On Medium Chemical Reaction in Diffusion-Based Molecular Communication: a Two-Way Relaying Example

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Abstract

Chemical reactions are a prominent feature of molecular systems, with no direct parallels in wireless communications. While chemical reactions may be used inside the transmitter nodes, receiver nodes or the communication medium, we focus on its utility in the medium in this paper. Such chemical reactions can be used to perform computation over the medium as molecules diffuse and react with each other (physical-layer computation). We propose the use of chemical reactions for the following purposes: (i) to realize molecular physical-layer network coding (molecular PNC) by performing the natural XOR operation inside the medium, and (ii) to reduce signal-dependent observation noise of molecular receptors by canceling out the remaining molecules from previous transmission. To make the ideas formal, we consider an explicit two-way relaying example with a ligand receiver (which has a signal-dependent noise). The proposed ideas are used to define a modulation scheme (which we call the PNC scheme). We compare the PNC with a previously proposed scheme for this problem where the XOR operation is performed at the relay node (using a molecular logic gate). We call the latter, the straightforward network coding (SNC). It is observed that in addition to the simplicity of the proposed PNC scheme, it outperforms the SNC scheme especially when we consider inter-symbol interference (ISI).

I. INTRODUCTION

While traditional wireless communication systems employ energy carriers (such as electromagnetic or acoustic waves) for communication, Molecular Communication (MC) utilizes physical molecules as its carriers of information. In diffusion-based MC, released molecules from the transmitter diffuse in the...
environment to reach the receiver. Electromagnetic waves and molecular diffusion share similarities and differences. Both the electromagnetic wave equation and the Fick’s second law of macro-scale diffusion are second-order linear partial differential equations. As a result, both lead to linear system models that satisfy the superposition property. The superposition property is used in the design of multi–carrier wireless systems. However, there are also differences between electromagnetic waves and molecular diffusion. Notably in MC, we can have multiple molecule types in the medium that may undergo chemical reactions as they diffuse in the environment. The reaction amongst the molecules is governed by the non-linear reaction–diffusion differential equations. Furthermore, while the measurement noise of a wireless receiver may be modeled by an additive Gaussian noise (the AWGN channel), some of the most promising molecular receptors have a signal-dependent measurement noise (i.e., their noise variance is higher when they are measuring a larger signal); see for instance [1] for a detailed discussion.

In a diffusion-based communication system, the transmitter and the receiver are biological or engineered cells that release or receive molecules, while the channel is assumed to be a gas or aqueous medium in which molecules can move. We might also have relay nodes to facilitate the communication between the transmitter and the receiver.

Chemical reaction is a key operation mechanism of biological molecular systems. As a result, chemical reactions are likely to be a fixture of future engineered molecular transmitters or receivers. For instance, [2], [3] consider the role of chemical reaction in transmitter and receiver design. However, the emphasis of this paper is on the challenges and opportunities of utilizing chemical reactions inside the communication medium (channel) rather than inside the transmitter or receiver nodes. We may view the diffusion-reaction process as a form of physical-layer computation that is performed over the medium (distinct from the operation of transceiver cells). While the superposition property has been utilized for “computation over the air” in the wireless literature [4]–[8], chemical reactions provide the possibility of more complicated interactions than a simple superposition. Although few existing works provide a number of ideas for exploiting chemical reactions in the medium for communication purposes, we still lack a full understanding. In this paper, we review the state of the art and give a number of new ideas. In particular, our emphasis is on the utility of chemical reactions by the relay nodes.

**Challenges and known techniques:** While linear chemical reactions can be readily utilized for signal shaping, the more interesting chemical reactions are non-linear and demonstrate complicated patterns [9]. The main challenge of utilizing chemical reactions is the non-linearity of the reaction-diffusion equations and lack of explicit analytical solutions. For instance, consider the following chemical reaction:

\[
A + B \xrightarrow{\gamma} C \tag{1}
\]
in which $\gamma$ is the rate of the reaction. Let $c_A$ and $c_B$ be the concentrations of A and B. The reaction-diffusion law can be expressed as

$$\frac{\partial c_A}{\partial t} = D_A \nabla^2 c_A - \gamma c_A c_B, \quad \frac{\partial c_B}{\partial t} = D_B \nabla^2 c_B - \gamma c_A c_B,$$

where $D_A$ and $D_B$ are the diffusion coefficients of A and B, respectively. The term $\gamma c_A c_B$ is the challenging non-linear term. Thus far, this challenge is mostly dealt with in the MC literature by noting that despite lack of analytical solutions, it may be still possible to intuitively predict the *qualitative behavior* of the solutions, in particular when the reaction is limited to a small neighbourhood [10] or is instantaneous (high reaction rate). The general approach is to use the high-level intuition to design signaling schemes, which may be backed up with numerical simulations or partial supporting analysis.

We may categorize the known ideas of utilizing chemical reactions in the medium as follows:

- **Memory degradation:** In [11], it is suggested to release enzymes throughout the environment. A chemical reaction between enzymes and information carrying molecules cancels out the involved molecules, and has the effect of shortening the lifetime distribution of all molecules in the environment. This reaction can put down inter-symbol interference (ISI) by reducing the remaining molecular concentration from previous transmissions, at the cost of weakening the desired signal.

- **Pattern formation:** In the above item, we gave a chemical reaction that simply reduces the concentration of the reactant molecules. However, more complicated dynamics and patterns (such as oscillating reactions or travelling waves) can arise from chemical reactions. Assuming that molecules of type A are used for communication, it has been suggested in [13] to fill the environment with molecules of type B whose reaction with molecules of type A produces such oscillating and propagating patterns. This may be utilized to increase the propagation range of the molecules (before they dissolve in the environment). The more complicated spatial-temporal patterns could increase the decoder’s ability to distinguish amongst them; this can effectively increase the information capacity of the system.

- **Simulating negative signals and ISI reduction:** Unlike electrical current and voltage that can take negative values, the density of molecules in an environment cannot go negative. Chemical reactions are proposed for simulating transmission of a negative signal by a molecular transmitter [10], [14], [15]. For instance, authors of [10] suggest using $H^+$ and $OH^-$ ions. Release of any of these ions reduces the concentration of the other one in the medium, and one can interpret release of $H^+$ ions as sending a positive, and release of $OH^-$ ions as sending a negative signal. Simulation of negative signals allows for design of precoders at the transmitter to combat the ISI (e.g. see [15]).

1While [11] assumes enzymes are released throughout the medium, [12] study its release in a limited area of the medium.
• **Relay Signal Amplification:** The degradation and attenuation of molecules limit the transmission distance between the transmitter and the receiver [16]. Relaying is an approach to increase the range of communication; it is also observed in intracellular communication in nature. Authors in [17] describe a chemical reaction that amplifies the incoming signals. However, we point out that signal amplification may be also performed blindly in the medium; assume that the information molecule is of type \( A \) and the relay releases a limited amount of molecules of type \( B \) such that

\[
A + B \xrightarrow{\gamma} 2C + D. \tag{3}
\]

This reaction produces molecules of type \( C \) whose concentration is twice the concentration of molecules of type \( A \) in the environment. Thus, the relay simply releases molecules of type \( B \) without having to sense the incoming density of molecules of type \( A \).

• **Molecular media-based modulation:** authors in [1] argue that information can be transmitted by changing the general physical properties of the communication medium (rather than directly changing the density of the released molecules). For instance, assume that we have two transmitters, called the \( A \)-transmitter and the \( B \)-transmitter, who release molecules of types \( A \) and \( B \) in the medium, respectively. There is a receiver who can only sense the density of molecules of type \( A \). If \( A \) and \( B \) react in the environment, the \( B \)-transmitter can communicate indirectly to the receiver (despite the receiver only has sensors that detect \( A \) molecules): the reason is that the actions of the \( B \)-transmitter influences the communication medium between the \( A \)-transmitter and the receiver.

Besides the above explicit ideas for medium chemical reactions, authors in [18] utilize an interesting feature of non-linear systems, namely harnessing noise for signal propagation in a cell-to-cell MC system. Unlike linear systems where noise plays a disruptive role, noise can increase information capacity of non-linear systems (this effect is known as the *stochastic resonance*).

**Our contribution:** Our main contribution in this work is to propose new ideas for utility of chemical reactions in a communication medium. These ideas are as follows:

1) **Receiver noise reduction:** as mentioned earlier, many molecular receivers have signal dependent noise. In particular, they face a smaller noise if they are sensing a smaller signal. Now, suppose the density of molecules around the receiver is \( y \) and the receiver wants to measure it. If a receiver can predict that \( y \) is at least \( \lambda \), it can locally release a different species of molecules that would react with the signal molecules around the receiver, and reduce the signal molecule density by \( \lambda \) in the vicinity of the receiver. Thus, instead of measuring \( y \), it measures \( y - \lambda \). This will incur a smaller signal dependent noise.

The receiver can predict a minimum for its upcoming measurement \( y \) by utilizing its previous
observations. For instance, if the receiver has measured a high density of molecules in the previous time slot, it expects the current density of molecules to be high in the current time slot as well. The reason is that diffusion is a slow process and it takes time for the effect of previous transmissions to disappear from the medium. As a result, the receiver may have an estimate that the molecule density is at least $\lambda$, where $\lambda$ is found adaptively from its previous observations. One should also consider the possibility that the estimate $\lambda$ is incorrect, \textit{i.e.}, $y$ is less than $\lambda$. In this case, the receiver observes $\min(0, y - \lambda) = 0$, and the information about $y$ will be lost. Receiver’s error in finding a suitable lower bound $\lambda$ for $y$ can result in an error, but the probability of this error can be small and compensate for the decrease in the signal-dependent measurement noise.

2) \textit{The dual purpose of transmission:} Thus far the literature assumes that a transmitter releases molecules to convey its own message. Consider a scenario where we have two nodes that are using molecules of types A and B for transmission, respectively. These transmitters also have receptors on their surface that allows them to obtain information about the other node’s transmissions. Assume that these molecules of types A and B can react and cancel out each other. Then, the first node can release molecules of type A for (i) encoding of its information bits, or (ii) for reducing the density of the other’s nodes molecule to reduce its measurement noise level.

3) \textit{Molecular physical-layer network coding (Molecular PNC):} Network coding in MC has been studied in [19], [20], where the relay uses an XOR logic gate [21], at the molecular level, to XOR the messages of the two transceivers. As we show later, one can improve upon the previously proposed schemes by realizing the XOR operation inside the medium via chemical reactions. This allows for removal of the XOR gate inside the relay node. The idea is as follows: suppose we have molecules of type A and B that react and cancel out each other. Then, if only one molecule type exists in the medium, it survives. However, the presence of both molecules results in the destruction of both.

\textbf{Example of a two-way relay network model:} To make the above ideas formal at once, we propose a specific setup with a certain signal-dependent receiver noise. We give an explicit modulation scheme that utilizes all the above-mentioned ideas in its design. More specifically, we consider a two-way molecular relay network, depicted in Fig. [1] where two nano-transceivers, $T_1$ and $T_2$, exchange their information through a nano-relay, $R$, in two phases. In phase 1, $T_1$ and $T_2$ send their messages to the relay $R$ using molecule types $M_1$ and $M_2$, respectively, and in phase 2, the relay sends a message back to both transceivers using a different molecule type $M_3$ (to avoid self-interference [22]). Multiple transmission...

\footnote{We have already used a simpler form of this idea in [15], but in that work the amount of release of molecules was not chosen adaptively by the receiver.}
options are possible in this network [8]:

1) (No network coding). The transceivers send their messages to the relay node simultaneously in one time slot using different molecule types $M_1$ and $M_2$ (or in two time slots using the same molecule type). Then, the relay takes two time slots to forward the message of one transceiver to the other and vice versa. This will take three (or four) time slots.

