

$$f(T_i;d,v,D)=\frac{d}{\left(4\pi D T_i{}^3\right)^{\frac{1}{2}}}\exp\left(\frac{-(vT_i-d)^2}{4DT_i}\right). \qquad (5)$$

For the observations $\{T_i\}_{i=1}^{N}$, we express the likelihood function as

$$\begin{aligned}L&\left(d,v,D;\{T_i\}_{i=1}^{N}\right)\\&=\prod_{i=1}^{N}f(T_i;d,v,D)\\&=\left(\frac{d^2}{4\pi D}\right)^{\frac{N}{2}}\prod_{i=1}^{N}T_i^{-\frac{3}{2}}\exp\left(-\frac{1}{4D}\sum_{i=1}^{N}\frac{(vT_i-d)^2}{T_i}\right)\end{aligned}$$

$$= \left(\frac{d^2}{4\pi D}\right)^{\frac{N}{2}} \prod_{i=1}^{N} T_i^{-\frac{3}{2}} \exp\left(-\frac{1}{4D}\sum_{i=1}^{N}\left(v^2 T_i - 2vd + \frac{d^2}{T_i}\right)\right), \tag{6}$$

where $\{T_i\}_{i=1}^{N}$ are the i.i.d. inverse Gaussian random variables. Taking the natural logarithm on both sides of the above equation, we have

$$\begin{aligned} \ln L(d, v, D) &= \frac{N}{2}\ln\left(\frac{d^2}{4\pi D}\right) - \frac{3}{2}\sum_{i=1}^{N}\ln T_i \\ &\quad - \frac{1}{4D}\sum_{i=1}^{N}\left(v^2 T_i - 2vd + \frac{d^2}{T_i}\right) \\ &= N\ln d - \frac{N}{2}\ln(4\pi D) - \frac{3}{2}\sum_{i=1}^{N}\ln T_i \\ &\quad - \frac{v^2}{4D}\sum_{i=1}^{N}(T_i) + \frac{Nvd}{2D} - \frac{d^2}{4D}\sum_{i=1}^{N}\left(\frac{1}{T_i}\right). \end{aligned} \tag{7}$$

MLE indicates that we can get the estimation of $\widehat{d}, \widehat{v}$ and $\widehat{D}$ by maximizing the log-likelihood function as

$$\left\{\widehat{d}, \widehat{v}, \widehat{D}\right\} = \arg\max_{d,v,D}\left[\ln L(d, v, D)\right]. \tag{8}$$

Taking the partial derivative of (7) with respect to parameters $d$, $v$, and $D$ respectively, we can get a group of equations for these parameters shown as below

$$\frac{\partial \ln L(d, v, D)}{\partial d} = \frac{N}{d} + \frac{Nv}{2D} - \frac{d}{2D}\sum_{i=1}^{N}\left(\frac{1}{T_i}\right), \tag{9}$$

$$\frac{\partial \ln L(d, v, D)}{\partial v} = -\frac{v}{2D}\sum_{i=1}^{N} T_i + \frac{Nd}{2D}, \tag{10}$$

$$\frac{\partial \ln L(d, v, D)}{\partial D} = -\frac{N}{2D} + \frac{v^2}{4D^2}\sum_{i=1}^{N} T_i - \frac{Nvd}{2D^2} + \frac{d^2}{4D^2}\sum_{i=1}^{N}\frac{1}{T_i}. \tag{11}$$

It is obvious that in the above formulas (9), (10) and (11) there are variables $d$, $v$, $D$ and observation set $\{T_i\}_{i=1}^{N}$. For different known conditions, we discuss several cases in the following.

### A. DIRECT ESTIMATION FOR THE PARAMETER d

#### 1) VELOCITY v AND DIFFUSION COEFFICIENT D ARE GIVEN, DISTANCE d IS THE QUANTITY TO BE ESTIMATED

The slope at the maximum point of (8) is zero. That is when $v$ and $D$ are known variables to the receiver, setting the result of (9) to zero can give us the estimated $\widehat{d}$. In order to ensure the reasonableness of the estimation, we add a constraint $d > 0$. Thus, the estimated $d$, denoted as $\widehat{d}_1$, is expressed as

$$\widehat{d}_1 = \frac{Nv + \sqrt{(Nv)^2 + 8ND\sum_{i=1}^{N}\left(\frac{1}{T_i}\right)}}{2\sum_{i=1}^{N}\left(\frac{1}{T_i}\right)}. \tag{12}$$

