A Framework to Study the Molecular Communication System

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***Abstract*—Communication between a transmitter and a receiver using electromagnetic waves does not scale to nano-sizes. To enable communication between nano-sized devices separated by a short distance, molecular communication has recently been proposed as a feasible scheme. The transmitter *disperses* molecules into the medium, which propagate to, and are sensed by, the receiver. In this paper, we wish to mathematically model such a system and subsequently characterize the information theoretic capacity of this channel. We present basic results on characterizing the mutual information between the transmitter and the receiver when information is encoded in the time of release of the molecule. To do so, we model the propagation of the molecule in this medium as Brownian motion, and derive the probability density function of the arrival time of the molecule at the receiver.**

I. Introduction

Communications research has largely focused on systems based on electromagnetic propagation. However, at scales considered in nano-technology it is not clear that these concepts apply. In this paper we consider communication based on molecules [1]. Specifically, we consider the propagation of individual molecules between closely spaced transmitters and receivers embedded in a fluid medium. The transmitter encodes information in the pattern of release of the molecules it disperses into the fluid medium. These molecules then propagate to the receiver, where they are detected. The receiver then tries to decode the information from the pattern of received molecules. For a comprehensive overview of the molecular communication system, refer to [2] and the references therein.

As in any communication system, the potential rate of communication is determined by the characteristics of the channel. Here, propagation is determined by a mean drift velocity and is uncertain due to the Brownian motion within the fluid. In this preliminary work, our goal is to analyze the mutual information between the transmitter and receiver and hence the capacity of the channel. We would like to emphasize that, in order to gain insight, and to make the problem mathematically tractable, we consider a fairly simple model of a molecular communication system.

In [3], the authors compute information theoretic bounds to capacity for a general diffusion channel. Our work is along similar lines, although we lay a greater emphasis on the mathematical modeling of the system. In [4], the authors study a system where the receiver chemically "reacts" with the molecules and forms "complexes". This is very different from the system model we consider. We assume that the receiver absorbs the molecule. Furthermore, we model the diffusion of the particle in the medium, and incorporate its effect in our calculations.

This paper is organized as follows. Section II describes the system under consideration. The propagation of the molecule in this medium is analyzed in Section III, wherein the probability distribution function of the absorption time is derived. The challenges involved in transmission of information in this media are discussed in Section III-C. In Section IV, we characterize the maximum information transfer per molecule for the case where information is encoded in the time of release of the molecule. We use numerical methods to compute the maximum mutual information between the transmitter and the receiver. The results are presented in Section IV-B. We conclude by presenting a list of interesting research problems in this area in Section V.

II. System Model

The system model we consider is shown in Figure 1. The subsystems which make up the molecular communication system are:

1) Transmitter: The transmitter is a source of identical molecules. We assume that the transmitter can control precisely the time of dispersal of each of these molecules. We further assume that the transmitter does not influence the propagation of these molecules once it disperses them.

2) Propagation medium: The medium between the transmitter and the receiver is a fluid medium. The medium is characterized by two parameters, drift velocity, and the diffusion constant. These in turn depend on the physical properties of the medium. The propagation of the molecule is assumed to be one dimensional (Figure 1 shows two dimensional motion for illustration only).

3) Receiver: The dispersed molecule, when arrives at the receiver, is absorbed by the receiver and is removed from the medium. The receiver makes an accurate measurement of the time when it absorbs the molecule. It uses this information to decode the information.

4) Transmission of Information: The transmitter can encode information in either the time of dispersal of the molecules, or the number of molecules it disperses or both.

We now proceed to derive the probability distribution function (pdf) of the absorption time of the molecule. We then use the pdf of the absorption time to characterize the information conveyed per molecule.

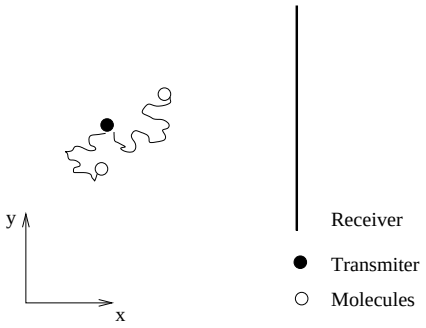

Fig. 1. System Model

III. Characterizing the diffusion process

The diffusion process is probabilistic. The motion of the dispersed molecule is effected by Brownian motion and hence, the propagation time to the receiver is random. In this work, we try to study the effect of this limitation, assuming everything else is perfect. This is because we expect the resulting uncertainty to be the dominant limiting factor to the information transfer per molecule. We now characterize the propagation of the molecule in a fluid medium, a key aspect of this communication system.

