Timing Information Rates for Active Transport Molecular Communication

Andrew W. Eckford

Dept. of Computer Science and Engineering, York University
4700 Keele Street, Toronto, ON, Canada M3J 1P3
aeckford@yorku.ca

Abstract. In this paper, active transport molecular communication is analyzed for microfluidic applications. It is shown how to adapt existing information-theoretic results to this new scenario. Achievable timing information rates, usable when all the molecules are indistinguishable, are obtained for microtubules propagating in a narrow kinesin-lined channel.

Keywords: Information theory, Kinesin, Microfluidics, Molecular communication.

1 Introduction

Molecular communication, in which information is encoded in the release times and identities of molecules, is a biologically inspired approach for communication at micro- and nano-scale dimensions [1]. This form of communication may be used in environments where electrical communication is not appropriate, such as where the terminals are small, in close proximity, and immersed in liquid. One such application is in lab-on-chip devices, where it is desirable to perform signal processing directly in the microfluidics, rather than electronically. For example, [2] proposed logic gates that can be implemented by manipulating beads of fluid in a microfluidic device.

Active transport is one method by which cargoes may propagate in microfluidics, and kinesin is one of many molecular motors that may facilitate such transport. Using kinesin, active transport is accomplished in conjunction with a polarized molecular *microtubule* (MT): the kinesin "walks" from site to site along the MT, while the polarity of the MT dictates the direction of the walk. In engineered systems, either the kinesin or the MT can be adapted to carry a cargo (e.g., a bead, or a vesicle). The possibility of using kinesin-transported MTs for molecular communication was previously identified in [3].

It is natural to consider the maximum rate at which information can be reliably transmitted over this type of molecular communication link. As such, the main contribution of this paper is to obtain achievable timing information rates for microtubules propagating in kinesin-lined channels, which is an appropriate setup for a microfluidic application. Related information-theoretic analysis has been performed in several recent works. Of particular relevance to the current paper is the work in [4,5], which gave a complete framework and family of

A. Schmid et al. (Eds.): Nano-Net 2009, LNICST 20, pp. 24–28, 2009.

bounds that may be used to analyze a wide variety of molecular communication systems; the analysis in this paper uses the fundamental results derived in those references. Related work has also been performed in [6,7], but those works used simpler models and scenarios that are not compatible with the current work.

In this paper, we consider microfluidic devices as engineered molecular communication systems, analogously to wired or wireless communication devices. The methods and theoretical framework from [4,5] (originally obtained for free-space diffusion) are adapted to this new channel, and used to calculate achievable information rates for active transport microfluidic systems.

2 System Model

In this paper, we deal with so-called *engines-down transport* [8], where a channel is lined with kinesin motors, and cargo-bearing MTs glide atop these motors, propagating along the channel (analogous to a conveyor belt). Since the movement of kinesin from site to site along the MT is random, the propagation of the MT in this channel is akin to a Brownian motion with drift. In [9], a stochastic model of this propagation was presented as a discrete-time random walk, characterized by spacial displacement Δr and angular displacement $\Delta\theta$ over time steps Δt. In this model, Δr is assumed to be a Gaussian random variable with mean and variance

$$\mu_{\Delta r} = v_{\text{avg}} \Delta t, \quad \sigma^2_{\Delta r} = 2 D_v \Delta t, \tag{1}$$

where v_{avg} is the average velocity and D_v is the motional diffusion coefficient. Further, $\Delta\theta$ is also assumed to be a Gaussian random variable with mean and variance

$$\mu_{\Delta\theta} = 0, \quad \sigma^2_{\Delta\theta} = \frac{v_{\text{avg}}}{L_p} \Delta t, \tag{2}$$

where L_p is the persistence length of the MT trajectory.

We use this model with values of $v_{\text{avg}} = 0.85\ \mu$m/s, $D_v = 2 \times 10^{-3}\ \mu\text{m}^2$/s, and $L_p = 111\ \mu$m are used, as these were given in [9] as physically realistic values. Furthermore, throughout this paper we use a step size of $\Delta t = 0.1s$. We make two further assumptions on MT motion. First, if two (or more) MTs are propagating simultaneously, their motions are independent of each other: although this assumption ignores any possible collisions between MTs, it is believed to be physically realistic due to the flexibility of MTs. Second, as in [9], the random walk is constrained by the size of the MT along which it is propagating – in the event of a collision with a wall, the MT finishes its propagation by hugging the wall.