2) (Straightforward network coding (SNC)). Here, the relay computes the XOR of the incoming messages and sends it back to the two transceivers in a single time slot. Each transceiver, having access to its own transmitted bits, uses the XOR to decode the other transceiver’s message. This will take two (or three) time slots.

3) (Physical-layer network coding (PNC)). The transceivers send their messages in the same time slot using different molecule types $M_1$ and $M_2$, and thus by canceling out/adding to each other in the communication medium, a physical-layer XOR is performed. This will take two time slots.

In this paper, we propose a new network coding scheme in MC parallel to the PNC in traditional wireless networks. The traditional PNC is based on the fact that the signals can be negative and thus they may cancel out each other physically when adding in the environment. Since in MC the transmitted signals cannot be negative, we suggest the use of molecular reaction to cancel out the signals. This covers our two new ideas (namely receiver noise reduction and molecular PNC) that we mentioned above. By making physical-layer XOR using reaction, the signal density reduces when both molecules arrive at the relay and hence the signal dependent noise at the relay is reduced. We show that our proposed PNC scheme outperforms previously proposed SNC schemes for MC.

A complication arises if the above molecular channels have ISI, and this is where we make use of our two new ideas (namely receiver noise reduction and the dual purpose of transmission). For point-to-point channels, ISI mitigating techniques have been introduced in [23], [24]. However, to the best knowledge, there is no study on the ISI-mitigating schemes in two-way relay channels. One natural way to tackle
this problem is to apply the point-to-point ISI mitigating techniques to each hop of the relay channel. For
the SNC scheme, we extend the existing ISI mitigating techniques of point-to-point channels proposed in
[23], [24] to each hop. However, for the PNC scheme we propose a novel ISI-mitigating scheme, which is
based on two observations: i) in two-way channels each transceiver has access to the previous messages
of the other transceiver, and thus knows an estimation of the other user’s ISI. ii) The molecular reaction
can be used to cancel out the ISI (or reduce the estimated ISI) by utilizing the “receiver noise reduction”
idea. It is important to point out that in a channel with ISI, a transmitter may release molecules even
when its bit is zero; this is to cancel out the ISI of the other receiver (dual purpose of transmission).

We make the following conclusions from our analysis of the proposed molecular PNC scheme. In the
no ISI case, our results (based on the derived closed form equations) show that the PNC outperforms the
SNC in terms of error probability thanks to the reaction among the molecules in the PNC scheme. In
fact, when the messages of both transceivers are 1, the number of the molecules bound to the receptors
is reduced compared to SNC scheme. This results in less error caused by the ligand-receptor binding
process. These results are confirmed by simulations. In presence of ISI, the error probability of both
ISI-mitigated PNC and SNC schemes are derived analytically (and confirmed by simulation); it is shown
that the PNC performs significantly better than the SNC. The main reason is that in the SNC, using
adaptive transmission rate at each transceiver mitigates its own ISI only when its message is 1. However,
in the PNC, using adaptive rates\(^3\) at the transceivers mitigates the ISI for all sent messages.

This paper is organized as follows: in Section II we present the physical model for the two-way relay
example. In Section III we describe the use of chemical reaction for molecular PNC and receiver noise
reduction, and in Section IV we explain the idea of chemical reaction for dual purpose of transmission
and receiver noise reduction. In Section V and VI the error performance of the two schemes in no ISI
and ISI cases are respectively investigated. In Section VII we present the numerical results, and finally,
we include concluding remarks in Section VIII.

Notation: We use the superscript \(T_iR\) for the parameters of the channel from the transceiver \(T_i\) to the
relay, \(RT_i\) for the parameters of the channel from the relay to the transceiver \(T_i\). The event \(E^c\) shows
the complement of the event \(E\) and \(\bar{i}\) denotes the complement of \(i\) in its defined set. The superscript “I”
denotes the parameters for the case with ISI. The random variables, error events, cumulative distribution
functions and diffusion coefficients are shown by upper cases while the realizations of random variables
are indicated by lower cases. The decoded value of the information bit \(B\) is denoted by \(\hat{B}\).

\(^3\)From now on by "adaptive rate", we mean "adaptive transmission rate"
II. PHYSICAL MODEL

We consider a diffusion-based nano-network consisting of two nano-transceivers and a nano-relay with the ability of both transmitting and receiving information in different time slots (see Fig. 1). A two-way communication between two nano-transceivers is established by a nano-relay. The distance of the relay from the transceiver $T_i$ is denoted as $d_i$. The transceiver $T_i$ for $i = 1, 2$ has a sequence of information bits $(B_{i,1}, B_{i,2}, \cdots)$ that wants to transmit to the other transceiver.

We assume that the time is slotted with duration $t_s$, and during any communication protocol, molecules are released by either the transceiver $T_i$ or relay $R$ at the beginning of the time slots. For instance, a protocol might utilize the on-off keying (OOK) modulation for transmission in which each transmitter releases a burst of molecules to send the information bit 1 at the beginning of each time slot, or stays silent to send the information bit 0. We assume that $T_1$ releases molecules of type $M_1$, $T_2$ releases molecules of type $M_2$, and the relay releases molecule type $M_3$ (to avoid self-interference). While molecules are released at the beginning of time slots of duration $t_s$, molecule density is measured by receptors on the surface of $T_1$, $T_2$ or $R$ at time instances $t_0, t_0 + t_s, t_0 + 2t_s, \ldots$ for some $t_0 \leq t_s$.

**Channel model:** For the diffusion of molecules, we use the deterministic model based on Fick’s second law of diffusion. According to this model, the impulse response of the channel for molecules of type $M_i$ with diffusion coefficient $D_i$, which is denoted by $h_{M_i}(r,t)$, for 3-D diffusion can be obtained as [25]

$$h_{M_i}(r,t) = \begin{cases} 1 & [t > 0] \frac{1}{(4\pi D_i t)^{3/2}} e^{-\frac{r^2}{4D_it}}, \end{cases} \tag{4}$$

This means that when a nano-transmitter releases $\zeta$ molecules at time $t = 0$, the concentration of molecules at distance $r$ from the transmitter will be $c(r,t) = \zeta h_{M_i}(r,t)$.

**Reception model:** Molecules released by $T_1$ and $T_2$ need to be measured by the relay $R$, and molecules released by the relay $R$ need to be measured by $T_1$ and $T_2$. The reception process is assumed to be the ligand-receptor binding process. More specifically, to measure the density of molecules of type $M_i$, we consider receptors of type $\Omega_i$ that react with molecules of type $M_i$ via the following reversible reaction:

$$M_i + \Omega_i \xrightleftharpoons{\gamma_i \eta_i}{\eta_i} M_i \Omega_i, \tag{5}$$

where $\gamma_i$ and $\eta_i$ are the association and dissociation rates of the molecule type $M_i$ to the receptors of its type, respectively. Since $T_1$ and $T_2$ use molecule types $M_1$ and $M_2$, respectively, the relay has two receptor groups for measuring density of molecules of type $M_1$ and $M_2$. Conversely, relay uses molecules of type $M_3$ and hence $T_1$ and $T_2$ each have a receptor group for measuring the density of molecules of type $M_3$. The number of receptors of type $\Omega_i$ on the surface of the relay is denoted by $n_{iR}$ for $i = 1, 2$. The number of receptors of type $T_3$ on the surface of $T_i$ is denoted by $n_{3T}$. 

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Equation (5) gives the reaction equation with \( M_i \) and \( \Omega_i \) only. Molecules of a different type \( M_j \) might also react and block the receptors of type \( \Omega_i \). The blocking effect caused by the molecules of the other types around the receptors of one type can be characterized by \( \gamma_{i,\text{Block},j} \) and \( \eta_{i,\text{Block},j} \), the blocking and unblocking rates, respectively, of the receptor type \( \Omega_i \) by the molecules of type \( M_j \) \([26]\). In this case, if the concentration of molecules of type \( M_i \) around a receptor type \( \Omega_i \) at a certain time is \( c_i \), the receptor binds with a molecule of type \( M_i \) with probability

\[
p_{b,i} = \frac{c_i}{c_i + \sum_{j \neq i} \frac{\eta_{i,\text{Block},j}}{\gamma_{i,\text{Diss},j}} + \kappa_{D,i}},
\]

where \( \kappa_{D,i} = \frac{\eta_i}{\gamma_i} \) and \( \kappa_{D,i,\text{Block},j} = \frac{\eta_{i,\text{Block},j}}{\gamma_{i,\text{Diss},j}} \) are the dissociation constants. As an example, consider the surface of the relay with \( n_i^R \) receptors of type \( \Omega_i \). Each receptor will be bound with probability \( p_{b,i} \) and the total number of bound receptors will follow a binomial distribution with parameters \((n_i^R, p_{b,i})\). The relay can read the number of receptors of type \( \Omega_i \) that are bound with molecules of type \( M_i \) as its output. The reception process at the transceivers \( T_1 \) and \( T_2 \) is similar.

### III. Chemical Reaction: Molecular PNC and Receiver Noise Reduction

Here, we demonstrate the benefit of chemical reaction for molecular PNC and receiver noise reduction (as discussed in the introduction) in the context of the above two-way communication channel. Previously, SNC was used for communication over this channel, \([19]\), \([20]\), in which the relay, after decoding the messages of both transceivers, forwards the XOR of the decoded messages to the transceivers. Now, we propose a new PNC scheme based on chemical reactions in the medium, which makes the physical-layer XORing possible by exploiting the reaction among different molecule types and thus it does not need a logic XOR gate at the relay. In this section, we consider a channel with no ISI. The case with ISI is considered in Section \( IV \) to illustrate the idea of the dual purpose of transmission.

#### A. The Previously Known SNC Scheme

For the transmission model, we restrict to protocols in which the transceivers and the relay alternate in becoming active. In other words, in each run of the protocol, the transceivers \( T_1 \) and \( T_2 \) first become active and transmit molecules. Then, \( T_1 \) and \( T_2 \) become silent and the relay \( R \) starts transmitting. During the \( k \)-th run of this protocol, \( T_i \) aims to communicate the bit \( B_{i,k} \) to the other transceiver for \( i = 1, 2 \). This protocol is run repeatedly so that \( T_1 \) reconstructs \((\hat{B}_{1,1}^{T_1}, \hat{B}_{1,2}^{T_1}, \cdots)\) while \( T_2 \) reconstructs \((\hat{B}_{1,1}^{T_2}, \hat{B}_{1,2}^{T_2}, \cdots)\). The transmission protocol in the SNC scheme has two communication phases described as follows:

- **Phase 1**: In the first phase, the transceivers, \( T_1 \) and \( T_2 \), send their information bits to the relay using OOK modulation. Due to using different molecule types by the transceivers, this phase consumes
only one time slot. Employing the OOK modulation, the transceivers $T_1$ and $T_2$ release $\xi^{T_1}$ and $\xi^{T_2}$ molecules of types $M_1$ and $M_2$, respectively, to send the information bit 1 and release nothing to send the information bit 0.

- **Phase 2:** In the second phase, the relay decodes the messages of $T_1$ and $T_2$ and transmits the XOR of the decoded bits to both transceivers using OOK modulation, i.e., the relay releases $\xi^R$ molecules of types $M_3$ to send the information bit 1 and stay silent to send the information bit 0. The relay consumes one time slot to forward its message to each transceiver. Each transceiver decodes the message of the relay and by XORing the decoded message and its own transmitted message finds the message sent by the other transceiver.