#### 2) GIVEN v, DISTANCE d AND DIFFUSION COEFFICIENT D ARE THE QUANTITIES TO BE ESTIMATED

If $v$ is given and the other two parameters ($d$ and $D$) are unknown, the two estimated parameters can be obtained by setting (9) and (11) to zero. In this subsection, we only estimate the distance. So only the distance $d$, denoted as $\widehat{d}_2$, is shown as

$$\hat{d}_2 = \frac{v\sum_{i=1}^{N} T_i}{N}. \tag{13}$$

#### 3) DIFFUSION COEFFICIENT D IS GIVEN, DISTANCE d AND VELOCITY v ARE QUANTITIES TO BE ESTIMATED

Assuming $D$ is given, and $v$ and $d$ are unknown. Equation (9) and (10) are set to zero. Then the estimated distance $d$, denoted as $\widehat{d}_3$, is expressed as

$$\hat{d}_3 = \sqrt{\frac{2ND\sum_{i=1}^{N} T_i}{\sum_{i=1}^{N} T_i \sum_{i=1}^{N}\frac{1}{T_i} - N^2}}. \tag{14}$$

In this part, we propose three different forms of the estimated $d = \{\widehat{d}_1, \widehat{d}_2, \widehat{d}_3\}$, which are shown in (12), (13) and (14). These expressions are suitable under different conditions.

### B. DIRECT ESTIMATION FOR THE PARAMETER v

#### 1) DISTANCE d AND DIFFUSION COEFFICIENT D ARE GIVEN, VELOCITY v IS THE QUANTITY TO BE ESTIMATED

Assuming that $d$ and $D$ are known by the receiver, we set the result of (10) to zero and then get the estimated velocity $\widehat{v}$. So the estimated $v$, denoted as $\widehat{v}_1$, can be written as

$$\widehat{v}_1 = \frac{Nd}{\sum_{i=1}^{N} T_i}. \tag{15}$$

#### 2) DISTANCE d IS GIVEN, v AND D ARE QUANTITIES TO BE ESTIMATED

If $d$ is given, $v$ and $D$ are unknown, the estimated medium velocity $v$ can be obtained by setting (10) and (11) to zero. Thus, the medium velocity $v$, denoted as $\widehat{v}_2$, can be formulated as

$$\widehat{v}_2 = \frac{Nd}{\sum_{i=1}^{N} T_i}. \tag{16}$$

#### 3) DIFFUSION COEFFICIENT $D$ IS KNOWN, VELOCITY $v$ AND DISTANCE $d$ ARE QUANTITIES TO BE ESTIMATED

Assuming $D$ is given, $d$ and $v$ are unknown, let the result of (9) and (10) to be zero. The estimated parameter medium velocity $v$, denoted as $\widehat{v}_3$, can be expressed as

$$\hat{v}_3 = \frac{N}{\sum_{i=1}^{N} T_i}\sqrt{\frac{2ND\sum_{i=1}^{N} T_i}{\sum_{i=1}^{N} T_i \sum_{i=1}^{N} \frac{1}{T_i} - N^2}}. \tag{17}$$

In this subsection, we have proposed three different forms of the estimated velocity $v = \{\widehat{v}_1, \widehat{v}_2, \widehat{v}_3\}$ in (15), (16) and (17). These expressions are used under different conditions.

### C. DIRECT ESTIMATION FOR THE PARAMETER D

#### 1) VELOCITY $v$ AND DISTANCE $d$ ARE GIVEN, DIFFUSION COEFFICIENT $D$ IS THE QUANTITY TO BE ESTIMATED

Assuming that for the receiver nanomachine, $d$ and $v$ are given. let the result of (11) to be zero, then we can get the estimated $\widehat{D}$. The expression for estimated $D$, denoted as $\widehat{D}_1$, is as follows,

$$D_1 = \frac{v^2 \sum_{i=1}^{N} T_i - 2Nvd + d^2 \sum_{i=1}^{N} \frac{1}{T_i}}{2N}. \tag{18}$$

#### 2) DISTANCE $d$ IS GIVEN, DIFFUSION COEFFICIENT $D$ AND VELOCITY $v$ ARE QUANTITIES TO BE ESTIMATED

If $d$ is given, $D$ and $v$ are unknown, we set (11) and (10) to zero. The expression for the estimated $D$, denoted as $\widehat{D}_2$, is written as

$$D_2 = \frac{d^2\left(\sum_{i=1}^{N} T_i \sum_{i=1}^{N} \frac{1}{T_i} - N^2\right)}{2N\sum_{i=1}^{N} T_i}. \tag{19}$$