Assume that a molecule is released in a static fluid medium at position x_o and time t_o. Let $X(t)$ denote the position of the particle at time t. Let $P_X(x,t;x_o,t_o)$ characterize the pdf of the position of the particle. If the fluid medium is static, the particle disperses in either of the directions with equal probability. The pdf of the position of the particle can then be characterized by the diffusion equation [5]

$$\frac{\partial}{\partial t}P_X(x,t;x_o,t_o) = D\frac{\partial^2}{\partial x^2}P_X(x,t;x_o,t_o), \qquad (1)$$

where D is the diffusion constant, whose value is dependent on the viscosity of the fluid medium.

A. Diffusion with drift

Equation (1) characterizes the pdf of the position of the particle in a static medium. Now suppose that the fluid is flowing with a constant drift velocity $v, v > 0$. We now derive the diffusion equation in this medium.

Consider a frame of reference which is moving with the same velocity velocity v. In this frame, the fluid medium is static and hence the diffusion of the particle obeys (1). Let

$$x^{'} = x + vt, \quad t^{'} = t$$

be the new coordinate system, and without loss of generality, assume $t_o = 0$. Also, without loss of generality, assume that the particle is dispersed at origin, i.e., $x_o = 0$. This assumption is made to simplify the notation, let $P(x,t)$ represent $P_X(x,t;0,0)$. This is equivalent to working in a new frame of reference with origin at x_o. Let

$$P_X(x,t) = P^{'}_{X'}(x^{'},t^{'}),$$

then

$$\frac{\partial}{\partial t'}P^{'}_{X'}(x^{'},t^{'}) = D\frac{\partial^2}{\partial x'^2}P^{'}_{X'}(x^{'},t^{'}).$$

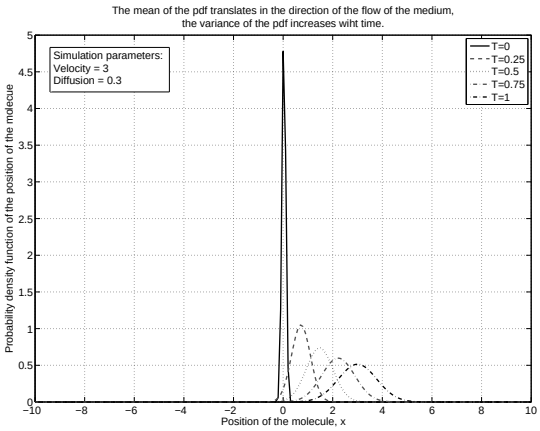

Fig. 2. This figure plots the diffusion of the particle as a function of time

In the static frame of reference, the differential equation can be written as

$$\frac{\partial}{\partial t}P_X(x,t) = \left(D\frac{\partial^2}{\partial x^2} + v\frac{\partial}{\partial x}\right)P_X(x,t) \qquad (2)$$

Assume that there is no absorbing boundary (receiver) and that the fluid medium extends from $-\infty$ to $+\infty$. The probability density function of the location of the particle can be obtained by solving the differential equation (2), with boundary conditions $P_X(x,0) = \delta(x)$ and $P_X(\pm\infty,t) = 0$.

For the sake of brevity, we do not give the details about solving the differential equation. The solution to the differential equation is

$$P(x,t) \quad = \quad \frac{1}{\sqrt{4\pi Dt}}\exp\left(-\frac{(x-vt)^2}{4Dt}\right). \qquad (3)$$

The pdf of the position of the particle, for every t, has a Gaussian distribution. The mean of the distribution drifts along the direction of flow of the fluid medium as vt, the variance increases as $2Dt$. Figure 2 plots $P(x,t)$, the units for velocity, diffusion and time are arbitrary.