This network coding scheme needs two time slots in total. We consider a super time slot which contains two time slots of equal duration of $t_s$. Throughout the paper, $k$ shows the index of the super time slot. $T_1$ and $T_2$ send their messages, $B_{1,k}$ and $B_{2,k}$, at the beginning of the $k$-th super time slot to the relay by releasing $X_{i,k} = B_{i,k} \xi^{T_i}$ molecules (phase 1) and then the relay decodes the message of each transceiver $T_i$ as $\hat{B}_{i,k}$ and sends the message $B_{R,k} = \hat{B}_{1,k} \oplus \hat{B}_{2,k}$, by releasing $X_{3,k} = B_{R,k} \xi^R$ molecules, in the phase 2 of the $k$-th super time slot to the transceivers. The number of bound molecules of type $M_i$ at the relay in the $k$-th super time slot is noted by $Y_{i,k}^R$ and the number of bound molecules of type $M_3$ at $T_i$ is noted by $Y_{3,i,k}^{T_i}$. The block diagram of the system is shown in Fig. 2. In the following, we explain the physical model of the SNC scheme in detail.

According to the channel model in the previous section, the channel impulse response from the transceiver $T_i$ to the relay $R$ is obtained as $h_{M_i}(d_i, t) = \frac{1}{(4\pi D_{i,t})^{3/2}} e^{-\frac{d_i^2}{4D_{i,t}}}$. The channel gains from $T_i$ to $R$ are obtained by sampling $h_{M_i}(d_i, t)$ at time instances $t_0, t_0 + t_s, t_0 + 2t_s, \ldots$ as follows:

$$\pi^{T_iR}_l = h_{M_i}(d_i, t_0 + (l - 1)t_s), \quad i \in \{1, 2\}, \quad \quad (7)$$

The channel gains from the relay $R$ to the transceiver $T_i$, $\pi^{RT_i}_l$, can be obtained similarly. We remark that the index $l$ refers to each time slot. When we have no ISI in the channels, the remaining molecules
of the previous super time time slot are died away before new molecules are released and hence the concentration of the molecules of type \( M_i \) measured by the relay in the \( k \)-th super time slot is

\[
C_{i,k} = X_{i,k} \pi_{1,R}^T = B_{i,k} \zeta_{1} \pi_{1,R}^T, \quad i \in \{1, 2\}. \tag{8}
\]

The concentration of molecules of type \( M_3 \) measured by each transceiver \( T_i \) can be obtained similarly.

### B. The Proposed PNC Scheme

Here, we propose to implement the physical-layer XOR using the molecular reaction, which reduces the receiver noise. Thus, we first choose two molecule types \( M_1 \) and \( M_2 \), to be sent by the transceivers \( T_1 \) and \( T_2 \), respectively, such that they can react with each other by an irreversible reaction as follows:

\[
M_1 + M_2 \xrightarrow{\gamma_{12}} M_{12}, \tag{9}
\]

where \( \gamma_{12} \geq 0 \) is the reaction rate of the molecules \( M_1 \) and \( M_2 \). The molecules of type \( M_{12} \) does not bind to the receptors of the relay, while the molecules of type \( M_i \) react with the receptors of the \( i \)-th type \( (\Omega_i) \) at the relay, by reversible reactions as given in (5). The two communication phases in this scheme are similar to the SNC scheme with the difference that the XOR is performed in the medium instead of the relay and the relay implicitly decodes the physically made XOR of the messages and sends it to the transceivers in the second phase. \( M_1 \) and \( M_2 \) are chosen such that \( \gamma_{12} \gg \gamma_1, \gamma_2 \). Hence, if both messages of the transmitters are 1, both molecules \( M_1 \) and \( M_2 \) arrive at the relay and react with each other as in (9) (much faster than binding to their receptors). As a result, the concentrations of both molecules decrease in the environment and almost no molecule binds to the receptors of the relay. When only \( M_1 \) or \( M_2 \) arrives at the relay, it binds to its corresponding receptors at the relay. The stimulated receptor group would release \( \zeta^R \) molecules of type \( M_3 \) in the next time slot. Thus, to make a physical-layer XOR, it is enough to choose the number of released molecules appropriately.

The physical model of the PNC scheme is similar to the SNC scheme, with the difference that in the PNC, (8) is the concentration of molecules of type \( M_i \) around the relay before reaction, i.e., the concentrations of molecules of types \( M_1 \) and \( M_2 \) around the relay before reaction are \( B_{1,k} \zeta_{1} \pi_{1,R}^T \) and \( B_{2,k} \zeta_{2} \pi_{2,R}^T \), respectively. Assuming perfect reaction, molecule type with lower concentration is completely canceled out, and a residual part of the one with higher concentration remains. In particular, the concentration of molecules of type \( M_1 \) and \( M_2 \) measured by the receptors of their type at the relay are \( C_{1,k} = \max\{B_{1,k} \zeta_{1} \pi_{1,R}^T - B_{2,k} \zeta_{2} \pi_{2,R}^T, 0\} \) and \( C_{2,k} = \max\{B_{2,k} \zeta_{2} \pi_{2,R}^T - B_{1,k} \zeta_{1} \pi_{1,R}^T, 0\} \), respectively. Each transceiver \( T_i \), knowing its own channel coefficient \( \pi_{1,R}^T \), chooses \( \zeta_{1}^T \) such that an almost equal concentration of molecules of both types arrives at the relay (when both transceivers send
**TABLE I: Used Notations**

| Notation | Description |
|----------|-------------|
| $B_{i,k}$ | The message of the transceiver $T_i$ in the $k$-th super time slot |
| $B_{R,k}$ | The sent message of the relay in the $k$-th super time slot |
| $B_{R,i,k}$ | A part of the message $B_{R,k}$, to be decoded by the $i$-th receptor group at the relay in the PNC in the $k$-th super time slot |
| $\hat{B}_{R,i,k}$ | The decoded message by the $i$-th receptor group at the relay in the PNC in the $k$-th super time slot |
| $\hat{B}_{i,k}^{R}$ | The decoded message by the $i$-th receptor group at the relay in the SNC in the $k$-th super time slot |
| $\hat{B}_{i,k}^{T}$ | The message of the relay, decoded at the transceiver $T_i$ in the $k$-th super time slot |
| $\hat{B}_{i,k}$ | The decoded message by the $i$-th receptor group at the relay in the SNC in the $k$-th super time slot |
| $\hat{B}_{T,i,k}$ | The message of the transceiver $T_i$, decoded by the transceiver $T_i$ in the $k$-th super time slot |
| $X_{i,k}$ | The number of released molecules of type $M_i$ in the $k$-th super time slot |
| $C_{i,k}$ | The concentration of molecules of type $M_i$ around its receptors in the $k$-th super time slot |
| $I_{i,k}$ | The concentration of remained molecules of type $M_i$ from the previous super time slots around its receptors in the $k$-th super time slot |
| $E_{i,k}$ | The error event at transceiver $T_i$ in the $k$-th super time slot ($\hat{B}_{i,k}^{T} \neq B_{i,k}$) |
| $E_{R,k}$ | The error event of the first communication phase in the $k$-th super time slot ($B_{R,k} \neq B_{1,k} \oplus B_{2,k}$) |
| $E_{R,i,k}$ | The error event of the $i$-th receptor group at the relay in the $k$-th super time slot (in PNC: $\hat{B}_{R,i,k} \neq B_{R,i,k}$, in SNC: $\hat{B}_{i,k}^{R} \neq B_{i,k}$) |
| $E_{T,i,k}$ | The error event of the second communication phase in the $k$-th super time slot ($\hat{B}_{R,i,k}^{T} \neq B_{R,k}$) |

The information bit $1$. This makes almost all molecules react with each other and thus realizes a physical-layer XOR. In this paper, we assume perfect reaction among molecules of types $M_1$ and $M_2$.

The error performances of the two schemes without ISI are investigated in Section V. It is shown analytically and later by simulation that the proposed PNC scheme outperforms the SNC scheme.

**Remark on notation**: While we have attempted to simplify the notation (both in the case with and without ISI) as much as possible, for the two phases of the communication, we needed to define messages sent and decoded in each phase by the transceivers and the relay; we needed to define error events for each phases. Furthermore, since we have two receptor groups at the relay we needed to define decoded messages of each receptor group and their corresponding error events. Table I summarizes our mostly used notations in this paper.

**IV. CHEMICAL REACTION: DUAL PURPOSE OF TRANSMISSION AND RECEIVER NOISE REDUCTION**

In this section, to illustrate the idea of the dual purpose of transmission and receiver noise reduction (as mentioned in the introduction), we consider the ISI case and using the reaction characteristic of the PNC scheme, we propose an ISI mitigating technique for the first communication phase of the PNC scheme. To have a fair comparison between the two schemes, we apply the existing ISI mitigating techniques to the SNC scheme. In our schemes, we assume that the transceivers know the channel coefficients of both transceivers to the relay, i.e., the distances and diffusion coefficients.
In the PNC scheme, the XOR is realized in the medium using the molecular reaction in the first communication phase. In the presence of ISI, there are remaining molecules from the previous transmissions. Using the idea of the dual purpose of transmission and receiver noise reduction, we use reaction to mitigate ISI in the first communication phase by releasing extra molecules from each transceiver to react with the remaining molecules of the other transceiver from the previous transmissions. Since each transceiver has access to the decoded version of the transmitted bits of the other transceiver in the previous super time slots, knowing its own channel coefficient and the channel coefficient of the other transceiver, it can estimate the concentration of the remaining molecules of the other transceiver from the previous transmissions and choose its transmission rate such that along with transmitting its own message, the concentration of the remaining molecules of the other transceiver is also canceled out. As an example, assume a two-way communication channel with one super time slot memory for the transceiver-relay channel. Also assume the messages of the transceivers $T_1$ and $T_2$ are 1 and 0, respectively, in the current super time slot. Because of the one super time slot memory in the channel, there may be concentrations of the remaining molecules of types $M_1$ and $M_2$ around the relay from the previous super time slot. The transceiver $T_1$ releases a constant number of molecules to send its information bit 1 and some extra molecules to cancel out the remaining molecules of the transceiver $T_2$ from the previous super time slot. Since the message of $T_2$ is 0, it does not release any molecules to send its message, but releases some molecules to cancel out the remaining molecules of $T_1$ around the relay from the previous super time slot. Hence, in this scheme, the transceivers may release some molecules even if their message is 0.

The transceivers do not know the very exact number of the released molecules of the other transceiver in the previous super time slots, but can estimate it. We show in Section IV-B that, for a unit super time slot memory, each transceiver can use the decoded message of the other transceiver in the $(k-1)$-th super time slot and the number of its own released molecules in the $(k-2)$-th super time slot to estimate the number of the released molecules of the other transceiver in the previous super time slot.

In the SNC scheme, we use the existing ISI mitigating techniques (as mentioned before, SNC in the presence of ISI has not been studied before). To mitigate ISI in a communication link, two approaches are possible: adapting transmission rate at the transmitter [24], and adapting threshold at the receiver [23]. Our proposed scheme for the first communication phase of the PNC scheme is based on using an adaptive rate at the transceivers along with a fixed threshold at the relay. Hence, we extend the method in [24] to the SNC scheme, i.e., each transceiver adapts its transmission rate to mitigate its own ISI. In this scheme, when the message of the transceiver is 0, it stays silent; otherwise, according to its transmission in the previous super time slot, it adapts its rate such that the concentration of molecules around the relay is a constant value. There is also ISI in the second communication phase of each scheme. To reduce the
complexity of the relay in both schemes, we put all complexity at the transceivers and take the second approach in phase 2 [23]. The adaptive thresholds in the second phase are derived in Section VI.