We may perform an information-theoretic analysis of this channel to determine rates at which reliable communication may be performed using the timing information (i.e., assuming that the MTs were indistinguishable), which is the most fundamental case to solve [5]. For n-fold vector channel inputs $\mathbf{x}$ and outputs $\mathbf{y}$, and given an input distribution $f(\mathbf{x})$, the maximum achievable information rate in any communication channel is given by

$$I(X;Y) := \lim_{n \to \infty} \frac{1}{n} E\left[\frac{f(\mathbf{y}|\mathbf{x})}{f(\mathbf{y})}\right]. \tag{3}$$

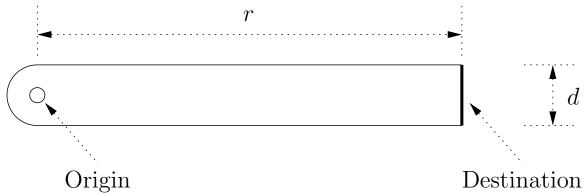

Fig. 1. Depiction of the propagation environment

An obvious question raised by (3) is how to formulate $\mathbf{x}$ and $\mathbf{y}$. Adapting the framework from [4,5], it is assumed that MTs propagate freely from the time of release until their arrival at the destination. As a result, it was shown that $\mathbf{x}$ is the vector of times at which each molecule departs the transmitter, and $\mathbf{y}$ is the vector of times at which each molecule arrives at the receiver. Thus, the system is completely characterized by the probability distribution function (pdf) of the *first passage time* at the destination: for a random walk $R(t)$ that begins at time $t = 0$, the first passage time t^* at a point r is the earliest time at which the random walk reaches r, i.e.,

$$t^* = \min\{t : R(t) = r\}. \tag{4}$$

The functions $f(\mathbf{y}|\mathbf{x})$ and $f(\mathbf{y})$ can then be obtained from the pdf of t^* and $f(\mathbf{x})$.

The pdf of t^* is dependent on the model of motion, given above in equations (1)-(2), as well as on the structure of the channel. For this work, we assume a "cigar-tube" channel, as in Figure 1: a rectangular channel of length r and width d, with a semi-circular end, centered on the origin. MTs are released at the origin; the detector takes up the rightmost wall of the rectangle, and MTs arriving at this wall are immediately removed from the system. Since the direction of MT propagation is determined by polarity, which is difficult to control in advance, we assume that the initial angle of propagation θ for each MT is either zero radians (i.e., left-to-right, directly towards the destination, or π radians (i.e., right-to-left, directly away from the destination); and the two possibilities are equiprobable. Under these circumstances, the first arrival time distribution is not available in closed form, but can be obtained by *Monte Carlo* simulation. Some examples are given in Figure 2.

As we mentioned above, $\mathbf{x}$ is a vector of n MT departure times, and $\mathbf{y}$ is a vector of n and MT arrival times. In the case of molecular communication, $I(X;Y)$ is difficult to calculate exactly. However, if $f(\mathbf{y}|\mathbf{x})$ is replaced by any approximation $g(\mathbf{y}|\mathbf{x})$, and letting $g(\mathbf{y}) = \int_{\mathbf{x}} g(\mathbf{y}|\mathbf{x}) f(\mathbf{x})$, it is known that

$$I(X;Y) \geq G(X;Y) := \lim_{n\to\infty} \frac{1}{n} E\left[\frac{g(\mathbf{y}|\mathbf{x})}{g(\mathbf{y})}\right], \tag{5}$$

and furthermore, the lower bound $G(X;Y)$ is achievable for a detector that assumes the approximation $g(\mathbf{y}|\mathbf{x})$ is correct.

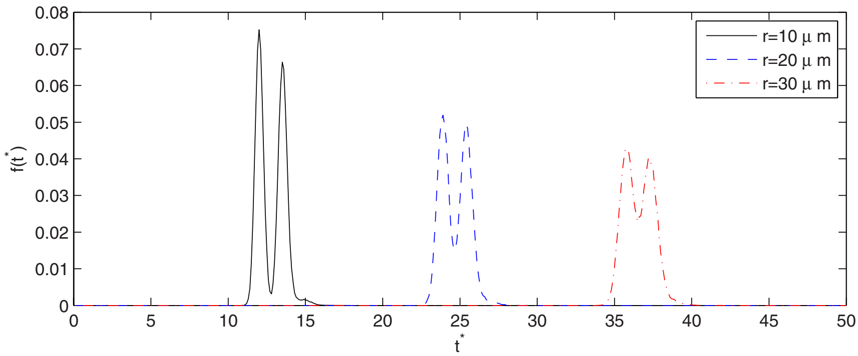

Fig. 2. First arrival time pdfs for various r, where $d = 1\mu m$

We use the *counting detector* from [5] to obtain $g(\mathbf{y}|\mathbf{x})$. Using this model, time is discretized into intervals. Transmitted messages $\mathbf{x}$ are encoded as $\{0, 1\}$ binary strings, with ones representing a single MT release, and zeros representing no release. MTs are (possibly) released at the beginning of each interval: for example, with an interval length of 1 second and $\mathbf{x} = [0, 1, 0, 0, 1, 1]$, three MTs would be released (at 1s, 4s, and 5s). Subsequently, $\mathbf{y}$ is formed by counting the number of arriving MTs in each interval: for example, again using an interval time of 1 second, if $\mathbf{y} = [0, 0, 1, 0, 0, 2]$, then one MT arrived between 2s and 3s, and two MTs arrived between 5s and 6s. The arrivals are modeled as a discrete Markov chain, and the reader is directed to the reference for full details.