#### 3) VELOCITY $v$ IS GIVEN, DIFFUSION COEFFICIENT $D$ AND DISTANCE $d$ ARE QUANTITIES TO BE ESTIMATED

When $v$ is given, $D$ and $d$ are unknown, let (9) and (11) be zero. The estimated diffusion coefficient $D$, denoted as $\widehat{D}_3$, can be expressed as

$$\hat{D}_3 = \frac{v^2 \sum_{i=1}^{N} T_i \left[\sum_{i=1}^{N} (T_i) \sum_{i=1}^{N}\left(\frac{1}{T_i}\right) - N^2\right]}{2N^3}. \tag{20}$$

In this subsection, we have proposed three different forms of the estimated parameter $D = \{\widehat{D}_1, \widehat{D}_2, \widehat{D}_3\}$ in (18), (19) and (20). Also, these are used under different conditions.

### D. ESTIMATION FOR THE PARAMETERS VIA $\lambda$ AND $\mu$

We have mentioned earlier that except for estimating the parameters directly with the log-likelihood function, we can also use the estimated parameters $\mu$ and $\lambda$ to obtain the channel parameters indirectly. In section II, $\mu$ and $\lambda$ have been presented as the inverse Gaussian distribution parameters. The likelihood function just with these two parameters can be expressed as

$$\begin{aligned} L(\mu, \lambda) &= \prod_{i=1}^{N} f(T_i; \mu, \lambda) \\ &= \left(\frac{\lambda}{2\pi}\right)^{N/2} \prod_{i=1}^{N} (T_i)^{-\frac{3}{2}} \exp\left[-\frac{\lambda}{2\mu^2}\sum_{i=1}^{N}\frac{(T_i-\mu)^2}{T_i}\right]. \end{aligned} \tag{21}$$

Taking natural logarithms on both sides of the equation, (21) becomes

$$\ln L(\mu,\lambda) = N\ln\left(\frac{\lambda}{2\pi}\right) - \frac{3}{2}\sum_{i=1}^{N}\ln T_i - \frac{\lambda}{2\mu^2}\sum_{i=1}^{N}\frac{(T_i-\mu)^2}{T_i}. \tag{22}$$

Taking the partial derivative of this logarithm of the likelihood function with respect to parameters $\mu$ and $\lambda$. Then we can get the expressions as (23) and (24). Still use the assumption that the slope at the maximum point is zero to get the estimation results,

$$\frac{\partial \ln L(\mu,\lambda)}{\partial \mu} = \frac{\lambda}{\mu^3}\sum_{i=1}^{N}\frac{(T_i-\mu)^2}{T_i} + \frac{\lambda}{\mu^2}\sum_{i=1}^{N}\frac{(T_i-\mu)}{T_i}, \tag{23}$$

$$\frac{\partial \ln L(\mu,\lambda)}{\partial \lambda} = \frac{N}{2\lambda} - \frac{1}{2\mu^2}\sum_{i=1}^{N}\frac{(T_i-\mu)^2}{T_i}. \tag{24}$$

Setting the result of (23) and (24) to zero, the estimators for $\mu$ and $\lambda$, denoted as $\widehat{\mu}$ and $\widehat{\lambda}$ can be calculated as

$$\widehat{\mu} = \frac{1}{N}\sum_{i=1}^{N} T_i, \tag{25}$$

$$\widehat{\lambda} = \frac{N}{\sum_{i=1}^{N}\left(\frac{1}{T_i} - \frac{N}{\sum_{i=1}^{N} T_i}\right)}. \tag{26}$$

Combining (2), (3) and (25), (26), we can obtain the estimated channel parameters.

#### 1) VELOCITY $v$ IS GIVEN, DISTANCE $d$ AND DIFFUSION COEFFICIENT $D$ ARE QUANTITIES TO BE ESTIMATED

If $v$ is known and $d$ and $D$ are unknown, then we estimate the parameters $d$ and $D$, denoted as $\widehat{d}_4$ and $\widehat{D}_4$, as

$$\begin{cases} \hat{d}_4 = \dfrac{v\sum_{i=1}^{N} T_i}{N} \\ \hat{D}_4 = \dfrac{v^2\sum_{i=1}^{N} T_i\left[\sum_{i=1}^{N}(T_i)\sum_{i=1}^{N}\left(\frac{1}{T_i}\right) - N^2\right]}{2N^3}. \end{cases} \tag{27}$$

