Stochastic Channel Modeling for Diffusive Mobile Molecular Communication Systems

Arman Ahmadzadeh, Student Member, IEEE, Vahid Jamali, Student Member, IEEE, and Robert Schober, Fellow, IEEE

Abstract

In this paper, we develop a mathematical framework for modeling time-variant stochastic channels in diffusive mobile molecular communication (MC) systems. In particular, we consider a diffusive mobile MC system consisting of a pair of transmitter and receiver nano-machines suspended in a fluid medium with a uniform bulk flow, where we assume that either the transmitter, or the receiver, or both are mobile and we model the mobility of the nano-machines by Brownian motion. The transmitter and receiver nano-machines exchange information via diffusive signaling molecules. Due to the random movements of the transmitter and receiver nano-machines, the statistics of the channel impulse response (CIR) change over time. In this paper, we introduce a statistical framework for characterization of the impulse response of time-variant MC channels. To this end, we derive closed-form expressions for the mean, the autocorrelation function, the cumulative distribution function (CDF), and the probability density function (PDF) of the time-variant CIR. Given the autocorrelation function, we define the coherence time of the time-variant MC channel as a metric for characterization of the variations of the impulse response. The derived CDF is employed for calculation of the outage probability of the system. We also show that under certain conditions, the PDF of the CIR can be accurately approximated by a Log-normal distribution. Given this approximation, we derive a simple model for outdated channel state information (CSI). Moreover, we derive an analytical expression for evaluation of the expected error probability of a simple detector for the considered MC system. In order to investigate the impact of CIR decorrelation over time, we compare the performances of a detector with perfect CSI knowledge and a detector with outdated CSI knowledge. The accuracy of the proposed analytical expressions is verified via particle-based simulation of the Brownian motion.

I. INTRODUCTION

Future synthetic nano-networks are expected to facilitate new revolutionary applications in areas such as biological engineering, healthcare, and environmental engineering [2], [3]. Molecular communication (MC), where molecules are the carriers of information, is one of the most promising candidates for enabling reliable communication between nano-machines in such

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future nano-networks due to its bio-compatibility, energy efficiency, and abundant use in natural biological systems.

Some of the envisioned application areas for synthetic MC systems may require the deployment of mobile nano-machines. For instance, in targeted drug delivery and intracellular therapy applications, it is envisioned that mobile nano-machines carry drug molecules and release them at the desired site of application, see [2, Chapter 1]. As another example, in molecular imaging, a group of mobile bio-nano-machines such as viruses carry green fluorescent proteins (GFPs) to gather information about the environmental conditions from a large area inside a targeted body, see [2, Chapter 1]. For these applications, communication among the nano-machines is needed for efficient operation. In order to establish a reliable communication link between nano-machines, knowledge of the channel statistics is necessary [4]. However, for mobile nano-machines, these statistics change with time, which makes communication even more challenging. Thus, it is crucial to develop a mathematical framework for characterization of the stochastic behaviour of the channel. Stochastic channel models provide the basis for the design of new modulation, detection, and/or estimation schemes for mobile MC systems.

In the MC literature, the problem of mobile MC has been considered in [5]–[13]. However, none of these previous works provided a stochastic framework for the modeling of time-variant channels. In particular, in [5]–[8] it is assumed that only the receiver node is mobile and the channel impulse response (CIR) either changes slowly over time, due to the slow movement of the receiver, as in [6], or it is fixed for a block of symbol intervals and may change slowly from one block to the next; see [7], [8]. In [9] and [10], a three-dimensional random walk model is adopted for modeling the mobility of nano-machines, where it is assumed that information is only exchanged upon the collision of two nano-machines. In particular, Förster resonance energy transfer and a neurospike communication model are considered for information exchange between two colliding nano-machines in [9] and [10], respectively. The authors of [11] proposed a leader-follower model for target detection applications in two-dimensional mobile MC systems. Langevin equations are used to describe the mobility of the nano-machines. There, it is assumed that the information molecules do not diffuse; the leader nano-machine releases signaling molecules that stick to the release site and form a path that the follower nano-machine follows. The mathematical modeling of this non-diffusion communication approach between leader and follower nano-machines is further analyzed in [12]. In the most recent work [13], a one-dimensional random walk model is adopted for modeling the mobility of a point source transmitter and a fully-absorbing point receiver, and the first hitting time distribution of the
released particles is evaluated. In our previous work [14], unlike [5]–[13], we have established the mathematical basis required for analyzing mobile MC systems. We have shown that by appropriately modifying the diffusion coefficient of the signaling molecules, the CIR of a mobile MC system can be obtained from the CIR of the same system with fixed transmitter and receiver.

In this paper, we consider a three-dimensional diffusion model to characterize the movements of both transmitter and receiver nano-machines, where unlike [9]–[12], we assume that nano-machines exchange information via diffusive signaling molecules. Furthermore, unlike [14], we develop a stochastic framework for characterizing the time-variant CIR of the mobile MC system. To the best of the authors’ knowledge, a stochastic channel model for mobile MC systems has not been reported, yet. In particular, this paper makes the following contributions:

1) Expanding upon our preliminary work in [1], we establish a mathematical framework for the characterization of the time-variant CIR of mobile MC systems as a stochastic process, i.e., we introduce a stochastic channel model.

2) We derive closed-form analytical expressions for the first-order (mean) and second-order (autocorrelation function) moments of the time-variant CIR of mobile MC systems. Here, unlike our preliminary work [1], we also include the impact of flow. Equipped with the autocorrelation function of the CIR, we define the coherence time of the channel as the time during which the CIR does not substantially change.

3) We derive a closed-form expression for the cumulative distribution function (CDF) of the CIR. The derived CDF can be employed for calculation of the outage probability of the considered system.

4) We propose a simple model for modeling outdated CSI in mobile MC systems. To this end, we derive a closed-form expression for the probability density function (PDF) of the impulse response of the channel. Subsequently, we show that in a certain regime, the PDF can be accurately approximated by a Log-normal distribution. We quantify the approximation regime and based on the approximated PDF, we derive the proposed model for outdated CSI in mobile MC systems.

5) To evaluate the impact of the CIR decorrelation occurring in mobile MC systems on performance, we derive the expected bit error probability of a simple detector for perfect and outdated CSI knowledge, respectively.

The rest of this paper is organized as follows. In Section II we introduce the system model. In Section III we develop the proposed stochastic channel model. In Section IV we derive closed-form expressions for the mean, the autocorrelation function, the CDF, and the PDF of
the time-variant CIR. Then, in Section V we calculate the expected bit error probability of the considered system for detectors with perfect and outdated CIR knowledge, respectively. Simulation and analytical results are presented in Section VI and conclusion are drawn in Section VII.

II. SYSTEM MODEL

We consider an unbounded three-dimensional fluid environment with constant temperature and viscosity. The receiver is modeled as a passive observer, i.e., as a transparent sphere with radius $a_{rx}$ that diffuses with constant diffusion coefficient $D_{rx}$. Furthermore, we model the transmitter as another transparent sphere with radius $a_{tx}$ that diffuses with constant diffusion coefficient $D_{tx}$. The transmitter employs type $A$ molecules, which we also refer to as $A$ molecules and also as information or signaling molecules, for conveying information to the receiver. We assume that the $A$ molecules are released in the center of the transmitter and that they can leave the transmitter via free diffusion. In particular, we assume that each signaling molecule diffuses with constant diffusion coefficient $D_A$ and the diffusion processes of individual $A$ molecules are independent of each other. Moreover, we assume that interfering $A$ molecules are uniformly distributed in the environment and impair the reception. These noise molecules may originate from natural sources in the environment. Furthermore, we assume that there exists a uniform
flow in the environment, denoted by \( \vec{v} = [v_x, v_y, v_z] \), where \( v_x \), \( v_y \), and \( v_z \) are the components of \( \vec{v} \) in the \( x \), \( y \), and \( z \) directions of a Cartesian coordinate system, respectively.

Due to the Brownian motion and flow, the positions of the transmitter and the receiver change over time. In particular, we denote the time-varying positions of the transmitter and the receiver at time \( t \) by \( \vec{r}_{tx}(t) \) and \( \vec{r}_{rx}(t) \), respectively. Then, we define vector \( \vec{r}(t) = \vec{r}_{rx}(t) - \vec{r}_{tx}(t) \) and denote its magnitude at time \( t \) as \( r(t) \), i.e., \( |\vec{r}(t)| = r(t) \), see Fig. 1. Furthermore, without loss of generality, we assume that at time \( t_0 = 0 \), the transmitter is located at the origin of the Cartesian coordinate system, i.e., \( \vec{r}_{tx}(t_0 = 0) = [0, 0, 0] \), and the receiver is at \( \vec{r}_{rx}(t_0 = 0) = [x_0, 0, 0] \). Thus, \( r(t_0 = 0) = r_0 = x_0 \).

We assume that the information that is sent from the transmitter to the receiver is encoded into a binary sequence of length \( L \), \( \mathbf{b} = [b_1, b_2, \ldots, b_L] \). Here, \( b_j \) is the bit transmitted in the \( j \)th bit interval with \( \Pr(b_j = 1) = P_1 \) and \( \Pr(b_j = 0) = P_0 = 1 - P_1 \), where \( \Pr(\cdot) \) denotes probability. We assume that transmitter and receiver are synchronized, see e.g. [15]. We adopt ON/OFF keying for modulation and a fixed bit interval duration of \( T \) seconds. In particular, the transmitter releases a fixed number of \( A \) molecules, \( N_A \), for transmitting bit “1” at the beginning of a modulation bit interval and no molecules for transmitting bit “0”.

### III. Stochastic Channel Model

In this section, we provide some preliminaries regarding the modeling of time-variant channels in diffusive mobile MC systems. In particular, in Section III-A, we introduce the terminology used for describing the time-variant CIR in the absence of flow. Subsequently, we present a mathematical expression for the CIR. Then, we investigate the impact of flow on the derived CIR expression in detail in Section III-B.