If the particle were to be released at $x = -\zeta$ instead of origin, and if it were to be released at time t_o, then the pdf of the position of the particle is given by

$$P_X(x,t;-\zeta,t_o) = \frac{1}{\sqrt{4\pi D(t-t_o)}}\exp\left(-\frac{(x+\zeta-v(t-t_o))^2}{4D(t-t_o)}\right). \qquad (4)$$

B. Solution to the diffusion equation in the presence of an absorbing boundary

Consider (4) for $t_o = 0$, and assume that the particle is released at $x_0 = -\zeta$. Assume that there exists an absorbing boundary at $x = 0$. For such a system, to solve for $P_X(x,t;-\zeta,0)$, we need to solve the differential equation (2) with the following boundary conditions.

- For $x < 0, \quad P_X(x,0;-\zeta,0) = \delta(x+\zeta)$. The probability density function has a physical interpretation only for

$x < 0$. In this region, we require it to be a delta function at $t = 0$ centered at $x = -\zeta$.
- $P_X(-\infty, t; -\zeta, 0) = 0, \quad \forall t$.
- $P_X(0, t; -\zeta, 0) = 0, \quad \forall t$. Condition imposed by the absorbing boundary.

The solution to this differential equation is the summation of two terms. The first term is the probability density in the absence of the absorbing boundary. To have the probability density at the origin to be zero for all time, the *method of images* gives the second term, a *negative probability density*. Consider the following equation

$$P_X(x,t;-\zeta,0) = \underbrace{\frac{1}{\sqrt{4\pi Dt}}\exp\left(-\frac{(x+\zeta-vt)^2}{4Dt}\right)}_{\text{first term}} - \underbrace{\frac{1}{\sqrt{4\pi Dt}}\exp\left(-\frac{(x-\zeta-vt)^2}{4Dt}\right)\exp\left(\frac{v\zeta}{D}\right)}_{\text{second term}} \quad (5)$$

It can be shown that (5) is the solution to the differential equation and satisfies all the boundary conditions.

At a given time t, the probability that the particle has not yet been absorbed is given by

$$\begin{aligned}\bar{F}(t) &= \int_{-\infty}^{0} P_X(x,t;-\zeta,0)dx \\ &= \left(1 - \int_{\frac{-(vt-\zeta)}{\sqrt{2Dt}}}^{\infty} \frac{1}{\sqrt{2\pi}} e^{\frac{-x^2}{2}} dx\right) - \\ &\quad \exp\left(\frac{v\zeta}{D}\right)\left(1 - \int_{\frac{-(vt+\zeta)}{\sqrt{2Dt}}}^{\infty} \frac{1}{\sqrt{2\pi}} e^{\frac{-x^2}{2}} dx\right)\end{aligned}$$

$\bar{F}$(t) is the probability that the particle has not been absorbed until time t. The probability that the particle has been absorbed before t is given by $F(t) = 1 - \bar{F}(t)$. Hence, the probability density function of the absorption time is $f(t) = F^{'}(t)$.

$$\begin{aligned}f(t) &= -\frac{d\bar{F}}{dt} \\ &= -\frac{1}{\sqrt{2\pi}}\exp\left(\frac{-(vt-\zeta)^2}{4Dt}\right)\left(\frac{-v}{\sqrt{2Dt}} + \frac{(vt-\zeta)}{2\sqrt{2Dt^3}}\right) + \\ &\exp\left(\frac{v\zeta}{D}\right)\frac{1}{\sqrt{2\pi}}\exp\left(\frac{-(vt+\zeta)^2}{4Dt}\right)\left(\frac{-v}{\sqrt{2Dt}} + \frac{(vt+\zeta)}{2\sqrt{2Dt^3}}\right) \\ &= \frac{\zeta}{\sqrt{4\pi Dt^3}}\exp\left(\frac{-(vt-\zeta)^2}{4Dt}\right) \quad (6)\end{aligned}$$

Equation (6) gives the probability density function of the absorption time of a particle.

Note that the pdf decays exponentially in the 'high velocity' regime and decays only as $t^{-\frac{3}{2}}$ in the 'low velocity' regime. Figure 3 plots pdf of the absorption time for different sets of drift velocities and diffusion constant.

