

Interference Mitigation in Large-Scale Multiuser Molecular Communication

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Abstract—In recent years, communicating information using molecules via diffusion has attracted significant interest in bio-medical applications. To date, most of the studies have concentrated on point-to-point molecular communication (MC), whereas in a realistic environment, multiple MC transmitters are likely to transmit molecular messages simultaneously sharing the same propagation medium, resulting in significant performance variation of the MC system. In this type of large-scale MC system, the collective signal strength at the desired receiver can be impaired by the interference caused by other MC transmitters, which may degrade the system reliability and efficiency. This paper presents the first tractable analytical framework for the collective signal strength at a partially absorbing receiver due to the desired transmitter under the impact of a swarm of interfering transmitters in a 3D large-scale MC system using stochastic geometry. To combat the multi-user interference and the intersymbol interference (ISI) in the multi-user environment, we propose Reed–Solomon (RS) error correction coding, due to its high effectiveness in combating burst and random errors, as well as the two types of information molecule modulating scheme, where the transmitted bits are encoded using two types of information molecules at consecutive bit intervals. We derive analytical expressions for the bit error probability (BEP) of the large-scale MC system with the proposed two schemes to show their effectiveness. The results obtained using Monte Carlo simulations, match exactly with the analytical results, justifying the accuracy of the derivations. Results reveal that both schemes improve the BEP by a factor of 3–4 compared with that of a conventional MC system without using any ISI mitigation techniques. Due to the implementation simplicity, the two-type molecule encoding scheme is better than the RS error correction coding scheme, as the RS error correction coding scheme involves additional encoding and decoding process at both the transmitter and receiver nodes. Furthermore, the proposed

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analytical framework can be generalized to the analysis of other types of receiver designs and performance characterization in multi-user large-scale MC systems. Also, the two types of information molecule modulating scheme can be extended to M-type of information molecule modulating scheme without loss of generality.

Index Terms—Large-scale molecular communication system, partially absorbing receiver, intersymbol interference, multi-user interference, 3D stochastic geometry, Reed Solomon codes.

I. INTRODUCTION

CONVEYING information over a distance in an environment where a set of interconnected micro and nanoscale devices are communicating, has been a challenge for decades. It requires classical communication methods to be revised to meet the requirements of very small dimensions and specific transmission mediums. Molecular communication (MC) is an emerging communication paradigm which has gained significant research attention in recent years as a solution for the aforementioned research question. It is inspired by nature and adopts the prevalent communication mechanism of living cells and organisms to achieve effective communication [1]. In MC, information is carried by chemical signals and based on the propagation channel characteristics, it is generally classified into walkway-based, flow-based, and diffusion-based MC types [2]. Recent work in MC research spans theoretical analysis of the performance of the communication channels, improved transmitter and the receivers designed to more practical design of suitable modulation and coding techniques [3]–[7]. The potential applications of MC in micro and nanoscale level systems, include: bio-medicine systems for detection, control and treatment of diseases, require robust and reliable communication capabilities.

In this paper, we limit ourselves to MC via diffusion (MCvD), as it is the simplest, general, and energy efficient MC paradigm. In a typical point-to-point MCvD system, the information is carried via so-called messenger molecules. The input information is modulated onto the physical properties of the messenger molecules, such as their types, quantity, or their release time, using different modulation techniques [3]. Then, the transmitter emits a number of messenger molecules in a time slotted fashion to convey the input bit sequence. Once emitted by the transmitter, these molecules propagate through the fluid medium via diffusion, where each molecule

undergoes a random walk following Brownian motion and propagation follows a Wiener process [8]. Finally, the receiver, demodulates the received signal based on the properties of the received molecules, such as the type, number or the receive times of the absorbed molecules during each bit interval. Here, we focus on the quantity of molecules for information modulation and demodulation. Due to the randomness in the arriving time of molecules, crossover between molecules from different bit intervals can occur. Thus, delayed molecules from previous symbols arriving at the current bit interval, cause intersymbol interference (ISI) at the receiver. As shown in [9], ISI has been regarded as one of the main bottlenecks exist in MC, which degrades the overall system performance and its reliability.

In a realistic 3D large-scale MC environment, there exists a swarm of MC transmitters which share the transmission medium and transmits molecular messages simultaneously. This type of large-scale MC system suffers not only from ISI, but also from multi-user interference (MUI) due to the interfering signals from the swarm of interfering transmitters on the desired signal. In [10], an analytical framework based on Poisson point process was presented to model the collective signal strength due to the joint transmission of all transmitters in a 3D large-scale MC system. In [11], the exact expressions of ISI and MUI of a MC system with the fully absorbing receiver were presented to reveal the theoretical limits on multi-user MC. While [10] and [11] only modeled the 3D large-scale MC system, active error mitigation in the presence of a swarm of interfering transmitters is not considered.

Existing works on interference mitigation in MC mostly focused on modeling the ISI in point-to-point MC system [9], [12]–[14], and inspired from conventional data communication networks, error correction codes (ECCs) were employed to overcome this bottleneck. In [12], the bit error performance of Hamming codes (HC), Euclidean Geometry Low Density Parity Check (EG-LDPC) codes, and Cyclic Reed-Muller (C-RM) codes were studied in diffusion-based MC systems. In [13], the self-orthogonal convolutional codes (SOCCs) with majority-logic decoding scheme was proposed as a low energy decoding technique for MC. Apart from the study of existing channel coding techniques mentioned above, Shih *et al.* [14] designed a low complexity ISI-free code based on the inherent characteristics of MC system, specifically for diffusion-based MC systems. Reference [15] presents a simple pre-coding technique to reduce the ISI in a MC system, with an intelligent transmitter consisting of M bits of Memory. In this proposed technique, the molecular diffusion rate is adjusted for each bit interval by taking advantage of the memory. Another ISI-free modulation scheme for a given maximum transmission delay is proposed in [16], where symbols of the same type are released sufficiently far apart to reduce the ISI in the system. Inspired by modern advancements in digital communication applications, Dissanayake *et al.* [9] proposed Reed Solomon (RS) codes as an error correction technique for a diffusion-based MC system, with a point transmitter and a fully absorbing receiver, as they are highly effective against burst and random errors. Their results also showed that the bit error rate performance improves with the help of RS codes compared

to both a no-coding scenario and that with HC. Moreover, in [3], following the biological behavior of a MC system, as an alternative solution for interference mitigation, a new type of molecule with kill effect on information carrying molecules, such as molecules with antibacterial behaviors, have been introduced to the system at regular intervals to destroy the accumulated information molecules.

From the analysis point of view, most prior works in the literature only consider ISI mitigation in a point-to-point single transmitter receiver pair, and they fail to address the inherent characteristics and requirements of large-scale multi-user environments in MC. Therefore, a proper analytical and simulation framework is required to precisely analyze the effect of ISI and MUI, and quantify the performance improvement of interference mitigation schemes in a 3D large-scale system with a partially absorbing receiver. In this work, we study the interfering effect of a swarm of point transmitters on the desired signal of a partially absorbing receiver in a large-scale MC system using stochastic geometry. We propose two schemes to mitigate the adverse effects of both ISI and MUI, which are the RS coding scheme and a two-molecule type encoding scheme. To the best of our knowledge, this is the first analytical consideration of MUI and ISI with a partially absorbing receiver in a large-scale multi-user MC system. Moreover, this is the first time that interference mitigation techniques are studied in a large scale MC system under a swarm of transmitters.

Our major contributions can be summarized as follows:

- 1) We present an analytical framework for a large-scale MC system with a point transmitter delivering information to its associated partially absorbing receiver under the interference from other transmitters. We model the interfering transmitters as a homogeneous Poisson point process (HPPP) and stochastic geometry is applied to obtain tractable analytical expressions for the average behavior of the large-scale MC system. To the best of our knowledge, this is the first attempt in the literature that analyzes the behavior of a partially absorbing receiver on large-scale MC systems with multi-users, and addresses the limitations that exist in the previous work [10], [11].
- 2) We derive a closed-form expression for the collective signal strength at the surface of the partially absorbing receiver under the adverse effects of a swarm of interfering point transmitters in 3D space. Based on these, we derive a tractable expression for the bit error probability (BEP) of a large-scale MC system with a partial absorbing receiver.
- 3) We analyze the impact of both ISI and MUI on the desired signal, and propose two novel schemes to mitigate the adverse effects of these interference, which are RS coding and two types of information molecular modulating schemes. In the first scheme, we apply RS codes which is a popular ECC in data communication to the MC system to improve the error recovery capacity of the system and analyze the performance improvement achieved in a 3D large-scale multiuser environment. The second scheme is to prevent the ISI and we propose

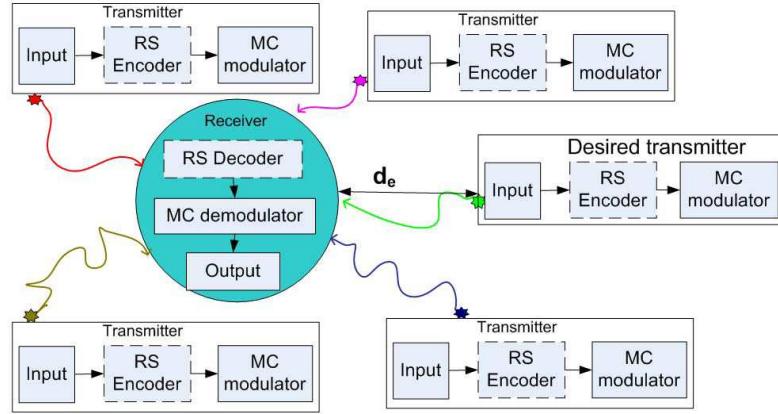


Fig. 1. Illustration of Our System Model, where the dotted lined boxes are only applicable for the system with RS coding and MC modulator/demodulator is differently configured for two types of molecular system.

the introduction of two types of information molecules to the system with the expectation of increasing the time interval between two molecular pulses of the same type. With this presumption, we analyze the feasibility of employing two types of information molecules to modulate the information, in alternative bit intervals to improve the system performance in error prone situations.

4) To evaluate the performance improvement, we derive the closed-form expressions for the strength of the collective signal at the receiver, tractable analytical expressions for the signal-to-interference ratio (SIR) at the receiver, and the BEP of the MC systems with the two proposed schemes. Our derived analytical results are verified via Monte Carlo simulations.