### 2) GIVEN THE DIFFUSION COEFFICIENT $D$, DISTANCE $d$ AND VELOCITY $v$ ARE QUANTITIES TO BE ESTIMATED

Under the condition that $D$ is known and $v$ is unknown, the estimated $d$ and $v$, denoted as $\widehat{d}_5$ and $\widehat{v}_5$, can be expressed as

$$\begin{cases} \hat{d}_5 = \sqrt{\dfrac{2ND\sum_{i=1}^{N} T_i}{\sum_{i=1}^{N} T_i \sum_{i=1}^{N} \frac{1}{T_i} - N^2}} \\ v_5 = \dfrac{N}{\sum_{i=1}^{N} T_i} \sqrt{\dfrac{2ND\sum_{i=1}^{N} T_i}{\sum_{i=1}^{N} T_i \sum_{i=1}^{N} \frac{1}{T_i} - N^2}}. \end{cases} \tag{28}$$

Comparing (13) with (14), (17) with (20), and (27) with (28), we can see that the estimated $\widehat{d}$, $\widehat{v}$ and $\widehat{D}$ based on these two schemes achieve the same results. So we can draw the conclusion that either the MLE method can solve the parameter estimation problem in this paper.

## IV. ANALYTICAL ANALYSIS OF ESTIMATION

If all the parameters of $D$, $d$, and $v$ are unknown, we set (9), (10) and (11) to zero. Then there are three unknown parameters and three equations. Theoretically, we can solve three equations for the three unknowns $D$, $d$ and $v$. Firstly, a system of equations is simplified. Secondly, we get a solution to the system which is a set of parameters for each unknown. These parameters together constitute a solution to each equation. However, based on (9) and (11), we can get a new equation that exists a linear problem with (10). The problem makes that the estimation has no single solution.

## V. CRAMER-RAO LOWER BOUND

In a parameter estimation problem, the Cramer-Rao lower bound (CRLB) [36], [37] determines a lower limit for any unbiased estimator of variance. It is a measure of the ability to estimate a parameter, this makes it a cornerstone of the statistical field. To ensure the effective estimator, the mean square error (MSE) can reach the CRLB on the condition of an unbiased estimator.

The CRLB of the estimated parameter can be computed by the inverse of the Fisher information. The Fisher information is a way of measuring the amount of information about the unknown parameter that is carried by the observable random variable, and it is widely used in optimal experimental design. We all know that the first derivative for the propagation distance $d$, the medium velocity $v$ and the diffusion coefficient $D$ are $\frac{\partial \ln L(d,v,D)}{\partial d}$, $\frac{\partial \ln L(d,v,D)}{\partial v}$ and $\frac{\partial \ln L(d,v,D)}{\partial D}$, respectively. Based on this first derivative, the second derivative for $d$, $v$ and $D$ can be expressed as

$$\frac{\partial^2 \ln L(d,v,D)}{\partial d^2} = -\frac{N}{d^2} - \frac{1}{2D}\sum_{i=1}^{N}\left(\frac{1}{T_i}\right), \tag{29}$$

$$\frac{\partial^2 \ln L(d,v,D)}{\partial v^2} = -\frac{1}{2D}\sum_{i=1}^{N} T_i, \tag{30}$$

$$\frac{\partial^2 \ln L(d,v,D)}{\partial D^2} = \frac{N}{2D^2} - \frac{v^2}{2D^3}\sum_{i=1}^{N} T_i + \frac{Nvd}{D^3} - \frac{d^2}{2D^3}\sum_{i=1}^{N}\frac{1}{T_i}. \tag{31}$$

The Fisher information can be expressed as

$$\begin{aligned} FIM\left(\widehat{d}\right) &= -E\left(\frac{\partial^2 \ln L(d,v,D)}{\partial d^2}\right) \\ &= E\left[\frac{N}{d^2} + \frac{1}{2D}\sum_{i=1}^{N}\left(\frac{1}{T_i}\right)\right] = \frac{N}{d^2} + \frac{1}{2D}\sum_{i=1}^{N} E\left(\frac{1}{T_i}\right), \end{aligned} \tag{32}$$

$$\begin{aligned} FIM\left(\widehat{v}\right) &= -E\left[\frac{\partial^2 \ln L(d,v,D)}{\partial v^2}\right] \\ &= E\left(\frac{1}{2D}\sum_{i=1}^{N} T_i\right) = \frac{1}{2D}\sum_{i=1}^{N} E(T_i), \end{aligned} \tag{33}$$

$$\begin{aligned} FIM\left(\widehat{D}\right) &= -E\left[\frac{\partial^2 \ln L(d,v,D)}{\partial D^2}\right] \\ &= -E\left(\frac{N}{2D^2} - \frac{v^2}{2D^3}\sum_{i=1}^{N} T_i + \frac{Nvd}{D^3} - \frac{d^2}{2D^3}\sum_{i=1}^{N}\frac{1}{T_i}\right) \\ &= -\frac{N}{2D^2} + \frac{v^2}{2D^3}\sum_{i=1}^{N} E(T_i) - \frac{Nvd}{D^3} + \frac{d^2}{2D^3}\sum_{i=1}^{N} E\left(\frac{1}{T_i}\right). \end{aligned} \tag{34}$$