A. The SNC Scheme

In this scheme, in the $k$-th super time slot, if $B_{i,k} = 0$, the transceiver $T_i$ stays silent and if $B_{i,k} = 1$, the transceiver transmits an adaptive number of molecules such that a constant concentration of molecules, $c_{\text{SNC}}$, arrives at the relay at each super time slot. We first need to explain the physical model for the ISI. We model the ISI in the channel of the transceiver $T_i$ to the relay $R$ by a $q_{T_i}^{R}$-slot memory [27], i.e., $\pi_{l}^{T_i,R} = 0$, for $l > q_{T_i}^{R} + 1$, where $\pi_{l}^{T_i,R}$ is defined in (7), and similarly, we model the channel of the relay $R$ to the transceiver $T_i$ by a $q_{RT_i}^{R}$-slot memory. In addition, since in our transmission protocol, the molecules of types $M_1$ and $M_2$ are released in odd time slots and the molecules of type $M_3$ are released in even time slots, the performance of the system is the same for $q = 2k'$ and $q = 2k' + 1$, $k' \in \{0, 1, 2, \ldots\}$, which means that the concentration of molecules of type $M_i$ around the relay in the $k$-th super time slot is given as

$$C_{i,k} = \sum_{l=0}^{\lfloor \frac{q_{T_i}^{R}}{2} \rfloor} \pi_{2l+1}^{T_i,R} \cdot X_{i,k-l} = X_{i,k}^{T_i,R} + I_{i,k}, \quad i \in \{1, 2\},$$

(10)

where $I_{i,k}$ denotes the ISI term, which is the concentration of molecules of type $M_i$ around the relay remained from the previous super time slots. The concentration of molecules around the transceivers can be obtained similarly. Each $T_i$ to send its message $B_{i,k} \in \{0, 1\}$ in the $k$-th super time slot transmits

$$X_{i,k} = B_{i,k}\left(\frac{c_{\text{SNC}}}{\pi_{1}^{T_i,R}} - I_{i,k}^{\text{SNC}}\right),$$

(11)

molecules such that

$$L_{i,k}^{\text{SNC}} = \frac{I_{i,k}}{\nu_{l}^{T_i,R}},$$

(12)

We first assume one super time slot memory for the transceiver-relay channel (i.e., $\lfloor \frac{q_{T_i}^{R}}{2} \rfloor = 1, i = 1, 2$). Then, we extend it to higher channel memories. We define the normalized channel gains as follows:

$$\nu_{l}^{T_i,R} = \frac{\pi_{l}^{T_i,R}}{\pi_{1}^{T_i,R}}, \quad i \in \{1, 2\}, \quad l > 1.$$

(13)

Using $I_{i,k} = \pi_{3}^{T_i,R}X_{i,k-1}$ and substituting (12) in (11), we obtain:

$$X_{i,k} = B_{i,k}\left(\frac{c_{\text{SNC}}}{\pi_{1}^{T_i,R}} - \frac{\pi_{3}^{T_i,R}X_{i,k-1}}{\pi_{1}^{T_i,R}}\right) = \frac{c_{\text{SNC}}}{\pi_{1}^{T_i,R}}B_{i,k} - \nu_{3}^{T_i,R}B_{i,k}X_{i,k-1}, \quad i \in \{1, 2\}.$$  

(14)

Remark 1. According to (14), each transceiver $T_i$ needs to save the number of its released molecules in the $(k-1)$-th super time slot, i.e., $X_{i,k-1}$ to determine $X_{i,k}$. Note that the number of released molecules
from $T_i$ in each super time slot has a maximum value which can be obtained from (14) when $X_{i,k-1} = 0$ and $B_{i,k} = 1$ as $X_{i,max}^{SNC} = \frac{c^{SNC}}{\pi_1^R}$. Hence, a finite memory is needed to save $X_{i,k-1}$.

**Extension to higher channel memories:** The results can be extended to a channel with arbitrary memory using (11) and (12):

$$X_{i,k} = \frac{c^{PNC}}{\pi_1^R} B_{i,k} - \sum_{l=1}^{\left\lfloor \frac{T_i^R}{2} \right\rfloor} \pi_2^R B_{i,k} X_{i,k-l}, \quad i \in \{1, 2\},$$

which shows that each transceiver $T_i$ has to save the number of its released molecules in previous $\left\lfloor \frac{T_i^R}{2} \right\rfloor$ super time slots. Similar to the channel with one super time slot memory, we have $X_{i,max}^{SNC} = \frac{c^{SNC}}{\pi_1^R}$.

**B. The Proposed PNC Scheme**

In this scheme, each transceiver $T_i$ releases extra molecules, denoted by $L_{i,k}$, in each super time slot to react with and cancel out the remained molecules of the other transceiver from the previous super time slots (dual purpose of transmission), i.e., for $i \in \{1, 2\}$,

$$X_{i,k} = B_{i,k} \frac{c^{PNC}}{\pi_1^R} + L_{i,k}^{PNC},$$

in which

$$L_{i,k}^{PNC} = \frac{\tilde{I}_{i,k}}{\pi_1^R},$$

where $\tilde{I}_{i,k}$ is the estimated value of the remained molecules of the transceiver $T_i$ around the relay in the $k$-th super time slot, which is calculated by the transceiver $T_i$ using its previously decoded messages. $c^{PNC}$ shows the fixed concentration of molecules that we wish to maintain around the relay. Note that the ISI model in this scheme is similar to the SNC scheme, with the difference that in the PNC, (10) is the concentration of molecules of type $M_i$ around the relay before reaction.

Similar to the SNC scheme, we first assume $\left\lfloor \frac{T_i^R}{2} \right\rfloor = 1$, $i = 1, 2$ and then extend it to higher channel memories. By substituting (17) in (16) and using $\tilde{I}_{i,k} = \pi_3^R X_i^{k-1}$ ($X_i^{k-1}$ is the approximated value of the number of released molecules from $T_i$ in the $(k-1)$-th super time slot, calculated by $T_i$), we have:

$$X_{i,k} = B_{i,k} \frac{c^{PNC}}{\pi_1^R} + \frac{\pi_3^R X_i^{k-1}}{\pi_1^R},$$

for $i \in \{1, 2\}$. We can write a similar equation for $X_{i,k-1}$ as follows

$$X_{i,k-1} = \tilde{B}_{i,k-1} \frac{c^{PNC}}{\pi_1^R} + \frac{\pi_3^R X_i^{k-2}}{\pi_1^R}.$$
Now, by substituting (19) in (18), we obtain:

\[
X_{i,k} = \frac{c_{\text{PNC}}}{\pi_1 \nu_1 T_i R} (B_{i,k} + \nu_3 T_i R \hat{B}_{i,k-1}) + \nu_3 T_i R \nu_3 T_i R X_{i,k-2}, \quad i \in \{1, 2\}. \tag{20}
\]

**Remark 2.** According to (20), each transceiver \(T_i\) needs to save the received message from the other transceiver in the \((k-1)\)-th super time slot (i.e., \(\hat{B}_{i,k-1}\)) along with the number of its released molecules in the two previous super time slots (i.e., \(\{X_{i,k-1}, X_{i,k-2}\}\)). Note that, we assume \(\nu_1 T_i R < 1\), for \(l > 1\), and hence, the number of released molecules from \(T_i\) in each super time slot has a maximum value. This means that the system is stable and a finite memory is needed to save \(X_{i,k-1}, X_{i,k-2}\). The maximum number of released molecules from \(T_i\) in each super time slot, \(X_{i,\text{max}}^{\text{PNC}}\), can be obtained from (20) by substituting \(X_{i,k} = X_{i,k-2} = X_{i,\text{max}}^{\text{PNC}}\) and \(B_{i,k} = \hat{B}_{i,k-1} = 1\):

\[
X_{i,\text{max}}^{\text{PNC}} = \frac{c_{\text{PNC}}}{\pi_1 \nu_1 T_i R} \cdot \frac{1 + \nu_3 T_i R}{1 - \nu_3 T_i R \nu_3 T_i R}, \quad i \in \{1, 2\} \tag{21}
\]

**Extension to higher channel memories:** The number of released molecules to mitigate ISI for higher channel memories can be obtained similar to the unit memory case from (16) and (17) as follows:

\[
X_{i,k} = \frac{c_{\text{PNC}}}{\pi_1 \nu_1 T_i R} (B_{i,k} + \sum_{l=1}^{\left\lfloor \frac{T_i R}{2} \right\rfloor} \nu_3 T_i R \hat{B}_{i,k-l}) + \sum_{l=1}^{\left\lfloor \frac{T_i R}{2} \right\rfloor} \sum_{l_1=1}^{\left\lfloor \frac{T_i R}{2} \right\rfloor} \nu_2 T_i R \nu_2 T_i R X_{i,k-l_1-l_2}, \quad i \in \{1, 2\}, \tag{22}
\]

which shows that each transceiver \(T_i\) has to save its decoded messages in previous \(\left\lfloor \frac{T_i R}{2} \right\rfloor\) super time slots and the number of its released molecules in previous \(\left\lfloor \frac{T_i R}{2} \right\rfloor + \left\lfloor \frac{T_i R}{2} \right\rfloor\) super time slots. If the channel coefficients are such that \(\sum_{l_1=1}^{\left\lfloor \frac{T_i R}{2} \right\rfloor} \sum_{l_2=1}^{\left\lfloor \frac{T_i R}{2} \right\rfloor} \nu_2 T_i R \nu_2 T_i R < 1\), the number of released molecules from \(T_i\) in each super time slot has a maximum value, which can be obtained similar to (21) as follows:

\[
X_{i,\text{max}}^{\text{PNC}} = \frac{c_{\text{PNC}}}{\pi_1 \nu_1 T_i R} \cdot \frac{1 + \sum_{l_1=1}^{\left\lfloor \frac{T_i R}{2} \right\rfloor} \nu_2 T_i R \nu_2 T_i R}{1 - \sum_{l_1=1}^{\left\lfloor \frac{T_i R}{2} \right\rfloor} \sum_{l_2=1}^{\left\lfloor \frac{T_i R}{2} \right\rfloor} \nu_2 T_i R \nu_2 T_i R}, \quad i \in \{1, 2\}. \tag{23}
\]

This guarantees the stability of the scheme.

**Remark 3.** In Section VII, for a fair comparison of the SNC and PNC schemes, we choose \(c_{\text{SNC}}\) and \(c_{\text{PNC}}\) such that \(\frac{1}{2} \sum_{i=1}^{2} X_{i,\text{avg}}^{\text{SNC}} = \frac{1}{2} \sum_{i=1}^{2} X_{i,\text{avg}}^{\text{PNC}}\), where \(X_{i,\text{avg}}^{\text{PNC}}\) and \(X_{i,\text{avg}}^{\text{SNC}}\) are the average number of the released molecules from the transceiver \(T_i\) in the PNC and SNC schemes, respectively. The average

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4In diffusion-based systems with channel memory, the sampling time \(t_0\) is chosen such that \(h(d, t)\) takes its maximum at \(t = t_0\), and thus \(\pi_1 < \pi_1\), for \(l > 1\). Hence, for a single transmitter-receiver channel, \(t_s = \frac{d^2}{\pi_1^2}\). Applying this strategy in our model, we set the maximum of \(h_{M_1}(d, t)\) at \(t = \frac{d^2}{\pi_1^2}\) for the T-R channels and the maximum of \(h_{M_3}(d, t)\) at \(t = \frac{d^2}{\pi_1^2}\) for the R-T channels. To make all channel coefficients to be reducing, we choose \(t_0 = \max\left\{\frac{d^2}{\pi_1^2}, \frac{d^2}{\pi_1^2}, \frac{d^2}{\pi_1^2}, \frac{d^2}{\pi_1^2}\right\}\).