II. SYSTEM MODEL

In this paper, we focus on a 3D large-scale diffusion-based MC system, where a typical point transmitter communicates with a spherical partially absorbing receiver separated by a distance of d_e , under the interference of a swarm of active point transmitter with density λ_a as illustrated in Fig. 1. The interfering point transmitters are spatially distributed outside the receiver in \mathbb{R}^3 , following an independent and HPPP, Φ_a , with density of λ_a , and the partially absorbing receiver with a radius r_r and volume $V_{\Omega_{r_r}}$ has a finite absorption rate of k_1 [10]. In the baseline MC system, each transmitter emits molecular signal pulse at the start of each bit interval, T_b and the first bit is emitted at $t = 0$. The emitted molecules diffuse randomly in the propagation medium until they hit the surface of the receiver. For simplification, we assume that the flow current is absent in the propagation medium and the extension for flow currents can be treated in future work. The absorbing receiver counts the number of molecules absorbed by its surface during each T_b interval. We have considered a partially absorbing receiver, where a fraction of the hitting molecules is absorbed by the receptors of the receiver and counted for the signal demodulation. Due to the fact that the receiver has no knowledge whether the received molecules are emitted

from the desired transmitter or from any other interfering transmitters, the molecules from the interfering transmitters cause MUI at the receiver. It is shown in [10] that the negative effects brought by the joint transmission on collective signal strength increases with time and is heavily dependent on the density of the swarm of active point transmitters and the amount of molecules from the past bits arriving at the current bit interval at the receiver. Further, due to the random nature of molecular propagation, the residual molecules from previous transmissions hitting the receiver surface during the current bit interval cause ISI in MC. Hence, in large-scale MC systems, heavy signal distortion could occur at the receiver due to MUI and ISI, causing erroneous signal demodulation and it is essential to incorporate interference mitigation techniques in these systems to facilitate error free transmission.

To address the aforementioned problems, this paper presents two different interference mitigation schemes for 3D large-scale MC system. Borrowing from the data communication, as our first method to overcome adverse effects of ISI and MUI, we propose channel coding techniques. Specifically we focus on the RS code as our previous results [9] shown that RS codes provide a considerable improvement in BER in a diffusion-based MC system with a point transmitter and a fully absorbing receiver compared to HC [12], [13]. This is because the RS codes have the capacity to correct an entire symbol error compared to the one bit error correction achieved by HC. Although, from the computational complexity point of view, a RS scheme costs more than a simple channel coding scheme, it provides flexibility in error correction capacity, and it is possible to tune n and k of the $RS(n, k)$ coder to match the system requirement.

The second method for interference mitigation is to design a modulation scheme employing two information bearing molecule types for the ISI and MUI reduction inspired from [17]. Note that these two types of molecules can be recognized separately at the receiver in practical scenario, for instance the GABA-Areceptors can distinguish different types of ligands [18]. In our proposed scheme, type A and B molecules are alternated as the messenger molecules between each consecutive bit interval, so that effectively there exist $2T_b$ gap

TABLE I
ILLUSTRATING THE ASSIGNMENT OF TYPE A MOLECULES, N_{tx}^A , AND TYPE B MOLECULES, N_{tx}^B , IN THE PROPOSED ENCODING TECHNIQUE WITH TWO TYPES OF INFORMATION MOLECULES, WHEN j^{th} BIT IS ODD AND $b_i \in \{1, 0\}$

Bit Sequence		b_1	b_2	b_3	b_4	...	b_{j-1}	b_j	
Single type of information molecules		$N_{tx}b_1$	$N_{tx}b_2$	$N_{tx}b_3$	$N_{tx}b_4$...	$N_{tx}b_{j-1}$	$N_{tx}b_j$	
Two types of information molecules	Even		$N_{tx}^B b_2$		$N_{tx}^B b_4$...	$N_{tx}^B b_{j-1}$		
	Odd	$N_{tx}^A b_1$		$N_{tx}^A b_3$...		$N_{tx}^A b_j$	

between the same type of molecules. This technique will reduce the ISI and MUI in the system and will act as a bit error mitigation technique. As shown in Table I, we first divide the input sequence into odd and even numbered sequences by considering the original position of the bit, then the entire even numbered sequence is modulated using type B molecules, whereas the odd numbered sequence is modulated using type A molecules. Since this modulation scheme introduces minimum $2T_b$ time gap between emission of each type of molecules to the medium, the ISI from the nearest previous bit, which contributes largely to the overall ISI, is not present in the system. Additionally, for an odd sequence, the ISI from the bits transmitted by the even sequence, and vice versa is also eliminated. Hence, the proposed system modulated with two types of information molecules, inherently exhibits lower levels of ISI and MUI. The other advantage of the proposed scheme is the low complexity associated with the implementation, at both transmitter and the receiver, as the proposed technique doesn't require prior knowledge of the molecular type assignment pattern to modulate and demodulate the current bit.

Even though this work considers only two types of information molecules, it provides the fundamental insights to enable extension to a M -type molecular modulation scheme. Having a larger value for M will complicate the design of the receiver in practice. This is because one of the key requirement of the propose system is the ability of the receiver to differentiate between the M -types of molecules. In such scenario, creating a receptor with different types of sensitivities to many types of molecules is not practically possible, compared to designing a receptor with two or three different types of sensitivities. Hence, there exist an optimum value for M depending on the application scenario.

Furthermore, we follow the global synchronization assumption as [10], [11], and [19], where all transmitters are assumed to be synchronous. This facilitates simple analysis and leads to tractable results. Yet, our system can be extended to asynchronous transmission by following [20]. In an asynchronous system, molecules will be emitted randomly within the bit duration, T_b . ISI can be significant in asynchronous transmission, due to the spreading of significant number of molecules from molecular pulses emitted nearer to the end of the bit interval to the next bit interval at the receiver. Moreover,

the ISI due to asynchronous transmission is higher in the system with no coding and with one type of molecules, compared to the system with two types of molecules. Yet, in the system with $RS(n, k)$ codes with one type of molecules, the n and k can be fine-tuned to recover from the bit errors caused by ISI. Hence, the effect of the synchronization errors on a RS coded system can be minimized. In the system with two types of molecules, as we alternate the type of molecules used in every other bit interval, the spreading of the molecules emitted towards the end of the bit interval may not affect the next bit when the synchronization error is less than T_b , as the carrier molecular type for the next bit will be different from the previous bit. Yet, if the synchronization error is more than T_b , the ISI becomes significant and the system would not have the capacity to correct these errors.

Our proposed MC system consists of three key modules as illustrated in Fig. 1; the transmitter with a modulator and RS encoder, the propagation channel, and the receiver with a demodulator and RS decoder, which are presented in details in the following subsections.

A. Transmitters

1) *Single Type of Information Molecule*: In terms of the modulation scheme, we adopt Binary Concentration Shift Keying (BCSK) as in [2], where information is conveyed through the number of type S molecules transmitted at the start of each bit interval, T_b . In order to transmit the bit-1 signal, N_{tx}^S number of type S molecules are transmitted, and bit-0 is delivered with the absence of type S molecules.

2) *Two Types of Information Molecules*: In this scheme, we introduce two distinguishable types of molecules as information carriers, namely, type A and type B molecules. As illustrated in Table I, the input bit sequence is divided into two sequences, where the bits in the odd numbered positions constitute the first sequence (odd sequence), and the bits in the even numbered positions constitute the second sequence (even sequence). Both sequences are modulated using BCSK as in [2]. In more detail, N_{tx}^B type B molecules are emitted at $t = (2m - 2)T_b$ time instance to represent the a bit-1 in the even bit sequence, whereas N_{tx}^A A molecules are emitted at $t = (2m - 1)T_b$ to represent a bit-1 in the odd

bit sequence, here m indicates the position of the bit in the even or odd sequence. Similar to the system with a single type of information molecule, bit-0 in either sequence is signaled using an absence of molecules.

B. Propagation

Brownian motion governs the movement of information molecules in fluid environment. In the system modeled, the collisions between molecules are ignored, which is a reasonable assumption when the fluid medium is significantly bigger compared to the size of the molecules, i.e. when the molecular density in the transmission medium is low [9]. The molecular propagation in these type of environment follows Fick's Second law [21], which is described using

$$\frac{\partial(rC(r, t|r_0))}{\partial t} = D \frac{\partial^2(rC(r, t|r_0))}{\partial r^2}, \quad (1)$$

where $C(r, t|r_0)$ is the molecule concentration at time t at distance r , r_0 is the distance between transmitter and the center of the receiver, and D is the diffusion coefficient. The value of D depends on the temperature, viscosity of the fluid, and the Stokes' radius of the molecule [3].

C. Receiver

From the perspective of receiver design in MC, the majority of prior works has considered two types of receivers, namely passive and active receivers. Passive receivers only observe and count the number of molecules inside the receiver without interfering with the molecule propagation, while active receivers absorb fraction of the molecules that hit the receiver surface. In nature, most receivers commonly remove information molecules from the propagation medium once they bind to a receptor. Further, some molecules which hit the receiver surface can bounce back without binding to the receptors [22]. Also, some molecules may get bound to inactive receptors. Hence, we consider a molecule as received by a receiver for the demodulation process, only if it binds to one of the active receptors on the surface of the receiver [22], [23]. This motivates us to employ a partially absorbing receiver, which absorbs only a fraction of the bound molecules in our system.

The reception process of an absorbing receiver can be described as [8]

$$D \frac{\partial C(r, t|r_0))}{\partial r} \Big|_{r=r_r^+} = k_1 C(r_r, t|r_0), \quad (2)$$

where k_1 is the absorption rate. Eq. (2) describes the boundary condition for the partially absorbing receiver when k_1 is a non zero finite constant. Further, when $k_1 \rightarrow \infty$, it defines the boundary condition for the fully absorbing receiver. Moreover, in the case of multiple absorbing receivers the number of molecules absorbed by the receiver depends on the total number of absorbing receivers present. In the work presented, we consider the single partially absorbing receiver, which can reduce to a fully absorbing receiver when the absorption rate, $k_1 \rightarrow \infty$.

1) Single Type of Information Molecules: The demodulation of the BCSK signal is performed at the receiver to identify the bit pattern being transmitted. The total number of molecules hitting the surface of the absorbing receiver during each $[(j-1)T_b, jT_b]$ interval is counted at the demodulator for information demodulation. For instance, to demodulate the j^{th} bit, the number of molecules received during $[(j-1)T_b, jT_b]$ interval N_{net}^S is compared against a predefined demodulation threshold value N_{th} . If $N_{\text{th}} < N_{\text{net}}^S$ the received bit is interpreted as bit-1, otherwise as bit-0.

2) Two Types of Information Molecules: The receiver is assumed to have the capability to differentiate between the type A molecule and the type B molecule. The partially absorbing receiver counts the net number of molecules absorbed at every T_b interval and compares it against a pre-set threshold level for each molecule type for information demodulation. More precisely the number of type B molecules absorbed during the time interval $[(2m-2)T_b, (2m-1)T_b]$, (N_{net}^B) , is compared against the threshold level N_{th}^B to demodulate the bits in the even bit sequence, whereas the number of type A molecules absorbed during $[(2m-1)T_b, (2m)T_b]$, (N_{net}^A) , is compared against the threshold level N_{th}^A to demodulate the bits in the odd bit sequence. If $N_{\text{th}}^A \leq N_{\text{net}}^A$ or $N_{\text{th}}^B \leq N_{\text{net}}^B$, the received bit is demodulated as bit-1, otherwise as bit-0.

D. Reed Solomon coder

According to [10], it is evident that a 3D large-scale MC system experiences a significant amount of bit errors and it requires a powerful error correcting mechanism, which has the capacity to correct more than one bit in a single codeword. As a conventional practice in data communication, ECCs are used to achieve an acceptable level of reliability for the received message, when information is transmitted through error prone transmission channels. Hence, to combat the negative impact brought by the high MUI and ISI, following the observations of [9], we propose RS codes [24], which is a non-binary Bose, Chaudhuri, and Hocquenghem (BCH) code, as an ECC for 3D MC systems with a swarm of interfering transmitters.