For clarification, we use the property of expectation to simply $FIM\left(\widehat{d}\right)$, $FIM\left(\widehat{v}\right)$ and $FIM\left(\widehat{D}\right)$. Because of the random variable $T_i$ on the denominator, it is difficult to calculate the final result. Then we combine the definition of the expectation and the property of the expectation to derive $FIM\left(\widehat{d}\right)$, $FIM\left(\widehat{v}\right)$ and $FIM\left(\widehat{D}\right)$

$$\begin{aligned} FIM\left(\widehat{d}\right) &= \frac{N}{d^2} + \frac{1}{2D}\sum_{i=1}^{N} E\left(\frac{1}{T_i}\right) = \frac{N}{d^2} \\ &\quad + \frac{1}{2D}\sum_{i=1}^{N}\sum_{i=1}^{N}\left(\frac{1}{T_i} \times \frac{d}{\left(4\pi D T_i^{\,3}\right)^{\frac{1}{2}}}\exp\left(\frac{-(vT_i-d)^2}{4\pi T_i}\right) \times \Delta t_i\right), \end{aligned} \tag{35}$$

$$FIM\left(\widehat{v}\right) = \frac{1}{2D}\sum_{i=1}^{N} E(T_i) = \frac{Nd}{2Dv}, \tag{36}$$

$$FIM\left(\widehat{D}\right) = -\frac{N}{2D^2} + \frac{v^2}{2D^3}\sum_{i=1}^{N} E(T_i) - \frac{Nvd}{D^3} + \frac{d^2}{2D^3}\sum_{i=1}^{N} E\left(\frac{1}{T_i}\right)$$

**TABLE 1. Simulation parameters.**

| Parameters | Symbol | Values |
|---|---|---|
| distance | $d$ | 0.1 - 30 $\mu$m |
| medium velocity | $v$ | 1 - 20 $\mu$m/ms |
| diffusion coefficient | $D$ | 1 - 10 $\mu$m$^2$/ms |

$$= -\frac{N}{2D^2} + \frac{Nvd}{2D^3} - \frac{Nvd}{D^3} + \frac{d^2}{2D^3}\sum_{i=1}^{N}\sum_{i=1}^{N}\left(\frac{1}{T_i}\times\frac{d}{\left(4\pi D{T_i}^3\right)^{\frac{1}{2}}}\exp\left(\frac{-(vT_i-d)^2}{4\pi T_i}\right)\times\Delta t_i\right). \quad (37)$$

The CRLB for the estimators can be obtained by taking multiplicative inverse of the Fisher information matrix, and the variance is equal to or greater than the CRLB as

$$var\left(\widehat{d}\right) \geq \frac{1}{FIM\left(\widehat{d}\right)}, \quad (38)$$

$$var\left(\widehat{v}\right) \geq \frac{1}{FIM\left(\widehat{v}\right)}, \quad (39)$$

$$var\left(\widehat{D}\right) \geq \frac{1}{FIM\left(\widehat{D}\right)}. \quad (40)$$

## VI. SIMULATION RESULTS AND DISCUSSIONS

In this section, we present the numerical simulations and the performances of the proposed channel parameter estimators that are validated in MATLAB. For the simulation setup, We use a pseudo-random sequence that follows an inverse Gaussian distribution, to generate $T_i$. Based on [14] and [18], we choose the diffusion coefficient from 1 $\mu$m$^2$/ms to 10 $\mu$m$^2$/ms, and choose the propagation distance from 0.1 $\mu$m to 30 $\mu$m, which the molecules spread from the transmitter to the receiver. The velocity of the diffusive medium is chosen from [38] as 1 $\mu$m/ms to 20 $\mu$m/ms. The summary of the simulation parameters is shown in Table 1.

We set the number of simulation runs $M$ to 1000. Each point on the curves in these figures is an average of $M$ simulation runs. The accuracy is measured by the mean squared error (MSE) at each point. In the remainder of this section, we present and discuss the performance of our proposed estimators respect to different observation numbers with different pre-defined values.

