Parameter Estimation of Inverse Gaussian Channel for Diffusion-Based Molecular Communication

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***Abstract*—Molecular communication is a very promising research field. It has a broad range of prospective potential applications in biomedical engineering, material manufacturing, etc. Getting the knowledge of the diffusive molecular channel is important for the design and analysis of the molecular communication system. This paper investigates the channel parameter estimation based on a typical inverse Gaussian distributed channel. The estimator of propagation distance, medium velocity and diffusion coefficient are derived by maximum likelihood estimation method. The simulation results validate the effectiveness of the proposed estimators.**

***Index Terms*—Molecular communication, channel estimation, maximum likelihood estimation, inverse Gaussian distribution**

I. Introduction

Molecular communication is a novel communication paradigm for the transmissions of information between nano scale devices[1, 2]. The information is modulated by the properties of the molecular particles. The molecules released by the transmitter nanomahchine propagate in the aqueous medium and reach the receiver nanomachine. The receiver nanomachine receives and demodulates the molecules [3]. Molecular communication has a broad range of potential applications such as drug delivery in biomedicine [4, 5], advanced manufacturing, and environmental monitoring [6].

There exist several channel and propagation models for molecular communication in the literatures. 1) Free diffusion channel describes a scenario in which the released molecular particles move randomly as a Brownian motion in the environment [7-9]. It collides with other molecules in its vicinity. There is no external energy except thermal energy for this propagation scheme. 2) Flow assisted propagation is another propagation scheme [10-12]. The molecular particles propagate by a Brownian motion in the fluid medium with flow velocity towards the receiver nanomachine. It is a directed propagation. For example, the cells in the human body secrete hormone substances and they flow in the blood stream to the distant target cell [13]. 3) Molecular motor is a way of short-range molecular communication, which already exists in the biological cells [14, 15]. The information molecules are carried by the molecular motors and the motors move along the rails called microtubules to the destination. In this paper we focus on the flow assisted propagation model.

During the design and analysis of the molecular communication system, the parameters of the communication channel always need to be known by the nanomachine. For example, in [12], the nanomachine needs to know the medium velocity and the distance between the transmitter nanomachine and the receiver nanomachine, to calculate the proper symbol intervals. In an application of bloodstream monitoring using a network of nanomachines mentioned in [16], the nanomachines need to know the distance separating themselves so that they can be mounted at regular intervals. The propagation delay of the information molecules can be used for clock synchronization by the nanomachines [17]. Therefore, using the observed and received molecules at the receiver nanomachine to estimate the channel parameters is always necessary and needed.

There are a few research works which investigate the channel parameters of the diffusion-based molecular channel. For distance estimation, it can be divided into two categories: one-way message exchange and two-way message exchange. In the one-way message exchange scheme, the receiver nanomachine observes and analyzes the releasing molecules and estimates the distance, while in the two-way message exchange scheme, the receiver sends a feedback to the transmitter and the transmitter estimates the distance. In [18, 19], the authors use two-way message exchange to obtain the round-trip time and further the propagation delay of molecules from the transmitter to the receiver. In the concentration-based modulation, the relationship between the transmission time and the distance can be obtained. Using the calculated propagation delay, one can estimate the distance. Reference [20] also uses concentration-based modulation and the receiver detects the concentration peak to determine the propagation time of molecules and calculates the distance. In [21], a similar system model is adopted as in [20], but the authors use the peak concentration of the molecules at the receiver to calculate the distance between the transmitter and the receiver. Another method is to utilize the residual tail of the concentration at the receiver, which is just the leading factor of the inter-symbol interference. The distance can be estimated by analyzing the time interval of two consecutive spikes at the receiver side. Both of the distance estimation methods do not require the clock synchronization between the transmitter and the receiver. In [16], the authors

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use maximum likelihood estimation to estimate more than one channel parameter together, including the time that molecules are released, the number of molecules released, the distance, the diffusion coefficient, etc., at the receiver side based on arriving molecules with Poisson distribution.

