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Transceiver Observations in Asymmetric and Symmetric Diffusive Molecular Communication Systems

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Abstract—To estimate the molecular communication (MC) parameters (e.g., diffusion coefficient, reaction rate, and absorption rate) via observations at the transmitter and the receiver, we present an analytical framework for a diffusive MC system with a partially absorbing receiver and a general first-order chemical reaction during propagation, in both spherically asymmetric and spherically symmetric scenarios. The time-varying spatial distributions and the expected numbers of messenger molecules and their first-order reaction products inside the transmitter, as well as at the surface of the partially absorbing receiver, are derived in both scenarios, which can be simplified in the special cases of a fully absorbing receiver. Importantly, our analytical expressions are verified by particle-based simulations, which showcase the effect of the reaction rate on the transmitter and the receiver observations. The analytical results of channel impulse responses at the absorbing receiver as well as that inside the transmitter are first treated and solved for spherically asymmetric scenario in this work.

I. INTRODUCTION

With the prominent development and ubiquitous usage of communications, electrical and electromagnetic signals have been a conventional solution to the problem of information delivery. However, these technologies are not effective in some challenging environments like seawater and human bodies or at ultra-small dimensions like microscale and nanoscale [1]. The widespread application in nanotechnology, whose devices are miniaturized and fabricated at nano-scale [2] and could cooperate as a nano-network to perform more complex tasks such as pollution control and drug delivery, could be achieved via a natural approach - molecular communication (MC). A comparison between MC and traditional communications has been studied in [3] and research challenges of MC were described in [1].

Information delivery is realized by the transportation of chemical signals between transmitters and receivers in MC. In diffusive MC system, molecules propagate via Brownian motion without any external energy, which reflects its simplification and energy efficiency. In the past several years, various theoretical studies of the diffusive MC system have sought to understand the channel and guide system design [4]–[8].

The receiver model can be classified into *active* and *passive* receivers, which exhibit two distinct channel responses. For an active receiver, arrived molecules will react with receptors on

the surface of the receiver with some absorption rate, whereas for a passive receiver arrived molecules will freely propagate through the receiver boundary without any impedance. The active receiver mechanism can be considerably more sophisticated but is practical for many bio-applications. In the domain of diffusive MC systems, theoretical studies of active receivers include channel modeling [4], [5], the receiver design [6], [9], transfer functions [7], [10].

In a diffusive MC system, messenger molecules could react with other chemical molecules or degrade during propagation (e.g. acid and base reaction [11], and enzymes [12]). Existing works have mainly focused on the observations at the receiver side with a passive receiver [12] [13], an absorbing receiver [14], or a receiver with reversible absorption [15]. However, observations at the transmitter side are also of interest. For example, this would be more convenient and cost-effective for parameter estimation, especially in an adverse environment. Further work at the transmitter side is required, such as the parameter estimation, to perceive the environment in advance and adjust the next information delivery for better performance. Moreover, chemical reactions during propagation can have a significant impact on the channel impulse response, thus the investigations of both messenger molecule and reaction product will provide a new perspective: using the combination of observations for both types of molecules to obtain an enhanced detection at the transmitter and the receiver.

Existing MC works [4], [5], [7]–[9] consider geometries that are limited to spherical symmetry where the transmitter is effectively a spherical shell and molecules are released from random points over the shell; the actual angle to the transmitter when a molecule hits the receiver is ignored, so this assumption cannot accommodate a flowing environment [9]. To capture a more general channel impulse response, this paper will address spherical asymmetry by considering the actual angle to the transmitter when a molecule hits the receiver. This can facilitate the study of more complex MC systems (e.g., with flow, multi-user scenario, etc.).

In this diffusive MC system model, we consider the channel impulses responses and observations for both messenger molecules and their first order reaction products at the trans-

mitter as well as the receiver in spherical asymmetry and spherical symmetry. Our main contributions are as follows:

1) We present an analytical framework for the diffusive MC system with a partially absorbing receiver and a general first-order chemical reaction during propagation in spherically asymmetric and spherically symmetric scenarios.

2) In both scenarios, we derive the time-varying spatial distributions of messenger molecules and their products with a partially absorbing receiver, and their expected numbers inside a passive transmitter and at the receiver surface. Furthermore, the spatial distributions and the expected numbers will be simplified in the special case of a fully absorbing receiver.

3) Our analytical results for observations of messenger molecules and their products at the transmitter and the receiver are verified by particle-based simulations. The effect of the reaction rate on observations of both types of molecules at the transmitter and the receiver are examined, which shows the potential difference on combination of observations for messenger molecules and their products between transmitter estimation and receiver estimation design.

The rest of this paper is organized as follows. The system model in spherically asymmetric and spherically symmetric scenarios are presented in Section II. In Section III, we demonstrate the time-varying spatial distribution and observations for messenger molecules and their products in two scenarios. In Section IV, we discuss verified analytical results. The conclusion are drawn in Section V.