3 Results

We provide results for the case where $d = 1\mu m$, and $r = 10$, 20, and $30\mu m$; thus, the first arrival time pdfs are the same as those found in Figure 2. We use the counting detector with intervals of 1.6 seconds, and an independent, identically distributed binary input distribution, with probability p_x of releasing an MT at the beginning of an interval, and probability $1 - p_x$ of not releasing an MT. Although the data rates per unit time are relatively low (peaking around 0.4 bits per second), this is typical and expected given the low propagation speeds involved. However, a striking feature of these results is that the achievable information rate is largely insensitive to the length r of the microtubule, in spite of the latency (in fact $r = 30\mu m$ seems to have better performance than $r = 20\mu m$, but this is an artifact of the quantization inherent in the counting detector). Furthermore, dividing each achievable rate by $p_x/1.6$ gives the average transmission rate per microtubule, which can be quite large: two bits per microtubule at $p_x = 0.05$.

In future work, we will consider nonbinary input distributions (i.e., releasing several MTs at once). Furthermore, we will consider the case where MTs are lost in transit (e.g., if they escape from the channel or stick to the walls).

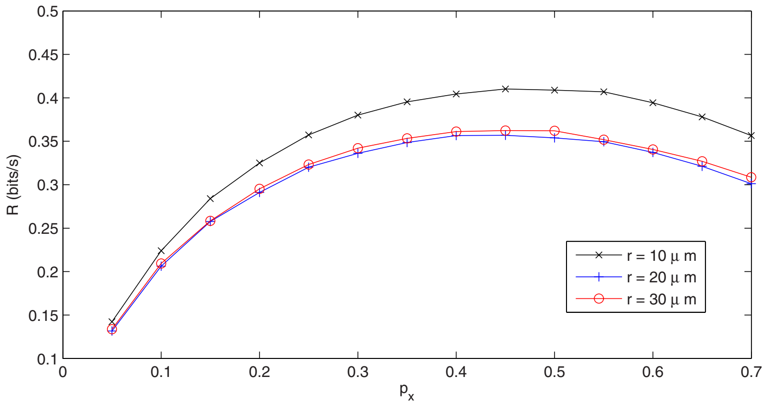

Fig. 3. Achievable rates R with respect to p_x, for various r

Acknowledgments

The author wishes to acknowledge Satoshi Hiyama and Yuki Moritani of NTT DOCOMO Inc., Japan, for their helpful discussions.

References

1. Hiyama, S., et al.: Molecular communication. In: Proc. 2005 NSTI Nanotechnology Conference, pp. 391–394 (2005)
2. Zhao, Y., Chakrabarty, K., Xu, T.: Digital microfluidic logic gates. In: Proc. 3rd Intl. Conf. on Nano-Networks, Boston, MA (2008)
3. Hiyama, S., Moritani, Y., Suda, T.: A biochemically engineered molecular communication system. In: Proc. 3rd Intl. Conf. on Nano-Networks, Boston, MA (2008)
4. Eckford, A.W.: Nanoscale communication with Brownian motion. In: Proc. Conference on Information Sciences and Systems, Baltimore, MD, pp. 160–165 (2007)
5. Eckford, A.W.: Molecular communication: Physically realistic models and achievable information rates. Submitted to IEEE Transactions on Information Theory (December 8, 2008) arXiv:0812.1554v1 [cs.IT]
6. Atakan, B., Akan, O.: An information theoretical approach for molecular communication. In: Proc. 2nd Intl. Conf. on Bio-Inspired Models of Network, Information, and Computing Systems, Budapest, Hungary (2007)
7. Moore, M.J., et al.: Simulating molecular motor uni-cast information rate for molecular communication. In: Proc. Conf. on Information Sciences and Systems, Baltimore, MD (2009)
8. Stewart, R.J., Limberis, L.: Engineering a molecular railroad. In: Shoseyov, O., Levy, I. (eds.) NanoBioTechnology: Bioinspired Devices and Materials of the Future, pp. 433–459. Humana Press, Totowa (2007)
9. Nitta, T., et al.: Simulating molecular shuttle movements: Towards computer-aided design of nanoscale transport systems. Lab. on a Chip 6, 881–885 (2006)