#### A. Impulse Response of Time-Variant MC Channel without Flow

In this subsection, in order to be able to focus on the impact of the mobility of the transmitter and receiver on the CIR, we assume \( \vec{v} = [0, 0, 0] \). We borrow the terminology and the notation for time-variant CIRs from [16, Ch. 5]. There, it is assumed that the impulse response of a classical wireless multipath channel can be characterized by a function \( h^\omega(t, \tau) \), where \( t \) represents the time variation due to the mobility of the receiver and \( \tau \) describes the channel multipath delay for a fixed \( t \). Here, we also adopt this notation and derive \( h^\omega(t, \tau) \) for the problem at hand. In the context of MC, the impulse response of the channel corresponds to the probability of observing a molecule released by the transmitter at the receiver [2].
Let us assume, for the moment, that at the time of release of a given \( A \) molecule at the transmitter, \( r(t) \) is known and given by \( r^* \). Then, the impulse response of the channel, i.e., the probability that a given \( A \) molecule, released at the center of the transmitter at time \( \tau = 0 \), is observed inside the volume of the transparent receiver at time \( \tau > 0 \) can be written as \([17, \text{Eq. (4)}]\)

\[
h^o(\tau|r^*) = \frac{V_{\text{obs}}}{(4\pi D_1 \tau)^{3/2}} \exp \left( \frac{-(r^*)^2}{4D_1 \tau} \right),
\]

where \( V_{\text{obs}} = \frac{4}{3} \pi a_{rx}^3 \) is the volume of the receiver and \( D_1 = D_A + D_{rx} \) is the effective diffusion coefficient capturing the relative motion of the signaling molecules and the receiver, see \([14, \text{Eq. (8)}]\). However, due to the random movements of both the transmitter and the receiver, \( \tilde{r}(t) \) (and consequently \( r(t) \)) change randomly. In particular, for the problem at hand, the PDF of random variable \( \tilde{r}(t) \) is given by

\[
f^{\circ}_{\tilde{r}(t)}(\tilde{r}) = \frac{1}{(4\pi D_2 t)^{3/2}} \exp \left( \frac{-|\tilde{r} - \tilde{r}_0|^2}{4D_2 t} \right),
\]

where \( D_2 = D_{rx} + D_{tx} \) is the effective diffusion coefficient capturing the relative motion of transmitter and receiver, see \([14, \text{Eq. (10)}]\). Thus, for a mobile transmitter and a mobile receiver, the CIR, denoted by \( h^o(t, \tau) \), can be written as

\[
h^o(t, \tau) = \frac{V_{\text{obs}}}{(4\pi D_1 \tau)^{3/2}} \exp \left( \frac{-|\tilde{r}(t)|^2}{4D_1 \tau} \right),
\]

where \( \tilde{r}(t) \) is distributed according to the PDF in \([2]\).

CIR \( h^o(t, \tau) \) completely characterizes the time-variant channel and is a function of both \( t \) and \( \tau \). Variable \( t \) represents the time of release of the molecules at the transmitter, whereas \( \tau \) represents the relative time of observation of the signaling molecules at the receiver for a fixed value of \( t \), cf. Fig. 1. We note that the movement of the receiver is accounted for in \([1]\) via \( D_1 \) as far as its effect on the \( A \) molecules is concerned, and in \([2]\) via \( D_2 \) as far as the relative motion of the transmitter and receiver is concerned. Both effects impact \( h^o(t, \tau) \) in \([3]\). For any given \( \tau \), \( h^o(t, \tau) \) is a stochastic process with random variables \( h^o(t_i, \tau) \), \( i \in \{1, 2, \ldots, n\} \). Specifically, \( h^o(t_i, \tau) \) can be interpreted as a function of random variable \( \tilde{r}(t) \).

**B. Impact of Flow**

In this subsection, we consider the impact of uniform bulk flow on the CIR \( h^o(t, \tau) \). We distinguish between three cases, based on the mobility of the transmitter and the receiver. Let us denote the \( x \), \( y \), and \( z \) coordinates of the position of the transmitter, i.e., the components
of vector \( \bar{r}_{\text{tx}}(t) \), at time \( t \) by \( X_{\text{tx}}(t) \), \( Y_{\text{tx}}(t) \), and \( Z_{\text{tx}}(t) \), respectively. Similarly, the \( x \), \( y \), and \( z \) coordinates of the position of the receiver, i.e., the components of vector \( \bar{r}_{\text{rx}}(t) \), at time \( t \) are denoted by \( X_{\text{rx}}(t) \), \( Y_{\text{rx}}(t) \), and \( Z_{\text{rx}}(t) \), respectively.

1) Mobile Transmitter and Mobile Receiver: In this case, both the transmitter and the receiver, along with the information molecules, move with the bulk flow in the environment. Using a moving reference frame that also moves with the bulk flow, it can be easily verified that the expressions for \( f_{\bar{r}(t)}(\bar{r}) \) and \( h^c(t, \tau) \), i.e., (2) and (3), respectively, are still valid.

2) Mobile Transmitter and Fixed Receiver: In this case, since the receiver is fixed, \( D_1 \) and \( D_2 \) are given by \( D_1 = D_A \) and \( D_2 = D_{\text{tx}} \), respectively. Due to the random walk of the transmitter, and according to the configuration of the transmitter and receiver as shown in Fig. [1] we can write

\[
X_{\text{tx}}(t) \sim \mathcal{N}(v_x t, 2D_{\text{tx}} t), \quad Y_{\text{tx}}(t) \sim \mathcal{N}(v_y t, 2D_{\text{tx}} t), \quad Z_{\text{tx}}(t) \sim \mathcal{N}(v_z t, 2D_{\text{tx}} t),
\]

\[
X_{\text{rx}}(t) = x_0, \quad Y_{\text{rx}}(t) = 0, \quad Z_{\text{rx}}(t) = 0,
\]

where \( \mathcal{N}(\mu, \sigma^2) \) denotes a Gaussian distribution with mean \( \mu \) and variance \( \sigma^2 \). Then, for the components of vector \( \bar{r}(t) = \bar{r}_{\text{tx}}(t) - \bar{r}_{\text{rx}}(t) \), we obtain

\[
X(t) = X_{\text{tx}}(t) - X_{\text{rx}}(t) \sim \mathcal{N}(x_0 - v_x t, 2D_2 t), \quad Y(t) = Y_{\text{tx}}(t) - Y_{\text{rx}}(t) \sim \mathcal{N}(-v_y t, 2D_2 t),
\]

\[
Z(t) = Z_{\text{tx}}(t) - Z_{\text{rx}}(t) \sim \mathcal{N}(-v_z t, 2D_2 t).
\]

Given (5), the PDF of random variable \( \bar{r}(t) \) can be written as

\[
f_{\bar{r}(t)}(\bar{r}) = \frac{1}{(4\pi D_{\text{tx}} t)^{3/2}} \exp \left( \frac{-|\bar{r} - (\bar{r}_0 - \bar{v} t)|^2}{4D_{\text{tx}} t} \right).
\]

In a similar way, the corresponding impulse response of the time-variant MC channel can be written as

\[
h^{\text{rx}}(t, \tau) = \frac{V_{\text{obs}}}{(4\pi D_A \tau)^{3/2}} \exp \left( \frac{-|\bar{r}(t) - \bar{v} \tau|^2}{4D_A t} \right).
\]

The superscript “rx” in \( f_{\bar{r}(t)}(\bar{r}) \) and \( h^{\text{rx}}(t, \tau) \) emphasizes that the receiver is fixed.

3) Fixed Transmitter and Mobile Receiver: In the third case, the transmitter node is fixed while the receiver is mobile, and, as a result, the corresponding effective diffusion coefficients are given by \( D_1 = D_A + D_{\text{rx}} \) and \( D_2 = D_{\text{rx}} \). Now, using a similar approach as in (4) and (5), we can write the PDF of random variable \( \bar{r}(t) \) as follows

\[
f_{\bar{r}(t)}(\bar{r}) = \frac{1}{(4\pi D_{\text{rx}} t)^{3/2}} \exp \left( \frac{-|\bar{r} - (\bar{r}_0 + \bar{v} t)|^2}{4D_{\text{rx}} t} \right),
\]
where the superscript “tx” indicates that the transmitter node is fixed. Furthermore, we denote the impulse response of the time-variant channel for this scenario by \( h^{tx}(t, \tau) \). For calculation of \( h^{tx}(t, \tau) \), however, since both the information molecules and the receiver are equally affected by the flow, by using a moving reference frame, it can be easily verified that \( h^{tx}(t, \tau) = h^\circ(t, \tau) \), i.e.,

\[
h^{tx}(t, \tau) = \frac{V_{\text{obs}}}{(4\pi D_1 \tau)^{3/2}} \exp \left( \frac{-|r(t)|^2}{4D_1 \tau} \right). \tag{9}
\]

By comparing the PDFs of random variable \( r(t) \) in (2), (6), and (8), and similarly, the impulse responses of the time-variant MC channel in (3), (7), and (9), we can observe that the major difference between the respective equations appears in the argument of the exponential functions. Thus, to facilitate our subsequent analysis, we introduce general expressions for the PDF of \( r(t) \) and the time-variant CIR unifying all considered cases. In particular, we model the PDF of random variable \( r(t) \) as

\[
f_{r(t)}(r) = \frac{1}{(4\pi D_2 t)^{3/2}} \exp \left( -\frac{|r - (r_0 - \bar{v}^* t)|^2}{4D_2 t} \right), \tag{10}
\]

and the impulse response of the time-variant MC channel as

\[
h(t, \tau) = \frac{V_{\text{obs}}}{(4\pi D_1 \tau)^{3/2}} \exp \left( -\frac{|r(t) - \bar{v}' \tau|^2}{4D_1 \tau} \right), \tag{11}
\]

where \( \bar{v}^*, \bar{v}', D_1, \) and \( D_2 \) are defined in Table I for different mobility scenarios. In Table I, “TX” and “RX” stand for transmitter and receiver, respectively. We also note that for the case of fixed TX and RX (with and without flow), \( f_{r(t)}(r) \to \delta(r - r_0) \), where \( \delta(\cdot) \) is the Dirac delta function. Furthermore, for conciseness of presentation, we introduce the following notations:

\[
\varphi = \frac{V_{\text{obs}}}{(4\pi D_1 \tau)^{3/2}}, \lambda(t) = \frac{1}{(4\pi D_2 t)^{3/2}}, \alpha = \frac{1}{4D_1 \tau}, \beta(t) = \frac{1}{4D_2 t}. \tag{12}
\]

**IV. Statistical Analysis of Time-Variant MC Channel**

In this section, we analyze the statistical averages of the considered time-variant channel, i.e., the statistical averages of the random process \( h(t, \tau) \). In particular, we derive closed-form expressions for the mean and autocorrelation function of \( h(t, \tau) \). Furthermore, we derive closed-form expressions for the CDF and the PDF of the time-variant CIR, and provide a mathematical model for outdated CSI.
TABLE I
VALUES OF $\bar{\mathbf{v}}^*, \bar{\mathbf{v}}', D_1,$ AND $D_2$

| Mobility Scenario                  | $\bar{\mathbf{v}}^*$ | $\bar{\mathbf{v}}'$ | $D_1$  | $D_2$  |
|-----------------------------------|-----------------------|-----------------------|--------|--------|
| No flow with fixed TX and fixed RX| $\vec{0}$             | $\vec{0}$             | $D_A$  | 0      |
| No flow with mobile TX and fixed RX| $\vec{0}$             | $\vec{0}$             | $D_A$  | $D_{tx}$|
| No flow with fixed TX and mobile RX| $\vec{0}$             | $\vec{0}$             | $D_A + D_{rx}$ | $D_{tx}$|
| No flow with mobile TX and mobile RX| $\vec{0}$             | $\vec{0}$             | $D_A + D_{rx}$ | $D_{tx} + D_{tx}$|
| Flow with fixed TX and fixed RX   | $\vec{0}$             | $\vec{0}$             | $D_A$  | 0      |
| Flow with mobile TX and fixed RX  | $\vec{v}$             | $\vec{0}$             | $D_A$  | $D_{tx}$|
| Flow with fixed TX and mobile RX  | $\vec{v}$             | $\vec{0}$             | $D_A$  | $D_{tx}$|
| Flow with mobile TX and mobile RX | $\vec{0}$             | $\vec{0}$             | $D_A + D_{rx}$ | $D_{tx} + D_{tx}$|

A. Statistical Averages of Time-Variant MC Channel

Let us start with the mean of $h(t, \tau)$ for arbitrary time $t$, denoted by $m(t)$. Then, $m(t)$ can be evaluated as

$$ m(t) = E\{h(t, \tau)\} = \int_{\mathbb{R}^3} h(t, \tau) \bigg|_{\mathbf{r}(t) = \mathbf{r}} \times f_{\mathbf{r}(t)}(\mathbf{r}) \, d\mathbf{r}, $$

where $E(\cdot)$ denotes expectation. The solution to (13) is provided in the following theorem.