In Fig. 2 we plot the MSE of the estimated distance respect to the number of observations. The distance is estimated from (13). We observe from Fig. 2 that regardless of the preset $\{v, D\}$ value, the MSE of the estimated distance $d$ decreases for the increasing number of observations $N$. It verifies the effectiveness of the proposed estimation schemes. Given $D$ with variable $v$, the MSE of the estimated distance decreases as $v$ increases. That is because a larger medium velocity can cause information molecules to move faster between the transmitter and the receiver. Thus, the effects of the Brownian motion have become less dominant. However, if $v$ is fixed and $D$ varies, there will be an opposite trend. Still observe Fig. 2 such as the curves with the same velocity $\{v = 10\,\mu\text{m/ms}\}$

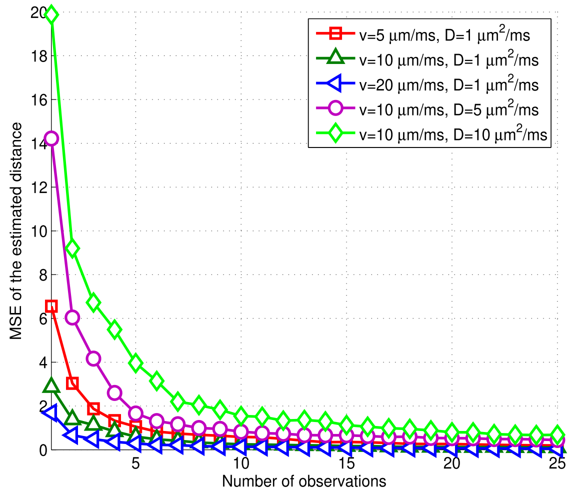


**FIGURE 2. Given *v* and *D*, the MSE of the estimated distance vs. the number of observations.**

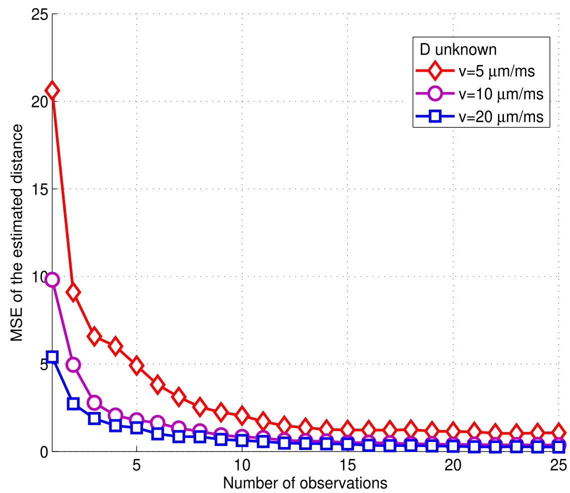


**FIGURE 3. Given different pre-defined medium velocity *v*, the MSE of the estimated distance vs. the number of observations.**

and different diffusion coefficient, it is obvious that when the coefficient $D$ increases, the MSEs of all these curves also increase. This is because the increase of the diffusion coefficient $D$ means that the molecules move more actively in the environment. More active molecular motion leads to more randomness, which is the reason that the estimator's performance deteriorates.

Fig. 3 shows the relationship between the MSE versus the estimated distance and different preset flow velocity of the diffusive medium. It reveals that as the observation number increases, the MSE of estimated $d$ decreases and finally tends to steady. The reason is obvious: the sample set of more observations will make the estimation more accurate. For all the curves in this figure, one can see that the curves with higher $v$ are below those with lower medium velocity, which has the same reason as we mentioned earlier. The larger flow velocity from the transmitter to the receiver reduces the effects of random motion.

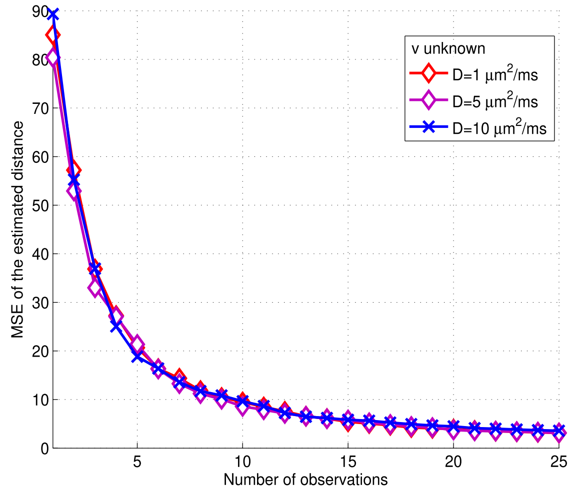


**FIGURE 4.** Given different pre-defined diffusive coefficient $D$, the MSE of the estimated distance vs. the number of observations.