In RS codes, the redundant data is embedded with the input message to facilitate the error recovery at the receiver. $RS(n, k)$ is defined over a Galois Field ($GF(p^m)$), where p is a prime, and m is a positive integer. The $RS(n, k)$ encoder, expands the input message (M) of k length into codeword (C) of n length by adding redundant parity bits (P) of $n-k$ length. These parity bits are generated, so that every codeword, C, is a multiple of the generator polynomial of the RS code, G. In special circumstances, the parity bits generated to satisfy the above condition, could be a null sequence. The RS decoder, first computes the syndrome (S) by multiplying the received codeword, C' by a predefined check polynomial [25]. If the syndrome computation results in a non zero value, it treats the received codeword as in error and attempts to correct the identified erroneous codeword, by first determining the symbol error locator polynomial using the Berlekamp-Massey algorithm, then finding the roots of the error locator polynomial using the Chien search algorithm, and then estimating the error magnitudes using Forney algorithm. Once the error location

and the error values are estimated, a correction is applied to the received codeword to recover from the error. An extensive review of RS codes is given in [24] and [25].

In general, a RS code with $n - k$ length of parity bits has the capacity to correct up to $\frac{n-k}{2}$ number of errors per codeword [25]. Hence, the higher the redundancy is, the more errors can be corrected. Due to the effectiveness of RS codes in combating both random multiple bit errors and burst errors, they are more popular in data communication applications compared to HC, which only provides single bit error correction. On the other hand, as the size of the codeword n increases, the implementation grows in complexity. Hence, the code length, n and the message length, k of the $RS(n, k)$ code should be carefully selected according to the channel error rate and the required level of BEP improvement.

III. CHANNEL IMPULSE RESPONSE

In this section, we derive the analytical expression for the channel impulse response at the partially absorbing receiver due to a j length bit stream emission at each point transmitter in a large scale MC system, where information is modulated using single type of information molecules.

A. Reaction Rate of the Receiver

As the stationary spherical receiver with radius r_r is located at the origin of an unbounded 3D space, the reaction can occur at anywhere on its surface. If the transmitter is located at \mathbf{r}_0 and emits an impulse signal at $t = t_0$, the reaction rate at distance $r = r_r$ in general is given as

$$K(t|\|\mathbf{r}_0\|, t_0) = 4\pi r_r^2 D \frac{\partial C(r, t|\|\mathbf{r}_0\|, t_0)}{\partial r} \Big|_{r=r_r}, \quad (3)$$

where $\|\mathbf{r}_0\|$ defines the norm of the vector \mathbf{r}_0 , and is a function that assigns a strictly positive length or size to the vector.

According to [8, eq. (3.99)], the concentration of molecules at distance r and time t in a MC system with a partially absorbing receiver is derived as

$$\begin{aligned} C(r, t|\|\mathbf{r}_0\|, t_0) &= \frac{1}{4\pi r \|\mathbf{r}_0\|} \frac{1}{\sqrt{4\pi D(t-t_0)}} \\ &\times \left(\exp \left\{ -\frac{(r - \|\mathbf{r}_0\|)^2}{4D(t-t_0)} \right\} - \exp \left\{ -\frac{(r + \|\mathbf{r}_0\| - 2r_r)^2}{4D(t-t_0)} \right\} \right) \\ &- \frac{1}{4\pi r \|\mathbf{r}_0\|} \alpha \left(\exp \left\{ \alpha^2 D(t-t_0) + \alpha(r + r_0 - 2r_r) \right\} \right. \\ &\times \left. \operatorname{erfc} \left\{ \alpha \sqrt{D(t-t_0)} + \frac{r + r_0 - 2r_r}{\sqrt{4D(t-t_0)}} \right\} \right), \end{aligned} \quad (4)$$

where $\alpha = \frac{k_1 r_r + D}{Dr_r}$. Substituting (4) into (3), we can derive the reaction rate with impulse signal emitted at t_0 as

$$\begin{aligned} K_{PA}(t|\|\mathbf{r}_0\|, t_0) &= \frac{k_1 r_r}{r_0} \left(1 + \operatorname{erf} \left\{ \frac{(r_r - \|\mathbf{r}_0\|)}{4D(t-t_0)} \right\} \right. \\ &- \left. \exp \left\{ \alpha^2 D(t-t_0) + \alpha(r_0 - r_r) \right\} \right. \\ &\times \left. \operatorname{erfc} \left\{ \alpha \sqrt{D(t-t_0)} + \frac{r_0 - r_r}{\sqrt{4D(t-t_0)}} \right\} \right), \end{aligned} \quad (5)$$

where $k_1 = \frac{D(r_r \alpha - 1)}{r_r}$.

In a fully absorbing receiver, complete absorption of molecules that collide with the surface of the receiver occurs. This is a special case of the partially absorbing receiver, and the boundary condition for the full absorption receiver is obtained from Eq. (2), when $k_1 \rightarrow \infty$. Hence, its rate of absorption can be obtained from (5) by employing the limit $k_1, \alpha \rightarrow \infty$ as

$$K_{FA}(t|\|\mathbf{r}_0\|, 0) = \frac{r_r}{\|\mathbf{r}_0\|} \frac{\|\mathbf{r}_0\| - r_r}{\sqrt{4\pi D t^3}} \exp \left(-\frac{(\|\mathbf{r}_0\| - r_r)^2}{4Dt} \right), \quad (6)$$

when $t_0 = 0$.

B. Channel Impulse Response

The fraction of absorbed molecules at the receiver during the $[(j-1)T_b, jT_b]$ sampling interval due to the desired transmitter located $\|\mathbf{d}_e\|$ distance from the origin with a single pulse emitted at every T_b interval is given as

$$\begin{aligned} F_D(\Omega_{r_r}, (j-1)T_b, jT_b | \|\mathbf{d}_e\|) &= F_D(\Omega_{r_r}, 0, jT_b | \|\mathbf{d}_e\|) \\ &- F_D(\Omega_{r_r}, 0, (j-1)T_b | \|\mathbf{d}_e\|), \end{aligned} \quad (7)$$

where $F_D(\Omega_{r_r}, 0, jT_b | \|\mathbf{d}_e\|)$ is the total fraction of molecules contributed by all the bits emitted by the transmitter till $t = jT_b$. In absence of molecular degradation, the $F_D(\Omega_{r_r}, 0, jT_b | \|\mathbf{d}_e\|)$ can be expressed as

$$\begin{aligned} F_D(\Omega_{r_r}, 0, jT_b | \|\mathbf{d}_e\|) &= \sum_{i=1}^j b_i \int_0^{jT_b} K((t - (i-1)T_b) | \|\mathbf{d}_e\|) dt, \end{aligned} \quad (8)$$

where b_i is the i^{th} bit of the transmitted sequence and $K((t - (i-1)T_b) | \|\mathbf{d}_e\|)$ is the reaction rate due to a transmitter located at \mathbf{d}_e , and it can be evaluated using (5) for a partially absorbing receiver, and (6) for a fully absorbing receiver, respectively.

Note that the propagation of each molecule is independent, thus the fraction of molecules absorbed at the receiver due to all the interfering transmitters located at a distance $\|\mathbf{x}\|$ from the origin in the 3D space \mathbb{R}^3 during $[(j-1)T_b, jT_b]$ interval can be written using Slivnyak Meekes' Theorem [26] as

$$\begin{aligned} F_I^{all}(\Omega_{r_r}, (j-1)T_b, jT_b | \|\mathbf{x}\|) &= \sum_{x \in \Phi_a} F_I(\Omega_{r_r}, (j-1)T_b, jT_b | \|\mathbf{x}\|), \end{aligned} \quad (9)$$

where $F_I^{all}(\Omega_{r_r}, (j-1)T_b, jT_b | \|\mathbf{x}\|)$ is the total fraction of molecules absorbed at the receiver due to a swarm of interfering transmitters, during the time interval $[(j-1)T_b, jT_b]$, and $F_I(\Omega_{r_r}, (j-1)T_b, jT_b | \|\mathbf{x}\|)$ is the fraction of molecules absorbed at the receiver due to single interfering transmitter at location \mathbf{x} , emitting j sequence of bits. $F_I(\Omega_{r_r}, (j-1)T_b, jT_b | \|\mathbf{x}\|)$ can be formulated similar to (8) with b_i being the value of the i^{th} bit of the interfering transmitter at \mathbf{x} position as

$$\begin{aligned} F_I(\Omega_{r_r}, (j-1)T_b, jT_b | \|\mathbf{x}\|) &= \sum_{i=1}^j b_i \int_{(j-1)T_b}^{jT_b} K((t - (i-1)T_b) | \|\mathbf{x}\|) dt. \end{aligned} \quad (10)$$

Depending on the type of receiver used, we can use either (5) or (6) to evaluate for $K((t - (i - 1)T_b)| \|\mathbf{x}\|)$.

Furthermore, the total fraction of molecules absorbed at the receiver due to both the desired and the interfering transmitters can be written as

$$\begin{aligned} F_{\text{all}}(\Omega_{r_r}, (j-1)T_b, jT_b) &= F_{\text{D}}(\Omega_{r_r}, (j-1)T_b, jT_b| \|\mathbf{d}_e\|) \\ &+ \sum_{x \in \Phi_a} F_{\text{I}}(\Omega_{r_r}, (j-1)T_b, jT_b| \|\mathbf{x}\|) \end{aligned} \quad (11)$$

where, $F_{\text{D}}(\Omega_{r_r}, (j-1)T_b, jT_b| \|\mathbf{d}_e\|)$ can be evaluated using (7) and $F_{\text{I}}(\Omega_{r_r}, (j-1)T_b, jT_b| \|\mathbf{x}\|)$ can be evaluated using (9).

IV. RECEIVER OBSERVATION

In this section, we focus on the receiver observation due to j length bit stream emitted by each active transmitter at T_b bit intervals, and derive the exact expression for the expected number of molecules at the absorbing receiver in a large-scale MC system.

A. Single Type of Information Molecule

When modulated using the single type of information molecule, due to independent propagation of each molecule in the medium, the expected net number of molecules absorbed during $[(j-1)T_b, jT_b]$ interval due to desired transmitter can be formulated as

$$\begin{aligned} \mathbb{E}_{\text{D}}^{\text{S}} \{ N_{\text{D}}^{\text{S}}(\Omega_{r_r}, (j-1)T_b, jT_b) \} &= N_{\text{tx}}^{\text{S}} \mathbb{E} \{ F_{\text{D}}^{\text{S}}(\Omega_{r_r}, (j-1)T_b, jT_b| \|\mathbf{d}_e\|) \} \\ &= N_{\text{tx}}^{\text{S}} \sum_{i=1}^j b_i \int_{(j-1)T_b}^{jT_b} K((t - (i-1)T_b)| \|\mathbf{d}_e\|) dt, \end{aligned} \quad (12)$$

where $K((t - (i-1)T_b)| \|\mathbf{d}_e\|)$ for a partially absorbing receiver is given in (5) and that of a fully absorbing receiver is given in (6).