**Theorem 1 (Mean of Time-variant MC Channel):** The mean of the impulse response of a time-variant MC channel including the effects of uniform bulk flow, and diffusive passive transmitter and receiver nano-machines with diffusion coefficients $D_{tx}$ and $D_{rx}$, respectively, which communicate via signaling molecules with diffusion coefficient $D_A$, is given by

$$ m(t) = \varphi \lambda(t) \int_{\mathbb{R}^3} e^{-\alpha|\mathbf{r}-\bar{\mathbf{v}}^*\tau|^2} \times e^{-\beta(t)|\mathbf{r}-\bar{\mathbf{v}}'|^2} \bigg|_{\mathbf{r}(t) = \mathbf{r}} \times f_{\mathbf{r}(t)}(\mathbf{r}) \, d\mathbf{r}, $$

where $\varphi \lambda(t)$ denotes the mean of the impulse response of the MC channel.

**Proof:** Substituting (10) and (11) in (13), we can write $m(t)$ as

$$ m(t) = \varphi \lambda(t) \int_{\mathbb{R}^3} e^{-\alpha|\mathbf{r}-\bar{\mathbf{v}}^*\tau|^2} \times e^{-\beta(t)|\mathbf{r}-\bar{\mathbf{v}}'|^2} \bigg|_{\mathbf{r}(t) = \mathbf{r}} \times f_{\mathbf{r}(t)}(\mathbf{r}) \, d\mathbf{r}, $$

where $\varphi \lambda(t)$ denotes the mean of the impulse response of the MC channel.
The three integrals in (15) can be solved independently. Now, using the following definite integral [18, Eq. (3.323.2.10)]

$$\int_{-\infty}^{+\infty} \exp \left(-p^2 x^2 \pm q x \right) \, dx = \exp \left(\frac{q^2}{4p^2}\right) \frac{\sqrt{\pi}}{p},$$

(16)

the integrals in (15) simplify to the expression in (14). This completes the proof.

**Remark 1:** Since \(m(t)\) is a function of \(t\), \(h(t, \tau)\) is a non-stationary stochastic process. In fact, this is due to the assumption of an unbounded environment, as on average the transmitter and the receiver diffuse away from each other and, ultimately, \(h(t, \tau)\) approaches zero as \(t \rightarrow \infty\).

Next, we derive a closed-form expression for the *autocorrelation function* (ACF) of \(h(t, \tau)\) for two arbitrary times \(t_1\) and \(t_2 > t_1\), denoted as \(\phi(t_1, t_2)\). To this end, we write \(\phi(t_1, t_2)\) as follows \(^1\)

$$\phi(t_1, t_2) = \mathbb{E}\{h(t_1, \tau)h(t_2, \tau)\} = \iint_{\bar{\mathcal{R}}_1, \bar{\mathcal{R}}_2 \in \mathbb{R}^3} h(t_1, \tau)|_{\bar{\mathcal{R}}(t) = \bar{\mathcal{R}}_1} \times h(t_2, \tau)|_{\bar{\mathcal{R}}(t) = \bar{\mathcal{R}}_2} \times f_{\bar{\mathcal{R}}(t_1), \bar{\mathcal{R}}(t_2)}(\bar{\mathcal{R}}_1, \bar{\mathcal{R}}_2) \, d\bar{\mathcal{R}}_1 \, d\bar{\mathcal{R}}_2,$$

(17)

where \(f_{\bar{\mathcal{R}}(t_1), \bar{\mathcal{R}}(t_2)}(\bar{\mathcal{R}}_1, \bar{\mathcal{R}}_2)\) is the joint distribution function of random variables \(\bar{\mathcal{R}}(t_1)\) and \(\bar{\mathcal{R}}(t_2)\), which can be written as

$$f_{\bar{\mathcal{R}}(t_1), \bar{\mathcal{R}}(t_2)}(\bar{\mathcal{R}}_1, \bar{\mathcal{R}}_2) = f_{\bar{\mathcal{R}}(t_1)}(\bar{\mathcal{R}}_1)f_{\bar{\mathcal{R}}(t_2)}(\bar{\mathcal{R}}_2 | \bar{\mathcal{R}}_1),$$

(18)

where we used the fact that free diffusion is a memoryless process and, as a result, \(f_{\bar{\mathcal{R}}(t_2)}(\bar{\mathcal{R}}_2 | \bar{\mathcal{R}}_1, \bar{\mathcal{R}}_0) = f_{\bar{\mathcal{R}}(t_2)}(\bar{\mathcal{R}}_2 | \bar{\mathcal{R}}_1)\). Given (18), a closed-form expression of \(\phi(t_1, t_2)\) is provided in the following theorem.

**Theorem 2 (ACF of Time-variant MC Channel):** The ACF of the impulse response of a time-variant MC channel including the effects of uniform bulk flow, and diffusive passive transmitter and receiver nano-machines with diffusion coefficients \(D_{tx}\) and \(D_{rx}\), respectively, which communicate via signaling molecules with diffusion coefficient \(D_A\), is given by

$$\phi(t_1, t_2) = \frac{(2\pi)^3 \varphi^2 \lambda(t_1) \lambda(t_2 - t_1) \exp (\kappa_x + \kappa_y + \kappa_z)}{\left(4 \left(\alpha + \beta(t_1)\right) \left(\alpha + \beta(t_2 - t_1)\right) + \alpha \beta(t_2 - t_1)\right)^{3/2}},$$

(19)

where \(t_1\) and \(t_2 > t_1\) are two arbitrary times and \(\kappa_\zeta\) is defined as \(\kappa_\zeta = \frac{G_\zeta}{W}\) where

$$G_\zeta = -\alpha \left(2\beta(t_2 - t_1) + \alpha \beta(t_1)(x_0 - v_\zeta^* t_1)^2 + \beta(t_2 - t_1) \left(\alpha + \beta(t_1)\right) \left(v_\zeta^*(t_2 - t_1)\right)^2\right)^2,$$

(20)

\(^1\)In our analysis, the definition of the ACF in (17) can be easily extended to \(\phi(t_1, t_2) = \mathbb{E}\{h(t_1, \tau_1)h(t_2, \tau_2)\}\). However, since in Section \(V\) we consider a detector that takes only one sample at a fixed time after the beginning of each modulation interval, for simplicity of presentation, we focus on the case of \(\tau_1 = \tau_2 = \tau\).
of time-variant MC channel. To this end, we first define the normalized autocorrelation

\[ \sigma^2 = \frac{V^2_{\text{obs}}}{(4\pi D_1 \tau)^{3/2} (4\pi (D_1 \tau + 2D_2 t_1))^{3/2}} \exp \left( \frac{-|\eta_0 - \bar{v}^* T - \bar{v}' \tau|^2}{2 (D_1 \tau + 2D_2 t_1)} \right). \] (21)

**Proof:** Please refer to Appendix A.

In the following corollary, we study a special case of \( \phi(t_1, t_2) \) where \( t_2 \to t_1 \), i.e., \( \phi(t_1, t_1) = \mathcal{E} \{ h(t_1, \tau)h(t_1, \tau) \} \), since \( \phi(t_1, t_1) \) cannot be directly obtained from (19) by substituting \( t_2 = t_1 \).

**Corollary 1 (ACF of Time-variant MC Channel for \( t_2 = t_1 \))** In the limit of \( t_2 \to t_1 \), the ACF of \( h(t, \tau) \), i.e., \( \phi(t_1, t_1) \), is given by

\[ \phi(t_1, t_1) = \frac{V^2_{\text{obs}}}{(4\pi D_1 \tau)^{3/2} (4\pi (D_1 \tau + 2D_2 t_1))^{3/2}} \exp \left( \frac{-|\eta_0 - \bar{v}^* T - \bar{v}' \tau|^2}{2 (D_1 \tau + 2D_2 t_1)} \right). \] (21)

**Proof:** In the limit of \( t_2 \to t_1 \), \( \phi(t_1, t_2) \) in (17) becomes

\[ \phi(t_1, t_1) = \mathcal{E} \left\{ h^2(t_1, \tau) \right\} = \int_{\mathbb{R}^3} h^2(t_1, \tau) \bigg|_{\mathbb{R}^3} \times f_{\tilde{r}_1}(\tilde{r}_1) \, d\tilde{r}_1. \] (22)

Substituting (10) and (11) in (22), leads to

\[ \phi(t_1, t_1) = \varphi^2 \lambda(t_1) \int_{\mathbb{R}^3} e^{-2\alpha |\eta_0 - \bar{v}' \tau|^2} \times e^{-\beta(t_1)|\eta_0 - \bar{v}^* n|^2} \, d\tilde{r}_1. \] (23)

Now, expanding the integrand in (23), similar to (15), and using (16), \( \phi(t_1, t_1) \) simplifies to (21).

Given (21), we define the variance of the time-variant MC channel as \( \sigma^2(t) = \phi(t, t) - m^2(t) \).

**B. Coherence Time of Time-variant MC Channel**

In this subsection, we provide an expression for evaluation of the coherence time of the considered time-variant MC channel. To this end, we first define the normalized autocorrelation function of random process \( h(t, \tau) \) as follow:

\[ \rho(t_1, t_2) = \frac{\mathcal{E} \{ h(t_1, \tau)h(t_2, \tau) \}}{\sqrt{\mathcal{E} \{ h^2(t_1, \tau) \} \mathcal{E} \{ h^2(t_2, \tau) \}}} = \frac{\phi(t_1, t_2)}{\sqrt{\phi(t_1, t_1)\phi(t_2, t_2)}}. \] (24)

Now, for time \( t_1 = 0 \), we define the coherence time of the time-variant MC channel, \( T^c \), as the minimum time \( t_2 \) after \( t_1 = 0 \) for which \( \rho(t_1, t_2) \) falls below a certain threshold value \( 0 < \eta < 1 \), i.e.,

\[ T^c = \arg \min_{\forall t_2 > 0} \left( \rho(0, t_2) < \eta \right). \] (25)
We note that the particular choice of $\eta$ is application dependent, as the coherence time of the channel refers to the time during which the channel does not change significantly and the definition of a significant change may vary from one application scenario to another. For example, typical values of $\eta$ reported in the traditional wireless communications literature span the range from 0.5 to 1, [19]–[21], e.g., smaller values of $\eta$ are often employed for resource allocation problems, while larger values of $\eta$ are used for channel estimation problems.