II. SYSTEM MODEL AND ANALYTICAL PRELIMINARIES

In this section, we present the system model and analytical framework for a diffusive MC system with a partially absorbing receiver and a general first-order chemical reaction during propagation in both spherically asymmetric and spherically symmetric scenarios. The passive transmitter (i.e., with transparent membrane) is assumed to be able to count and observe the number of molecules inside it in real time, whereas the molecules at the surface of an absorbing receiver bind to receptors to activate the counting mechanism. Receptors are uniformly distributed at the receiver surface and only one molecule can bind to a receptor at a time [15]. The binding between the molecules and the receptors is independent of the binding between other molecules and other receptors and the number of the receptors is assumed to be unlimited to absorb all arrived molecules. Both the transmitter and receiver can identify two types of molecules: **A** molecule is the emitted message molecule and **B** molecule is its reaction product. The synchronization between the transmitter and the receiver is assumed to be perfect. The system model in spherically asymmetric and spherically symmetric scenarios, as shown in Fig. 1, will be demonstrated in the following respectively.

A. Spherically Asymmetric Scenario

The spherical receiver with radius r_r is assumed to be stationary at the origin of spherical coordinates (r, θ, λ) when the centre of the transmitter is located at $(r_0, 0, 0)$ where $r_0 > r_r$ [16]. The angular distribution, which is with respect

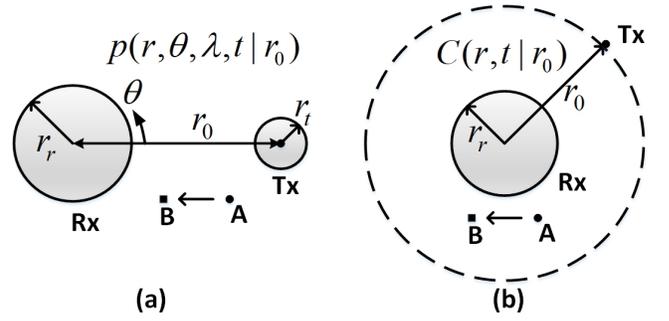


Fig. 1. (a) System model in spherically asymmetric scenario; (b) System model in spherically symmetric scenario

to the initial spatial direction connecting the centre of the transmitter and the receiver [16], is measured via θ . This scenario is explicitly more realistic but also more complex due to the lack of spherical symmetry.

1) *Emission*: We set $\theta_0 = 0$ to get “ λ -independence” [16]. A fixed number of **A** molecules are released into the channel from the centre of the transmitter with radius r_t at initial time $t_0 = 0$. From [17], the initial conditions for an **A** molecule and a **B** molecule can be expressed as

$$p_A(r, \theta, t \rightarrow 0 | r_0) = \delta(\vec{r} - \vec{r}_0), \text{ and } p_B(r, \theta, t \rightarrow 0 | r_0) = 0, \quad (1)$$

where $p_A(r, \theta, t | r_0)$ and $p_B(r, \theta, t | r_0)$ are the probability densities of finding an **A** molecule and a **B** molecule located at (r, θ, λ) and time t with its original coordinates $(r_0, \theta_0, \lambda_0)$. The first boundary conditions for an **A** molecule and a **B** molecule are given as

$$\lim_{r \rightarrow \infty} p_A(r, \theta, t | r_0) = 0, \text{ and } \lim_{r \rightarrow \infty} p_B(r, \theta, t | r_0) = 0. \quad (2)$$

2) *Diffusion*: Once released in the environment, molecules will diffuse via random collisions with other molecules [18]. The diffusion coefficient D (m^2s^{-1}) is assumed to be constant for a sufficiently low concentration of messenger molecules [15]. During the propagation, **A** molecules will undergo the first-order chemical reaction $A \rightarrow B$ with reaction rate k_F (s^{-1}), and the expected dynamics are then [16, Eq. (5)]

$$\frac{\partial p_A(r, \theta, t | r_0)}{\partial t} = D \nabla^2 p_A(r, \theta, t | r_0) + g(r_0, \theta_0, t_0) - k_F p_A(r, \theta, t | r_0), \quad (3)$$

and

$$\frac{\partial p_B(r, \theta, t | r_0)}{\partial t} = D \nabla^2 p_B(r, \theta, t | r_0) + g(r_0, \theta_0, t_0) + k_F p_A(r, \theta, t | r_0), \quad (4)$$

where

$$g(r_0, \theta_0, t_0) = -\frac{\delta(r - r_0)\delta(\cos\theta - 1)\delta(t - 0)}{2\pi r_0^2}. \quad (5)$$

3) *Reception*: Arrived molecules are absorbed by receptors at the surface of the receiver with absorption rate k_1 (ms^{-1}). No molecule has arrived at the receiver at $t = 0$, thus, the second initial conditions for an **A** molecule and a **B** molecule at $r = r_r$ are written as

$$p_A(r_r, \theta, 0|r_0) = 0, \text{ and } p_B(r_r, \theta, 0|r_0) = 0. \quad (6)$$

The second boundary conditions for an **A** molecule and a **B** molecule at $r = r_r$ [16, Eq. (7)] are

$$D \frac{\partial p_A(r, \theta, t|r_0)}{\partial \vec{n}} \Big|_{r=r_r^+} = k_1 p_A(r_r, \theta, t|r_0), \quad (7)$$

and

$$D \frac{\partial p_B(r, \theta, t|r_0)}{\partial \vec{n}} \Big|_{r=r_r^+} = k_1 p_B(r_r, \theta, t|r_0), \quad (8)$$

where \vec{n} is the unit normal vector on the surface of the receiver.