In this paper, the channel parameter estimation in an inverse Gaussian distributed channel is studied. The channel in which a molecule move as a Brownian motion with a positive drift is considered to be an inverse Gaussian channel [11]. The inverse Gaussian random variable is used to model the time a Brownian motion with positive drift takes to reach a fixed positive level. An example of the inverse Gaussian channel is the blood vessel. We focus on the channel parameters including the distance between the transmitter and the receiver, the fluid flow velocity, and the diffusion coefficient of the medium. Obtaining the knowledge of these parameters is very useful in the practical applications. For example, the nanomachines in a nanonetwork for drug delivery in blood stream need to know the distance separating themselves so as to decide the amount of the released drug at each time. The fluid flow velocity in a blood stream can be used for analyzing the blood pressure. The diffusion coefficient can be used for determine the blood composition. To the best of the authors knowledge, there is no research work so far, which focus on parameter estimation based on the inverse Gaussian channel. The main contributions of this paper include:

1) Using a inverse Gaussian distribution to model a Brownian motion in a diffusive channel;

2) Using the maximum likelihood estimation to estimate the parameters such as the propagation distance, the drift velocity, and the diffusion coefficient in the molecular communication system.

The rest of this paper is organized as follows. Section II presents the system model. The maximum likelihood estimation method for the channel parameters in the inverse Gaussian channel is presented in Section III. Single channel parameter estimation and joint estimation of multiple channel parameters are discussed separately. Section V gives the simulation results and finally the conclusion is drawn in Section VI.

II. System Model

Molecular communication from a transmitter nanomancine to a receiver nanomanchine takes place in aqueous medium which uses chemical or biological molecules as the information carriers, shown as Fig. 1. The whole communication process includes the transmission process, the propagation process and the reception process, where a one-way message exchange is used. The term "one-way" means one-directional, which is defined in [16]. The transmitter nanomachine sends information molecules into the channel. *M*-ary digital modulation scheme, such as *M*-ary IMoSK proposed in [22], is assumed to be used, so that the information molecules can contain multiple-bit information, e.g., time instant in this paper. These information molecules propagate based on a Brownian motion in a 1-D diffusive channel with drift. It is assumed that the receiver nanomachine can successfully receive, absorb, and

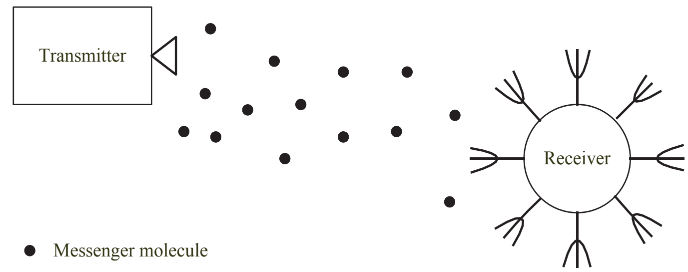

Fig. 1. Diffusive communication model with drift.

demodulate the information molecules. We also assume that all the information molecules have identical properties with respect to their shapes and sides no matter in the transmission process, propagation process, or reception process.

Because the molecular propagation is affected by the Brownian motion with medium velocity, a random propagation delay is incurred. The propagation delay in the diffusive channel with Brownian motion has been described by an inverse Gaussian distribution [11]. The probability density function (PDF) $f\left(t;\mu,\lambda\right)$ can be expressed as

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

where t is the propagation delay from the transmitter nanomachine to the receiver nanomachine. μ is the mean of t and λ is the shape parameter.

The relationship between the parameters $\{\mu,\ \lambda\}$ and the communication channel parameters have been presented in [12]. μ and λ can be expressed as

$$\mu=\frac{d}{v} \tag{2}$$

$$\lambda=\frac{d^{2}}{2D} \tag{3}$$

where d, v and D represent the propagation distance, the medium velocity and the diffusion coefficient, respectively.

The objective of the channel parameter estimation is to estimate d, v and D. For this purpose, we consider a one-way message exchange mechanism from the transmitter nanomachine to the receiver nanomachine. The transmitter nanomachine sends totally N messages. For each message, the transmitter nanomachine records its sending time instant $T_{1,i}$, and put this value into the message. After the propagation in the aqueous channel, the information molecules arrive at the receiver nanomachine. The receiver nanomachine records the arriving time $T_{2,i}$. It is assumed that the two nanomachines are perfectly synchronized. This assumption has been widely made in many literatures [8], [10], [11]. $\{T_{1,i},T_{2,i}\}_{i=1}^{N}$ will be used to estimate d, v and D.