C. CDF of Impulse Response of Time-Variant MC Channel

Now, we are interested in calculating the CDF of the time-variant CIR $h(t, \tau)$ in (11), denoted as $F_{h(t,\tau)}(h)$. Thus, we need to calculate $Pr(h(t, \tau) \leq h)$. The result of this calculation is provided in the following theorem.

**Theorem 3 (CDF of Time-variant MC Channel):** The CDF of the impulse response of a time-variant MC channel including the effects of uniform bulk flow, and diffusive passive transmitter and receiver nano-machines with diffusion coefficients $D_{tx}$ and $D_{rx}$, respectively, which communicate via signaling molecules with diffusion coefficient $D_A$, is given by

\[
F_{h(t,\tau)}(h) = \frac{1}{2} \text{erfc} \left( \frac{\sqrt{\ln \left( \frac{\phi}{\pi} \right) + r_{eq}(t) \sqrt{\alpha}}}{\sqrt{4D_2t\alpha}} \right) + \frac{1}{2} \text{erfc} \left( \frac{\sqrt{\ln \left( \frac{\phi}{\pi} \right) - r_{eq}(t) \sqrt{\alpha}}}{\sqrt{4D_2t\alpha}} \right) \] 
\[+ \frac{\sqrt{D_2t}}{r_{eq}(t)\sqrt{\pi}} \left\{ \exp \left( -\frac{\left( \sqrt{\ln \left( \frac{\phi}{\pi} \right) - r_{eq}(t) \sqrt{\alpha}} \right)^2}{4D_2t\alpha} \right) - \exp \left( -\frac{\left( \sqrt{\ln \left( \frac{\phi}{\pi} \right) + r_{eq}(t) \sqrt{\alpha}} \right)^2}{4D_2t\alpha} \right) \right\}, \tag{26} \]

where erfc($\cdot$) denotes the complementary error function, and we define the equivalent distance $r_{eq}(t) = |\vec{r}_0 - \vec{v}^*t - \vec{v}'\tau|$ for compactness.

**Proof:** Please refer to Appendix B.

**Remark 2:** One immediate application of the derived CDF is the calculation of the outage probability of the considered system. In particular, the outage probability, $P_{\text{out}}$, can be defined as $Pr(h(t, \tau) < h_{\text{min}})$, i.e., the probability that the value of the impulse response of the time-variant channel falls below a minimum threshold. Different criteria can be used for selecting $h_{\text{min}}$, e.g., $h_{\text{min}}$ can be chosen such that it guarantees a minimum bit error probability at the receiver nano-machine. As another application, the derived CDF can be employed for calculation of the average number of successfully transmitted information bits before an outage occurs, denoted by $\bar{n}_{\text{out}}$. 

Let us define \( t_{\text{max}} = \arg \max_{t > 0} (\Pr (h(t, \tau) < h_{\text{min}})) \). Then, \( \hat{n}^\text{out}_b = t_{\text{max}} / T \), where \( T \) is the duration of the modulation bit interval.

**Remark 3:** Assuming independent diffusion for each information molecule \( A \), we can write the observed signal at the receiver as \( N(t, \tau) = N_A h(t, \tau) \). Now, given \( F_{h(t, \tau)}(h) \), the CDF of \( N(t, \tau) \) can be evaluated as \( F_{N(t, \tau)}(n) = F_{h(t, \tau)}(n/N_A) \).

### D. PDF of Impulse Response of Time-Variant MC Channel

In this subsection, we calculate the PDF of the impulse response of the time-variant MC channel, and provide a corresponding simple approximation.

**Corollary 2 (PDF of Time-variant MC Channel):** Given (26), the PDF of the impulse response of the considered time-variant MC channel, \( f_{h(t, \tau)}(h) \), can be expressed as

\[
f_{h(t, \tau)}(h) = \frac{1}{4 \alpha r_{\text{eq}}(t) h \sqrt{\pi D_2 t}} \exp \left( -\frac{\ln \left( \frac{\xi}{h} \right) - r_{\text{eq}}(t) \sqrt{\alpha}}{4D_2 t \alpha} \right) - \exp \left( -\frac{\ln \left( \frac{\xi}{h} \right) + r_{\text{eq}}(t) \sqrt{\alpha}}{4D_2 t \alpha} \right)
\]

(27)

**Proof:** \( f_{h(t, \tau)}(h) \) can be straightforwardly calculated by taking the partial derivative of \( F_{h(t, \tau)}(h) \) in (26) with respect to \( h \).

The derived expression for the PDF of the time-variant CIR can be used for the design of new detection and/or estimation algorithms at the receiver nano-machines [22], [23]. However, (27) might be too complicated for some design and/or analysis problems. In the remainder of this section, we first show how (27) can be approximated by a Log-normal distribution. Then, we specify the necessary condition that has to be met for this approximation to be accurate. To this end, we start with the following Lemma.

**Lemma 1:** It has been shown in [24, Ch. 1] that if random variable \( U \) is noncentral chi-squared distributed, i.e., \( U \sim \chi^2_k(\gamma) \), the asymptotic distribution of

\[
\frac{U - (k + \gamma)}{\sqrt{2k + 4\gamma}} \sim N(0, 1)
\]

(28)

follows a standard Normal distribution as either \( k \to \infty \) for a fixed \( \gamma \), or \( \gamma \to \infty \) for a fixed \( k \).

Given the result of Lemma 1, we provide the asymptotic distribution of \( h(t, \tau) \) in the following proposition.
Proposition 1: The asymptotic PDF of $h(t, \tau)$ in (27), denoted by $f_{h(t, \tau)}^*(h)$, in the regime of $\frac{(r_{eq}(t))^2}{2D_2t} \to \infty$ follows a Log-normal distribution, i.e.,

$$f_{h(t, \tau)}^*(h) \sim \text{Lognormal} \left( \mu^*, \sigma^*^2 \right),$$

(29)

$$\mu^* = -2D_2\alpha \left( 3 + \frac{(r_{eq}(t))^2}{2D_2t} \right) + \ln (\varphi), \quad \sigma^*^2 = (2D_2\alpha)^2 \times \left( 6 + \frac{2(r_{eq}(t))^2}{D_2t} \right).$$

(30)

Proof: We have shown in Appendix B that $h(t, \tau) = \varphi \exp \left( -2D_2\alpha r^2(t) \right)$, where $r^2(t) \sim \chi^2_k(\gamma(t))$ with $k = 3$ and $\gamma(t) = (r_{eq}(t))^2/(2D_2t)$. Employing Lemma 1 for the case where $k$ is fixed, in the limit of $\gamma(t) \to \infty$, we obtain $r^2(t) \sim \mathcal{N} \left( (k + \gamma(t)), 2k + 4\gamma(t) \right)$, i.e.,

$r^2(t) \sim \mathcal{N} \left( 3 + \frac{(r_{eq}(t))^2}{2D_2t}, 6 + \frac{2(r_{eq}(t))^2}{D_2t} \right)$.

(31)

Now, given (31), it is straightforward to show that $f_{h(t, \tau)}^*(h)$ follows a Log-normal distribution.

Fig. 2. NMSE between the PDF of random variable $U \sim \chi^2_k(\gamma)$ and its Gaussian approximation as a function of $\gamma$. The key step in the derivation of the asymptotic PDF, $f_{h(t, \tau)}^*(h)$, is the approximation of the PDF of $r^2(t) \sim \chi^2_k(\gamma(t))$ with a Normal distribution employing (28). Theoretically, this approximation becomes valid when $\gamma(t) \to \infty$. In order to evaluate the accuracy of the approximation introduced in (28), in Fig. 2, we show the normalized mean square error (NMSE) between the PDF of $U \sim \chi^2_k(\gamma)$, denoted by $f_U(x|k, \gamma)$, and the approximated PDF of a Gaussian random variable with mean $\mu = (k + \gamma)$ and variance $\sigma^2 = (2k + 4\gamma)$, denoted by $g_U(x|\mu, \sigma^2)$. As can be observed, values of $\gamma \geq 100$ lead to an NMSE of approximately less than $10^{-10}$, which provides an accurate approximation for (31). Taking this into account, we establish a necessary condition
for approximating the PDF of the impulse response of a time-variant MC channel by a Log-
normal distribution as $\gamma(t) \geq 100$, i.e.,
\[
\frac{(r_{\text{eq}}(t))^2}{2D_2t} \geq 100 \quad \text{or} \quad D_2t \leq \frac{(r_{\text{eq}}(t))^2}{200}.
\] (32)

*Remark 4:* In the literature of conventional (non-molecular) communication, a similar approach for approximating the distribution of a noncentral chi-squared random variable with normal distribution can be found. There, usually the case where $k \to \infty$ is considered. For example, in his seminal work [25], Urkowitz showed that values of $k \geq 250$ provide an accurate approximation. Later, Urkowitz’ criterion has been widely used in the spectrum sensing literature, see e.g. [26]–[28]. In this work, we have a fixed $k = 3$ and adopt the approximation based on $\gamma \to \infty$.

**E. Outdated CSI Model**

As one application of the expression derived for the PDF of $h(t, \tau)$, in this subsection, we propose a simple analytical model for outdated CSI in time-variant MC channels. In particular, for the problem at hand, knowledge of the CSI is equivalent to knowledge of the CIR. Due to the mobility of the nano-machines, the CIR decorrelates over time, which may limit the performance of detection algorithms that require instantaneous knowledge of the CIR. Similar to conventional wireless communication systems, one possible approach would be to organize the transmitted symbols into blocks, estimate the CIR at the beginning of each block based on pilot symbols, and use the estimated CIR for detection/decoding of the symbols in the block, where the CIR changes within the transmission block due to the mobility of the transmitter and receiver. On the other hand, there is a trade-off between block length and CSI quality, i.e., by increasing the block length, the CSI becomes more outdated but the training overhead is reduced. Thus, a simple yet accurate model for the outdated CSI is desirable.