In a MC system, all the transmitters are located outside the surface of the spherical receiver, in contrast to a wireless communication system where the transmitter can be located randomly. Hence, in a MC system, there exists a minimum distance r_r between a point transmitter and the receiver center. Therefore, we express the expected number of molecules observed at the receiver due to interfering transmitters for the time interval $[(j-1)T_b, jT_b]$ as

$$\begin{aligned} \mathbb{E}_{\text{I}}^{\text{S}} \{ N_{\text{I}}^{\text{S}}(\Omega_{r_r}, (j-1)T_b, jT_b) \} &= N_{\text{tx}}^{\text{S}} \mathbb{E} \left\{ \sum_{x \in \Phi_a} F_{\text{I}}^{\text{S}}(\Omega_{r_r}, (j-1)T_b, jT_b| \|\mathbf{x}\|) \right\} \\ &= \lambda_a N_{\text{tx}}^{\text{S}} \int_{\mathbb{R}} F_{\text{I}}^{\text{S}}(\Omega_{r_r}, (j-1)T_b, jT_b| \|\mathbf{x}\|) dx, \end{aligned} \quad (13)$$

which can be further simplified applying Campbell's theorem in 3D space as [26, eq. (1.18)]

$$\begin{aligned} \mathbb{E}_{\text{I}}^{\text{S}} \{ N_{\text{I}}^{\text{S}}(\Omega_{r_r}, (j-1)T_b, jT_b) \} &= 4\pi \lambda_a N_{\text{tx}}^{\text{S}} \int_{r_r}^{\infty} \sum_{i=1}^j b_i \\ &\times \int_{(j-1)T_b}^{jT_b} K((t - (i-1)T_b)| \|\mathbf{x}\|) dt r^2 dr. \end{aligned} \quad (14)$$

B. Two Types of Information Molecules

In this section, we analyze the receiver observation of the MC system modulating using two types of information molecules.

1) *Odd Numbered Bits*: The bits emitted at odd T_b bit intervals are transmitted using type A molecules, with N_{tx}^{A} number of molecules to signal bit-1 and an absence of molecules to signal bit-0. Taking this into account, the expression for the expected number of molecules at the partially absorbing receiver derived in (12) and (14) can be modified as

$$\begin{aligned} \mathbb{E}_{\text{D}}^{\text{A}} \{ N_{\text{D}}^{\text{A}}(\Omega_{r_r}, (j-1)T_b, jT_b) \} &= N_{\text{tx}}^{\text{A}} \sum_{i=1}^{\lceil j/2 \rceil} b_{(2i-1)} \int_{(j-1)T_b}^{jT_b} K((t - (i-1)2T_b)| \|\mathbf{d}_e\|) dt, \end{aligned} \quad (15)$$

and

$$\begin{aligned} \mathbb{E}_{\text{I}}^{\text{A}} \{ N_{\text{I}}^{\text{A}}(\Omega_{r_r}, (j-1)T_b, jT_b) \} &= 4\pi \lambda_a N_{\text{tx}}^{\text{A}} \int_{r_r}^{\infty} \sum_{i=1}^{\lceil j/2 \rceil} b_{(2i-1)} \\ &\times \int_{(j-1)T_b}^{jT_b} K((t - (i-1)2T_b)| \|\mathbf{x}\|) dt r^2 dr, \end{aligned} \quad (16)$$

where $K((t - (i-1)2T_b)| \|\mathbf{d}_e\|)$ and $K((t - (i-1)2T_b)| \|\mathbf{x}\|)$ can be evaluated using (5) for a partially absorbing receiver and (6) a fully absorbing receiver.

2) *Even Numbered Bits*: The expression for the expected number of molecules at the receiver due to an even numbered sequence, with the knowledge that bit-1 is represented using N_{tx}^{B} number of type B molecules and bit-0 by the absence of molecules, can be formulated as

$$\begin{aligned} \mathbb{E}_{\text{D}}^{\text{B}} \{ N_{\text{D}}^{\text{B}}(\Omega_{r_r}, (j-1)T_b, jT_b) \} &= N_{\text{tx}}^{\text{B}} \sum_{i=1}^{\lfloor j/2 \rfloor} b_{2i} \\ &\times \int_{(j-1)T_b}^{jT_b} K((t - (2i-1)T_b)| \|\mathbf{d}_e\|) dt, \end{aligned} \quad (17)$$

and

$$\begin{aligned} \mathbb{E}_{\text{I}}^{\text{B}} \{ N_{\text{I}}^{\text{B}}(\Omega_{r_r}, (j-1)T_b, jT_b) \} &= 4\pi \lambda_a N_{\text{tx}}^{\text{B}} \int_{r_r}^{\infty} \sum_{i=1}^{\lfloor j/2 \rfloor} b_{2i} \\ &\times \int_{(j-1)T_b}^{jT_b} K((t - (2i-1)T_b)| \|\mathbf{x}\|) dt r^2 dr. \end{aligned} \quad (18)$$

where $K((t - (2i-1)T_b)| \|\mathbf{d}_e\|)$ and $K((t - (2i-1)T_b)| \|\mathbf{x}\|)$ can be evaluated using (5) for a partially absorbing receiver and (6) for a fully absorbing receiver.

C. Cumulative Expectation

1) *Single Type of Information Molecule*: The total expected net number of absorbed molecules at the receiver in the MC system with a single type of information molecule, during the

time interval $[(j-1)T_b, jT_b]$ due to j length bit sequence can be written by combining (12) and (14) as

$$\begin{aligned} \mathbb{E}_{\text{all}}^S \{ N_{\text{all}}^S(\Omega_{rr}, (j-1)T_b, jT_b) \} \\ = \mathbb{E}_{\text{D}}^S \{ N_{\text{D}}(\Omega_{rr}, (j-1)T_b, jT_b) \} \\ + \mathbb{E}_{\text{I}}^S \{ N_{\text{I}}(\Omega_{rr}, (j-1)T_b, jT_b) \} \end{aligned} \quad (19)$$

2) *Two Types of Information Molecules*: The cumulative expected number of molecules at the receiver in the MC system with two types of information molecules, can be formulated as

$$\begin{aligned} \mathbb{E}_{\text{all}}^{A+B} \{ N(\Omega_{rr}, (j-1)T_b, jT_b) \} \\ = N_{\text{tx}}^A [\mathbb{E} \{ F_{\text{D}}^A(\Omega_{rr}, (j-1)T_b, jT_b | \| \mathbf{d}_e \|) \} \\ + \mathbb{E} \{ F_{\text{I}}^A(\Omega_{rr}, (j-1)T_b, jT_b | \| \mathbf{x} \|) \}] \\ + N_{\text{tx}}^B [\mathbb{E} \{ F_{\text{D}}^B(\Omega_{rr}, (j-1)T_b, jT_b | \| \mathbf{d}_e \|) \} \\ + \mathbb{E} \{ F_{\text{I}}^B(\Omega_{rr}, (j-1)T_b, jT_b | \| \mathbf{x} \|) \}], \end{aligned} \quad (20)$$

where $\mathbb{E} \{ F_{\text{D}}^A(\Omega_{rr}, (j-1)T_b, jT_b | \| \mathbf{d}_e \|) \}$, $\mathbb{E} \{ F_{\text{I}}^A(\Omega_{rr}, (j-1)T_b, jT_b | \| \mathbf{x} \|) \}$, $\mathbb{E} \{ F_{\text{D}}^B(\Omega_{rr}, (j-1)T_b, jT_b | \| \mathbf{d}_e \|) \}$, and $\mathbb{E} \{ F_{\text{I}}^B(\Omega_{rr}, (j-1)T_b, jT_b | \| \mathbf{x} \|) \}$ can be evaluated using (15), (16), (17) and (18) respectively.

D. Signal to Interference Ratio

The Signal to Interference Ratio (SIR) for the MC system presented in this paper is defined as the ratio of molecules that arrive in the current symbol duration from the desired transmitter to the ratio of interfering molecules from the swarm of transmitters. Hence, the impact of the proposed system can be further realized through analysis of the SIR for the bit interval $[(j-1)T_b, jT_b]$.

1) *Single Type of Information Molecule*: The SIR of the MC system using a single type of information molecule is defined as

$$SIR^S[j] = \frac{N_{\text{tx}}^S \mathbb{E} \{ F_{\text{D}}^S(\Omega_{rr}, (j-1)T_b, jT_b | \| \mathbf{d}_e \|) \}}{N_{\text{tx}}^S \mathbb{E} \{ \sum_{x \in \Phi_a} F_{\text{I}}^S(\Omega_{rr}, (j-1)T_b, jT_b | \| \mathbf{x} \|) \}}, \quad (21)$$

where $\mathbb{E} \{ F_{\text{D}}^S(\Omega_{rr}, (j-1)T_b, jT_b | \| \mathbf{d}_e \|) \}$ and $\mathbb{E} \{ \sum_{x \in \Phi_a} F_{\text{I}}^S(\Omega_{rr}, (j-1)T_b, jT_b | \| \mathbf{x} \|) \}$ can be evaluated using (12) and (14), respectively.

2) *Two Types of Information Molecules*: The SIR of the MC system modulating using two types of information molecules changes with the position of the j^{th} bit in the sequence. Hence, the SIR can be written as

$$SIR_{\text{A}}^{A+B}[j] = \frac{N_{\text{tx}}^A \mathbb{E} \{ F_{\text{D}}^A(\Omega_{rr}, (j-1)T_b, jT_b | \| \mathbf{d}_e \|) \}}{N_{\text{tx}}^A \mathbb{E} \{ \sum_{x \in \Phi_a} F_{\text{I}}^A(\Omega_{rr}, (j-1)T_b, jT_b | \| \mathbf{x} \|) \}}, \quad (22)$$

when j^{th} bit is in an odd numbered position, and as

$$SIR_{\text{B}}^{A+B}[j] = \frac{N_{\text{tx}}^B \mathbb{E} \{ F_{\text{D}}^B(\Omega_{rr}, (j-1)T_b, jT_b | \| \mathbf{d}_e \|) \}}{N_{\text{tx}}^B \mathbb{E} \{ \sum_{x \in \Phi_a} F_{\text{I}}^B(\Omega_{rr}, (j-1)T_b, jT_b | \| \mathbf{x} \|) \}}, \quad (23)$$

when j^{th} bit is in an even numbered position. The $\mathbb{E} \{ F_{\text{D}}^A(\Omega_{rr}, (j-1)T_b, jT_b | \| \mathbf{d}_e \|) \}$, $\mathbb{E} \{ F_{\text{I}}^A(\Omega_{rr}, (j-1)T_b, jT_b | \| \mathbf{x} \|) \}$, $\mathbb{E} \{ F_{\text{D}}^B(\Omega_{rr}, (j-1)T_b, jT_b | \| \mathbf{d}_e \|) \}$ and

$\mathbb{E} \{ F_{\text{I}}^B(\Omega_{rr}, (j-1)T_b, jT_b | \| \mathbf{x} \|) \}$ can be evaluated using (15), (16), (17) and (18), respectively. It should be noted that, the interference is caused by molecules of same type only, and molecules from two different types don't create interference at the receiver. For instance, if the desired signal is transmitted using type A molecules, the interference is only from the type A molecules transmitted by the swarm of interfering transmitters.

