Noise Modeling for Molecular Communication via Chemical Reactions and Diffusion

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***Abstract*—Reaction and diffusion are two fundamental phenomena defining the production and propagation dynamics of information molecules in molecular communication. Under the effects of the reaction and diffusion, the channel can be modeled via systems of partial differential equations. However, obtaining tractable closed form solutions of the corresponding partial differential equations is in general not possible. Moreover, randomness due to a finite number of molecules and finite sampling times is inherently present. In this paper, we address these issues by presenting probabilistic model of signals in molecular communication channels in the presence of both reaction and diffusion.**

I. Introduction

Molecular communications has been proposed as an effective communication mechanism in nanonetworks and more widely as a framework for understanding information processing in biochemical systems [1]. There are various attempts to define realistic models for this class of communication [2]. One of the most popular is molecular communication via diffusion (MCvD) [3]. Due to the slow and uncertain transport of information molecules in MCvD, inter-symbol interference is the major problem. Furthermore, the impact of the information molecule production process is not explicitly described.

An alternative method to MCvD is molecular communication modeled via the diffusion dynamics induced by chemical reactions. As proposed in [4] reaction-based communication has several advantages: i) the production of information molecules is explicitly modeled; ii) long-term behavior of the system can often be tractably characterized via a deterministic model; and iii) feedback mechanisms based on reversible reaction are naturally present.

Although reaction-based communication models are promising due to its deterministic nature, they are only valid when the channel is reaction-limited [4]. In other words, the proposed communication method is only applicable when dynamics due to chemical reactions dominate and the effects of the diffusion are negligible. Furthermore, the deterministic model may not be applicable and a noisy observation may be expected when the number of information molecules are limited and/or when diffusion is not negligible. Although there are some approximate solutions for the channels under the effects of both reactions and diffusion [5], exact and general solutions are not presently available. In this paper, our aim is to determine the distribution of the noise when the effects of diffusion and other limiting factors such as sampling times and the number of transmitted molecules are accounted for.

II. System Model

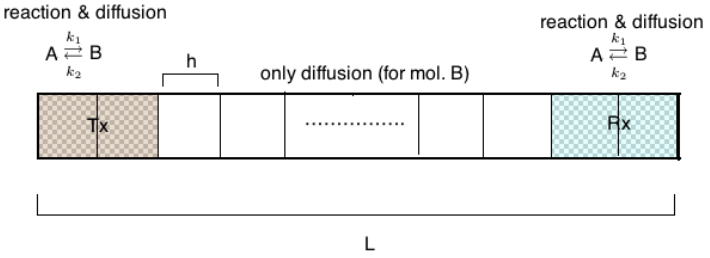


Fig. 1: The system is simulated by dividing the environment into voxels with length h [6].

The system model is illustrated in Fig. 1. In this paper, we focus on a one dimensional model, which can be nevertheless easily extended to higher dimensions [6]. As shown in Fig. 1, both the transmitter in region T and the receiver in region R are able to generate information molecules (B) via a chemical reaction involving species A.

$$\mathsf{A} \underset{k_2}{\overset{k_1}{\rightleftarrows}} \mathsf{B} \tag{1}$$

Once a transmission starts, both the transmitter and the receiver generate information molecules according to (1) and only information molecules (B) are allowed to permeate from the device surface and diffuse in the environment freely. The molecules of species A cannot diffuse outside of the device.

Let D be the diffusion coefficient of the molecule and $k = k_1 = k_2$ (this a simplifying assumption, which can also be generalized) are the reaction rates and L is the length of the channel. A general rule of thumb [4] is that the corresponding channel can be approximated as reaction-limited if the Damköhler number ($D_a = kL^2/D$) satisfies $D_a \ll 1$ and it can be treated as diffusion-limited if $D_a \gg 1$. For the other cases, both the reaction and the diffusion have non-negligible effects on the dynamics of the molecules. The concentrations $[\mathsf{A}], [\mathsf{B}]$ of A and B molecules, respectively, in the system in Fig.1 can be modeled by a system of partial differential equations as

$$\frac{\partial [\mathsf{B}]}{\partial t} = D\frac{\partial^2 [\mathsf{B}]}{\partial x^2} - f(x)k_1[\mathsf{B}] + f(x)k_2[\mathsf{A}], \tag{2}$$

where $f(x) = 1$ if $x \in T, R$ and 0 otherwise. In this paper, however, we use the next reaction algorithm proposed in [6] to examine the stochastic characteristics of the channel due to the limiting factors.