To summarize, we have derived the pdf of the absorption time of a molecule when released in a fluid medium with diffusion constant D, at a distance ζ from the absorption boundary, with the fluid flowing with a constant velocity $v, v > 0$.

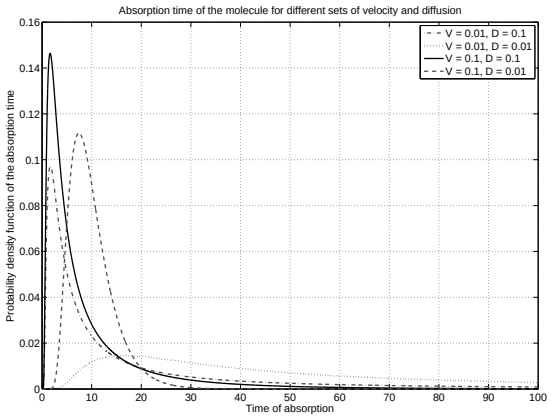

Fig. 3. The probability distribution function of the absorption time for different sets of velocity and diffusion

C. Communication in fluid media

In this section, we list the differences between a traditional wireline communication system and a molecular communication system, and the new challenges involved. In a molecular communication system, the transmitter encodes the message in the number of molecules released and the time of release of these molecules. Based on the number and the time of absorption of the molecules, the receiver decodes the transmitted information.

In a traditional wireline communication system, receiver noise limits the maximum rate at which information can be conveyed. It may be a similar case with the system model considered above, where the receiver might record the number and time of absorption of the molecules incorrectly. However, as discussed before, the uncertainty in the propagation time is a major bottleneck to the information transfer. This uncertainty in the propagation time also means that the order in which molecules are received at the receiver need not be the order in which they were transmitted. This will result in 'inter block interference'. This is a serious impairment in the low velocity regime, where the pdf of the absorption time decays only as $t^{-\frac{3}{2}}$. However, to *cancel this interference*, we do not have an equivalent of a negative voltage, the number of molecules released can only be zero at least.

Achieving time synchronization between the transmitter and the receiver is not as straightforward as in the case of a wireline communication system. In a wireline system, the transmitter sends a known signal to the receiver to mark the start of transmission. The same principle can obviously not be used as is. One way to synchronize the clocks is to do so before installing the transmitter and receiver. If the data rates are slow enough, the clocks need not be re-synchronized (to correct for difference in the oscillator frequencies) very often. We assume that that the clocks are synchronized.

Given these fundamental differences, designing a reliable communication system is challenging. We look at a very basic communication system here and analyze it. We hope that the

framework developed therein can be reused in designing more sophisticated and better systems.

IV. Message encoded in the time of release of the molecule

We analyze the case of the transmitter having just a single molecule. In such a scenario, it can encode information only in the time of release of the molecule. We discretize time into slots of duration T_s. The transmitter releases the molecule in the beginning of one of the N time slots. This molecule then propagates through the medium and is absorbed by the receiver in a later time slot. The receiver then estimates the time slot in which the molecule was released.

The transmitter releases the molecule in one of the N time slots, or can choose not to release the molecule at all. Hence, it can encode a maximum of $\log_2(N+1)$ bits of information. Suppose the velocity of the fluid medium is high enough, so that the particle gets absorbed by the boundary in M time slots with very high probability. For such a system, we can transmit information at a rate *lower* than $\log_2(N+1)/M$ bits per time slot. We study the degradation in the mutual information at low velocity and for different values for diffusion.

There are various parameters which characterize this scheme, and which influence the mutual information, and hence the rate.