V. ERROR PROBABILITY

In this section, we derive the bit error probability of a 3D large-scale MC system defined in Section II with the two schemes to reduce the effect of MUI and ISI interference. The net number of absorbed molecules at the surface of the partially absorbing receiver and the fully absorbing receiver is sampled at the detector and one sample per bit is used for information demodulation.

A. Bit Error Probability of the MC System

The net number of absorbed molecules at the receiver in the j^{th} bit interval due to all the transmitters in the space \mathbb{R}^3 with multiple transmitted bit sequences can be written as

$$N_{\text{net}}[j] = N_{\text{net}}^{\text{D}}[j] + N_{\text{net}}^{\text{I}}[j], \quad (24)$$

where

$$N_{\text{net}}^{\text{D}}[j] \sim B(N_{\text{tx}}, F_{\text{D}}(\Omega_{rr}, (j-1)T_b, jT_b | \| \mathbf{d}_e \|)), \quad (25)$$

$$N_{\text{net}}^{\text{I}}[j] \sim \sum_{x \in \Phi_a} B(N_{\text{tx}}, F_{\text{I}}(\Omega_{rr}, (j-1)T_b, jT_b | \| \mathbf{x} \|)), \quad (26)$$

For the simplicity of the analysis, (25) and (26) can be approximated using a Poisson model as in [2]. Therefore Eq. (24) can be expressed using a Poisson approximation as

$$\begin{aligned} N_{\text{net}}[j] \sim P(N_{\text{tx}} F_{\text{D}}(\Omega_{rr}, (j-1)T_b, jT_b | \| \mathbf{d}_e \|) \\ + N_{\text{tx}} \sum_{x \in \Phi_a} F_{\text{I}}(\Omega_{rr}, (j-1)T_b, jT_b | \| \mathbf{x} \|)). \end{aligned} \quad (27)$$

The BEP of the large-scale MC system, for the j^{th} bit can be written as

$$\begin{aligned} P_e[j] = P_r[e | b_j = 0, b_{1:j-1}] P_r[b_j = 0] \\ + P_r[e | b_j = 1 b_{1:j-1}] P_r[b_j = 1], \end{aligned} \quad (28)$$

where $P_r[e | b_j = 0, b_{1:j-1}]$ and $P_r[e | b_j = 1 b_{1:j-1}]$ are the conditional probabilities.

1) *Single Type of Information Molecule*: For the MC system using a single type of information molecule, the net number of absorbed molecules at the receiver in the j^{th} bit interval due to all the transmitters in the space \mathbb{R}^3 with multiple transmitted bit sequences can be approximated as

$$N_{\text{net}}^S[j] \sim P(N_{\text{tx}}^S R_{\text{Tot}}^S(\Omega_{rr}, j)), \quad (29)$$

where

$$\begin{aligned} R_{\text{Tot}}^S(\Omega_{rr}, j) &= F_{\text{D}}(\Omega_{rr}, (j-1)T_b, jT_b | \| \mathbf{d}_e \|) \\ &+ \sum_{x \in \Phi_a} F_{\text{I}}(\Omega_{rr}, (j-1)T_b, jT_b | \| \mathbf{x} \|), \\ &= R_{\text{D}}^S(\Omega_{rr}, j | \| \mathbf{d}_e \|) + \sum_{x \in \Phi_a} R_{\text{I}}^S(\Omega_{rr}, j | \| \mathbf{x} \|). \end{aligned} \quad (30)$$

Closed-form expressions for conditional probabilities in (28) for single type of information molecules are derived in the following lemma.

Lemma 1: The conditional probabilities in (28) in the j^{th} bit are written as

$$P_r[e | b_j = 1, b_{1:j-1}] = P_r[N_{\text{net}}^S[j] < N_{\text{th}}^S], \quad (31)$$

and

$$\begin{aligned} P_r[e | b_j = 0, b_{1:j-1}] &= P_r[N_{\text{net}}^S[j] \geq N_{\text{th}}^S] \\ &= 1 - P_r[N_{\text{net}}^S[j] < N_{\text{th}}^S], \end{aligned} \quad (32)$$

where

$$\begin{aligned} P_r[N_{\text{net}}^S[j] < N_{\text{th}}^S] \\ &= \mathbb{E}\left\{\exp\left\{-N_{\text{tx}}^S R_{\text{Tot}}^S\right\} \sum_{n=0}^{N_{\text{th}}^S-1} \frac{[N_{\text{tx}}^S R_{\text{Tot}}^S]^n}{n!}\right\}. \end{aligned} \quad (33)$$

Proof: See Appendix A for the derivation of the closed-form expression for $P_r[N_{\text{net}}^S[j] < N_{\text{th}}^S]$. ■

By substituting (31) and (32) into (28), we can obtain the expression for the bit error probability for the uncoded system with a single type of information molecule.

2) *Two Types of Information Molecules:* The net number of absorbed molecules at the receiver in the j^{th} bit interval due to all the transmitters with multiple transmitted bit sequences modulated using type A and B information molecules, can be expressed using a Poisson approximation as

$$N_{\text{net}}^{A+B}[j] \sim P(N_{\text{tx}}^{A+B} R_{\text{Tot}^{A+B}}(\Omega_{rr}, j)), \quad (34)$$

where

$$\begin{aligned} R_{\text{Tot}}^{A+B}(\Omega_{rr}, j) &= (F_D^A(\Omega_{rr}, (j-1)T_b, jT_b | \|\mathbf{d}_e\|)) \\ &+ \sum_{x \in \Phi_a} F_I^A(\Omega_{rr}, (j-1)T_b, jT_b | \|\mathbf{x}\|) \\ &+ (F_D^B(\Omega_{rr}, (j-1)(T_b), j(T_b) | \|\mathbf{d}_e\|)) \\ &+ \sum_{x \in \Phi_a} F_I^B(\Omega_{rr}, (j-1)(T_b), j(T_b) | \|\mathbf{x}\|) \\ &= R_{\text{Tot}}^A(\Omega_{rr}, j) + R_{\text{Tot}}^B(\Omega_{rr}, j). \end{aligned} \quad (35)$$

With the assumption of no interaction and reaction between type A and type B information molecules, the conditional probabilities given in (28) can be rewritten as

$$P_r[e | b_j = 1, b_{1:j-1}] = P_r[N_{\text{net}}^{A+B}[j] < N_{\text{th}}], \quad (36)$$

and

$$P_r[e | b_j = 0, b_{1:j-1}] = P_r[N_{\text{net}}^{A+B}[j] > N_{\text{th}}], \quad (37)$$

where N_{th} can be either N_{th}^A or N_{th}^B depending on the position of the j^{th} bit in the input sequence.

Let us first evaluate the conditional probability for the even numbered sequence, when j is an even number and $N_{\text{th}} = N_{\text{th}^B}$.

$$\begin{aligned} P_r[e | b_j = 1, b_{1:j-1}] \\ &= P_r[N_{\text{net}}^{A+B}[j] < N_{\text{th}}^B], \\ &= P_r[N_{\text{net}}^B[j] < N_{\text{th}}^B], \\ &= \mathbb{E}\left\{\exp\left\{-N_{\text{tx}}^B R_{\text{Tot}_{\text{even}}}^B\right\} \sum_{n=0}^{N_{\text{th}}^B-1} \frac{[N_{\text{tx}}^B R_{\text{Tot}_{\text{even}}}^B]^n}{n!}\right\}. \end{aligned} \quad (38)$$

Proof: Eq.(38) can be further simplified as in Lemma 1. ■

We can follow a similar method to derive $P_r[e | b_j = 0, b_{1:j-1}]$ for the even numbered sequence, which can be written as

$$\begin{aligned} P_r[e | b_j = 0, b_{1:j-1}] &= P_r[N_{\text{net}}^{A+B}[j] \geq N_{\text{th}}^B] \\ &= P_r[N_{\text{net}}^B[j] \geq N_{\text{th}}^B] \\ &= 1 - P_r[N_{\text{net}}^B[j] < N_{\text{th}}^B]. \end{aligned} \quad (39)$$

By substituting (38) and (39) into (28), we obtain the expression for the bit error probability of the uncoded MC system for the even numbered sequence. As the evaluation of conditional probabilities of the odd numbered sequence takes a similar approach as that of even numbered sequence, we can derive the BEP of the odd numbered sequence by following the same procedure as that presented above by accounting for the bit interval of the odd sequence as $(2n-1)T_b$. Note that our derivations can be easily generalized for any type of receiver, by evaluating the term $K((t-(i-1)T_b) | \|\mathbf{x}\|)$ in Eq. (7) and (9), which defines the reaction rate at the receiver due to a transmitter located at \mathbf{x} , considering the type of receiver used. For instance, we can expand this derivation for a reversible adsorption receiver, simply by using, [2, eq. (8)] for $K((t-(i-1)T_b) | \|\mathbf{x}\|)$ to determine the fraction of information molecules received.

B. Bit Error Probability of the Reed Solomon Coded System

We propose RS codes as channel codes to mitigate the interference caused by the interfering transmitters and previously transmitted bits. Following [25], the BEP for the j^{th} bit of a $RS(n, k)$ coded system can be written as

$$P_b[j] = \sum_{i=t_e+1}^n \binom{n}{i} P_e[j]^i (1 - P_e[j])^{n-i}, \quad (40)$$

where $t_e = \frac{n-k}{2}$ is the error correction capacity, and $P_e[j]$ is the bit error probability for the uncoded system given by (28).

VI. RESULTS AND ANALYSIS

This section examines the expected number of molecules observed and the bit error probability at the partially absorbing receiver with the proposed two distortion mitigation techniques. It has been shown in [10], that results obtained from both Monte Carlo simulations and Particle-Based simulations are well matched in a 3D large-scale molecular communication system with an absorbing receiver. Due to the extensive computational capability required to simulate a large scale MC environment in particle-based simulations, in this paper, we use Monte Carlo simulation to validate the analytical derivations presented in earlier sections. In all the figures presented in this paper, analytical curves are abbreviated as “Ana” and that of Monte Carlo simulations as “Sim”. Furthermore, the results of the MC system modulated with single type of information molecules is abbreviated as “One” and that of type A and B information molecules as “Two”.

In Fig. 2-11, the simulation results are obtained using the Monte Carlo simulation method, which was performed by averaging the expected number of observed molecules due

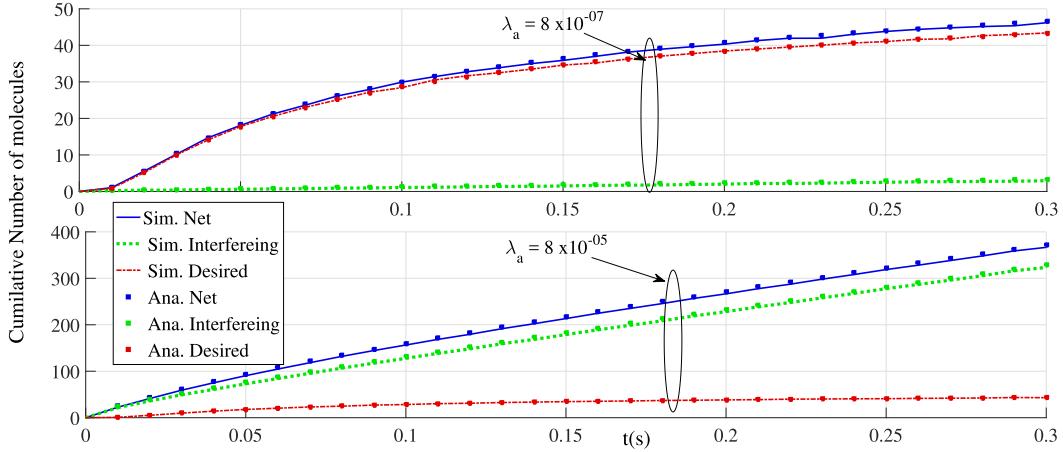


Fig. 2. Expected number of molecules observed at the Full absorption Receiver with parameters $N_{tx} = 200$, $t_b = 0.1s$, $R = 100\mu m$, $d_e = 15\mu m$, $r_r = 5\mu m$, and $D = 800\mu m^2/s$.