5This condition can be assured by decreasing \(\nu_1 T_i R\)s which needs increasing the \(t_s\) and decreasing the sampling rate accordingly.
values can be obtained from (15) and (22) by substituting $X_{i,k}$ and $X_{i,k-1}$ with their average values ($X_{i,avg}^{PNC}$ or $X_{i,avg}^{SNC}$), and $B_{i,k}$ and $B_{i,k-1}^{k-1}$ with their average values, $\frac{1}{2}$, as follows:

$$X_{i,avg}^{SNC} = \frac{c^{SNC}}{\pi T_{i,R}} \cdot \frac{1}{2 + \sum_{l=1}^{\lfloor \frac{T_{i,R}}{2} \rfloor} \nu_{2l+1}^{T_{i,R}}} \cdot X_{i,avg}^{PNC} = \frac{c^{PNC}}{\pi T_{i,R}} \cdot \frac{1 + \sum_{l=1}^{\lfloor \frac{T_{i,R}}{2} \rfloor} \nu_{2l+1}^{T_{i,R}}}{2(1 - \sum_{l=1}^{\lfloor \frac{T_{i,R}}{2} \rfloor} \sum_{l=2}^{\lfloor \frac{T_{i,R}}{2} \rfloor} \nu_{2l+1}^{T_{i,R}})},$$

(24)

V. ERROR PERFORMANCE ANALYSIS WITH NO ISI

In this section, we derive the probabilities of error at the transceivers $T_1$ and $T_2$, noted by $p_{e,1}$ and $p_{e,2}$, respectively. Throughout this paper, we consider the average bit error probability (Avg-BEP) as follows:

$$\text{Avg-BEP} = \frac{1}{2}(p_{e,1} + p_{e,2}).$$

First, we investigate the error probabilities of the proposed PNC scheme. Then, using a similar approach, we derive the error probabilities of the SNC scheme. Since the error probability without ISI in the current super time slot does not depend on the error probabilities of the previous super time slots and is the same for all super time slots, we drop the index $k$ of the bits and error events in this section.

A. The proposed PNC scheme

Each transceiver $T_i$ sends its message $B_i \in \{0, 1\}$ to the relay through releasing $X_i = \zeta^RB_i$ molecules of type $M_i$. When both transceivers send the information bit 1, almost all molecules react with each other and we have a physical-layer XOR. That is, the relay implicitly decodes the physically made XOR of the messages, $B_1 \oplus B_2$, and sends it to the transceivers through releasing $X_3$ molecules of type $M_3$.

We define an auxiliary variable $B_{R_i}$ as the part of the message $B_1 \oplus B_2$ which corresponds to $B_i$. Each receptor group $i$ at the relay decodes the message $B_{R_i} = B_i(B_1 \oplus B_2)$, the part of the message $B_1 \oplus B_2$ which corresponds to $B_i$, as $\hat{B}_{R_i}$. For $\hat{B}_{R_1} = \hat{B}_{R_2} = 0$, the relay stays silent; otherwise (when $\hat{B}_{R_1} = 1$ or $\hat{B}_{R_2} = 1$), it releases $\zeta^R$ molecules of type $M_3$ and hence, $X_3 = (\hat{B}_{R_1} + \hat{B}_{R_2})\zeta^R = B_{R_3}\zeta^R$. Due to the perfect reaction assumption, $\hat{B}_{R_1}$ and $\hat{B}_{R_2}$ cannot be 1 at the same time and thus, $X_3 \in \{0, \zeta^R\}$.

We remark that these notations are used for the ease of error analysis. In fact, the message sent by the relay ($B_{R_i}$) implicitly shows the $B_1 \oplus B_2$ and it is realized through $\hat{B}_{R_1}$ and $\hat{B}_{R_2}$ in our scheme. Furthermore, the system naturally adds up $\hat{B}_{R_1}$ and $\hat{B}_{R_2}$, because the encoder would release molecules when it is stimulated by the active receptor group (at most one active receptor group exists in each time slot). Finally, each transceiver $T_i$ decodes the message of the relay as $\hat{B}_{R_i}^T$ and, by XORing it with its own sent message, finds the message sent by the other transceiver, i.e., $\hat{B}_{i}^T = B_i \oplus \hat{B}_{R_i}^T$, $i \in \{1, 2\}$.

Define $E_i$ as the error event at the transceiver $T_i$, i.e., $\hat{B}_{i}^T \neq B_i$. The probability of the event $E_i$ is shown by $P(E_i) = p_{e,i}$. $E_i$ consist of two error events corresponding to two communication phases:
Each receptor group $M_i$ according to the physical model, the conditional distribution of the number of bound molecules of type $\hat{B}_i \neq M_i$.  

In the following, we compute the error probabilities of the two communication phases, i.e., $E_{T_i}$ for $i \in \{1, 2\}$. The relay can be obtained from (6) as
\[
\mathbb{P}(E_{1}|B_1 = b_1, B_2 = b_2) = \mathbb{P}(\hat{B}_{T_1} \neq b_1, b_2)
\]
\[
= \mathbb{P}(\hat{B}_{T_1} = B_R, B_R \neq b_1 \oplus b_2|b_1, b_2) + \mathbb{P}(\hat{B}_{T_1} \neq B_R, B_R = b_1 \oplus b_2|b_1, b_2)
\]
\[
= \mathbb{P}(E_{1}|b_1, b_2)(1 - \mathbb{P}(E_{T_1}|B_R = b_1 \oplus b_2)) + (1 - \mathbb{P}(E_{1}|b_1, b_2))\mathbb{P}(\hat{E}_{T_1}|B_R = b_1 \oplus b_2),
\]
for $i \in \{1, 2\}$. By taking average over $B_1$ and $B_2$, the total probability of error at the transceiver $T_i$ can be easily obtained for $i \in \{1, 2\}$ as
\[
p_{b_i} = \mathbb{P}(E_{i}) = \frac{1}{4} \sum_{b_1, b_2} \mathbb{P}(E_{i}|B_1 = b_1, B_2 = b_2)
\]
\[
= \frac{1}{2} \sum_{b_1, b_2} \mathbb{P}(E_{T_1}|B_R = b_1) + \frac{1}{4} [1 - \sum_{b_1, b_2} \mathbb{P}(E_{T_1}|B_R = b_1)] \sum_{b_1, b_2} \mathbb{P}(E_{1}|b_1, b_2).
\]

In the following, we compute the error probabilities of the two communication phases, i.e., $\mathbb{P}(E_{1}|B_1 = b_1, B_2 = b_2)$ and $\mathbb{P}(E_{T_1}|B_R = b_1)$. 

**Phase 1:** When both transceivers send the same information bit 1 or 0, the concentrations of molecules of types 1 and 2 around the relay are $C_1 = C_2 = 0$ (thanks to perfect reaction) and when the transceiver $T_i, i \in \{1, 2\}$, sends the information bit 1 and the transceiver $T_i$ sends the information bit 0, the concentrations are $C_i = \zeta^{T_1}_{T_1} \pi^{T_1}_{T_1}$ and $C_i = 0$. Hence, when $B_{R_i} = b_{R_i}$, the concentration of the molecule type $M_i$ around the relay is $C_i = b_{R_i} \zeta^{T_1}_{T_1} \pi^{T_1}_{T_1}$ and the probability of binding for the receptor type $\Omega_{i}$ at the relay can be obtained from (6) as
\[
\gamma_{b_i}^{R, PNC}(b_{R_i}) = \frac{b_{R_i} \zeta^{T_1}_{T_1} \pi^{T_1}_{T_1}}{b_{R_i} \zeta^{T_1}_{T_1} \pi^{T_1}_{T_1} + \kappa_{D_i}}, \quad i \in \{1, 2\}.
\]

According to the physical model, the conditional distribution of the number of bound molecules of type $M_i$ at the relay, $Y_i^{R}$, given $B_{R_i} = b_{R_i}$, is Binomial\left(n_i^{R}, p_{b_i}^{R, PNC}(b_{R_i})\right).$ Since $p_{b_i}^{R, PNC}(0) = 0$, we have
\[
\mathbb{P}\{Y_i^{R} = y|B_{R_i} = 0\} = \delta[y], \quad i \in \{1, 2\}.
\]

Each receptor group $i$ uses a threshold, $\tau_{i}^{R}$, to decode $B_{R_i}$; if $Y_i^{R}$ is lower than $\tau_{i}^{R}$, then $B_{R_i}$ is decoded as $\hat{B}_{R_i} = 0$; otherwise, $\hat{B}_{R_i} = 1$. The maximum-a-posteriori (MAP) decision rule is used as follows:
\[
\mathbb{P}\{B_{R_i} = 1\} \mathbb{P}(y_i^{R}|B_{R_i} = 1) \overset{\hat{B}_{R_i} = 1}{\geq} \mathbb{P}\{B_{R_i} = 0\} \mathbb{P}(y_i^{R}|B_{R_i} = 0) = \mathbb{P}\{B_{R_i} = 0\} \delta[y_i^{R}],
\]
(30)
which results in $\tau_i^R = 0, i \in \{1, 2\}$.

We define $E_{R_i}$ as the event $\{\hat{B}_{R_i} \neq B_{R_i}\}$. Hence, $\mathbb{P}(E_{R_i})$ is the probability of error when $B_{R_i}$ is decoded with error at the $i$-th receptor group of the relay. Note that $B_{R_i} = 0$ is decoded without error at the relay, due to the noiseless assumption. Hence, for $i \in \{1, 2\}$,

$$\mathbb{P}(E_{R_i} | B_{R_i} = 0) = \mathbb{P}\{Y_i > \tau_i^R | B_{R_i} = 0\} = 0,$$

$$\mathbb{P}(E_{R_i} | B_{R_i} = 1) = \mathbb{P}\{Y_i \leq \tau_i^R | B_{R_i} = 1\} = (1 - p_{b_i}^{R,\text{PNC}}(1))^{n_i^R}.$$

Recall that the number of released molecules of type $M_3$ equals to $X_3 = 0$ when the transceivers send the same messages and $X_3 = \zeta^R$ when one of the transceivers send the information bit 1 and the corresponding receptor group at the relay decodes it correctly (see Table III). Thus, when $(B_1, B_2) \in \{(0, 0), (1, 1)\}$, $B_{R_1}$ and $B_{R_2}$ equal to zero and are decoded without error at the relay. When $(B_1, B_2) = (1, 0)$, we have $B_{R_1} = 1$ and $B_{R_2} = 0$. Hence, $B_{R_2}$ is decoded without error at the relay and we get

$$\mathbb{P}(E_{R_i} | B_1 = 1, B_2 = 0) = \mathbb{P}(E_{R_1} | B_1 = 1, B_2 = 0).$$

Similarly, we get $\mathbb{P}(E_{R_i} | B_1 = 1, B_2 = 0) = \mathbb{P}(E_{R_2} | B_1 = 0, B_2 = 1)$. Therefore,

$$\mathbb{P}(E_{R_i} | B_1 = 0, B_2 = 0) = \mathbb{P}(E_{R_i} | B_1 = 1, B_2 = 1) = 0,$$

$$\mathbb{P}(E_{R_i} | B_1 = 1, B_2 = 0) = (1 - p_{b_1}^{R,\text{PNC}}(1))^{n_i^R}, \quad \mathbb{P}(E_{R_i} | B_1 = 1, B_2 = 1) = (1 - p_{b_2}^{R,\text{PNC}}(1))^{n_i^R}.\quad \text{(32)}$$

**Phase 2:** The binding probability for the receptors at each transceiver $T_i$ when $B_R = b_R$ is:

$$p_{b_i}^{T_i}(b_R) = \frac{b_R \kappa_i^{R, \text{RT}_i} \zeta_R}{b_R \kappa_i^{R, \text{RT}_i} + \kappa_D}, \quad i \in \{1, 2\}. \quad \text{(33)}$$