Let us assume that the receiver obtains a perfect estimate of the CIR at time $t_s$, where we denote the estimated CIR by $\hat{h}(t_s, \tau)$ and the estimated $\bar{r}(t_s)$ by $\hat{\bar{r}}(t_s)$. Now, given (31), for $t > t_s$, we can write
\[
h(t', \tau) = \varphi \exp \left( -2D_2t' \alpha \bar{r}^2(t') \right) = \varphi \exp \left( -2D_2t' \alpha \left( 3 + \frac{(r_{\text{eq}}(t'))^2}{2D_2t'} \right) + \sqrt{6 + \frac{2(r_{\text{eq}}(t'))^2}{D_2t'}} \times \epsilon \right),
\] (33)

\(^2\)We note that based on the expression for the CIR in ([1]), knowing $h(t_s, \tau)$ is equivalent to knowing $\bar{r}(t_s)$, if all other system parameters are known at the receiver.
where \( t' = t - t_s \) and \( \epsilon \sim N(0, 1) \). Now, substituting \( r_{eq}(t') = \sqrt{|\hat{r}_s - \bar{v}' t' - \bar{v}' \tau|^2} \) into (33), it can be easily verified that \( h(t', \tau) \) can be written as
\[
h(t', \tau) = C\hat{h}(t_s, \tau)M^\Theta,
\]
where \( M \sim \text{Lognormal}(0, 1) \), and \( C \) and \( \Theta \) are defined as
\[
C = \exp\left(-6D_2t'\alpha - 2\alpha \left(\bar{v}' t' \odot (\hat{r}_s - \bar{v}' \tau)\right)\right), \quad \Theta = -2D_2t'\alpha\sqrt{6 + \frac{2|\hat{r}_s - \bar{v}' t' - \bar{v}' \tau|^2}{D_2t'}}.
\]
and \( \odot \) denotes the inner product of two vectors. In (34), \( C \) and \( \Theta \) are two time-dependent variables. In the limit of \( t \to t_s \) \( (t' \to 0) \), \( C \) and \( \Theta \) approach 1 and 0, respectively, and \( h(t', \tau) \to \hat{h}(t_s, \tau) \). On the other hand, as \( t' \) increases, \( C \) decreases and \( \Theta \) increases, which reflects the decorrelation of \( h(t', \tau) \) and \( \hat{h}(t_s, \tau) \). Furthermore, we note that the accuracy of (34) depends on the accuracy of the approximation introduced in (31).

V. Error Rate Analysis for Perfect and Outdated CSI

In this section, we first calculate the expected error probability of a single-sample threshold detector. Then, we discuss the choice of the detection threshold of the detector. Finally, in order to investigate the impact of CIR decorrelation, we calculate the expected error probability of the considered detector for perfect and outdated CSI.

A. Expected Bit Error Probability

We consider a single-sample threshold detector, where the receiver takes one sample at a fixed time \( \tau_s \) after the release of the molecules at the transmitter in each modulation bit interval, counts the number of signaling \( A \) molecules inside its volume, and compares this number with a detection threshold. In particular, we denote the received signal, i.e., the number of molecules observed inside the volume of the receiver in the \( j \)th bit interval, \( j \in \{1, 2, \ldots, L\} \), at the time of sampling by \( N(\tau_{j,s}) \), where \( \tau_{j,s} = (j - 1)T + \tau_s \). Furthermore, we assume that the detection threshold of the receiver, \( \xi_j \), can be adapted from one bit interval to the next. The choice of \( \xi_j \) is discussed in the next subsection. Thus, the decision of the single-sample detector in the \( j \)th bit interval, \( \hat{b}_j \), is given by
\[
\hat{b}_j = \begin{cases} 
1 & \text{if } N(\tau_{j,s}) \geq \xi_j, \\
0 & \text{if } N(\tau_{j,s}) < \xi_j.
\end{cases}
\]
For the decision rule in (36), we showed in [14] that the expected error probability of the jth bit, $\overline{P}_e(b_j)$, can be calculated as [14, Eq. (12)]

$$\overline{P}_e(b_j) = \int \cdots \int_{r \in \mathcal{R}} \sum_{b \in \mathcal{B}} f_{\tilde{r}}(r) \Pr(b) P_e(b_j|b, r) \, d\tilde{r}_1 \cdots d\tilde{r}_{L-1},$$

(37)

where $f_{\tilde{r}}(r)$ is the $(L - 1)$-dimensional joint PDF of vector $\tilde{r} = [\tilde{r}(T), \tilde{r}(2T), \cdots, \tilde{r}((L - 1)T)]$ that can be evaluated as

$$f_{\tilde{r}}(r) = f_{\tilde{r}(T)}(\tilde{r}_1|\tilde{r}_0) \times \cdots \times f_{\tilde{r}((L-1)T)}(\tilde{r}_{L-1}|\tilde{r}_{L-2}, \cdots, \tilde{r}_0)$$

(38)

Here, $r = [\tilde{r}_1, \tilde{r}_2, \cdots, \tilde{r}_{L-1}]$ is one sample realization of $\tilde{r}$ and equality (a) holds as free diffusion is a memoryless process, i.e., $f_{\tilde{r}(jT)}(\tilde{r}_j|\tilde{r}_{j-1}, \cdots, \tilde{r}_0) = f_{\tilde{r}(jT)}(\tilde{r}_j|\tilde{r}_{j-1})$. Furthermore, $\mathcal{R}$ and $\mathcal{B}$ are the sets containing all possible realizations of $r$ and $b$, respectively, and $\Pr(b)$ denotes the likelihood of the occurrence of $b$ and $P_e(b_j|b, r)$ is the conditional bit error probability of $b_j$. In [14], we considered a reactive receiver [29] and showed how $P_e(b_j|b, r)$ can be calculated for a single-sample detector using a fixed detection threshold $\xi$. Here, we provide $P_e(b_j|b, r)$ for a passive receiver [17] employing a single-sample detector with an adaptive detection threshold $\xi_j$.

Let us assume that $b$ and $r$ are known. It has been shown in [17] that the number of observed molecules, $N(\tau_{j,s})$, can be accurately approximated by a Poisson random variable. The mean of $N(\tau_{j,s})$, denoted by $\overline{N}(\tau_{j,s})$, due to the transmission of all bits up to the current bit interval can be written as

$$\overline{N}(\tau_{j,s}) = N_A \sum_{i=1}^{j} b_j h(iT, (j-i)T + \tau_s) \bigg| \tilde{r}(iT) = \tilde{r}_0 + \overline{N}_{A},$$

(39)

where $\overline{N}_{A}$ is the mean number of noise molecules inside the volume of the receiver at any given time. Now, given $\overline{N}(\tau_{j,s})$ and the decision rule in (36), $P_e(b_j|b, r)$ can be written as

$$P_e(b_j|b, r) = \begin{cases} 
\Pr(N(\tau_{j,s}) < \xi_j) & \text{if } b_j = 1, \\
\Pr(N(\tau_{j,s}) \geq \xi_j) & \text{if } b_j = 0,
\end{cases}$$

(40)

where $\Pr(N(\tau_{j,s}) < \xi_j)$ can be calculated from the cumulative distribution function of a Poisson distribution as

$$\Pr(N(\tau_{j,s}) < \xi_j) = \exp\left(-\overline{N}(\tau_{j,s})\right) \sum_{\omega=0}^{\xi_j-1} \frac{\left(\overline{N}(\tau_{j,s})\right)^\omega}{\omega!},$$

(41)
and \( \Pr(N(\tau,j,s) \geq \xi_j) = 1 - \Pr(N(\tau,j,s) < \xi_j) \). Given \( P_e(b_j|b, r) \) in (40), \( \bar{P}_e(b_j) \) can be calculated based on (37). Subsequently, we can obtain the expected error probability as \( \overline{P}_e = \frac{1}{L} \sum_{j=1}^{L} \bar{P}_e(b_j) \).

### B. Choice of Detection Threshold

In this subsection, we discuss the choice of the adaptive detection threshold for the considered single-sample detector. Let us assume for the moment that sequence \( \{b_1, b_2, \ldots, b_{j-1}\} \) and \( r \) are known, and we are interested in finding the optimal detection threshold, \( \xi_{j}^{\text{opt}} \), that minimizes the instantaneous error probability \( P_e(b_j) \). Then, we have shown in [30] that for any threshold detector whose received signal can be modeled as a Poisson random variable, \( \xi_{j}^{\text{opt}} \) is given by [30, Eq. (25)]

\[
\xi_{j}^{\text{opt}} = \left\lceil \ln \left( \frac{P_0}{P_1} \right) + (\lambda_1 - \lambda_0) \right\rceil \ln \left( \frac{\lambda_1}{\lambda_0} \right),
\]

(42)

where \( \lambda_1 = \bar{N}(\tau,j,s|b_j = 1) \), \( \lambda_0 = \bar{N}(\tau,j,s|b_j = 0) \), and \( \lceil \cdot \rceil \) denotes the ceiling function.

**Remark 5:** We note that the evaluation of \( \xi_{j}^{\text{opt}} \) requires knowledge of the previously transmitted bits up to the current bit interval, which is not available in practice. Thus, for practical implementation, we propose a suboptimal detector whose detection threshold, \( \hat{\xi}_{j}^{\text{subopt}} \), is evaluated according to (42) after replacing \( \{b_1, b_2, \ldots, b_{j-1}\} \) in (39) with the estimated previous bits, i.e., \( \{\hat{b}_1, \hat{b}_2, \ldots, \hat{b}_{j-1}\} \).

**Remark 6:** It has been shown in [31] that when the effect of inter-symbol interference (ISI) is negligible compared to \( \bar{n}_A \), the combination of (36) and (42) constitutes the optimal maximum likelihood (ML) detector. We note that, in this regime, knowledge of previously transmitted bits is not required for calculation of \( \xi_{j}^{\text{opt}} \).

### C. Detectors with Perfect and Outdated CSI

In this subsection, we distinguish between the cases of perfect CSI and outdated CSI knowledge, and explain how the corresponding expected error probabilities of the single-sample detector can be evaluated.

**Perfect CSI:** For the case of a single-sample detector with perfect CSI, we assume that for any given modulation bit interval, \( r(t) \) is known at the receiver for all previous bit intervals up to the current bit interval, i.e., for the \( j \)th bit interval, \( [\tilde{r}(0), \tilde{r}(T), \ldots, \tilde{r}(jT)] \) is known at the receiver. Thus, \( \hat{\xi}_{j}^{\text{subopt}} \) can be directly obtained from (11), (39), and (42).

**Outdated CSI:** For the case of a single-sample detector with outdated CSI, we assume that only the initial distance between transmitter and receiver at time \( t_0 = 0 \), i.e., \( r_0 \), is known at the
TABLE II  
SIMULATION PARAMETERS

| Parameter | Value  | Parameter | Value  |
|-----------|--------|-----------|--------|
| $N_A$     | 30000  | $T$       | 0.5 ms |
| $D_A$     | $5 \times 10^{-9}$ m$^2$/s | $\tau = \tau_s$ | 0.035 ms |
| $D_{tx}$  | $10^{-13}$ m$^2$/s | $L$       | 50     |
| $r_0$     | 1 $\mu$m  | $P_1$    | 0.5    |
| $a_{tx}$  | 0.15 $\mu$m | $P_0$    | 0.5    |
| $\bar{n}_A$ | 10     | $\Delta t$ | 5 $\mu$s |

receiver. As a result, in any modulation bit interval, the receiver evaluates $\hat{\xi}_{j,\text{subopt}}$ via (42) with the mean given by

$$\overline{N}(\tau_{j,s}) = N_A \sum_{i=1}^{j} b_i h \left(t_0, (j-i)T + \tau_s\right) + \bar{n}_A. \tag{43}$$

Finally, for both cases, $P_e(b_j|b, r)$ is obtained from (40).