B. Spherically Symmetric Scenario

In the spherically symmetric scenario, the emitting point transmitter is treated as a random point over the shell of radius r_0 concentric with the receiver. Thus, the molecules are released from any direction at a distance r_0 from the centre of the fixed receiver with equal likelihood [19].

1) *Emission*: For simplification, we assume $t_0 = 0$, and a fixed number of **A** molecules are released into the channel from the transmitter with radius r_t at time $t = 0$. The initial conditions for an **A** molecule and a **B** molecule are expressed as [19, Eq. (3.61)]

$$C_A(r, t \rightarrow 0|r_0) = \frac{1}{4\pi r_0^2} \delta(r - r_0), \text{ and } C_B(r, t \rightarrow 0|r_0) = 0, \quad (9)$$

where $C_A(r, t|r_0)$ and $C_B(r, t|r_0)$ are the probability densities of finding an **A** molecule and a **B** molecule at time t and the distance r with initial distance r_0 . The first boundary conditions for an **A** molecule and a **B** molecule are written as [8, Eq. (2)]

$$\lim_{r \rightarrow \infty} C_A(r, t|r_0) = 0, \text{ and } \lim_{r \rightarrow \infty} C_B(r, t|r_0) = 0. \quad (10)$$

2) *Diffusion*: During propagation, the **A** molecules will react with reaction rate k_F (s^{-1}) to generate **B** molecules. From Fick's Second Law [19, Eq. (3.67)], the expected propagation channel model can be expressed as

$$\frac{\partial(r \cdot C_A(r, t|r_0))}{\partial t} = D \frac{\partial^2(r \cdot C_A(r, t|r_0))}{\partial r^2} - k_F r C_A(r, t|r_0), \quad (11)$$

and

$$\frac{\partial(r \cdot C_B(r, t|r_0))}{\partial t} = D \frac{\partial^2(r \cdot C_B(r, t|r_0))}{\partial r^2} + k_F r C_A(r, t|r_0). \quad (12)$$

C. Reception

Arrived molecules are absorbed by receptors on the surface of the receiver with absorption rate k_1 (ms^{-1}). From [8, Eq. (4)], the second initial conditions for an **A** molecule and a **B** molecule at $r = r_r$ are expressed as

$$C_A(r_r, 0|r_0) = 0, \text{ and } C_B(r_r, 0|r_0) = 0. \quad (13)$$

From [8, Eq. (5)], the second boundary conditions are

$$D \frac{\partial(C_A(r, t|r_0))}{\partial r} \Big|_{r=r_r^+} = k_1 C_A(r_r, t|r_0), \quad (14)$$

and

$$D \frac{\partial(C_B(r, t|r_0))}{\partial r} \Big|_{r=r_r^+} = k_1 C_B(r_r, t|r_0). \quad (15)$$

III. OBSERVATIONS AT TRANSMITTER & RECEIVER

In this section, the time-varying spatial distributions and the expected numbers of **A** molecules and **B** molecules with a general first-order chemical reaction during propagation, inside the transmitter as well as at the surface of the partially absorbing receiver, are derived in both spherically asymmetric and spherically symmetric scenarios. Furthermore, the spatial distributions and the expected numbers of **A** molecules and **B** molecules are simplified for the special case of a fully absorbing receiver.

A. Transmitter Observations with Spherical Asymmetry

The time-varying spatial distributions of messenger molecules and their products are crucial to capture the molecule observations for a diffusive MC system and are solved in the following theorem.