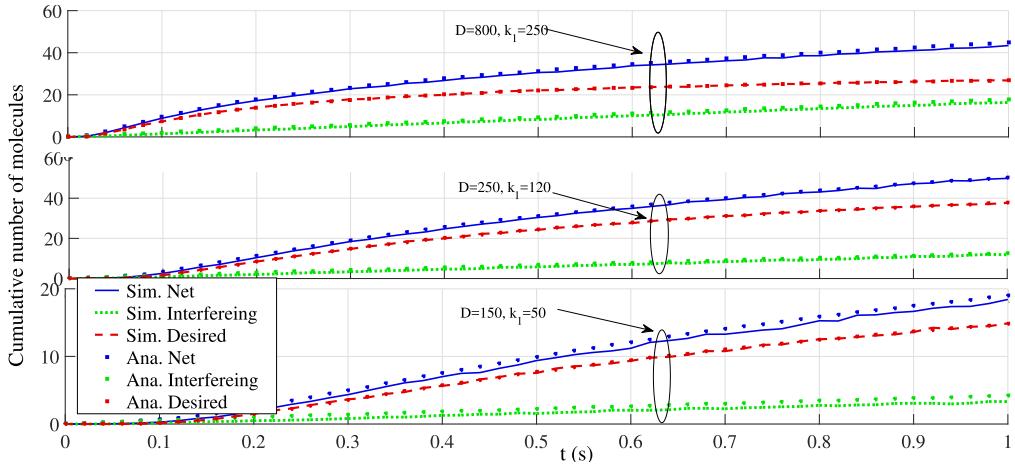


Fig. 3. Expected number of molecules observed at the Partial absorption Receiver with parameters $N_{tx} = 1000$, $t_b = 0.5s$, $R = 100\mu m$, $\lambda_a = 8 \times 10^{-6}$, $d_e = 20\mu m$, and $r_r = 5\mu m$.

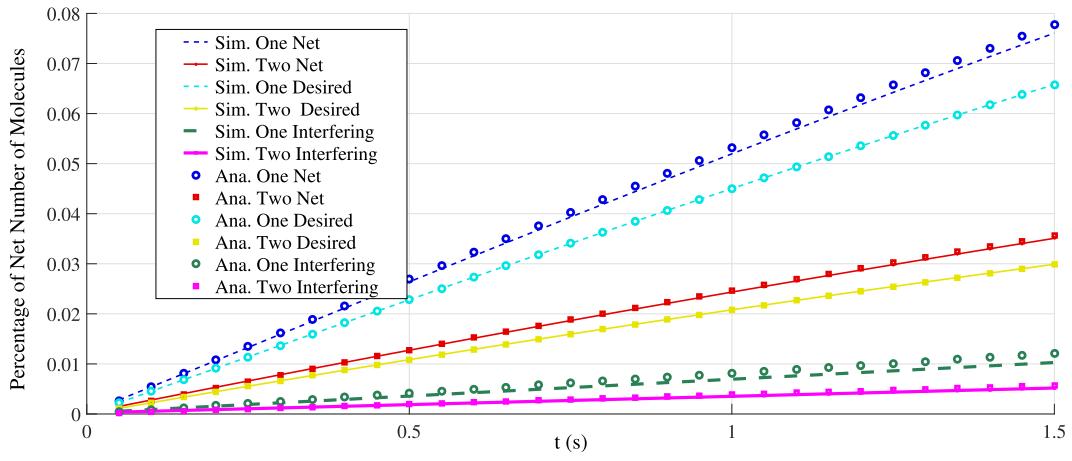


Fig. 4. Expected number of molecules observed at the Full Absorption Receiver with parameters $N_{tx} = 1$, $t_b = 1s$, $R = 100\mu m$, $\lambda_a = 5 \times 10^{-7}$, $d_e = 15\mu m$, $r_r = 5\mu m$ and $D = 800\mu m^2/s$.

to all active interfering transmitters with randomly generated locations and a desirable transmitter located at a predefined position, \mathbf{d}_e , as calculated from (5) and (6) over 10^6 real-

izations. In Fig. 2 and Fig. 3, the analytical curves of the expected net number of absorbed molecules at the receiver in the MC system with single type of information molecule,

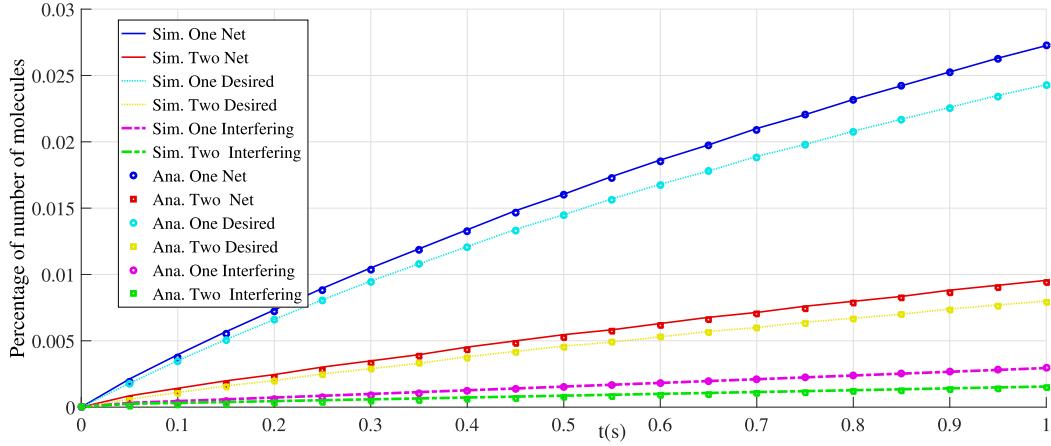


Fig. 5. Expected number of molecules observed at the Partial Absorption Receiver with parameters $N_{tx} = 1$, $t_b = 1s$, $R = 100\mu m$, $k_1 = 60\mu m/s$, $\lambda_a = 5 \times 10^{-7}$, $d_e = 15\mu m$, $r_r = 5\mu m$ and $D = 120\mu m^2/s$.

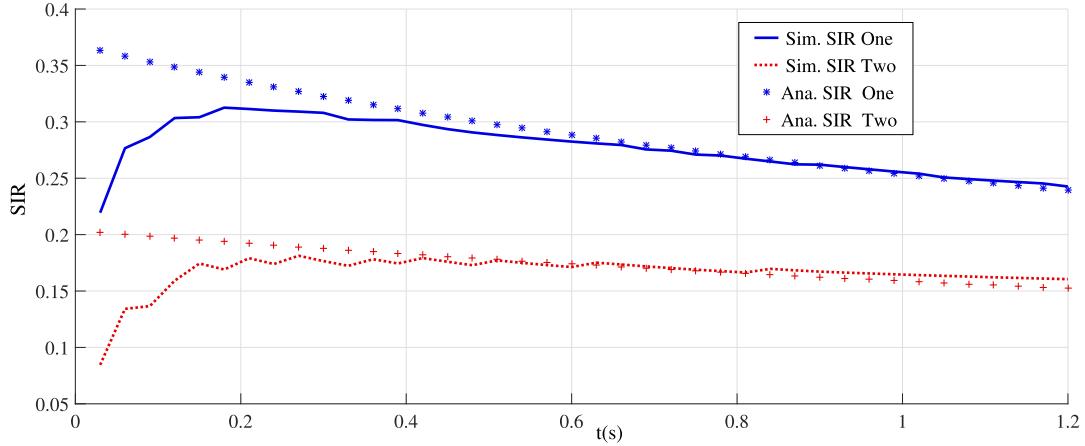


Fig. 6. SIR for Partial Absorption Receiver with parameters $t_b = 1.2s$, $R = 100\mu m$, $k_1 = 120\mu m/s$, $\lambda_a = 5 \times 10^{-7}$, $d_e = 15\mu m$, $r_r = 5\mu m$, and $D = 250\mu m^2/s$.

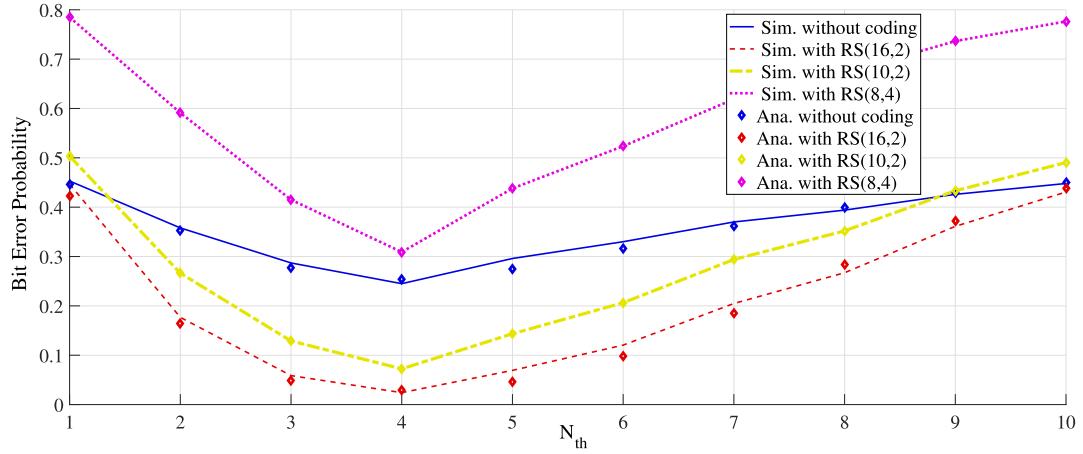


Fig. 7. Bit error probability for Full Absorption Receiver with parameters $N_{tx} = 15$, $t_b = 0.1s$, $R = 100\mu m$, $\lambda_a = 8 \times 10^{-6}$, $d_e = 15\mu m$, $r_r = 5\mu m$, and $D = 800\mu m^2/s$.

during the time interval $[(j-1)T_b, jT_b]$ are plotted using (12) for desirable transmitter, (14) for interfering transmitter, and (19) for the entire system and are abbreviated as “Ana.