VI. SIMULATION RESULTS

In this section, we present simulation and analytical results to assess the accuracy of the derived analytical expressions for the mean and the ACF of the time-variant CIR and the expected error probability of the considered mobile MC system. For simulation, we adopted a particle-based simulation of Brownian motion, where the precise locations of the signaling molecules, transmitter, and receiver are tracked throughout the simulation environment. In particular, in the simulation algorithm, time is advanced in discrete steps of $\Delta t$ seconds. In each step of the simulation, each $A$ molecule, the transmitter, and the receiver undergo random walks, and their new positions in each Cartesian coordinate are obtained by sampling a Gaussian random variable with mean $v_\zeta \Delta t$, $\zeta = \{x, y, z\}$, and standard deviation $\sqrt{2D_A \Delta t}$, $\sqrt{2D_{tx} \Delta t}$, and $\sqrt{2D_{rx} \Delta t}$, respectively. Furthermore, we used Monte-Carlo simulation for evaluation of the multi-dimensional integral in (37).

For all simulation results, we chose the set of simulation parameters provided in Table II unless stated otherwise. For all simulation results in Sections VI-A and VI-B, we assume that $\bar{n}_A = 0$. Furthermore, we considered an environment with the viscosity of blood plasma ($\approx 4$ mPa $\cdot$ s) at 37 $^\circ$C and we used the Stokes–Einstein equation [2 Eq. (5.7)] for calculation of $D_A$ and $D_{tx}$. The only parameters that were varied are $D_{tx} = \{0.1, 1, 5, 20, 100\} \times 10^{-13}$ m$^2$/s (corresponding to
In Fig. 3 and its inset, we investigate the impact of time $t$ on the mean and the normalized variance of the received signal in the absence of flow, i.e., $N_A m(t)$ and $\sigma^2(t)/m^2(t)$, respectively, for $D_{tx} = \{5, 20, 100\} \times 10^{-13} \text{ m}^2/\text{s}$. Fig. 3 shows that as time $t$ increases, $N_A m(t)$ decreases. This is due to the fact that as $t$ increases, on average $r(t)$ increases as transmitter and receiver diffuse away and, consequently, $m(t)$ decreases. The decrease is faster for larger values of $D_{tx}$, since for larger $D_{tx}$, the transmitter diffuses away faster. The normalized variance of the received signal is shown in the inset of Fig. 3. We observe that for all considered values of $D_{tx}$, the normalized variance of the received signal is an increasing function of time. This is because as time increases, due to the Brownian motion of transmitter and receiver, the variance of their movements increases, which leads to an increase in the normalized variance of the received signal. As expected, this increase is faster for larger values of $D_{tx}$, since the displacement variance of the transmitter, $2D_{tx}t$, is larger.

In Fig. 4, the normalized ACF, $\rho(t_1, t_2)$, is evaluated as a function of $t_2$ in the absence of flow for a fixed value of $t_1 = 0$ and transmitter diffusion coefficients $D_{tx} = \{0.1, 1, 5, 20, 100\} \times 10^{-13} \text{ m}^2/\text{s}$. We observe that for all considered values of $D_{tx}$, $\rho(t_1, t_2)$ decreases with increasing $t_2$. This is due to the fact that as $t_2$ increases, on average $r(t_2)$ increases as transmitter and receiver diffuse away, and, consequently, $m(t_2)$ decreases. The decrease is faster for larger values of $D_{tx}$, since for larger $D_{tx}$, the transmitter diffuses away faster.

The very small values of $a_{tx}$ (in the order of a few nm) have been used only to consider the full range of $D_{tx}$ values.

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**A. First- and Second-order Moments of CIR**

In Fig. 3 and its inset, we investigate the impact of time $t$ on the mean and the normalized variance of the received signal in the absence of flow, i.e., $N_A m(t)$ and $\sigma^2(t)/m^2(t)$, respectively, for $D_{tx} = \{5, 20, 100\} \times 10^{-13} \text{ m}^2/\text{s}$. Fig. 3 shows that as time $t$ increases, $N_A m(t)$ decreases. This is due to the fact that as $t$ increases, on average $r(t)$ increases as transmitter and receiver diffuse away and, consequently, $m(t)$ decreases. The decrease is faster for larger values of $D_{tx}$, since for larger $D_{tx}$, the transmitter diffuses away faster. The normalized variance of the received signal is shown in the inset of Fig. 3. We observe that for all considered values of $D_{tx}$, the normalized variance of the received signal is an increasing function of time. This is because as time increases, due to the Brownian motion of transmitter and receiver, the variance of their movements increases, which leads to an increase in the normalized variance of the received signal. As expected, this increase is faster for larger values of $D_{tx}$, since the displacement variance of the transmitter, $2D_{tx}t$, is larger.

In Fig. 4, the normalized ACF, $\rho(t_1, t_2)$, is evaluated as a function of $t_2$ in the absence of flow for a fixed value of $t_1 = 0$ and transmitter diffusion coefficients $D_{tx} = \{0.1, 1, 5, 20, 100\} \times 10^{-13} \text{ m}^2/\text{s}$. We observe that for all considered values of $D_{tx}$, $\rho(t_1, t_2)$ decreases with increasing $t_2$. This is due to the fact that as $t_2$ increases, on average $r(t_2)$ increases as transmitter and receiver diffuse away, and, consequently, $m(t_2)$ decreases. The decrease is faster for larger values of $D_{tx}$, since for larger $D_{tx}$, the transmitter diffuses away faster. The normalized variance of the received signal is shown in the inset of Fig. 4. We observe that for all considered values of $D_{tx}$, the normalized variance of the received signal is an increasing function of time. This is because as time increases, due to the Brownian motion of transmitter and receiver, the variance of their movements increases, which leads to an increase in the normalized variance of the received signal. As expected, this increase is faster for larger values of $D_{tx}$, since the displacement variance of the transmitter, $2D_{tx}t$, is larger.

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3The very small values of $a_{tx}$ (in the order of a few nm) have been used only to consider the full range of $D_{tx}$ values.
Fig. 5. Expected received signal, $N_Am(t)$, as a function of time $t$ for a fixed receiver.

Fig. 6. Normalized ACF, $\rho(t_1, t_2)$, as a function of $t_2$, for $\tau = \tau_s$, $D_{tx} = \{5, 20\} \times 10^{-13} \text{ m}^2/\text{s}$, and $v = \{0, 10^{-5}, -10^{-5}\} \text{ m/s}$ for a fixed receiver.

is due to the fact that by increasing $t_2$, on average $r(t)$ increases, and the CIR becomes more decorrelated from the CIR at time $t_1 = 0$. Furthermore, as expected, for larger values of $D_{tx}$, $\rho(t_1, t_2)$ decreases faster, as for larger values of $D_{tx}$, the transmitter diffuses away faster. For $\eta = 0.9$, the coherence time, $T_c$, for $D_{tx} = 20 \times 10^{-13} \text{ m}^2/\text{s}$ and $D_{tx} = 5 \times 10^{-13} \text{ m}^2/\text{s}$ is 7 ms and 23 ms, respectively. The coherence time is a measure for how frequently CSI acquisition has to be performed.

In Figs. 5 and 6, we investigate the impact of flow on $N_Am(t)$ and the normalized ACF. In Fig. 5, $N_Am(t)$ is depicted as a function of time $t$ for system parameters $D_{tx} = \{20, 100\} \times 10^{-13} \text{ m}^2/\text{s}$ and $v = \{0, 10^{-5}, -10^{-5}\} \text{ m/s}$, where we assumed $v_x = v_y = v_z = v$ and a fixed receiver. Fig. 5 shows that for positive $v$, $N_Am(t)$ first increases, as a positive flow carries the transmitter towards the receiver, and then decreases, since the transmitter eventually passes the receiver. Moreover, the increase of $N_Am(t)$ is larger for smaller values of $D_{tx}$. This is because, when $D_{tx}$ is small, flow is the dominant transport mechanism. However, when $D_{tx}$ is large, diffusion becomes the dominant transport mechanism and, as discussed before, on average $r(t)$ increases, which reduces $N_Am(t)$. For the case when the flow is negative, $N_Am(t)$ decreases quickly. This behaviour is expected, as for $v < 0$, the flow carries the transmitter away from the receiver.

In Fig. 6, the normalized ACF, $\rho(t_1, t_2)$, is evaluated as a function of $t_2$ for a fixed value of $t_1 = 0$, a fixed receiver, and system parameters $D_{tx} = \{5, 20\} \times 10^{-13} \text{ m}^2/\text{s}$ and $v = \{0, 10^{-5}, -10^{-5}\} \text{ m/s}$, where $v_x = v_y = v_z = v$. We observe that, for both considered values of $D_{tx}$, if $v = 10^{-5}$ ($v = -10^{-5}$) $\text{ m/s}$, $\rho(0, t_2)$ is larger (smaller) than the corresponding value when $v = 0$. This has
the following reason. On the one hand, the variance of the movements of the transmitter in each Cartesian coordinate, $\sigma_{tx}^2 = 2D_{tx}t_2$, is an increasing function of time $t_2$ and independent of $v$. On the other hand, for $v = 10^{-5}$ ($v = -10^{-5}$ $\text{m/s}$), on average the transmitter is closer to (farther from) the receiver than for $v = 0$ $\text{m/s}$. Thus, at any given time $t_2$, $\sigma_{tx}^2$ leads to relatively smaller (larger) variations of $h(t_2, \tau_s)$ for the case when $v = 10^{-5}$ ($v = -10^{-5}$) $\text{m/s}$ compared with the case when $v = 0$ $\text{m/s}$. This leads to a larger (smaller) value of $\rho(0, t_2)$ for $v = 10^{-5}$ ($v = -10^{-5}$) $\text{m/s}$ than for $v = 0$ $\text{m/s}$.

We note the excellent match between simulation and analytical results in Figs. 3-6.