The conditional distribution of the number of bound molecules of type $M_3$ at the transceiver $T_i$, $Y_3^{T_i}$, given $B_R = b_R$, is Binomial$(n_i^{T_i}, p_{b_i}^{T_i}(b_R))$. We have $\mathbb{P}\{Y_3^{T_i} = 0 | B_R = 0\} = \delta[y]$ since $p_{b_i}^{T_i}(0) = 0.$

To decode $B_R$, each transceiver $T_i$ uses a threshold, $\tau_i^{T_i}$. Using MAP decision rule, the optimum value of $\tau_i^{T_i}$ can be obtained similar to (30) as $\tau_i^{T_i} = 0$. Hence,

$$\mathbb{P}(E_{T_i}^{\hat{B}_R} | B_{R_i} = 0) = 0, \quad \mathbb{P}(E_{T_i}^{\hat{B}_R} | B_{R_i} = 1) = (1 - p_{b_i}^{T_i}(1))^{n_i^{T_i}}. \quad \text{(34)}$$

**Note:** Note that here we have, $\mathbb{P}\{B_{R_i} = 1\} = \mathbb{P}\{B_i = 1, B_i = 0\} = \frac{1}{2}$, $\mathbb{P}\{B_{R_i} = 0\} = \mathbb{P}\{B_i = 0, B_i = 0\} + \mathbb{P}\{B_i = 0, B_i = 1\} + \mathbb{P}\{B_i = 1, B_i = 1\} = \frac{3}{4}$, and thus, $\mathbb{P}(B_{R_i} = 1) < \mathbb{P}(B_{R_i} = 0)$ and (30) result in $\tau_i^{R} = 0$. However, if $\mathbb{P}(B_{R_i} = 1) \geq \mathbb{P}(B_{R_i} = 0)$, since the threshold is non-negative, we would still obtain $\tau_i^{R} = 0.$
Now, by substituting the error probabilities of the two phases from (32) and (34) in (27), we obtain
\[
p_{i,b} = \frac{1}{2}(1 - p_b^R(1))^{n_2} \left[ \frac{1}{4} \left( 1 - (1 - p_b^R(1))^{n_1} \right) \right] \left( 1 - p_b^{R,SNC}(1) \right) \left( 1 - p_b^{R,SNC}(1) \right) \right] + \left( 1 - p_b^{R,SNC}(1) \right) \right]
\]
for \( i \in \{1, 2\} \), and thus the Avg-BEP can be obtained from (25).

**B. The SNC scheme**

In the SNC scheme, the \( i \)-th receptor group at the relay decodes \( B_i \) (the message of the transceiver \( T_i \)) as \( \hat{B}_i \). The relay XORs the decoded messages and sends the message \( B_R = \hat{B}_1^R \oplus \hat{B}_2^R \) to the transceivers using \( X^R_3 = B_R \zeta^R \) molecules of type M3. The error probability of the second communication phase can be obtained from (34). In the following, we derive the error probability of the first phase. Here, we define \( E_R = \{ B_R \neq B_1 \oplus B_2 \} \) to show the error event at the relay. The total error probability at the transceiver \( T_i \) can be obtained from (27). Now, we compute \( \mathbb{P}(E_R|B_1 = b_1, B_2 = b_2) \). When \( B_1 = b_1 \) and \( B_2 = b_2 \), the probability of binding for the receptor type \( \Omega_i \) at the relay can be obtained from (6) as
\[
p_{i,b}^{R,SNC}(b_1, b_2) = \frac{\bar{\zeta}_{i,T_i}^{R,SNC}(b_1, b_2)}{\zeta_{i,T_i}^{R,SNC}(b_1, b_2)} \quad ; \quad i \in \{1, 2\}.
\]

The conditional distribution of \( Y_i^R \) (given \( B_1 = b_1 \) and \( B_2 = b_2 \)) is Binomial \( (n_i^R, p_{i,b}^{R,SNC}(b_1, b_2)) \). Since \( p_{i,b}^{R,SNC}(0, b_2) = p_{i,b}^{R,SNC}(b_1, 0) = 0 \), we have \( \mathbb{P}(Y_i^R = y|B_1 = 0) = \delta[y] \), \( i \in \{1, 2\} \).

The relay uses a threshold \( \tau_i^R \) to decode \( B_i \). Similar to the PNC scheme, we obtain the optimum thresholds using MAP decision rule as \( \tau_i^R = \tau_i^R = 0 \). We also define \( E_i^R = \{ \hat{B}_i^R \neq B_i \} \) to denote the event where \( B_i \) is decoded with error at the relay. Hence,
\[
\mathbb{P}(E_i^R|B_1 = 0, B_2 = 0) = \mathbb{P}(Y_i^R = y|B_1 = 0, B_2 = 0) = 0, \quad (37)
\]
\[
\mathbb{P}(E_i^R|B_1 = 1, B_2 = 0, B_2 = 0) = \mathbb{P}(Y_i^R = y|B_1 = 1, B_2 = 0, B_2 = 0) = (1 - p_{i,b}^{R,SNC}(1, b_2))^{n_1^R}.
\]

\( \mathbb{P}(E_2^R|B_1 = b_1, B_2 = b_2) \) can be obtained similarly. Due to XORing at the relay, the event \( E_R \) is equivalent to the event that one of the messages \( B_1 \) or \( B_2 \) is decoded with error at the relay. Hence,
\[
\mathbb{P}(E_R|B_1 = b_1, B_2 = b_2) = \mathbb{P}(E_i^R|b_1, b_2)(1 - \mathbb{P}(E_2^R|b_1, b_2)) + (1 - \mathbb{P}(E_i^R|b_1, b_2))\mathbb{P}(E_2^R|b_1, b_2). \quad (38)
\]

By substituting \( \mathbb{P}(E_i^R|b_1, b_2) \) and \( \mathbb{P}(E_2^R|b_1, b_2) \) from (37) in (38) we obtain:
\[
\mathbb{P}(E_R|B_1 = 1, B_2 = 0) = (1 - p_{i,b}^{R,SNC}(1, 0))^{n_1^R}, \quad \mathbb{P}(E_R|B_1 = 0, B_2 = 1) = (1 - p_{i,b}^{R,SNC}(0, 1))^{n_2^R}, \quad (39)
\]
\[
\mathbb{P}(E_R|B_1 = 0, B_2 = 0) = 0, \quad \mathbb{P}(E_R|B_1 = 1, B_2 = 1) = (1 - p_{i,b}^{R,SNC}(1, 1))^{n_1^R} + (1 - p_{i,b}^{R,SNC}(1, 1))^{n_2^R}
\]
\[
- 2(1 - p_{i,b}^{R,SNC}(1, 1))^{n_1^R} (1 - p_{i,b}^{R,SNC}(1, 1))^{n_2^R}.
\]
Finally, by substituting the error probabilities of the two communication phases (from (39) and (44)) in (27), we obtain $p_{e,i}$, $i \in \{1, 2\}$, as

$$p_{e,i} = \frac{1}{2}(1 - p_{b}^{T}(1))^{n_{T}^{i}} + \frac{1}{4} \left[ 1 - (1 - p_{b}^{T}(1))^{n_{T}^{i}} \right] \left[ (1 - p_{b,1}^{R,SNC}(1, 0))^{n_{R}^{b}} + (1 - p_{b,2}^{R,SNC}(0, 1))^{n_{R}^{b}} \right]$$

$$+ (1 - p_{b,1}^{R,SNC}(1, 1))^{n_{R}^{b}} + (1 - p_{b,2}^{R,SNC}(1, 1))^{n_{R}^{b}} - 2(1 - p_{b,1}^{R,SNC}(1, 1))^{n_{R}^{b}} (1 - p_{b,2}^{R,SNC}(1, 1))^{n_{R}^{b}} \right].$$

**Remark 4.** Comparing (35) and (40), it can be seen that the error probability at each transceiver and thus the Avg-BEP of the PNC scheme is lower than or equal to that of the SNC: since $p_{b,i}^{T}$ is the same for both schemes, the first two terms of (35) and (40) are equal; the second two terms of (40) are lower than those in (35) according to the fact that $p_{b,1}^{R,PNC}(1) \geq p_{b,1}^{R,SNC}(1, 0)$, $p_{b,2}^{R,PNC}(1) \geq p_{b,2}^{R,SNC}(0, 1)$ due to the blocking effect in the SNC scheme; the sum of the other terms in (40) is $P(E_{1}|B_{1} = 1, B_{2} = 1) \geq 0$.

**VI. ERROR PERFORMANCE ANALYSIS IN THE PRESENCE OF ISI**

We assume the transceiver-relay and the relay-transceiver channels to have unit super time slot memory. In Section VII we simulate the system for higher channels memories.

**A. The PNC scheme**

Similar to the no ISI case, from (26), we define two error events in each super time slot corresponding to each communication phase: (i) $E_{R,k} = \{\hat{B}_{R,k} \neq B_{R,k}\}$, and (ii) $E_{k}^{T} = \{\hat{B}_{R,k}^{T} \neq \hat{B}_{R,k}\}$. In the following, we obtain recursive equations for the error probabilities of both communication phases.

**Phase 1:** According to (20), the transceiver $T_i$ uses the decoded message of the other transceiver in the $(k - 1)$-th super time slot ($\hat{B}_{1,k-1}^{T}$) and the number of its own released molecules in the $(k - 2)$-th super time slot ($X_{i,k-2}$) to determine the number of released molecules in the $k$-th super time slot. $X_{1,k-2}$ and $X_{2,k-2}$, themselves, depend on the previous decoded messages and hence, they may contain error. We consider the error effect in $(k - 1)$-th super time slot and neglect the error effect in $X_{1,k-2}$ and $X_{2,k-2}$ to obtain an approximate value for the error probability of the first communication phase (however, in Section VII we simulate this system and obtain the error probability considering the effect of error in $X_{i,k-2}$). With this assumption, the error probability of phase 1 in the $k$-th super time slot is obtained as

$$P(E_{R,k}|B_{1,k} = b_{1,k}, B_{2,k} = b_{2,k}) = \frac{1}{4} \sum_{\hat{b}_{1,k-1},\hat{b}_{2,k-1} \in \{0,1\}, \hat{b}_{1,k-1},\hat{b}_{2,k-1} \in \{0,1\}} \left[ P(\hat{B}_{1,k-1}^{T} = \hat{b}_{1}, \hat{B}_{2,k-1}^{T} = \hat{b}_{2}|b_{1,k}, b_{2,k}, b_{1,k-1}, b_{2,k-1}) \right]$$

$$\times P(E_{R,k}|B_{1,k}, B_{2,k}, B_{1,k-1}, B_{2,k-1}, \hat{B}_{1,k-1}^{T}, \hat{B}_{2,k-1}^{T}) = (b_{1,k}, b_{2,k}, b_{1,k-1}, b_{2,k-1}, \hat{b}_{1}, \hat{b}_{2}) \right].$$
The first term in the summation of \((41)\) is the joint decoding probability at the transceivers, which is independent of the current messages \((b_{1,k}, b_{2,k})\) and can be derived as a function of the error probabilities in the \((k-1)\)-th super time slot as

\[
P(\hat{B}_{1,k-1}^{T_1} = \hat{b}_1, \hat{B}_{2,k-1}^{T_1} = \hat{b}_2 | b_{1,k}, b_{2,k}, b_{1,k-1}, b_{2,k-1}) = (1 - P(E_{R,k-1} | b_{1,k-1}, b_{2,k-1})) P(\hat{B}_{1,k-1}^{T_2} = \hat{b}_1, \hat{B}_{2,k-1}^{T_2} = \hat{b}_2 | b_{1,k-1}, b_{2,k-1}, E_{R,k-1}^{c})
\]

\[
+ P(E_{R,k-1} | b_{1,k-1}, b_{2,k-1}) P(\hat{B}_{1,k-1}^{T_2} = \hat{b}_1, \hat{B}_{2,k-1}^{T_2} = \hat{b}_2 | b_{1,k-1}, b_{2,k-1}, E_{R,k-1}).
\]