Theorem 1: The time-varying distributions of **A** molecules and **B** molecules, with a first-order chemical reaction during propagation and a partially absorbing receiver, located at (r, θ, λ) and time t are expressed as

$$\begin{aligned} p_A(r, \theta, t|r_0) &= \frac{e^{-k_F t}}{2\pi^2 r_r^2} \sum_{l=0}^{\infty} (2l+1) P_l(\cos(\theta)) \int_0^{\infty} \frac{\psi_l(r) \psi_l(r_0)}{N_{l^2}} e^{-Dz^2 t} dz, \end{aligned} \quad (16)$$

and

$$\begin{aligned} p_B(r, \theta, t|r_0) &= \frac{1 - e^{-k_F t}}{2\pi^2 r_r^2} \sum_{l=0}^{\infty} (2l+1) P_l(\cos(\theta)) \times \\ &\quad \int_0^{\infty} \frac{\psi_l(r) \psi_l(r_0)}{N_{l^2}} e^{-Dz^2 t} dz, \end{aligned} \quad (17)$$

with

$$\begin{aligned} \psi_l(r) &= (zr_r)^2 \left\{ [j_l(zr) y_l'(zr_r) - y_l(zr) j_l'(zr_r)] \right. \\ &\quad \left. - \frac{k_1}{Dz} [j_l(zr) y_l(zr_r) - y_l(zr) j_l(zr_r)] \right\}, \end{aligned} \quad (18)$$

and

$$\begin{aligned} N_{l^2} &= (zr_r)^2 \left\{ \left[\frac{k_1}{Dz} j_l(zr_r) - j_l'(zr_r) \right]^2 \right. \\ &\quad \left. + \left[\frac{k_1}{Dz} y_l(zr_r) - y_l'(zr_r) \right]^2 \right\}, \end{aligned} \quad (19)$$

where the Legendre polynomials are

$$P_n(x) = \frac{1}{2^n n!} \frac{d^n}{dx^n} [(x^2 - 1)^n], \quad (20)$$

and the spherical Bessel functions j_l and y_l are

$$j_l(x) = (-x)^l \left(\frac{1}{x} \frac{d}{dx} \right)^l \frac{\sin x}{x}, \text{ and } y_l(x) = -(-x)^l \left(\frac{1}{x} \frac{d}{dx} \right)^l \frac{\cos x}{x}. \quad (21)$$

Proof: See the Appendix.

Lemma 1: In the case of perfect absorption, i.e., as $k_1 \rightarrow \infty$, the time-varying distributions of **A** molecules and **B** molecules are given by

$$p_A(r, \theta, t|r_0) = \frac{e^{-k_{\text{FT}}t}}{2\pi^2} \sum_{l=0}^{\infty} (2l+1) P_l(\cos(\theta)) \times \int_0^{\infty} \frac{\Phi(r)\Phi(r_0)}{[j_l(zr_r)]^2 + [y_l(zr_r)]^2} z^2 e^{-Dz^2t} dz, \quad (22)$$

and

$$p_B(r, \theta, t|r_0) = \frac{1 - e^{-k_{\text{FT}}t}}{2\pi^2} \sum_{l=0}^{\infty} (2l+1) P_l(\cos(\theta)) \times \int_0^{\infty} \frac{\Phi(r)\Phi(r_0)}{[j_l(zr_r)]^2 + [y_l(zr_r)]^2} z^2 e^{-Dz^2t} dz, \quad (23)$$

where

$$\Phi(r) = [j_l(zr)y_l(zr_r) - y_l(zr)j_l(zr_r)]. \quad (24)$$

Compared with the distance between the transmitter and the receiver, the radius of the transmitter is assumed to be small enough to ignore the change of time-varying spatial distributions for **A** molecules and **B** molecules inside it. In other words, the time-varying spatial distribution inside the transmitter can be approximated as the time-varying spatial distribution at the centre of the transmitter.

Based on the multiplexing between their time-varying spatial distributions and the sphere volume formula $V = \frac{4}{3}\pi r_t^3$ (V is the sphere-volume), the expected numbers of molecules inside the transmitter can be derived in the following theorem.

Theorem 2: The expected numbers of **A** molecules and **B** molecules, with a first-order chemical reaction during propagation, inside a passive transmitter with a partially absorbing receiver at time t are expressed as

$$N_A^{\text{TX}}(t|r_0) = e^{-k_{\text{FT}}t} \frac{2N_{\text{TX}}r_t^3}{3\pi r_r^2} \sum_{l=0}^{\infty} (2l+1) \times \int_0^{\infty} \frac{[\psi_l(r_0)]^2}{N_l^2} e^{-Dz^2t} dz, \quad (25)$$

and

$$N_B^{\text{TX}}(t|r_0) = (1 - e^{-k_{\text{FT}}t}) \frac{2N_{\text{TX}}r_t^3}{3\pi r_r^2} \sum_{l=0}^{\infty} (2l+1) \times \int_0^{\infty} \frac{[\psi_l(r_0)]^2}{N_l^2} e^{-Dz^2t} dz, \quad (26)$$

where $P_l(\cos(\theta_0)) = 1$ and N_{TX} is the number of molecules released.