III. Maximum Likelihood Estimation

Maximum likelihood estimation (MLE) can be implemented for any estimation problem where the PDF of the random variables is known [23]. As the number of observations increases, i.e., $n \to \infty$, the estimator becomes unbiased. Here we use MLE to estimate the channel parameters d, v and D. The observations are $\{T_{1,i}, T_{2,i}\}_{i=1}^{N}$. Because the transmitter nanomachine and the receiver nanomachine are assumed to be synchronized. the propagation delay of the ith message exchange, T_i, can be expressed as

$$T_i = T_{2,i} - T_{1,i} \tag{4}$$

where $\{T_i\}_{i=1}^{N}$ is modeled as independent and identical distributed (i.i.d) inverse Gaussian random variables with the parameters $\{\mu,\lambda\}$.

The goal is to estimate the parameters d, v and D based on a set of observations. There are two schemes: A) use the MLE to estimate the parameters d, v and D directly, and B) use the MLE to estimate the parameters $\{\mu, \lambda\}$ and then use (2) and (3) to calculate d, v and D. They are discussed below.

A. Direct Estimation for the Parameters d, v and D

The diffusive channel has been mentioned and described by the inverse Gaussian distribution in Section II. Putting (2), (3) and (4) into (1), we can obtain the PDF with the parameters d, v and D as following [12].

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

For the observations $\{T_i\}_{i=1}^{N}$, the likelihood function can be expressed as

$$\begin{aligned} &L\left(d, v, D; \{T_i\}_{i=1}^{N}\right) = \prod_{i=1}^{N} f\left(T_i; d, v, D\right) \\ &= \left(\tfrac{d^2}{4\pi D}\right)^{\frac{N}{2}} \prod_{i=1}^{N} T_i^{-\frac{3}{2}} \exp\left(-\tfrac{1}{4D}\sum_{i=1}^{N} \tfrac{\left(vT_i - d\right)^2}{T_i}\right) \\ &= \left(\tfrac{d^2}{4\pi D}\right)^{\frac{N}{2}} \prod_{i=1}^{N} T_i^{-\frac{3}{2}} \exp\left(-\tfrac{1}{4D}\sum_{i=1}^{N} \left(v^2 T_i - 2vd + \tfrac{d^2}{T_i}\right)\right) \end{aligned} \tag{6}$$

where $\{T_i\}_{i=1}^{N}$ follows the i.i.d. inverse Gaussian distribution. Taking natural logarithms on both sides, we can get

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

The estimated parameters $\widehat{d}$, $\widehat{v}$ and $\widehat{D}$ can be calculated by maximizing the logarithm of the likelihood function.

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

Based on (7) and (8), we take the partial derivative of the log-likelihood function with respect of d, v and D, respectively. A system of equations for d, v and D are shown as in (9), (10) and (11).

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

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

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

It is clear that (9), (10) and (11) include d, v, D and $\{T_i\}_{i=1}^{N}$. Several cases are discussed as follows.

1) d is unknown, v and D are known: If v and D are known by the receiver nanomachine, the estimated $\widehat{d}$ can be obtained by setting the result of (9) to zero. In order to guarantee the calculation reasonable, we give the condition $d > 0$. Then the estimated d, denoted as $\widehat{d_1}$, can be expressed as

$$\widehat{d_1} = \frac{Nv + \sqrt{\left(Nv\right)^2 + 8ND\sum\limits_{i=1}^{N}\left(\frac{1}{T_i}\right)}}{2\sum\limits_{i=1}^{N}\left(\frac{1}{T_i}\right)} \tag{12}$$

2) v is known, d and D are unknown: Assuming that v is known and d and D are unknown, we set (9) and (11) to zero. The two estimated d and D, denoted as $\widehat{d_2}$ and $\widehat{D}_2$ respectively, can be expressed as

$$\begin{cases} \widehat{d_2} = \dfrac{v\sum\limits_{i=1}^{N} T_i}{N} \\ \widehat{D}_2 = \dfrac{v^2\sum\limits_{i=1}^{N} T_i\left[\sum\limits_{i=1}^{N}\left(T_i\right)\sum\limits_{i=1}^{N}\left(\frac{1}{T_i}\right) - N^2\right]}{2N^3} \end{cases} \tag{13}$$