Desired”, “Ana. Interfering”, and “Ana. Net”, respectively. Similarly in Fig. 4 and Fig 5, analytical curves “Ana. Desired”, “Ana. Interfering”, and “Ana. Net” are generated using (15)

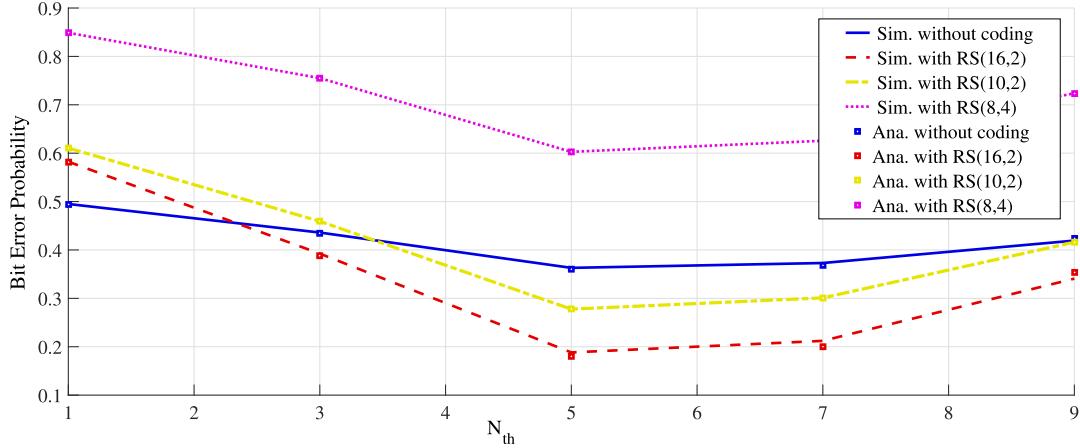


Fig. 8. Bit error probability for Partial Absorption with parameters $N_{tx} = 100$, $t_b = 0.25s$, $R = 100\mu m$, $k_1 = 120\mu m/s$, $\lambda_a = 8 \times 10^{-7}$, $d_e = 20\mu m$, $r_r = 10\mu m$, and $D = 250\mu m^2/s$.

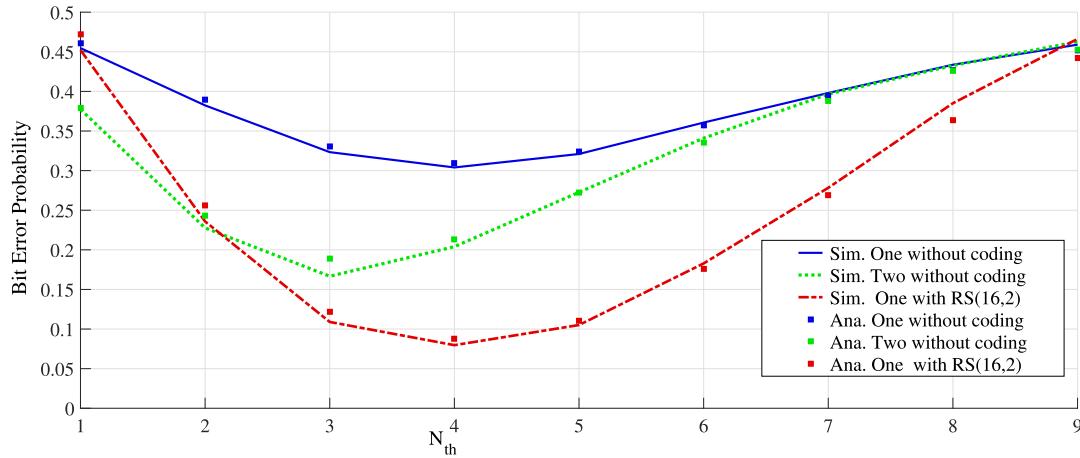


Fig. 9. Bit error probability for Full Absorption Receiver with parameters $N_{tx} = 5$, $t_b = 0.1s$, $R = 100\mu m$, $D = 1000\mu m^2/s$, $\lambda_a = 8 \times 10^{-6}$, $d_e = 20\mu m$, $r_r = 5\mu m$, and input bit stream of $[1101\times]$.

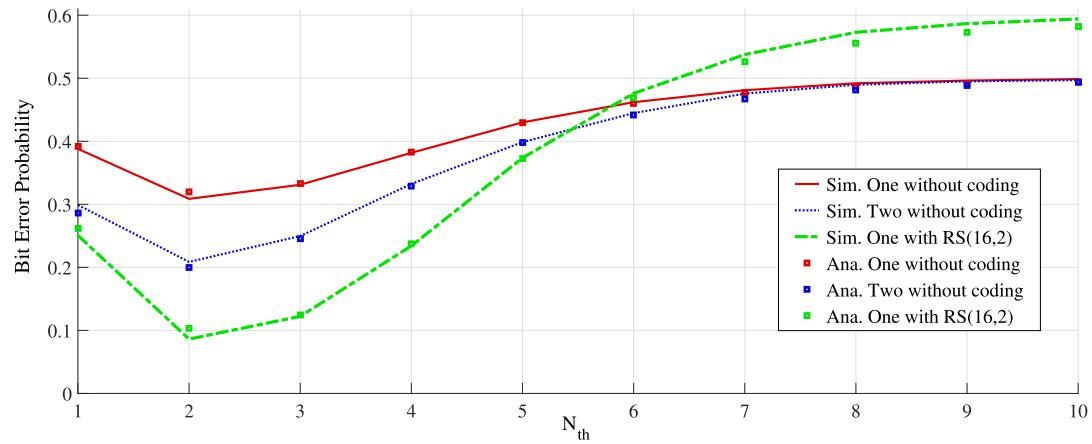


Fig. 10. Bit error probability for Partial Absorption Receiver with parameters $k_1 = 350\mu m/s$, $N_{tx} = 25$, $t_b = 0.1s$, $R = 100\mu m$, $D = 600\mu m^2/s$, $\lambda_a = 5 \times 10^{-5}$, $d_e = 20\mu m$, $r_r = 10\mu m$, and input bit stream of $[1001\times]$.

with (16), (17) with (18), and (20) respectively. Eq. (21), and (22) with (23), are used in Fig. 6 to generate analytical curves for the SIR for partially absorption receiver and are

abbreviated as “Ana. SIR One” and “Ana. SIR Two”. The analytical curves of the BEP due to single type of information molecules without coding, two types of information molecules

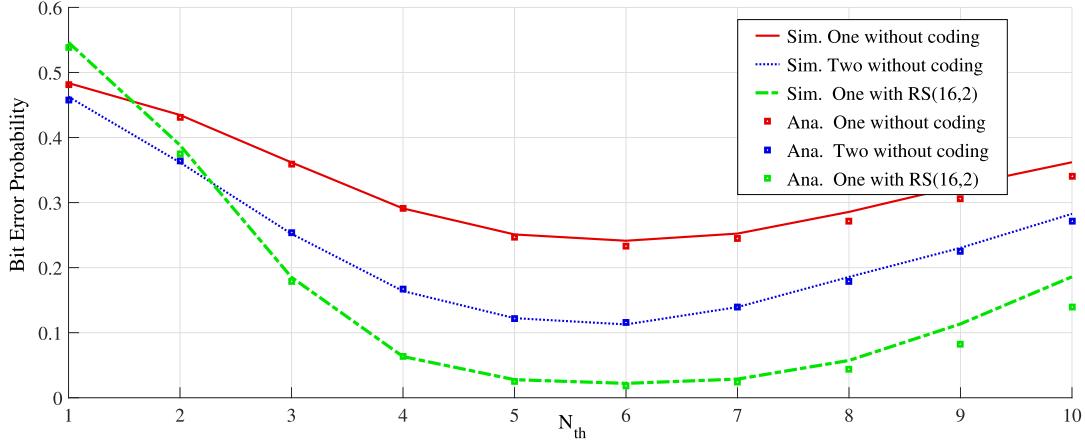


Fig. 11. Bit error probability for Partial Absorption Receiver with parameters $k_1 = 500\mu\text{m}^2/\text{s}$, $N_{\text{tx}} = 50$, $t_b = 0.1\text{s}$, $R = 100\mu\text{m}$, $D = 1000\mu\text{m}^2/\text{s}$, $\lambda_a = 5 \times 10^{-6}$, $d_e = 20\mu\text{m}$, $r_r = 10\mu\text{m}$, and input bit stream of $[1001\times]$.

without coding and RS coding with single type of information molecules, are plotted in Fig. 7-11 using, (28) with (31) and (32), (28) with (38) and (39), and (40) with (28),(31) and (32), and are abbreviated as “Ana. One without coding”, “Ana. Two without coding”, and “Ana. One with $RS(n, k)$ ”, respectively.

For the results presented in this paper, we set the receiver radius as $r_r = 10\mu\text{m}$ for Fig. 8, 10 and 11, and $r_r = 5\mu\text{m}$ for the rest of the figures. The desired transmitter is fixed at $d_e = 20\mu\text{m}$ for Fig. 3,7, 9, 10, and 11, and at $d_e = 15\mu\text{m}$ for the rest of the figures. The density of interfering transmitters is set in the range of $5 \times 10^{-7} < \lambda_a < 5 \times 10^{-5}$, with these transmitters positioned randomly outside the receiver surface in a 3D space of radius, $R = 100\mu\text{m}$. All the parameter values used in both theoretical and simulation results are set similar as in [2], [9]–[11], and [27].

A. Expected Number of Molecules

1) *Single Type of Information Molecule*: Fig. 2 and Fig. 3 plot the cumulative number of molecules observed at both fully absorbing and partially absorbing receivers, when the input sequence takes the form of $[1\ 0\ 0\ 0\ \dots]$. It can be seen from Fig. 2 that as the density of the swarm of transmitters, λ_a , increases, the strength of interference increases relative to the desired signal. This interference can create a significant error at demodulation especially when decoding bit-0.

According to Fig. 3, we can see that for a partially absorbing receiver, the interference from the swarm of transmitters in the 3D space remains high at all the absorption rates, k_1 , used. Furthermore, we notice that the cumulative number of molecules received at the receiver increases gradually with time, with a sharp increase at the beginning of the bit interval. As illustrated in the Fig. 3 top subplot, although the molecules from the desired transmitter tend to stabilize with time, that of interfering transmitters increase gradually. Hence, from these observations, it can be concluded that in 3D large-scale MC system the interference from rest of the transmitters is significantly high, and it is necessary to introduce error recovery techniques to facilitate error free information reception at the receiver. To solve this bottleneck,

we have applied channel coding as well as a novel molecular modulation technique based on two distinguishable types of molecules as information carriers.

2) *Two Types of Information Molecules*: Fig. 4 and 5 plot the expected number of molecules observed at the receiver as a function of time averaged over the number of molecules transmitted to signal bit-1, N_{tx}^A or N_{tx}^B , for both full absorption and partial absorption receivers. According to Fig. 2 and Fig. 3, it is evident that the interference causes maximum distortion to the desired signal at the receiver when the transmitter emits bit-0 preceded by series of bit-1s. Therefore, we have used $[1\ 1\ 0\ 0\ 0\ \dots]$ as the input sequence, and have observed the receiver response from the 3rd bit interval onwards. It is observed that the percentage net number of molecules at both full absorbing and partial absorbing receivers is nearly halved for the MC system based on two types of information molecules compared to that of the system with single type of information molecules, thereby reducing the ISI significantly and improving the system reliability by a notable level.