Lemma 2: In the case of perfect absorption, i.e., as $k_1 \rightarrow \infty$, the expected numbers of **A** molecules and **B** molecules are given by

$$N_A^{\text{TX}}(t|r_0) = e^{-k_{\text{FT}}t} \frac{2N_{\text{TX}}r_t^3}{3\pi} \sum_{l=0}^{\infty} (2l+1) \times \int_0^{\infty} \frac{z^2 e^{-Dz^2t} [\Phi(r_0)]^2}{[j_l(zr_r)]^2 + [y_l(zr_r)]^2} dz, \quad (27)$$

and

$$N_B^{\text{TX}}(t|r_0) = (1 - e^{-k_{\text{FT}}t}) \frac{2N_{\text{TX}}r_t^3}{3\pi} \sum_{l=0}^{\infty} (2l+1) \times \int_0^{\infty} \frac{z^2 e^{-Dz^2t} [\Phi(r_0)]^2}{[j_l(zr_r)]^2 + [y_l(zr_r)]^2} dz. \quad (28)$$

B. Receiver Observations with Spherical Asymmetry

The time-varying spatial distributions of **A** molecule and **B** molecule over the surface of the partially absorbing receiver based on (16) and (17) are

$$p_A(r_r, \theta, t|r_0) = \frac{e^{-k_{\text{FT}}t}}{2\pi^2 r_r^2} \sum_{l=0}^{\infty} (2l+1) P_l(\cos(\theta)) \times \int_0^{\infty} \frac{\psi_l(r_0)}{N_l^2} e^{-Dz^2t} dz, \quad (29)$$

and

$$p_B(r_r, \theta, t|r_0) = \frac{1 - e^{-k_{\text{FT}}t}}{2\pi^2 r_r^2} \sum_{l=0}^{\infty} (2l+1) P_l(\cos(\theta)) \times \int_0^{\infty} \frac{\psi_l(r_0)}{N_l^2} e^{-Dz^2t} dz, \quad (30)$$

where $\psi_l(r_r) = 1$ in [16, Eq. (12)].

The hitting probabilities of molecules is the reaction rate when the molecules hit the surface of the receiver and are absorbed. The hitting probability of the molecules over the surface of an absorbing receiver is [19, Eq. (3.106)]

$$K(\theta, t|r_0) = 4\pi r_r^2 k_1 p(r_r, \theta, t|r_0), \quad (31)$$

where $4\pi r_r^2$ is the area of the receiver's surface. The hitting probabilities of **A** molecule and **B** molecule over the surface of an absorbing receiver are expressed as

$$K_A(\theta, t|r_0) = \frac{2k_1}{\pi} \int_0^{\infty} \frac{\psi_0(r_0)}{N_0^2} e^{-(Dz^2 + k_{\text{FT}})t} dz, \quad (32)$$

and

$$K_B(\theta, t|r_0) = \frac{2k_1}{\pi} \int_0^{\infty} \frac{\psi_0(r_0)}{N_0^2} (1 - e^{-k_{\text{FT}}t}) e^{-Dz^2t} dz, \quad (33)$$

where the Legendre polynomials have the orthogonality property over the sphere.

The expected numbers of molecules over the surface of a partially absorbing receiver can be calculated using the following equation [19, Eq. (3.109)]

$$N(t|r_0) = N_{\text{TX}} \int_0^t K(\theta, t'|r_0) dt'. \quad (34)$$

By substituting (32) and (33) into (34), the expected numbers of **A** molecules and **B** molecules at the surface of the receiver can be solved in the following theorem.

Theorem 3: The expected numbers of **A** molecules and **B** molecules, with a first-order chemical reaction during propagation, at the surface of a partially absorbing receiver at time t are given by

$$N_A^{\text{RX}}(t|r_0) = \frac{2N_{\text{TX}}k_1}{\pi} \int_0^\infty \frac{\psi_0(r_0)}{N_{0^2}} \frac{1 - e^{-(Dz^2+k_F)t}}{Dz^2 + k_F} dz, \quad (35)$$

and

$$N_B^{\text{RX}}(t|r_0) = \frac{2N_{\text{TX}}k_1}{\pi} \int_0^\infty \frac{\psi_0(r_0)}{N_{0^2}} \times \left[\frac{1 - e^{-Dz^2t}}{Dz^2} - \frac{1 - e^{-(Dz^2+k_F)t}}{Dz^2 + k_F} \right] dz. \quad (36)$$

Lemma 3: In the case of perfect absorption, i.e., as $k_1 \rightarrow \infty$, the expected numbers of **A** molecules and **B** molecules are given by

$$N_A^{\text{RX}}(r_r, \theta, t|r_0) = \frac{2N_{\text{TX}}Dr_r}{\pi r_0} \int_0^\infty z \sin[z(r_0 - r_r)] \frac{1 - e^{-(Dz^2+k_F)t}}{Dz^2 + k_F} dz, \quad (37)$$

and

$$N_B^{\text{RX}}(r_r, \theta, t|r_0) = \frac{2N_{\text{TX}}Dr_r}{\pi r_0} \int_0^\infty z \sin[z(r_0 - r_r)] \times \left[\frac{1 - e^{-Dz^2t}}{Dz^2} - \frac{1 - e^{-(Dz^2+k_F)t}}{Dz^2 + k_F} \right] dz. \quad (38)$$

C. Receiver Observations with Spherical Symmetry

In the spherical symmetry scenario, we can simplify the analytical results, as they are special cases for the spherically asymmetric scenario. The time-varying spatial distributions of messenger molecules and their products are solved in the following theorem.