3) D is known, d and v are unknown: If D is known and d and v are unknown, we set (9) and (10) to zero. The two estimated d and v, denoted as $\widehat{d}_3$ and $\widehat{v}_3$, can be expressed as

$$\begin{cases} \widehat{d}_3 = \sqrt{\dfrac{2ND\sum\limits_{i=1}^{N} T_i}{\sum\limits_{i=1}^{N} T_i\sum\limits_{i=1}^{N}\frac{1}{T_i} - N^2}} \\ \widehat{v}_3 = \dfrac{N}{\sum\limits_{i=1}^{N} T_i}\sqrt{\dfrac{2ND\sum\limits_{i=1}^{N} T_i}{\sum\limits_{i=1}^{N} T_i\sum\limits_{i=1}^{N}\frac{1}{T_i} - N^2}} \end{cases} \tag{14}$$

From (12), (13) and (14), we can see that the estimated $d = \{\widehat{d_1}, \widehat{d_2}, \widehat{d_3}\}$ have different forms under different conditions. They can be used for different situations.

B. Estimation for the Parameters via μ and λ

The inverse Gaussian distribution including μ and λ has been presented in Section II. The likelihood function without d, v and D can be expressed as

$$\begin{aligned} L(\mu,\lambda) &= \prod_{i=1}^{N} f(T_i;\mu,\lambda) \\ &= \left(\tfrac{\lambda}{2\pi}\right)^{N/2} \prod_{i=1}^{N} (T_i)^{-\frac{3}{2}} \exp\left[-\tfrac{\lambda}{2\mu^2}\sum_{i=1}^{N}\tfrac{(T_i-\mu)^2}{T_i}\right] \end{aligned} \tag{15}$$

Taking natural logarithms on both sides, we have

$$\ln L(\mu,\lambda) = N\ln\left(\frac{\lambda}{2\pi}\right) - \frac{3}{2}\sum_{i=1}^{N}\ln T_i - \frac{\lambda}{2\mu^2}\sum_{i=1}^{N}\frac{(T_i-\mu)^2}{T_i} \tag{16}$$

Based on (16), the parameters μ and λ can be obtained by differentiating the logarithm of maximum likelihood function, as (17) and (18).

$$\frac{\partial \ln L(\mu,\lambda)}{\partial\mu} = \frac{\lambda}{\mu^3}\sum_{i=1}^{N}\frac{(T_i-\mu)^2}{T_i} + \frac{\lambda}{\mu^2}\sum_{i=1}^{N}\frac{(T_i-\mu)}{T_i} \tag{17}$$

$$\frac{\partial \ln L(\mu,\lambda)}{\partial\lambda} = \frac{N}{2\lambda} - \frac{1}{2\mu^2}\sum_{i=1}^{N}\frac{(T_i-\mu)^2}{T_i} \tag{18}$$

Setting the result to zero, we can obtain the estimators for μ and λ, denoted as $\widehat{\mu}$ and $\widehat{\lambda}$.

$$\widehat{\mu} = \frac{1}{N}\sum_{i=1}^{N} T_i \tag{19}$$

$$\widehat{\lambda} = \frac{N}{\sum\limits_{i=1}^{N}\left(\frac{1}{T_i} - \frac{N}{\sum\limits_{i=1}^{N} T_i}\right)} \tag{20}$$

Combining (2), (3) and (19), (20), we can calculate the channel parameters.

1) v is known, D is unknown: Assuming that v is known and D are unknown, the estimated d, denoted as $\widehat{d_4}$ can be expressed as

$$\left\{\ \widehat{d_4} = \frac{v\sum\limits_{i=1}^{N} T_i}{N}\right. \tag{21}$$

2) D is known, v is unknown: In the condition of known D and unknown v, the estimated d, denoted as $\widehat{d_5}$, can be expressed as

$$\widehat{d_5} = \sqrt{\frac{2ND\sum\limits_{i=1}^{N} T_i}{\sum\limits_{i=1}^{N} T_i \sum\limits_{i=1}^{N}\frac{1}{T_i} - N^2}} \tag{22}$$

The comparison of (13) / (14) and (21) / (22) shows that the estimated $\widehat{d}$ based on the two MLE methods have the same results. Any MLE method can be used to solve the parameter estimation problem.