Now, considering the independent decoding at the transceivers, as well as the independent channels from the relay to the transceivers, we obtain

\[
P(\hat{B}_{1,k-1}^{T_2} = \hat{b}_1, \hat{B}_{2,k-1}^{T_2} = \hat{b}_2 | b_{1,k-1}, b_{2,k-1}, E_{R,k-1})
\]

\[
= P(\hat{B}_{1,k-1}^{T_2} = \hat{b}_1 | b_{1,k-1}, b_{2,k-1}, E_{R,k-1}) P(\hat{B}_{2,k-1}^{T_2} = \hat{b}_2 | b_{1,k-1}, b_{2,k-1}, E_{R,k-1})
\]

where the above probabilities would be the error probability when \(\hat{b}_i \neq b_{i,k-1}\), for \(i \in \{1, 2\}\), and thus:

\[
P(\hat{B}_{1,k-1}^{T_1} = \hat{b}_1 | b_{1,k-1}, b_{2,k-1}, E_{R,k-1}) = \begin{cases} P(E_{k-1} | B_{R,k-1} = b_{1,k-1} \oplus b_{2,k-1}), & \text{if } \hat{b}_i \neq b_{i,k-1} \\ 1 - P(E_{k-1} | B_{R,k-1} = b_{1,k-1} \oplus b_{2,k-1}), & \text{if } \hat{b}_i = b_{i,k-1} \end{cases}
\]

Similar equations can be derived for \(P(\hat{B}_{1,k-1}^{T_2} = \hat{b}_1, \hat{B}_{2,k-1}^{T_2} = \hat{b}_2 | b_{1,k-1}, b_{2,k-1}, E_{R,k-1})\). Combining \((42)-(44)\) gives the first term in the summation of \((41)\). To obtain the second term in the summation of \((41)\), i.e., \(P(E_{R,k} | B_{1,k}, B_{2,k}, B_{1,k-1}, B_{2,k-1}, \hat{B}_{1,k-1}^{T_2}, \hat{B}_{2,k-1}^{T_2}) = (b_{1,k}, b_{2,k}, b_{1,k-1}, b_{2,k-1}, \hat{b}_1, \hat{b}_2)\), one must obtain the concentration of each molecule type around the relay after reaction for all \(2^6\) realizations of \(b_{1,k}, b_{2,k}, b_{1,k-1}, b_{2,k-1}, \hat{b}_1, \hat{b}_2\). Then, the error probability at the relay for each case can be derived based on the corresponding binding probabilities. The details are given in Appendix A where the second term in the summation of \((41)\) is derived. Combining all these equations, a set of recursive equations is obtained for the error probability of the relay in Appendix A.

**Phase 2:** Here, using fixed transmission rate, the probability of binding for molecules of type \(M_3\) at the transceiver \(T_i\) (when \(B_{R,k} = b_{R,k}\) and \(B_{R,k-1} = b_{R,k-1}\)) is given as

\[
p_{b}(\hat{b}_{R,k}, b_{R,k-1}) = \frac{b_{R,k} \xi_t R_{\pi_1} + b_{R,k-1} \xi_t R_{\pi_3} + b_{R,k} \xi_t R_{\pi_2} + \kappa_D, i}{b_{R,k} \xi_t R_{\pi_1} + b_{R,k-1} \xi_t R_{\pi_3} + \kappa_D, i}, \quad i \in \{1, 2\}.
\]

To mitigate ISI in this phase, the transceiver \(T_i\) uses the decoded message of the relay in the \((k-1)\)-th super time slot, i.e., \(\hat{b}_{R,k-1}\) and obtains the adaptive threshold in the \(k\)-th super time slot using Maximum Likelihood (ML) decision rule as follows:

\[
P(\hat{y}_{3,k} | B_{R,k} = 1, B_{R,k-1} = \hat{b}_{R,k-1}^{T_1}) \begin{array}{c} \hat{b}_{R,k}^{T_1} = 1 \\ \hat{b}_{R,k}^{T_1} = 0 \end{array} \geq \frac{p(\hat{y}_{3,k} | B_{R,k} = 0, B_{R,k-1} = \hat{b}_{R,k-1}^{T_1}),}{p(\hat{y}_{3,k} | B_{R,k} = 1, B_{R,k-1} = \hat{b}_{R,k-1}^{T_1})}
\]
For the above decision rule, the error probability at previous decoded message is zero, our ISI mitigating technique gives the zero threshold (i.e., $\tau^{T_i,1}(0) = 0$). Hence, which gives the adaptive threshold used at $T_i$ (that is $\tau^{T_i,1}(\hat{i}^{T_i}_{R,k-1})$). It can be easily seen that when previous decoded message is zero, our ISI mitigating technique gives the zero threshold (i.e., $\tau^{T_i,1}(0) = 0$).

For the above decision rule, the error probability at $T_i$, for $b_{R,k} \in \{0, 1\}$ is obtained as

$$P(E^T_k | B_{R,k} = b_{R,k}) = \sum_{b_{R,k-1}, \hat{b}_{R,k-1} \in \{0, 1\}} \left[ P(B_{R,k-1} = b_{R,k-1}) \cdot P(\hat{b}^{T}_{R,k-1} = b_{R,k-1} | b_{R,k-1}) \right. \
\left. \times P(Y^T_{3,k} > \tau^{T_i,1}(\hat{i}^{T_i}_{R,k-1}) | b_{R,k}, b_{R,k-1}, \hat{b}^{T}_{R,k-1}) \right]$$

(48)

for $i \in \{1, 2\}$, where $P(B_{R,k-1} = 0) = \frac{1}{4}[2 - P(E_{R,k-1} | B_{1,k-1} = 0, B_{2,k-1} = 0) - P(E_{R,k-1} | B_{1,k-1} = 1, B_{2,k-1} = 1) + P(E_{R,k-1} | B_{1,k-1} = 0, B_{2,k-1} = 1) + P(E_{R,k-1} | B_{1,k-1} = 1, B_{2,k-1} = 0)]$ and

$$P(\hat{b}^{T}_{R,k-1} = b_{R,k-1} | b_{R,k-1}) = \begin{cases} P(E^T_k | b_{R,k-1}), & \text{if } \hat{b}^{T}_{R,k-1} \neq b_{R,k-1}, \\ 1 - P(E^T_k | b_{R,k-1}), & \text{if } \hat{b}^{T}_{R,k-1} = b_{R,k-1}. \end{cases}$$

(49)

Hence, $P(E^T_k | B_{R,k} = b_{R,k})$ can be obtained recursively from (48). Since we have two linear equations in (48) with two unknowns, a closed form equation can be easily obtained for $P(E^T_k | B_{R,k} = b_{R,k})$.

**Remark 5.** To further simplify the error performance results, we consider the case where there is no error in the decoded messages of the previous super time slots (i.e., we ignore the error propagation). Then, the error probability of phase 1 will be equal to the no ISI case. For the error probability of phase 2, we take the average of (48) over $\hat{b}^{T_i,1}_{R,k-1} = B_{R,k-1}$ and use (27) to obtain the error probability at the transceiver $T_i$ as follows:

$$P_{c,i}^{\text{NoE}} = \frac{1}{16}(4 - u^2)w_{i,1} + \frac{1}{16}(2-u)^2w_{i,2} + \frac{1}{4}u,$$

(50)

for $i \in \{1, 2\}$, where

$$w_{i,1} = (1 - p^{T_i,J(1,0)})^{n_{T_i}} + \sum_{l=\tau^{T_i,J}(1)+1}^{n_{T_i}} \binom{n_{T_i}}{l} \left( p^{T_i,J(0,1)} \right)^{l} \left( 1 - p^{T_i,J(0,1)} \right)^{n_{T_i} - l},$$

(51)

$$w_{i,2} = \sum_{l=0}^{\tau^{T_i,J}(1)} \binom{n_{T_i}}{l} \left( p^{T_i,J(1,1)} \right)^{l} \left( 1 - p^{T_i,J(1,1)} \right)^{n_{T_i} - l},$$

(50) $w_{i,1}$ and $w_{i,2}$ are defined in (28) and (45), respectively. Note that, ignoring the error propagation gives lower bounds on the error probabilities of each hop, while the overall error probability cannot be proved to necessarily be a lower bound. However, in our simulation results, it is always a lower bound.
B. The SNC scheme

Here, the error probability of the second phase is the same as that of the PNC given in (48), with the difference that \( P(B_{R,k-1} = 0) \) must be computed separately, since the error probabilities of the first phase are not equal for two schemes. Thus, we only analyze the error probability of the first phase. According to (14), the transceiver \( T_i \) uses the number of released molecules in the \((k-1)\)-th super time slot to determine the number of released molecules in the \(k\)-th super time slot: if its message is 1, the transceiver \( T_i \) releases some molecules such that the concentration of molecules of type \( M_i \) at the relay will be equal to \( e_{SNC} \) and if its message is 0, it stays silent (concentration of the molecules of type \( M_i \) at the relay will be equal to the concentration of the remaining molecules from the previous super time slot, i.e., \( X_{i,k-1} = \pi_{3}^{T_i,R} \)). Hence, the concentration of molecules of type \( M_i \) around the relay is \( C_{i,k} = B_{i,k} e_{SNC} + (1 - B_{i,k}) X_{i,k-1} \pi_{3}^{T_i,R} \) and the binding probability for molecules of type \( M_i \) at the relay can be obtained from (6). It is just straightforward to show from (14) that the probability distribution function (PDF) of \( X_{i,k} \) for \( i \in \{1, 2\} \) is as follows:

\[
 p_{X_i,k}(x) = \frac{1}{2^m} \delta(x - x_{i,m}), \quad x_{i,m} = \frac{e_{SNC}}{\pi_{1}^{T_i,R}} l \sum_{l=0}^{m-2} (-1)^l \pi_{3}^{T_i,R}, \quad m \in \mathbb{N}. \tag{52}
\]

The relay uses MAP decision rule to decode the message of the transceiver \( T_i, i \in \{1, 2\} \) as

\[
 \frac{1}{2} P(y_{i,k}^R | B_{i,k} = 1) = \frac{1}{2} P(y_{i,k}^R | B_{i,k} = 0). \tag{53}
\]

Hence,

\[
 \sum_{b_{i,k} \in \{0,1\}} \int P(X_{1,k-1} = x_1) P(X_{2,k-1} = x_2) \left[ p_{y_{i,k}^R | b_{i,k}, x_1, x_2} (y_{i,k}^R) - p_{y_{i,k}^R | 0, b_{i,k}, x_1, x_2} (y_{i,k}^R) \right] dx_1 dx_2 \gtrless \sum_{B_{i,k} \in \{0,1\}} \frac{1}{2} P(y_{i,k}^R | B_{i,k} = 0), \tag{54}
\]

where \( p_{y_{i,k}^R | b_{i,k}, x_1, x_2} (y_{i,k}^R) = P(y_{i,k}^R | B_{i,k} = b_{i,k}, B_{i,k} = b_{i,k}, X_{1,k-1} = x_1, X_{2,k-1} = x_2) \). By substituting \( P(X_{i,k-1} = x_i) \) from (52), we obtain the MAP decision rule in the \( i \)-th receptor group as

\[
 \sum_{b_{i,k} \in \{0,1\}} \sum_{m_1, m_2=0}^{\infty} \left( \frac{1}{2} \right)^{m_1+m_2} \left[ p_{y_{i,k}^R | b_{i,k}, x_1, m_1, x_2, m_2} (y_{i,k}^R) - p_{y_{i,k}^R | 0, b_{i,k}, x_1, m_2, x_2, m_2} (y_{i,k}^R) \right] \gtrless \sum_{B_{i,k} \in \{0,1\}} \frac{1}{2} P(y_{i,k}^R | B_{i,k} = 0). \tag{55}
\]

which its solution gives the optimum threshold at the relay (shown by \( \tau_i^R \)) and can be found numerically.