Theorem 4: The time-varying distributions of **A** molecule and **B** molecule, with a first-order chemical reaction during propagation and a partially absorbing receiver, at a distance r and time t are expressed as

$$C_A(r_r, t|r_0) = \frac{e^{-k_F t}}{4\pi r r_0} \times \left\{ \frac{1}{\sqrt{4\pi D t}} \left[e^{-\frac{(r-r_0)^2}{4Dt}} + e^{-\frac{(r+r_0-2r_r)^2}{4Dt}} \right] - \frac{D + k_1 r_r}{Dr_r} e^{\left(\frac{D+k_1 r_r}{Dr_r}\right)^2 Dt + \frac{D+k_1 r_r}{Dr_r} (r+r_0-2r_r)} \times \operatorname{erfc} \left(\frac{D + k_1 r_r}{Dr_r} \sqrt{Dt} + \frac{r + r_0 - 2r_r}{\sqrt{4Dt}} \right) \right\}, \quad (39)$$

and

$$C_B(r_r, t|r_0) = \frac{1 - e^{-k_F t}}{4\pi r r_0} \times \left\{ \frac{1}{\sqrt{4\pi D t}} \left[e^{-\frac{(r-r_0)^2}{4Dt}} + e^{-\frac{(r+r_0-2r_r)^2}{4Dt}} \right] - \frac{D + k_1 r_r}{Dr_r} e^{\left(\frac{D+k_1 r_r}{Dr_r}\right)^2 Dt + \frac{D+k_1 r_r}{Dr_r} (r+r_0-2r_r)} \times \operatorname{erfc} \left(\frac{D + k_1 r_r}{Dr_r} \sqrt{Dt} + \frac{r + r_0 - 2r_r}{\sqrt{4Dt}} \right) \right\}. \quad (40)$$

Proof: Analogous to Appendix A in [8].

Lemma 4: In the case of perfect absorption, i.e., as $k_1 \rightarrow \infty$, the time-varying distributions of **A** molecules and **B** molecules are given by

$$C_A(r, t|r_0) = \frac{e^{-k_F t}}{4\pi r r_0 \sqrt{4\pi D t}} \left[e^{-\frac{(r-r_0)^2}{4Dt}} - e^{-\frac{(r+r_0-2r_r)^2}{4Dt}} \right], \quad (41)$$

and

$$C_B(r, t|r_0) = \frac{1 - e^{-k_F t}}{4\pi r r_0 \sqrt{4\pi D t}} \left[e^{-\frac{(r-r_0)^2}{4Dt}} - e^{-\frac{(r+r_0-2r_r)^2}{4Dt}} \right]. \quad (42)$$

The hitting probabilities of **A** molecule and **B** molecule at the fully absorbing receiver surface are derived based on (31)

$$K_A(\Omega_r, t|r_0) = e^{-k_F t} \frac{r_r}{r_0} \frac{r_0 - r_r}{t} \frac{1}{\sqrt{4\pi D t}} e^{-\frac{(r_0-r_r)^2}{4Dt}}, \quad (43)$$

and

$$K_B(\Omega_r, t|r_0) = (1 - e^{-k_F t}) \frac{r_r}{r_0} \frac{r_0 - r_r}{t} \frac{1}{\sqrt{4\pi D t}} e^{-\frac{(r_0-r_r)^2}{4Dt}}. \quad (44)$$

By substituting (43) and (44) into (34), the expected numbers of **A** molecules and **B** molecules at the receiver are solved in the following theorem.

Theorem 5: The expected numbers of **A** molecules and **B** molecules, with a first-order chemical reaction during propagation, at the surface of a fully absorbing receiver at time t are given by

$$N_A^{\text{Sym}}(\Omega_r, t|r_0) = N_{\text{TX}} \left\{ \frac{r_r}{r_0} e^{-\sqrt{\frac{k_F}{D}}(r_0-r_r)} - \frac{r_r}{2r_0} e^{-(r_0-r_r)\sqrt{\frac{k_F}{D}}} \operatorname{erfc} \left(\sqrt{k_F t} - \frac{r_0 - r_r}{\sqrt{4Dt}} \right) + \frac{r_r}{2r_0} e^{+(r_0-r_r)\sqrt{\frac{k_F}{D}}} \operatorname{erfc} \left(\sqrt{k_F t} + \frac{r_0 - r_r}{\sqrt{4Dt}} \right) \right\}, \quad (45)$$

and

$$N_B^{\text{Sym}}(\Omega_r, t|r_0) = N_{\text{TX}} \left\{ \frac{r_r}{r_0} \operatorname{erfc} \left(\frac{r_0 - r_r}{\sqrt{4Dt}} \right) - \frac{r_r}{r_0} e^{-\sqrt{\frac{k_F}{D}}(r_0-r_r)} + \frac{r_r}{2r_0} e^{-(r_0-r_r)\sqrt{\frac{k_F}{D}}} \operatorname{erfc} \left(\sqrt{k_F t} - \frac{r_0 - r_r}{\sqrt{4Dt}} \right) - \frac{r_r}{2r_0} e^{+(r_0-r_r)\sqrt{\frac{k_F}{D}}} \operatorname{erfc} \left(\sqrt{k_F t} + \frac{r_0 - r_r}{\sqrt{4Dt}} \right) \right\}, \quad (46)$$

respectively.