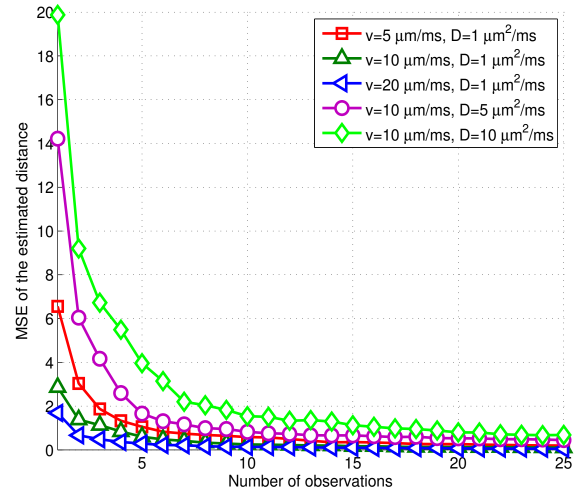

Fig. 2. The MSE of the estimated distance vs. the number of observations under known v and D.

IV. Simulation Results and Discussions

In this section, numerical simulations in MATLAB are performed to validate the performances of our channel parameter estimators. In the simulation we focus on the estimation process which is at the upper layer above the physical layer [24]. So for the simulation setup, pseudorandom sequences based on inverse Gaussian distribution are used to generate T_i. The propagation distance between the transmitter and the receiver is set from 0.1 μm to 30 μm and the medium velocity between the transmitter and the receiver is set from 1 μm/ms to 20 μm/ms [16]. The diffusion coefficient is set from 1 μm^2/ms to 10 μm^2/ms. Table I summarizes the simulation parameters.

TABLE I
System Parameters

Parameters	Symbol	Values
distance	d	0.1 μm - 30 μm
medium velocity	v	1 μm/ms - 20 μm/ms
diffusion coefficient	D	1 μm^2/ms - 10 μm^2/ms

Each point in the figure is an average of M simulation runs, where M is set to 1000. Mean squared error (MSE) at each point is calculated to measure the accuracy. The performance of estimators with respect to the number of observations for different pre-defined values are presented and discussed as following.

Fig. 2 describes the relationship between the MSE of the estimated distance and the number of observations. It is computed from (13). For all the pre-defined $\{v, D\}$, the MSE of the estimated distance d decreases as the number of observations N increases. It proves the effectiveness of our proposed estimation. If v varies and D is fixed, the larger the v is, the smaller the MSEs of the estimated distance is. That's because the larger medium velocity v can cause a faster

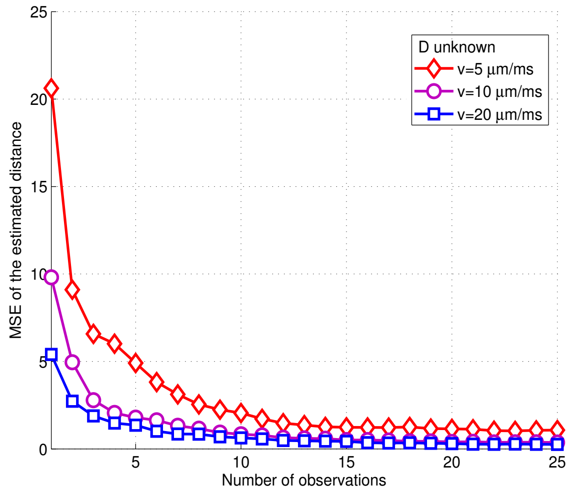

Fig. 3. The MSE of the estimated distance vs. the number of observations with pre-defined medium velocity v.