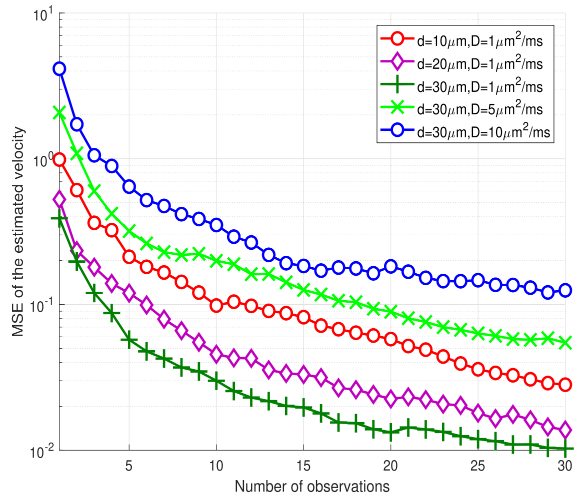


**FIGURE 6.** Given $d$ and $D$, the MSE of the estimated velocity vs. the number of observations.

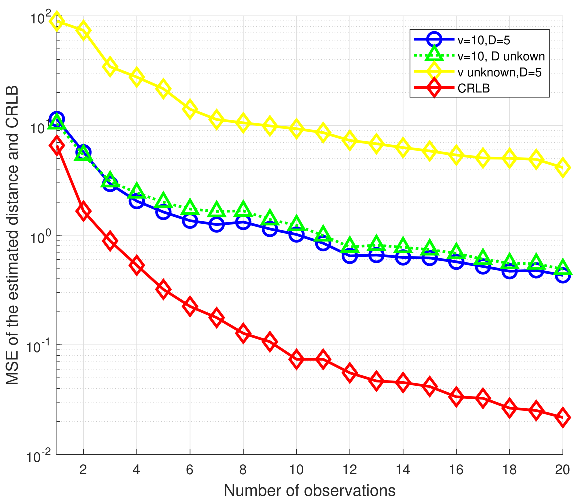


**FIGURE 5.** The comparison between the MSEs for the estimated distance under different pre-defined conditions and CRLB.

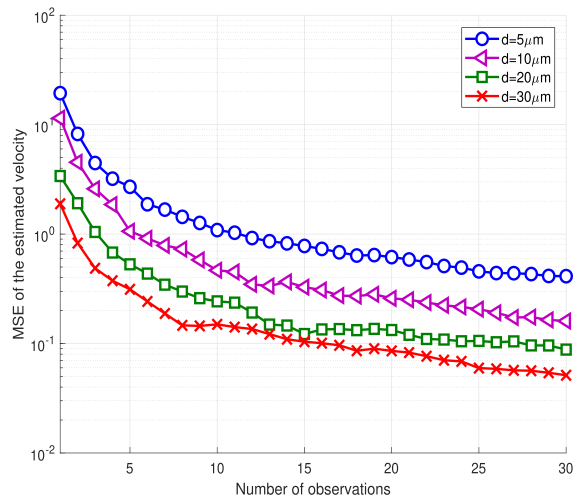


**FIGURE 7.** Given pre-defined distance $d$, the MSE of the estimated velocity vs. the number of observations.

In Fig. 4, the curves of the MSE of the estimated distance with different preset diffusion coefficient $D$ is plotted. The trend of the curve is the same as that shown in Fig. 2 and Fig. 3. The MSE of the estimated distance decreases with the number of observations increasing and eventually stabilizes. Also, comparing Fig. 4 and Fig. 2 we can find that if the velocity $v$ is unknown, the change of the diffusion coefficient has little effect on the accuracy of the estimation. Whereas in Fig. 2, if the flow velocity $v$ is known, the coefficient's influence is obvious.

Fig. 5 compares the MSEs of the estimated distance under different pre-defined conditions and CRLB. These conditions include$\{v = 10\,\mu\text{m/ms}, D = 5\,\mu\text{m}^2/\text{ms}\}$, $\{v = 10\,\mu\text{m/ms}, D$ unknown$\}$ and $\{v$ unknown, $D = 5\,\mu\text{m}^2/\text{ms}\}$. We observe from Fig. 5 that the MSEs of estimated distance decrease for increasing observations for all these conditions. Except for the curve under the condition $\{v$ unknown, $D = 5\,\mu\text{m}^2/\text{ms}\}$, the other three curves are almost the same. These three curves are all below the curve $\{v$ unknown, $D = 5\,\mu\text{m}^2/\text{ms}\}$. This reveals that the velocity $v$ has a greater impact on estimation accuracy than diffusive coefficient $D$. Furthermore, the CRLB for the estimator $d$ is also presented in this figure. All the three other curves are above the CRLB curve, which validates the effectiveness of our proposed estimator.