### B. CDF and PDF of CIR

In Fig. 7, the CDF of the impulse response of a time-variant MC channel, $F_{h(t, \tau)}(h)$, is shown for system parameters $D_{tx} = \{10^{-12}, 10^{-13}\}$ $\text{m}^2$/s, $v_x = v_y = v_z = v = \{0, 10^{-5}, -10^{-5}\}$ $\text{m}/\text{s}$, a fixed receiver, and time $t = 5$ ms, i.e., $t = 10T$. We observe that for all considered values of $v$, increasing $D_{tx}$ makes the CDF wider, as for larger values of $D_{tx}$ the variance of the movements of the transmitter and, as a result, the variance of $\tilde{r}(t)$ increase, which leads to an increase in the variance of $h(t, \tau)$. Furthermore, Fig. 7 shows that for a given $D_{tx}$ and a fixed receiver, a positive and a negative flow shift the CDF of the CIR to the right and the left, respectively, compared to the case without flow. This is because, e.g. in the presence of a positive flow, the transmitter is pushed towards the receiver and hence, $\tilde{r}(t)$ decreases. As a result, larger values of $h$ are more likely to occur. Furthermore, the solid black line in Fig. 7 denotes $h = h_{\text{min}} = 10^{-3}$, which corresponds to an average error probability of approximately $10^{-3}$. Fig. 7 reveals that

![Fig. 7. CDF of the CIR, $F_{h(t, \tau)}(h)$, at $t = 5$ ms.](image1)

![Fig. 8. PDF of the CIR, $f_{h(t, \tau)}(h)$, for $v = \{0, -10^{-5}\}$ $\text{m/s}$ and $t = \{25, 100\}$ ms.](image2)
after 5 ms, i.e., after transmission of 10 bits, the outage probability is higher for $v = 0 \text{ m/s}$ and $v = -10^{-5} \text{ m/s}$ compared to $v = 10^{-5} \text{ m/s}$, as for $v = \{0, -10^{-5}\} \text{ m/s}$, transmitter and receiver are on average further apart after 5 ms. We note again the excellent matched between simulation and analytical results.

In Fig. 8, the PDF of the time-variant CIR, $f_{ht}(h)$, is evaluated for system parameters $t = \{25, 100\} \text{ ms}$, $v_x = v_y = v_z = v = \{0, -10^{-5}\} \text{ m/s}$, $D_{tx} = 10^{-13} \text{ m}^2/\text{s}$, and a fixed transmitter. For the case of a fixed transmitter, in the presence of a negative flow, e.g., $v = -10^{-5} \text{ m/s}$, the receiver first moves towards the transmitter before passing it. Thus, as shown in Fig. 8, first, for $t = 25 \text{ ms}$, $f_{ht}(h)$ is shifted to the right, and later for $t = 100 \text{ ms}$, when the receiver is far away from the transmitter, $f_{ht}(h)$ is shifted to the left. We note the excellent agreement of the derived expression for $f_{ht}(h)$ i.e., (27) with the simulation results. We also observe that the Log-normal distribution provides a good approximation for the PDF of the CIR in Fig. 8, as for all three considered cases, the necessary condition (32) is satisfied.

In Fig. 9, $f_{ht}(h)$ is depicted for system parameters $t = \{5, 25\} \text{ ms}$, $v_x = v_y = v_z = v = \{0, -10^{-5}\} \text{ m/s}$, $D_{tx} = 10^{-12} \text{ m}^2/\text{s}$, and a fixed receiver. In Fig. 9, since the receiver is fixed, in the presence of a positive flow $v = 10^{-5} \text{ m/s}$, the transmitter moves towards the receiver, and hence, $f_{ht}(h)$ shifts to the right compared to the case without flow, see e.g. for time $t = 5 \text{ ms}$. As time increases, the transmitter passes the receiver and $r(t)$ starts to increase, and hence, $f_{ht}(h)$ starts to shift to the left. However, in Fig. 9, the effective diffusion coefficient $D_2 = D_{tx} = 10^{-12} \text{ m}^2/\text{s}$ is greater than the effective diffusion coefficient $D_2 = D_{rx} = 10^{-13} \text{ m}^2/\text{s}$ in Fig. 8. As a result, the Log-normal distribution approximation starts to deviate from the actual PDF sooner, i.e., at
In order to evaluate the accuracy of the proposed approximate PDF, \( f_\star(h,t) \), in Fig. 10 the NMSE of the PDF of the received signal, defined as \( \text{NMSE} = \left( \int |1/N_A f_{h(t)}(n/N_A) - 1/N_A f_\star h(t,\tau) (n/N_A)|^2 \, dn / \int |1/N_A f_{h(t)}(n/N_A)|^2 \, dn \right) \), is evaluated as a function of normalized time, \( t/T \), for system parameters \( D_2 = \{10^{-12}, 10^{-13}, 10^{-14}\} \text{ m}^2 \text{s} \) and \( v = \{0, 10^{-5}, -10^{-5}\} \text{ m} \text{s} \) for a fixed receiver. Fig. 10 shows that, for a given time \( t \), the NMSE grows with the effective diffusion coefficient of transmitter and receiver, \( D_2 \). This is because condition (32) is inversely proportional to \( D_2 \). In other words, for smaller values of \( D_2 \), the maximum time, \( t_{\text{max}} \), that satisfies (32) is larger than for larger values of \( D_2 \). For example, in Fig. 10, for \( D_2 = 10^{-13} \text{ m}^2 \text{s} \) and \( v = 0 \text{ m} \text{s} \), \( t_{\text{max}} \approx 33.5 \text{ ms} \). Furthermore, we can observe that for the considered values of \( D_2 \), when \( v < 0 \), NMSE is smaller compared to the case when \( v \geq 0 \). This is because for \( v < 0 \), \( r_{\text{eq}}(t) \) in (32) increases more quickly over time, which yields smaller values of NMSE.

C. Error Rate Analysis

In Fig. 11 the expected error probability, \( \mathbb{P}_e(b_j) \), is shown as a function of bit interval \( j \) in the absence of flow for system parameters \( D_{tx} = \{0.1, 5, 20, 100\} \times 10^{-13} \text{ m}^2 \text{s} \) as well as for the conventional case of fixed transmitter and fixed receiver, i.e., \( D_{tx} = D_{rx} = 0 \). As expected, when transmitter and receiver are fixed, the performances of the detectors with perfect and outdated CSI are identical, as the channel does not change over time. On the other hand, when \( D_{tx} > 0 \), the performances of both detectors deteriorate over time. This is due to the fact that as time increases,
i) $\sigma^2(t)$ increases and ii) $m(t)$ decreases. Furthermore, the gap between the BERs of the detector with perfect CSI and the detector with outdated CSI increases over time since the impulse response of the channel decorrelates (see Fig. 4), and, as a result, the CSI becomes outdated. Moreover, the CSI becomes outdated faster for larger values of $D_{tx}$. Hence, for a given time (bit interval), the absolute value of the performance gap between both cases, highlighted by solid black lines in Fig. 11, increases. For instance, for $j = 37$, the absolute values of the performance gap between the detectors with perfect and outdated CSI for $D_{tx} = \{0.1, 5, 20, 100\} \times 10^{-13}$ m$^2$/s are $\{0.0013, 0.0212, 0.0624, 0.08\}$, respectively.

In Fig. 12, $P_e(b_j)$ is evaluated as a function of bit interval $j$ for two sets of system parameters. For the first set, we consider a mobile transmitter and receiver in the absence of flow, and adopt $D_{tx} = \{0.1, 20\} \times 10^{-13}$ m$^2$/s, $D_{rx} = 10^{-13}$ m$^2$/s, and $v_y = v_z = v_x = 0$ m/s. For the second set, we consider a mobile transmitter and a fixed receiver in the presence of flow, and assume $D_{rx} = 0$ m$^2$/s, $v_y = v_z = 0$ m/s, and $v_x = 10^{-5}$ m/s. Furthermore, in order to have a fair comparison between both sets with respect to $D_2$, for the second set, we adopt $D_{tx} = \{1.1, 21\} \times 10^{-13}$ m$^2$/s such that the same values of $D_2$ results for both sets. First of all, Fig. 12 shows that for both considered values of $D_2$, by increasing $v_x$ the performance of both detectors improves. This is because in the presence of positive flow $v_x = 10^{-5}$ m/s, $r(t)$ increases on average later in time compared to the case without flow, since the transmitter is moved towards the receiver, and, as a result, the performance of both detectors improves. Furthermore, we can see that the performance gap between the two detectors becomes larger as $D_{tx}$ decreases. This is because for the detector with outdated CSI, the channel does not only decorrelate over time, but the mean of the channel also changes drastically for smaller values of $D_2$ in the presence of positive flow compared with the case without flow, and as a result, the performance gap between the two detectors is larger for smaller values of $D_2$.

In Fig. 13, the impact of flow on $P_e(b_j)$ is investigated for system parameters $D_{tx} = 5.1 \times 10^{-13}$ m$^2$/s, $v_y = v_z = 0$ m/s, and $v_x = \{0.4, 1, 2.5\} \times 10^{-5}$ m/s. Interestingly, Fig. 13 reveals that when diffusion is dominant over the flow ($v_x = 0.4 \times 10^{-5}$ m/s), the performance of both detection schemes deteriorates over time, as on average $r(t)$ increases. In the intermediate regime ($v_x = 1 \times 10^{-5}$ m/s), diffusion and flow essentially cancel out each others’ impact and $r(t)$ remains on average approximately constant. Thus, the BERs of both detectors also remain approximately constant over time. However, in a flow dominated regime ($v_x = 2.5 \times 10^{-5}$ m/s), since $r(t)$ decrease on average over time for the duration of the considered bit intervals, the BER for perfect CSI decreases over time but the BER for outdated CSI still increases because of the inaccurate
Fig. 13. Expected error probability, $P_e(b_j)$, as a function of bit interval $j$.

decision threshold.

VII. CONCLUSIONS

In this paper, we established a mathematical framework for the statistical characterization of the time-variant CIR of mobile MC channels. In particular, we derived closed-form expressions for the mean, the ACF, the CDF, and the PDF of the time-variant CIR. Furthermore, we approximated the PDF of the CIR by a Log-normal distribution, quantified the regime where this approximation is valid, and proposed a simple model for outdated CSI. Our analytical and simulation results reveal that (1) the coherence time of the channel decreases when transmitter and/or receiver diffuse faster; (2) outages are more likely to occur when flow causes the transmitter and receiver to drift apart and/or transmitter and receiver diffuse faster; (3) the accuracy of the Log-normal approximation of the PDF of the CIR decreases slower over time for smaller effective diffusion coefficients of transmitter and receiver; (4) both CIR decorrelation over time and flow influence the performance gap between detectors employing perfect and outdated CSI, respectively; (5) new modulation, detection, and estimation techniques have to be developed to enable reliable communication of time-variant mobile MC channels.