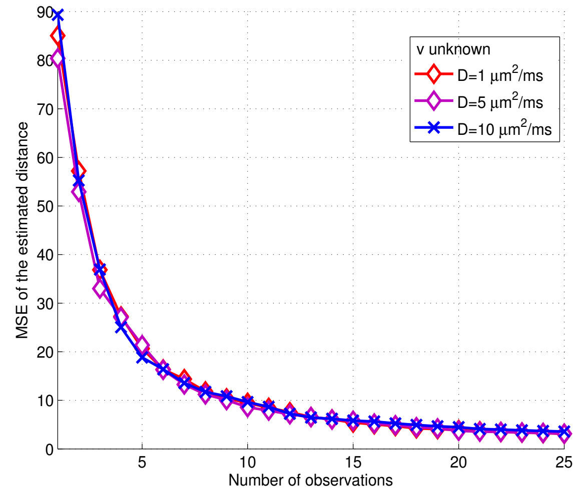

Fig. 4. The MSE of the estimated diffusive coefficient vs. the number of observations with pre-defined diffusive coefficient D.

motion of information molecules in propagation process. The influence of the Brownian motion becomes less significant. While if v is fixed and D varies such as the curves of $\{v = 10$ μm/ms, $D = 1$ μm^2/ms$\}$, $\{v = 10$ μm/ms, $D = 5$ μm^2/ms$\}$ and $\{v = 10$ μm/ms, $D = 10$ μm^2/ms$\}$, it is obvious that the MSE of the estimated distance increases as D increases. This is because larger D the diffusion coefficient D means more active molecular motion. More active motion leads to more serious randomness, and therefore the poor accuracy of the estimation.

Fig. 3 gives an example of the MSE of the estimated distance for different pre-defined medium velocity v. It is clear that the MSE of the estimated distance decreases and tends to steady as the number of observations increases. The reason is simple: large sample size achieves accurate estimation. For all the curves $\{v = 5$ μm/ms, $v = 10$ μm/ms, $v = 20$ μm/ms$\}$, the larger v is, the smaller the MSE of the estimated distance is. The reason is the same as stated in Fig. 2. The larger velocity makes the random motion less significant.

Fig. 4 shows the MSE of the estimated distance vs. the number of observations with pre-defined diffusion coefficient D. Similar to Fig. 2 and Fig. 3, the MSE of the estimated distance decreases and tends to steady with the increase of the number of the observations. We can also find that the different diffusion coefficient has a little effect on the accuracy for the distance estimation if the velocity v is unknown. This is different from the case where v is known in shown in Fig. 2.

Fig. 5 describes the comparison of the MSEs of the estimated distance with different conditions $\{v = 10$ μm/ms, $D = 5$ μm^2/ms$\}$, $\{v = 10$ μm/ms, D unknown$\}$ and $\{v$ unknown, $D = 5$ μm^2/ms$\}$. As the number of the observations increases, the MSEs of the estimated distance decrease for all the conditions. The curves $\{v = 10$ μm/ms, $D = 5$ μm^2/ms$\}$ and $\{v = 10$ μ m/ms, D unknown$\}$ are almost the same. They are smaller than the curve $\{v$ unknown, $D = 5$ μm^2/ms$\}$. The conclusion can be drawn that the influence of v is more severe the influence of D.

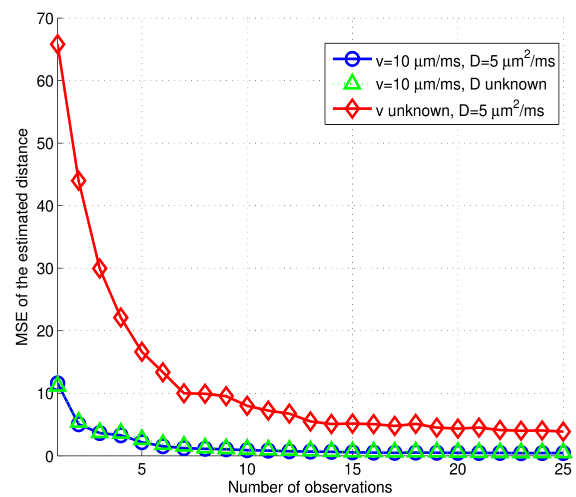

Fig. 5. The comparison of the MSEs for the estimated distance under different pre-defined conditions.

V. Conclusion

This paper has discussed the channel parameter estimation for molecular communication system. An one-way molecular communication in nanonetworks has been used to estimate the propagation distance d, the medium velocity v and the diffusion coefficient D. These channel parameters have been estimated by the MLE. The simulation results demonstrate that our estimated scheme achieves a good performance. This work lays a foundation for the complex cooperation of nanomachines in the molecular communication system.

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