- Number of transmit time slots (N). As stated before, the information conveyed grows with N as $\log_2(N)$ whereas the duration of one block of transmission grows linearly in N. Therefore, the maximum rate of communication when N transmit time slots are used grows as $\log_2 N/(N+W)$, where W is a constant. Depending on the value of W, this function is an increasing function of N for small N and then decreases to zero.
- Duration of a time slot (T). We have set T to be one unit. We do not explore the variation of mutual information with T.
- Waiting time at the receiver (M time slots). Theoretically, we need to wait for an infinite amount of time to guarantee that the molecule which has been released gets absorbed. However, it is impractical to do so for two reasons. First, this would induce an infinite delay between encoding and decoding of the message. Second, we would like to use the same channel repeatedly. On the other hand, if the receiver only waits for a finite time, it will lead to molecules from different blocks interfering with each other. We set M to be long enough to ensure that all the transmitted molecules in a block get absorbed by the receiver with a probability greater than 0.999. We do not consider the effect of inter-block interference.
- Sampling rate at the receiver. We have assumed so far that the receiver makes an accurate measurement of the time of absorption of the molecule and uses it to estimate the time slot in which the molecule was released. We now relax this assumption. We assume that the receiver only uses the time slot in which the molecule was absorbed, and not the exact time. Essentially, the time at the receiver is discretized. However, the duration of each time slot at the receiver need not be the same as that at the transmitter. The receiver could use a smaller duration of the time slot. For the sake of clarity, we set the duration of a time slot at the receiver to be the same as that at the transmitter. It is straightforward to change it to a different value.

In the following section, we derive the mutual information between the transmitter and the receiver as a convex optimization problem.

A. The mutual information as an optimization problem

Define a random variable X to denote the time slot in which the transmitter releases the molecule. Assume that the transmitter releases the particle at the beginning of the i^{th} slot ($1 \leq i \leq N$) with probability p_i, with $\sum_{i=1}^{N} p_i = 1 - p_0$. With probability p_0, the transmitter does not release any molecule. Let Y denote the time slot in which the receiver absorbs the molecule. For the time being, we allow Y to range between 1 and ∞, though we will see shortly that this is not required. Also, let $Y = 0$ denote the event that the molecule is never received. When we wait for an infinite time at the receiver, the event $Y = 0$ occurs only when the molecule is not transmitted. Assume that the duration of the time slot is T. From Section III-B, let $F(t)$ denote the probability that the particle gets absorbed before time t, given that it was released at the beginning of the first time slot, at time 0. Denote by α_j the probability that the particle arrives in the j^{th} time slot, given that it was released at time 0, which is equal to $F(jT) - F((j-1)T)$, with $\alpha_j = 0$ for $j \leq 0$. Let $\mathrm{entr}(x)$ denote $-x\log_2(x)$, the binary entropy function. We now proceed to calculate the mutual information between the random variables X and Y.

$$
\begin{aligned}
I(X;Y) &= H(Y) - H(Y|X) \\
H(Y|X) &= H(Y|X=0)p_0 + \sum_{i=1}^{N} H(Y|X=i)p_i \\
&= 0 \times p_0 + \sum_{i=1}^{N} p_i \sum_{j=i}^{\infty} \mathrm{entr}\left(P(Y=j|X=i)\right) \\
&= \sum_{i=1}^{N} p_i \sum_{j=i}^{\infty} \mathrm{entr}\left(\alpha_{j-i+1}\right) \\
&= (1-p_0) \sum_{k=1}^{\infty} \mathrm{entr}\left(\alpha_k\right), \qquad (7) \\
H(Y) &= \mathrm{entr}(P(Y=0)) + \sum_{j=1}^{\infty} \mathrm{entr}(P(Y=j)) \\
&= \mathrm{entr}(p_0) + \sum_{j=1}^{\infty} \mathrm{entr}\left(\sum_{i=1}^{N} P(Y=j|X=i)p_i\right) \\
&= \mathrm{entr}(p_0) + \sum_{j=1}^{\infty} \mathrm{entr}\left(\sum_{i=1}^{N} \left(\alpha_{j-i}\right) p_i\right) \qquad (8)
\end{aligned}
$$

$$I(X;Y) \quad = \text{entr}(p_0) + \sum_{j=1}^{\infty} \text{entr}\left(\sum_{i=1}^{N} p_i \alpha_{j-i}\right) - (1-p_0)\sum_{j=1}^{\infty} \text{entr}\left(\alpha_j\right) \tag{9}$$

The sequence $\{\alpha_j\}$ is a decreasing sequence. The rate of decay depends on the values of the drift velocity v and the diffusion coefficient D. The summations in (9) can therefore be terminated for some large enough j.