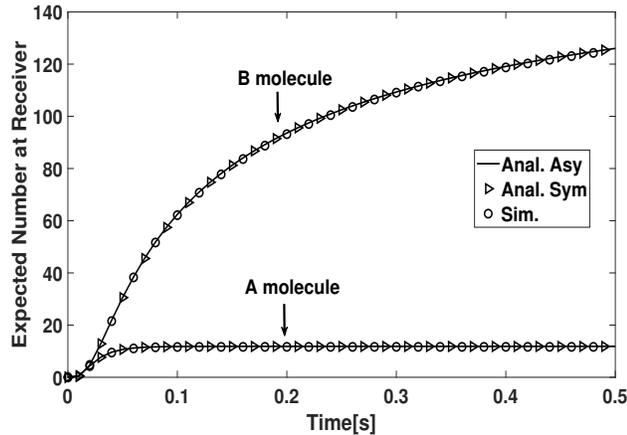
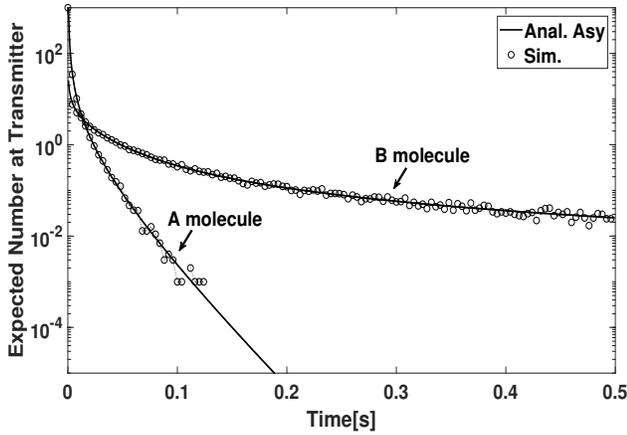


Fig. 2. The expected numbers of **A** molecules and **B** molecules at the transmitter and the receiver.

IV. NUMERICAL RESULTS

We verify the analytical results of the expected numbers of **A** molecules and **B** molecules inside the passive transmitter as well as at the surface of the fully absorbing receiver in the spherically asymmetric scenario and that at the fully absorbing receiver surface in both spherically asymmetric and spherically symmetric scenarios via particle-based simulation [20]. For all figures in this section, we set the fixed parameters as: $r_0 = 5 \mu\text{m}$, $r_r = 1 \mu\text{m}$, $r_t = 0.5 \mu\text{m}$, $D = 10^{-10} \text{m}^2\text{s}^{-1}$ and $N = 10^3$. Each figure contains two subplots for the transmitter and the receiver respectively. In Fig. 2, the analytical results of the expected numbers of molecules in spherically asymmetric and spherically symmetric scenarios are abbreviated as “Anal. Asy.” and “Anal. Sym.”, while the corresponding simulation results are abbreviated as “Sim.”, with arrows indicating **A** molecule and **B** molecule. In Fig. 3, the analytical results of expected numbers of **A** molecules and **B** molecules are abbreviated as “Anal. A” and “Anal. B” with arrows indicating different reaction rates in the two subplots.

Fig. 2 plots the expected numbers of **A** molecules and **B** molecules inside the passive transmitter as well as at the surface of the fully absorbing receiver in both spherically