APPENDIX A

PROOF OF THEOREM 2

Given (18), substituting $h(t_1, \tau)|_{\bar{r}(t)=\bar{r}_1}$ and $h(t_2, \tau)|_{\bar{r}(t)=\bar{r}_2}$ from (11) in (17), we can write $\phi(t_1, t_2)$ as

$$
\phi(t_1, t_2) = \varphi^2 \lambda(t_2 - t_1) \lambda(t_1) \int_{\bar{r}_1, \bar{r}_2 \in \mathbb{R}^3} e^{-a|\bar{r}_1 - \bar{v}'_1\tau|^2} e^{-a|\bar{r}_2 - \bar{v}'_2\tau|^2} e^{-\beta(t_1)|\bar{r}_1 - (\bar{r}_0 - \bar{v}^* t_1)|^2}
$$
Expanding the integrands in (44) leads to
\[
\phi(t_1, t_2) = \varphi^2 \lambda(t_2 - t_1) \lambda(t_1) \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} e^{-\alpha(x_1 - v_1^* \tau)^2 - \alpha(x_2 - v_2^* \tau)^2 - \beta(t_2 - t_1)(x_2 - x_1 + v_2^*(t_2 - t_1))^2} \\
\times \ e^{-\beta(t_1)(x_1 - x_0 + v_1^* \tau)^2} \times e^{-\alpha(x_1 - v_1^* \tau)^2 - \alpha(y_2 - v_2^* \tau)^2 - \beta(t_2 - t_1)(y_2 - y_1 + v_2^*(t_2 - t_1))^2} \times e^{-\alpha(z_1 - v_1^* \tau)^2 - \alpha(z_2 - v_2^* \tau)^2 - \beta(t_2 - t_1)(z_2 - z_1 + v_2^*(t_2 - t_1))^2} \\
\times \ e^{-\alpha(y_1 - v_1^* \tau)^2 - \beta(t_1)(y_1 + v_1^* \tau)^2} \right) d\tau_1 d\tau_2 d\tau_3 d\tau_4.
\]

(45)

To solve the multiple integrals in (45), we use the PDF integration formula for multivariate Gaussian distributions. In particular, let us assume that vector \( \mathbf{X} = [x_1, y_1, z_1, x_2, y_2, z_2]^T \) has a multivariate Gaussian distribution with mean vector \( \mu = E(\mathbf{X}) \in \mathbb{R}^6 \) and covariance matrix \( \Sigma = E((\mathbf{X} - \mu)(\mathbf{X} - \mu)^T) \). Then, the well-known PDF of \( \mathbf{X} \) is given by
\[
f_{\mathbf{X}}(x_1, y_1, z_1, x_2, y_2, z_2) = \frac{\exp \left(-\frac{1}{2} (\mathbf{X} - \mu)^T \Sigma^{-1} (\mathbf{X} - \mu) \right)}{(2\pi)^3 \sqrt{\det(\Sigma)}},
\]
(46)

where \( \det(\cdot) \) denotes the determinant. It can be easily verified that for mean vector \( \mu = [\mu_{x_1}, \mu_{y_1}, \mu_{z_1}, \mu_{x_2}, \mu_{y_2}, \mu_{z_2}] \) and inverse covariance matrix
\[
\Sigma^{-1} = \begin{bmatrix}
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
\end{bmatrix},
\]
(47)

where
\[
\vartheta = 2 \left( \alpha + \beta(t_2 - t_1) \right), \quad \varepsilon = 2 \left( \alpha + \beta(t_2 - t_1) \right), \quad \psi = -2\beta(t_2 - t_1) \\
\mu_{x_1} = \frac{2 \left[ \frac{\varepsilon - \psi}{\varepsilon} (\alpha v_x^* \tau) + \frac{\varepsilon + \psi}{\varepsilon} \left( \beta(t_2 - t_1)v_x^*(t_2 - t_1) \right) + \beta(t_1)(x_0 - v_x^* t_1) \right]}{\vartheta - \psi^2 / \varepsilon}, \\
\mu_{y_1} = \frac{2 \left[ \frac{\varepsilon - \psi}{\varepsilon} (\alpha v_y^* \tau) + \frac{\varepsilon + \psi}{\varepsilon} \left( \beta(t_2 - t_1)v_y^*(t_2 - t_1) \right) - \beta(t_1)v_y^* t_1 \right]}{\vartheta - \psi^2 / \varepsilon}, \\
\mu_{z_1} = \frac{2 \left[ \frac{\varepsilon - \psi}{\varepsilon} (\alpha v_z^* \tau) + \frac{\varepsilon + \psi}{\varepsilon} \left( \beta(t_2 - t_1)v_z^*(t_2 - t_1) \right) - \beta(t_1)v_z^* t_1 \right]}{\vartheta - \psi^2 / \varepsilon}, \\
\mu_{x_2} = \frac{2 \varepsilon \alpha v_x^* \tau - 2\beta(t_2 - t_1)v_x^*(t_2 - t_1) - \psi \mu_{x_1}}{\varepsilon}, \quad \mu_{y_2} = \frac{2 \varepsilon \alpha v_y^* \tau - 2\beta(t_2 - t_1)v_y^*(t_2 - t_1) - \psi \mu_{y_1}}{\varepsilon}, \\
\mu_{z_2} = \frac{2 \varepsilon \alpha v_z^* \tau - 2\beta(t_2 - t_1)v_z^*(t_2 - t_1) - \psi \mu_{z_1}}{\varepsilon},
\]
(48)
exp\left(-\frac{1}{2}(X - \mu)^T \Sigma^{-1}(X - \mu)\right) \times \exp(\kappa_x + \kappa_y + \kappa_z) \text{ (with } \kappa_x, \kappa_y, \kappa_z \text{ as given in (20)) is equal to the integrands in (45).}

Now, given that \(\int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} f_X(x_1, y_1, z_1, x_2, y_2, z_2) \, dx_1 \cdots dz_2 = 1\), \(\phi(t_1, t_2)\) can be written as

\[
\phi(t_1, t_2) = \varphi^2 \lambda(t_2 - t_1) \lambda(t_1) \exp(\kappa_x + \kappa_y + \kappa_z)(2\pi)^3 \sqrt{\det(\Sigma)}. \tag{49}
\]

Given \(\Sigma^{-1}\) in (47), after some calculations, it can be shown that

\[
\det(\Sigma) = \frac{1}{(\theta \times \varepsilon - \psi^2)^3}. \tag{50}
\]

Finally, substituting (50) into (49) leads to (19).

**APPENDIX B**

**PROOF OF THEOREM 3**

For calculation of \(F_{h(t, \tau)}(h)\), we first find the distribution of \(|\tilde{r}(t) - \tilde{v}'\tau|^2\). Given the PDF of random variable \(\tilde{r}(t)\) in (10), we obtain for the elements of the vector \(\tilde{r}(t) - \tilde{v}'\tau = [X(t), Y(t), Z(t)]\)

\[
X(t) \sim \mathcal{N}(x_0 - v_x^* t - v_x' \tau, 2D_2 t), \quad Y(t) \sim \mathcal{N}(-v_y^* t - v_y' \tau, 2D_2 t), \quad Z(t) \sim \mathcal{N}(-v_z^* t - v_z' \tau, 2D_2 t). \tag{51}
\]

We can rewrite \(|\tilde{r}(t) - \tilde{v}'\tau|^2\) as follows

\[
|\tilde{r}(t) - \tilde{v}'\tau|^2 = X^2(t) + Y^2(t) + Z^2(t) = 2D_2 t \times \left(\tilde{X}^2(t) + \tilde{Y}^2(t) + \tilde{Z}^2(t)\right) = 2D_2 t \times \tilde{r}^2(t), \tag{52}
\]

where \(\tilde{X}(t) \sim \mathcal{N}\left((x_0 - v_x^* t - v_x' \tau)/\sqrt(2D_2 t), 1\right), \quad \tilde{Y}(t) \sim \mathcal{N}\left((-v_y^* t - v_y' \tau)/\sqrt(2D_2 t), 1\right), \quad \text{and} \quad \tilde{Z}(t) \sim \mathcal{N}\left((-v_z^* t - v_z' \tau)/\sqrt(2D_2 t), 1\right)\). Given (52), we can rewrite the CIR in (11) as \(h(t, \tau) = \varphi \exp(-2 \times D_2 t \alpha \tilde{r}^2(t))\), where \(\tilde{r}^2(t)\) follows a noncentral chi-square distribution with \(k = 3\) degrees of freedom and noncentrality parameter \(\gamma(t) = |\tilde{r}_0 - \tilde{v}'\tau|^2/2D_2 t\), i.e., \(\tilde{r}^2(t) \sim \chi^2_3(\gamma(t))\). Therefore, we can calculate the CDF of the CIR of the mobile MC channel as follows

\[
F_{h(t, \tau)}(h) = \Pr(\{h(t, \tau) < h\}) = \Pr(\varphi \exp\left(-2D_2 t \alpha \tilde{r}^2(t)\right) \leq h) = \Pr\left(\tilde{r}^2(t) \geq \frac{\ln(\varphi/h)}{2D_2 t \alpha}\right) = 1 - \Pr\left(\tilde{r}^2(t) < \frac{\ln(\varphi/h)}{2D_2 t \alpha}\right), \tag{53}
\]

where \(\ln(\cdot)\) denotes the natural logarithm. The last term on the right-hand side of (53) is the CDF of random variable \(\tilde{r}^2(t)\). The CDF of a random variable \(U \sim \chi^2_3(\gamma)\), i.e., \(\Pr(U \leq u)\), is given by \(1 - Q_{k/2}(\sqrt{\gamma}, \sqrt{u})\), where \(Q_{m}(a, b)\) denotes the generalized Marcum Q-function of order \(m\) \([32, \text{Eq. (4.33)}]\)

\[
Q_{m}(a, b) = \frac{1}{a^{m-1}} \int_{b}^{\infty} x^m \exp\left(-\frac{x^2 + a^2}{2}\right) I_{m-1}(ax) \, dx, \tag{54}
\]
where $I_m(\cdot)$ is the $m$th-order modified Bessel function of the first kind. Given (53) and (54), we obtain

$$F_{h(t,\tau)}(h) = Q_{3/2} \left( \frac{r_{eq}(t)}{\sqrt{2D_2 t}} \sqrt{\frac{\ln(\varphi/h)}{2D_2 t \alpha}} \right).$$  

(55)

In order to further simplify the expression derived in (55), we use the closed-form representation of $Q_m(a, b)$ proposed in [33]. There, it has been shown that for the case of $m = 0.5n$, where $n$ is an odd positive integer, $Q_m(a, b)$ is given by [33, Eq. (11)]

$$Q_m(a, b) = \frac{1}{2} \text{erfc} \left( \frac{a + b}{\sqrt{2}} \right) + \frac{1}{2} \text{erfc} \left( \frac{b - a}{\sqrt{2}} \right) + \frac{1}{a \sqrt{2\pi}} \sum_{k=0}^{m-0.5} \frac{b^{2k}}{2^k} \sum_{q=0}^{k} \frac{(-1)^q (2q)!}{(k-q)! q!} \times \left\{ \sum_{i=0}^{2q} \frac{1}{(ab)^{2q-i} i!} \left[ (-1)^i \exp \left( -\frac{(b - a)^2}{2} \right) - \exp \left( -\frac{(b + a)^2}{2} \right) \right] \right\}, \quad a > 0, b \geq 0.$$  

(56)

After substituting $m = 3/2 = 0.5 \times 3$, $a = r_{eq}(t)/\sqrt{2D_2 t}$, and $b = \sqrt{\ln(\varphi/h)/2D_2 t \alpha}$ from (55) into (56), $F_{h(t,\tau)}(h)$ simplifies to (26).

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