The expression for mutual information is a non-negative weighted sum of concave functions plus a constant. Hence, the mutual information is a concave function of the input distribution $\{p_i, i = 1, \ldots, N\}$. Standard optimization packages like CVX [6] can be used to solve for the input probability distribution which maximizes the mutual information.

Suppose that we were to convey information only in the time of release of the molecule, that is, we do not allow for the case of no transmission. The derivation of mutual information is very similar to the derivation above. Mutual information can then be expressed as

$$I(X;Y) = \sum_{j=1}^{M} \text{entr}\left(\sum_{i=1}^{N} p_i \alpha_{j-i}\right) - \sum_{j=1}^{M} \text{entr}\left(\alpha_j\right) \tag{10}$$

B. Simulation Results

Using numerical methods, we find the input distribution that maximizes (9). In Figure 4, we plot the mutual information as a function of velocity, for two different sets of diffusion coefficients, 0.05, representing the low diffusion scenario, and a high diffusion constant 0.2. We have two sets of plots in the figure, one for the case where we have two slots in which we can release the molecule, or choose not to release it, and another, where we have four time slots. Also, we give the input distribution $(p_0, p_1, p_2, p_3, p_4)$ at which the mutual information is maximized at the two extreme values of velocity.

From the figure, it is evident that the mutual information increases with an increase in velocity and saturates to a maximum of $\log_2(N+1)$ bits. This trend is expected. The mutual information maximizing input probability distribution is the uniform probability distribution. At high velocities, the receiver can detect error free the slot in which the transmitter disperses the molecule. Also, because we wait for a sufficiently long time at the receiver, we can detect error free if a molecule was transmitted or not. Therefore, a lower limit on the mutual information is one bit. At lower velocities, the mutual information is marginally greater than one bit.

The diffusion constant is a measure of the uncertainty in the propagation time. Hence, we would expect the mutual information to be lower when the diffusion constant is high. This is indeed the case at high velocities. However, it is surprising that higher diffusion constant results in higher mutual information at low velocities. This is because, at low velocities, it is the diffusion in the medium which aids the propagation of the molecule from the transmitter towards the receiver. This is illustrated in the pdf of the absorption time,

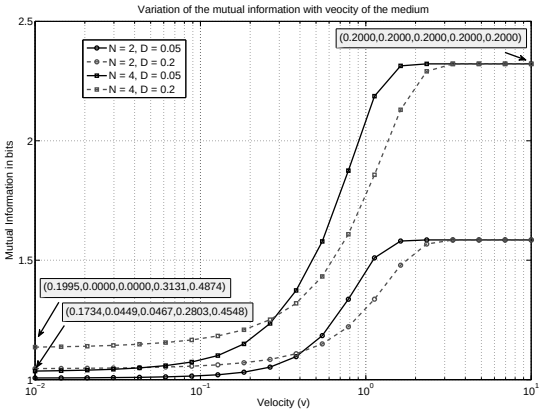

Fig. 4. Variation of mutual information with velocity.

shown in Figure 3. Compared to the case when the diffusion in the medium is low, the probability distribution function is more "concentrated" when the diffusion in the medium is higher.

Next, we find the input distribution which maximizes (10). The mutual information in this case is plotted in Figure 5. The maximum mutual information is now $\log_2(N)$ bits, which is achieved at high velocities. However, it is in the low velocity regime where the mutual information is significantly lower than the case where the transmitter is allowed to not transmit the molecule. Figure 6 compares the two scenarios.

From the results, we see that the velocity-diffusion region can be roughly classified into two regimes:

- A diffusion dominated region, where mutual information is relatively insensitive to the velocity. This corresponds to $v < 10^{-1}$ and $v > 3$ in Figure 4.
- A velocity dominated regime, where the mutual information is highly sensitive to the velocity of the medium, $10^{-1} < v < 3$ in Figure 4.

In the low velocity regime, we see no significant improvement in the mutual information when we increase the number of time slots in which we can release the molecules. As expected, very little information can be conveyed in the time of release of the molecule when there is high uncertainty in the propagation time. Hence, we need to explore alternative ways of encoding message in this regime.