III. Simulation Results and Discussion

Let $A_T(t)$ and $B_T(t)$ be the number of corresponding molecules at time t at the transmitter and $A_R(t)$ and $B_R(t)$ are the number of molecules at the receiver in time t. For conducting simulations, without loss of generality, the reactions are assumed balanced as $k_1 = k_2 = 1$, $A_T(0) = B_T(0) = 2M$ and $A_R(0) = B_R(0) = M$. The length of the transmitter and the receiver is chosen as $L/10$. *The goal of this study is to characterize the quantity of molecules of type* B *(B_R) in the receiver at the equilibrium.*

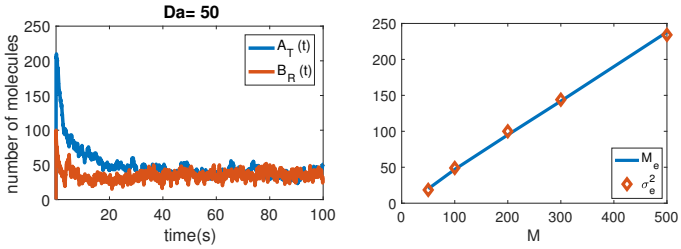
A. Steady-State Behavior

In [4] it has been shown that steady-state concentrations can be used to characterize the impact of initial conditions in the reaction-limited regime. On the other hand, when both diffusion and reaction are not negligible, it may not be possible to determine the steady-state conditions analytically.

Let $X(t) = \{A_T(t), B_T(t), A_R(t), B_R(t)\}$ be the state variable that defines the number of molecules at the receiver and the transmitter at time t. Based on Fig. 2, and verified using several other choices of model parameters, the distribution for the number of molecules converges to a stationary distribution; i.e.,

$$\lim_{t\to\infty} \Pr(A_R(t) = x) = \Pr(A_{R,\infty} = x),\ x \in \mathbb{Z}_{\geq 0}. \quad (3)$$

Moreover, $A_{R,\infty}$ can be written as $A_{R,\infty} = M_e + \epsilon$ where M_e is the mean and ϵ can be viewed as a noise term. This is expected since at the steady-state, the number of molecules are spatially homogeneous. Furthermore, since $k_1 = k_2$, the statistics for the quantity of molecules for B and A are the same in the both the receiver and in the transmitter in the long-term, demonstrated in Fig. 2a.

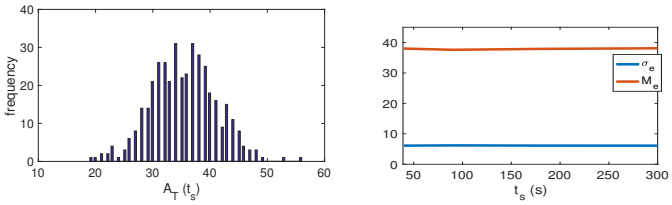


(a) $D_a = 50$ (b) Effects of M

Fig. 2: a)Number of molecules at the receiver and the transmitter with respect to time. Initially: $A_T(0) = B_T(0) = 200$ and $A_R(0) = B_R(0) = 100$. At steady-state $A_T(\infty) = B_T(\infty) = A_R(\infty) = B_R(\infty) = M_e$. Due to the spatial homogeneity there are $8M_e$ B molecules diffusing in the channel. Therefore the total number of molecules for this setup is $12M_e$ and it should be equal to the initial total number of molecules (600). Hence $M_e = 50$ can be easily obtained. b) Effect of the initial number of molecules M.

B. Effect of the Sampling Time

In a practical communication system, it is not possible to observe the stationary distribution. In other words, it is not reasonable to wait for $t \to \infty$ and instead a finite sampling time t_s^* should be used. Fig. 3a, shows that the distribution of the molecules for a given t_s can be modelled as normal distribution as $\epsilon \sim \mathcal{N}(0, \sigma_e^2)$. Moreover, in Fig. 3b the variance and the mean of the distribution are not changing significantly as t_s changes, if $t_s > t_s^*$.



(a) Samples from the steady-state (b) Distribution parameters for different t_s

Fig. 3: Approximate Steady-State Distribution

C. Impact of Initial Concentrations

It is clear that, as in reaction-limited regime, the number of molecules in the steady-state depends on the initial number of molecules in the system. When both reactions and diffusion are present, there is a linear relation between the initial number of molecules M and the number of molecules at the steady-state as can be observed in Fig. 2b. Furthermore, observe that the variance σ_e^2 is equal to M_e and as such the steady-state distribution of $A_R(t)$ can be modelled as $\beta M + \mathcal{N}(0, \beta M)$ by taking $M_e = \beta M$ where β can be easily calculated by using channel parameters as shown in Fig. 2a.

IV. Conclusion and Future Works

In this work, we have performed a preliminary study of noise in molecular communication systems with both reactions and diffusion. A key observation is that the long-term expected number of molecules can readily characterized. Our future aim is perform an analytical study to describe the impact of the sampling time, t_s^*, in terms of channel parameters and to explore the molecular communication aspects under the effects if reaction and diffusion.

References

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