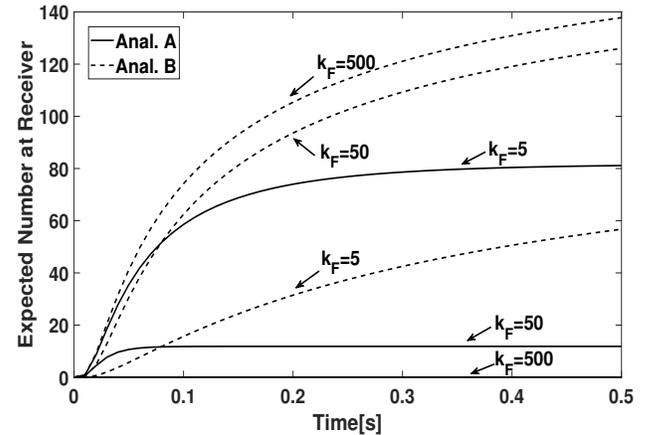
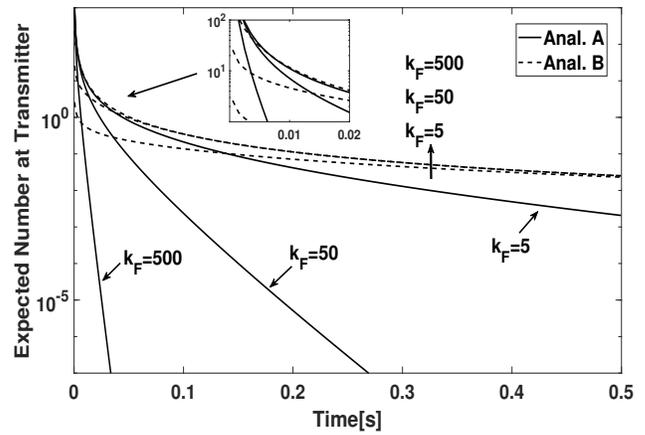


Fig. 3. The expected numbers of **A** molecules and **B** molecules for various reaction rate at the transmitter and the receiver. For $k_F = 500$, the stable value of **A** molecule is as small as 0.05.

asymmetric and spherically symmetric scenarios. We fix the reaction rate to be $k_F = 50\text{s}^{-1}$. As shown in the figure, the expected number of both molecules in two scenarios using analytical results are close to the simulation curves. The expected numbers of **A** molecules and **B** molecules decrease inside the transmitter and increase at the surface of the receiver with increasing time, as predicted by (27), (28), (37), (38), (45) and (46). Compared with **B** molecules, the expected number of **A** molecules has a shorter tail at the transmitter and lower stable value at the receiver due to the first-order chemical reaction during propagation.

Fig. 3 examines the impact of the reaction rate on the expected numbers of **A** molecules and **B** molecules inside the passive transmitter as well as at the surface of the fully absorbing receiver. At the transmitter side, the expected number of **A** molecules decreases faster whereas **B** molecules decreases slower with increasing reaction rate k_F . At the receiver side, the expected number of **A** molecules reaches a lower stable value within shorter time whereas the expected number of **B** molecules undergoes a higher growing rate with increasing reaction rate k_F . At both sides, the gap between **A** molecules and **B** molecules becomes larger with growing reaction rate

k_F and growing time. The different impact of the reaction rate k_F on **A** molecules and **B** molecules reveals the potential difference in transmitter parameter estimation and receiver parameter estimation by using the combination of observations of both types of molecules.

V. CONCLUSION

In this paper, we modeled a diffusive MC system with a partially absorbing receiver and a general first-order chemical reaction during propagation in both spherically asymmetric and spherically symmetric scenarios. We characterized the time-varying spatial distributions and the expected numbers of messenger molecules and their products inside the passive transmitter as well as at the surface of the partially absorbing receiver in both scenarios. The spatial distributions and the expected numbers were simplified and derived in the special case of a fully absorbing receiver. Our analytical expressions were validated by using particle-based simulations and revealed the effect of the reaction rate on the transmitter and the receiver observations. Our ongoing work is to estimate the environmental parameters at the transmitter as well as at the receiver and considering the usage of both types of molecules in a dynamic environment. The analytical framework presented in this paper can also be a foundation for the precise design of an adaptive diffusive molecular communication system in more complex environments.

APPENDIX

Proof of Theorem 1

The time-varying spatial distributions of molecules for a diffusive MC system with a partially absorbing receiver and without first-order chemical reaction during propagation is presented as [16, eq.(9)]

$$\begin{aligned} p(r, \theta, t|r_0) &= \frac{1}{2\pi^2 r_r^2} \sum_{l=0}^{\infty} (2l+1) P_l(\cos(\theta)) \int_0^{\infty} \frac{\psi_l(r)\psi_l(r_0)}{N_l^2} e^{-Dz^2 t} dz. \end{aligned} \quad (47)$$

During propagation, the first-order chemical reaction during propagation is given by

$$\frac{dp_A(r, \theta, t|r_0)}{dt} = -k_F p_A(r, \theta, t|r_0), \quad (48)$$

and none of the **A** molecule undergo the first-order chemical reaction during propagation process as $t \rightarrow 0$, so

$$p_A(r, \theta, t \rightarrow 0|r_0) = p(r, \theta, t|r_0), \quad (49)$$

Hence, the time-varying spatial distribution of **A** molecule is solved as below

$$\begin{aligned} p_A(r, \theta, t|r_0) &= e^{-k_F t} p_A(r, \theta, t \rightarrow 0|r_0) \\ &= e^{-k_F t} p(r, \theta, t|r_0), \end{aligned} \quad (50)$$

and the time-varying spatial distribution of **B** molecule is solved based on the equation

$$p(r, \theta, t|r_0) = p_A(r, \theta, t|r_0) + p_B(r, \theta, t|r_0). \quad (51)$$

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