3) *Signal to Interference Ratio*: Fig. 6 presents the SIR for partially absorption receiver. It compares the SIR of both ISI mitigation systems discussed in this manuscript. From the results presented it is clear that the MC system with single type of molecules experiences heavy SIR level than the MC system with two types of information molecules. Hence, the MC system with two types of information molecules yields a significant reduction of ISI at the receiver, thus achieving an improved BEP performance versus that with a single molecule type.

B. Bit Error Probability

1) *Single Type of Information Molecule*: Fig. 7 and Fig. 8 plot the BEP of the fully and partially absorbing receivers respectively, in the proposed 3D large-scale MC system based on single type of information molecules, with $RS(n, k)$ codes. In both figures we see a good match between the theoretical and the simulation results, validating our derivations. Furthermore, we observe that there exists an optimal N_{th} threshold level for a given set of system parameters of the 3D large-scale

MC system. Fig. 7 and 8 shown that, systems with $RS(16, 2)$ and $RS(10, 2)$ clearly outperforms the system with no coding in terms of improvement achieved in BEP, while $RS(8, 4)$ exhibits a severe loss of performance in terms of BEP. The severe high BEP of RS(8,4) when the decision threshold level is set to a smaller value like $N_{th} = 1$ is because, in this case almost all the bits in the received signal are demodulated as bit 1 due to a low N_{th} . Further, the error correction capacity, denoted by $t_e = \frac{n-k}{2}$, of $RS(8, 4)$ is not sufficient to handle the requirement of this particular system. In such scenarios, incorporation of RS codes only increase system degradation due to the extra redundant data introduced to the system by the channel coding. In overall, it is evident from results presented in Fig. 7 and 8, that the RS codes are capable of providing an acceptable level of improvement to the BEP. Hence, the code length, n and the message length, k of the $RS(n, k)$ code should be carefully selected according to the system settings and the required BEP.

2) *Two Types of Information Molecules*: Fig. 9, 10 and 11 plot the variation of the BEP with N_{th} for both fully and partially absorbing receivers, for the three systems: two types of information molecules without coding, single type of information molecules without coding, and $RS(16, 2)$ coding with single type of information molecules. According to Fig. 10 and Fig. 11 the proposed MC system based on two types of information molecules exhibits a significant improvement in BEP performance compared to the system which employs only one type of information molecule. Furthermore, the proposed system outperforms the MC system with single type of information molecules and RS(16,2) coding, at certain N_{th} levels in the case of a partially absorbing receiver and till the threshold level reach $N_{th} = 3$ in the case of a fully absorbing receiver. It should be noted that in terms of complexity, it is easier to implement the new MC system based on two types of information carrier molecules with simple modification at transmitter and receiver, compared to the MC system with RS coding which requires significant processing power at the receiver to perform the error recovery process. Additionally, RS coding introduces $n - k$ amount of redundancy for each codeword of n length, whereas the MC system based on two types of information molecules does not introduce any redundancy to the transmitted data stream. In a word, compared to MC system with single type of information molecules and RS codes as ECCs, the MC system based on two types of information molecules achieves a sufficient level of BEP improvement with a considerable level of low complexity, low redundancy, and low memory management.

VII. CONCLUSIONS AND FUTURE WORK

In this paper, we proposed RS coding based error correction, and a novel molecular modulating scheme which employs two distinguishable types of information molecules as information carriers, as interference mitigation schemes for ISI and MUI mitigation in a large-scale molecular communication system with a swarm of interfering transmitters. We first provided an analytical framework to quantify the performance improvement with the help of the proposed two

schemes using stochastic geometry. We then derived closed-form expressions for the collective signal strength and the BEP at a partially absorbing receiver due to desired transmitter in the presence of swarm of interfering transmitters. We have extended our analytical derivations to analyze the performance gain achieved in terms of BEP, with the proposed two schemes, and validated via Monte Carlo simulation. We observed that there exists an optimal demodulation threshold level for a given set of system parameters of our proposed 3D large-scale MC system. Furthermore, in comparison to MC system with single type of information molecules and RS codes as ECCs, the MC system modulating with two types of information molecules achieves a sufficient level of BEP improvement with a considerable level of low complexity, low redundancy, and low memory management. Yet, RS coding provides flexibility in error correction capacity, cause it is possible to tune the parameters of the RS coder to match the system requirement.

APPENDIX A PROOF OF LEMMA1

In order to derive a closed-form expression for the BEP of the uncoded system defined by (28), the expressions for conditional probabilities in (31) and (32) should be evaluated using (33). Based on the fact that

$$\frac{\partial^n (\exp \{-N_{tx}^S \phi x \tau\})}{\partial x^n} \Big|_{x=\phi^{-1}} = \exp \{-N_{tx}^S \tau\} (-N_{tx}^S \phi \tau)^n, \quad (A.1)$$

we further simplify (31) as

$$\begin{aligned} P_r [N_{net}^S[j] < N_{th}^S] &= \int_0^\infty \exp \{-N_{tx}^S \tau\} f_{R_{Tot}^S}(\tau) d\tau + \sum_{n=1}^{N_{th}^S-1} \frac{1}{(-\phi)^n n!} \\ &\quad \times \int_0^\infty \frac{\partial^n (\exp \{-N_{tx}^S \phi x \tau\})}{\partial x^n} \Big|_{x=\phi^{-1}} f_{R_{Tot}^S}(\tau) d\tau \\ &= \mathcal{L}_{R_{Tot}^S}(N_{tx}^S) + \sum_{n=1}^{N_{th}^S-1} \frac{1}{(-\phi)^n n!} \frac{\partial^n [\mathcal{L}_{R_{Tot}^S}(N_{tx}^S \phi x)]}{\partial x^n} \Big|_{x=\phi^{-1}}, \end{aligned} \quad (A.2)$$

where $f_{R_{Tot}^S}(\tau)$ is the PDF of R_{Tot}^S , and $\mathcal{L}_{R_{Tot}^S}(\cdot)$ is the Laplace transform of R_{Tot}^S . Using the definition of R_{Tot}^S presented in (30), the Laplace transform of R_{Tot}^S can be evaluated as

$$\begin{aligned} \mathcal{L}_{R_{Tot}^S}(N_{tx}^S) &= \mathbb{E} \left[\exp \left\{ -N_{tx}^S \left\{ R_D^S(\Omega_{rr}, j | \|\mathbf{d}_e\|) \right. \right. \right. \\ &\quad \left. \left. \left. + \sum_{x \in \Phi_a} R_I^S(\Omega_{rr}, j | \|\mathbf{x}\|) \right\} \right\} \right], \\ &= \exp \left\{ -N_{tx}^S R_D^S(\Omega_{rr}, j | \|\mathbf{d}_e\|) \right\} \\ &\quad \times \exp \left\{ -\lambda_a \int_{r_r}^\infty (1 - \exp \{-N_{tx}^S R_I^S(\Omega_{rr}, j | r)\}) 4\pi r^2 dr \right\}, \\ &= \mathcal{L}_{R_D^S}(N_{tx}^S) \cdot \mathcal{L}_{R_I^S}(N_{tx}^S). \end{aligned} \quad (A.3)$$

Based on (A.3), we can express $\left. \frac{\partial^n \left[\mathcal{L}_{R_{\text{Tot}}^j} (N_{\text{tx}} \phi x) \right]}{\partial x^n} \right|_{x=\phi^{-1}}$ as

$$\begin{aligned}
 & \left. \frac{\partial^n \left[\mathcal{L}_{R_{\text{Tot}}^j} (N_{\text{tx}} \phi x) \right]}{\partial x^n} \right|_{x=\phi^{-1}} \\
 &= \left. \frac{\partial^n \left[\begin{aligned} & \exp \left\{ -N_{\text{tx}} \phi x R_{\text{D}}^j (\Omega_{r_r}, j | \| \mathbf{d}_e \|) \right\} \\ & \times \exp \left\{ -4\pi r^2 \lambda_a \int_{r_r}^{\infty} (1 \right. \\ & \left. - \exp \left\{ N_{\text{tx}} \phi x R_{\text{I}}^j (\Omega_{r_r}, j | r) \right\} \right) dr \right\} \end{aligned} \right]}{\partial x^n} \right|_{x=\phi^{-1}}, \quad (\text{A.4})
 \end{aligned}$$

which can be further simplified using General Leibniz rule [28] as

$$\begin{aligned}
 & \left. \frac{\partial^n \left[\mathcal{L}_{R_{\text{Tot}}^S} (N_{\text{tx}}^S \phi x) \right]}{\partial x^n} \right|_{x=\phi^{-1}} \\
 &= \sum_{l=0}^n \binom{n}{l} \left. \frac{\partial^l \left[\mathcal{L}_{R_{\text{I}}^S} (N_{\text{tx}}^S \phi x) \right]}{\partial x^l} \right|_{x=\phi^{-1}} \\
 & \quad \times \exp \left\{ -N_{\text{tx}}^S R_{\text{D}}^S (\Omega_{r_r}, j | \| \mathbf{d}_e \|) \right\} \\
 & \quad \times (-N_{\text{tx}}^S \phi R_{\text{D}}^S (\Omega_{r_r}, j | \| \mathbf{d}_e \|))^{(n-l)}, \quad (\text{A.5})
 \end{aligned}$$

where $\left. \frac{\partial^l \left[\mathcal{L}_{R_{\text{I}}^S} (N_{\text{tx}}^S \phi x) \right]}{\partial x^l} \right|_{x=\phi^{-1}}$ can be further simplified using Faàdi Bruno's formula [29] as

$$\begin{aligned}
 & \left. \frac{\partial^l \left[\mathcal{L}_{R_{\text{I}}^S} (N_{\text{tx}}^S \phi x) \right]}{\partial x^l} \right|_{x=\phi^{-1}} \\
 &= \exp \left\{ -\lambda_a \int_{r_r}^{\infty} (1 - \exp \left\{ -N_{\text{tx}}^S R_{\text{I}}^S (\Omega_{r_r}, j | r) \right\}) 4\pi r^2 dr \right\} \\
 & \quad \times \sum_{k=1}^l \frac{l!}{\prod_{k=1}^l k! k!} \prod_{k=1}^l \left[-\lambda_a \int_{r_r}^{\infty} \left[-(-N_{\text{tx}}^S \phi R_{\text{I}}^S (\Omega_{r_r}, j | r)) \right]^k \right. \\
 & \quad \left. \times \exp \left\{ -N_{\text{tx}}^S R_{\text{I}}^S (\Omega_{r_r}, j | r) \right\} 4\pi r^2 dr \right]^{l_k}, \quad (\text{A.6})
 \end{aligned}$$

where the summation \sum_l is over all l -tuples of non-negative integers (l_1, \dots, l_l) satisfying the constraint $1 \cdot l_1 + 2 \cdot l_2 + \dots + k \cdot l_k + \dots + l \cdot l_l = l$. Noting that $\prod_{k=1}^l (-\phi)^{k l_k} = (-\phi)^l$, we finally derive $P_r [N_{\text{net}}^S[j] < N_{\text{th}}^S]$ by first substituting (A.6) into (A.5) and then using the resulting expression and (A.3) in (A.2).

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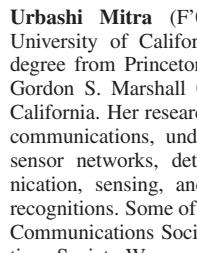
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