Fig. 6 and Fig. 7 focus on the estimation of the medium velocity. Similar to Fig. 2, the curves in Fig. 6 also decrease with the increasing of observation numbers. Furthermore, for a given distance $d$, the MSEs of the estimated value increase as $D$ becomes larger. For a given $D$, the MSE of the estimated velocity becomes smaller as the distance $d$ increases. So the curve with the longest distance and the smallest diffusion coefficient $\{d = 30\,\mu\text{m}, D = 1\,\mu\text{m}^2/\text{ms}\}$ is the lowest one. In the case of $D$ unknown, the MSE curves of the estimated velocity are depicted in Fig. 7. It is observed that the MSE has an obvious relationship with $d$, in more detail, it becomes smaller with the increase of the

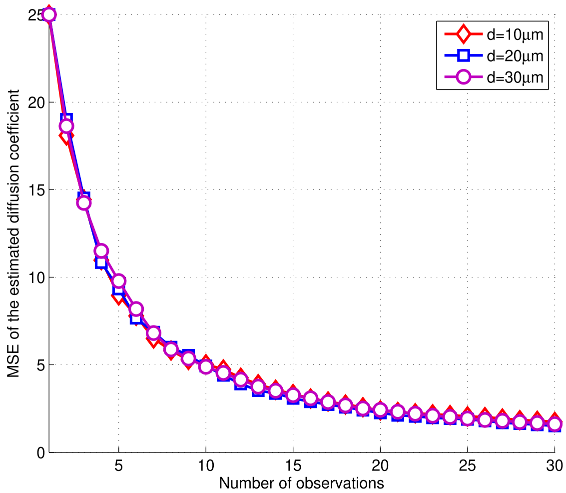


**FIGURE 8.** The MSE of the estimated diffusion coefficient vs. the number of observations with pre-defined distance $d$.

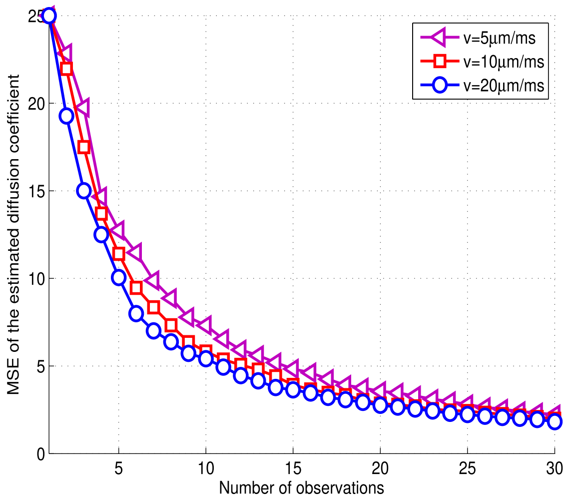


**FIGURE 9.** The MSE of the estimated diffusion coefficient vs. the number of observations with pre-defined medium velocity $v$.

distance $d$. The reason is like this: if the distance is smaller, then a random propagation delay would lead to severe estimation inaccuracy of the velocity. If the distance becomes larger, then the influence of random movement of the molecule would be alleviated, therefore the estimation of the velocity becomes more accurate.

Fig. 8 to Fig. 9 focus on the estimation of the diffusion coefficient. Fig. 8 is under the condition of given $d$, whereas Fig. 9 is under the condition of given $v$. In Fig. 8, we can see that when the velocity is unknown, the change in $d$ has little effect on the MSE. This is consistent with the conclusion of Fig. 4. In fact, Fig. 4 is drawn based on (14) and Fig. 8 is drawn based on (19). These two equations are actually the same, except that one represents $d$ by $D$ and the other one represents $D$ by d. In Fig. 9, when the distance is unknown, one can observe a trend that the MSE of the estimated diffusion coefficient decreases as the velocity increases. The conclusions in Fig. 9 and Fig. 3 are consistent.

## VII. CONCLUSION

In this paper, the channel parameter estimation for the molecular communication system with flow drift has been proposed. The propagation distance $d$, the diffusion coefficient $D$ and the medium velocity $v$ are estimated by using the single-directional molecular communication scheme. The MLE methods are used to estimate these parameters. The Cramer-Rao lower bound is derived. The simulation results demonstrate the effectiveness of our proposed estimator. The influence of different conditions to the estimation accuracy is analyzed. Future work would investigate more realistic model like three-dimensional environment and consider more practical situations by relaxing the assumptions about sampling times.

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