V. Conclusions and Future work

In this paper, we construct a framework to study data rates that can be achieved in a molecular communication system. We start by studying the propagation of the molecule in a fluid medium. We consider a simple model for the communication system, consisting of a transmitter and receiver separated in space, immersed in a fluid medium. We derive the pdf of the propagation time of the released molecule. This pdf characterizes the data rate completely. We then proceed to analyze the rates achieved by a simple communication protocol, where information is encoded in the time of release of the molecule.

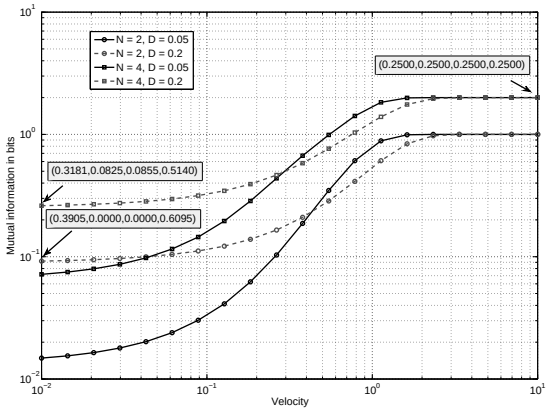

Fig. 5. Variation of mutual information with velocity when the transmitter is not allowed to not disperse the molecule.

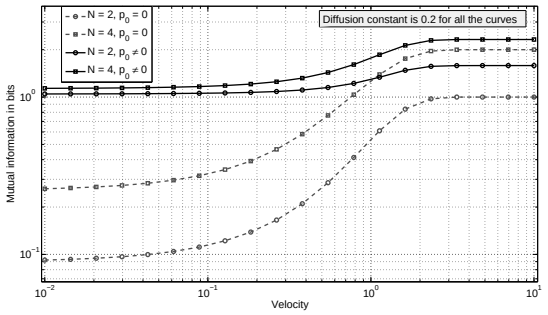

Fig. 6. A comparison of the mutual information between the two cases, when the transmitter is allowed not to transmit the molecule at all, and the case when it is not.

In the framework constructed here, many interesting problems arise. We list a few of them.

In this paper, we considered only the case where information is encoded in the time of release of the molecule. We could also potentially encode information in the number of molecules released in a time slot. Also, in the analysis so far, we have assumed that we can control very precisely the number of molecules (one in this paper) we release and the time of their release. It might not be possible to do so. Molecules might be generated as a product of a chemical reaction, in which case, the number of molecules released might be a random variable with a certain probability distribution function. Hence, at the transmitter, we might be able to release only a discreet set of number of molecules, say 0, 100 and 200. Associated with each of these levels will then be an uncertainty in the number of molecules released, a *signal dependent transmitter noise*. It would be interesting to compute the mutual information and the data rates for this scenario.

Assuming that the receiver can record the exact time of absorption of every molecule might also not be valid. We have avoided one of these two assumptions by quantizing the absorption time and noting only the time slot in which a molecule is absorbed. However, we have so far assumed that the receiver is sensitive enough to detect the absorption of every molecule. However, it might not be possible to design such receivers. *Receiver quantization, in time, and in the number of molecules it absorbs* needs to be accounted for. Also, we have not considered any receiver noise in our model. The number of molecules that the receiver detects might be modeled as a random variable and its effect accounted for when calculating the mutual information.

In this paper, we have assumed that the waiting time is long enough to ensure that the released molecule is absorbed. However, in practical systems, this time has to be truncated to allow for the reuse of the channel. This will then result in an inter-block-interference wherein molecules released in earlier blocks might arrive "late" and confuse the receiver. Also, there is a probability that the receiver absorbs no molecules even when the transmitter disperses them. The system model is equivalent to a *Z-channel with memory.* It would be interesting to study capacity of such channels.

We have computed information theoretic bounds for the maximum data rate. Another interesting research problem would be to devise "error detection or error correction" mechanisms for a molecular communication system. In particular, designing codes with very low encoding and decoding complexity will be a key challenge.

A complete departure from the framework of releasing finite number of molecules is to consider the case where the transmitter controls the *concentration of the molecules* it releases. Concentration being a real number, optimization has to be done over continuous valued probability distribution functions.

In conclusion, we believe that the area of molecular communication presents many interesting research problems. Most of these problems do not arise in the context of wireline communication, making the problems even more challenging.

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