Then, the error probability at the \( i \)-th receptor group \((i \in \{1, 2\})\) of the relay is obtained as

\[
 P(E_{i,k}^R | B_{i,k} = 0, B_{i,k} = b_{i,k}) = 1 - \sum_{m_1, m_2=0}^{\infty} \left( \frac{1}{2} \right)^{m_1+m_2} F_{Y_{i,k}^R | 0, b_{i,k}, x_1, m_1, x_2, m_2} (\tau_i^R), \tag{56}
\]

\[
 P(E_{i,k}^R | B_{i,k} = 1, B_{i,k} = b_{i,k}) = \sum_{m_1, m_2=0}^{\infty} \left( \frac{1}{2} \right)^{m_1+m_2} F_{Y_{i,k}^R | 1, b_{i,k}, x_1, m_1, x_2, m_2} (\tau_i^R),
\]

\[
 DRAFT
\]
where \( F_{\tau_i}^{\text{R}}(b_{i,k}, b_{i,k,x_{1,m_1}}, x_{2,m_2}) = \mathbb{P}\{Y_{i,k}^{\text{R}} \leq \tau_i^{\text{R}} \} \) = \( \mathbb{P}\{X_{i,k} = b_{i,k}, X_{1,k-1} = x_{1,m_1}, X_{2,k-1} = x_{2,m_2} \} \). Now, \( \mathbb{P}(E_{R,k}|B_{1,k} = b_{1,k}, B_{2,k} = b_{2,k}) \) can be obtained by substituting (56) in (38).

**Remark 6.** The error probability can be further simplified assuming that the message of the relay is decoded without error at the transceivers in the previous super time slot:

\[
p_{e,i}^{\text{NoE}} = \frac{1}{16} ((2 - u_1)^2 - u_2^2) w_{i,1} + \frac{1}{16} ((2 - u_2)^2 - u_1^2) w_{i,2} + \frac{1}{4} (u_1 + u_2),
\]

for \( i \in \{1, 2\} \), where \( u_1 = \mathbb{P}(E_{R,k}|B_{1,k} = 0, B_{2,k} = 0) + \mathbb{P}(E_{R,k}|B_{1,k} = 1, B_{2,k} = 1) \), \( u_2 = \mathbb{P}(E_{R,k}|B_{1,k} = 0, B_{2,k} = 1) + \mathbb{P}(E_{R,k}|B_{1,k} = 1, B_{2,k} = 0) \) can be computed from (56) and (38), and \( w_{i,1}, w_{i,2} \) are defined in (51). This provides a lower bound on the error probability of the SNC scheme. Because, we have \( p_{e,i} = \mathbb{P}(E_R) + (1 - 2\mathbb{P}(E_R))\mathbb{P}(E^{T_i}) \) from (27). By ignoring the error propagation we obtain a lower bound on \( \mathbb{P}(E^{T_i}) \). Since \( \mathbb{P}(E_R) < 0.5 \), this is a lower bound on \( p_{e,i} \).

VII. Simulation and Numerical Results

In this section, we evaluate the performance of the PNC and SNC schemes in terms of the probability of error. We consider the parameters in Table III (consistent with prior works [26], [29]). For the SNC scheme, we consider no, low, and high blocking cases, specified in Table III as in [26]. In the no ISI case, we choose \( t_s = t_0 = 1.67 \text{ s} \) which is the time that the impulse responses of the channels take their maximum. In the ISI case, we assume \( t_0 = 1.67s \) and \( t_s \) is chosen such that \( \nu_{q+2} = 0.05 \).

Fig. 3 shows the Avg-BEP versus \( \zeta^{T_1} = \zeta^{T_2} = \zeta^R = \zeta \) for the two schemes without ISI using (25), (35), and (40) along with the Avg-BEP using simulation. It can be seen that the proposed PNC scheme outperforms the SNC scheme in all blocking cases. This is due to the reduction in the number of the molecules bound to the receptors (thanks to reaction). Also, the simulations confirm the analytical results.

Fig. 4 shows the Avg-BEP versus the average number of transmitted molecules (i.e., \( \frac{1}{2} \sum_{i=1}^{2} X_{i,\text{avg}}^{\text{PNC}} = \frac{1}{2} \sum_{i=1}^{2} X_{i,\text{avg}}^{\text{SNC}} = X_{\text{avg}} \)) in the presence of ISI using analysis and simulation along with the Avg-BEP using NoE approximations given in (50) and (57) for the channels with memory of 3. It can be seen that the error performance of the SNC scheme, for which we adopt the existing ISI mitigating techniques, is considerably worse than the error performance of the PNC scheme, for which we propose a reaction-based ISI mitigating technique. The reason is that in the SNC scheme, using adaptive rate at each transceiver mitigates the ISI only when the message of the transceiver is 1. But, in the PNC scheme, using adaptive rates at the transceivers mitigates the ISI in all cases of the sent messages. It is also seen that the NoE approximation of error probability of the PNC scheme is a lower bound.

Fig. 5 shows the Avg-BEP versus the channel memory \( (q^{T,R} = q^{RT_i} = q, i = 1, 2) \), in the presence of ISI. Here, we assume \( \frac{1}{2} \sum_{i=1}^{2} X_{i,\text{avg}}^{\text{PNC}} = \frac{1}{2} \sum_{i=1}^{2} X_{i,\text{avg}}^{\text{SNC}} = 1 \times 10^{-22} \text{ mol} \). It can be observed that the error
Fig. 3: Average bit error probability with respect to $\zeta^1 = \zeta^2 = \zeta^R = \zeta$ without ISI.

Fig. 4: Avg-BEP with respect to the average number of transmitted molecules in the presence of ISI ($q_i^{T,R} = q_i^{RT}, i = 3, i = 1, 2$).

Fig. 5: Avg-BEP with respect to channel memory ($q_i^{T,R} = q_i^{RT}, i = q_i, i = 1, 2$), in the presence of ISI ($X_{avg} = 1 \times 10^{-22}$ mol).

probability increases by channel memory. However, the PNC scheme using the proposed ISI mitigating technique performs much better than the SNC scheme using the existing ISI mitigating techniques.

VIII. CONCLUDING REMARKS

In this paper, we proposed the physical-layer network coding (PNC) for molecular communication (MC) called the reaction-based PNC scheme, where we used different molecule types, reacting with each other by a fast irreversible reaction. Hence, we constructed a physical-layer XOR in this scheme without requiring an XOR gate at the relay. This results in a simple implementation for the proposed...
scheme. To mitigate the ISI, we also used the reaction characteristics of the PNC scheme and proposed a reaction-based ISI mitigating technique for this scheme, where each transceiver using its previously decoded messages, cancels out the ISI of the other transceiver using the reaction of molecules. Considering the ligand-receptor binding process at the receivers, we investigated the error probabilities of the straightforward and the proposed network coding schemes. As expected and confirmed by simulations, the reaction-based scheme decreases the overall error probability in two-way relay MC, while having less complexity. Further, the proposed ISI mitigating technique for the PNC scheme has significantly better performance compared to the existing techniques applied to each hop of the system. Our scheme also handled the receptors blocking problem.

*Channel state information (CSI)*: We assumed that the transceivers know the channel coefficients of both transceivers to the relay channels. This is justified if the nodes have fixed distance, where the channel coefficients can be computed from the diffusion equation. Studying the network coding schemes with limited (or no) CSI is an interesting future work.

*Deterministic model*: We considered the deterministic model for our analysis which ignores the channel noise. In the presence of noise, the derivations would be much more complex but the methods do not change.

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Consider the set of all 16 cases of the sent and decoded messages of the transceivers in the previous super time slot (i.e., the set $\mathcal{A} = \{(b_{1,k-1}, b_{2,k-1}, \hat{b}_1, \hat{b}_2)|b_{1,k-1}, b_{2,k-1}, \hat{b}_1, \hat{b}_2 \in \{0, 1\}\}$). We partition $\mathcal{A}$ into nine subsets shown by $\mathcal{A}_g, g = 1, ..., 9$ (see Table IV), based on the same error probability at the relay. In fact, in each subset (group), the concentration of molecules (of each type) around the relay is the same after reaction and thus the error probability is the same. Therefore, we rewrite the error probability at the relay, given in (41), as

$$\mathbb{P}(E_{R,k}|B_{1,k} = b_{1,k}, B_{2,k} = b_{2,k}) = \frac{1}{4} \sum_{g=1}^{9} f_g p_g(b_{1,k}, b_{2,k}),$$

(58)

where $f_g = \sum_{(b_{1,k-1}, b_{2,k-1}, b_1, b_2) \in \mathcal{A}_g} \mathbb{P}(\hat{B}_{1,k-1}^T = \hat{b}_1, \hat{B}_{2,k-1}^T = \hat{b}_2|b_{1,k-1}, b_{2,k-1})$, in which $\mathbb{P}(\hat{B}_{1,k-1}^T = \hat{b}_1, \hat{B}_{2,k-1}^T = \hat{b}_2|b_{1,k-1}, b_{2,k-1})$ is given in (42), and

$$p_g(b_{1,k}, b_{2,k}) = \mathbb{P}(E_{R,k}|B_{1,k} = b_{1,k}, B_{2,k} = b_{2,k}, (B_{1,k-1}, B_{2,k-1}, \hat{B}_{1,k-1}^T, \hat{B}_{2,k-1}^T) \in \mathcal{A}_g).$$

In group 1, the previous messages at the transceivers are decoded without error and all interference is canceled out at the relay. Thus, $C_{1,k} = b_{R,k}c^{PNC}$. In group 2, the previous message of $T_1$ is 0 which is decoded with error as 1 at $T_2$, while the previous message of $T_2$ is decoded without error at $T_1$. According to (20), the concentration of molecule type $M_1$ before reaction is $c^{PNC}(B_{1,k} + \nu_3 T_{3R} B_{2,k-1}^T + B_{1,k-1} + \nu_3 T_{3R} B_{2,k-2}^T + \nu_3 T_{3R} B_{1,k-1}^T X_{1,k-2} T_{1R}^T + X_{1,k-3} T_{3R}^T)$. The concentration of $M_2$ before reaction is similar. By considering the decoding error of the previous messages at the transceivers, we obtain $C_{1,k} = \max\{0, (B_{1,k} - B_{2,k} - \nu_3 T_{3R})c^{PNC}\}$ and $C_{2,k} = \max\{0, (B_{2,k} - B_{1,k} + \nu_3 T_{3R})c^{PNC}\}$. The concentration of molecules after reaction for the other groups can be obtained similarly (see Table IV).

We assume the fixed thresholds at the relay as $\tau_{1}^R = \tau_{2}^R = 0$. For group 1, since all interference is canceled out, the probability of error at the relay is equal to the no ISI case (obtained in (32)). For group 2, according to Table IV when $(B_{1,k}, B_{2,k}) \in \{(0, 0), (1, 1)\}$, $C_{1,k} = 0$ and $C_{2,k} = \nu_3 T_{3R} c^{PNC}$, and therefore, $\mathbb{P}(E_{R_1,k}) = 0$ and the error probability at the relay equals to $\mathbb{P}(E_{R_2,k})$. When $B_{1,k} = 1, B_{2,k} = 0$
TABLE IV: Concentration of molecules around the relay after reaction (PNC scheme with ISI)

| group $g$ | $A_g$ | $C_{1,k}$ | $C_{2,k}$ |
|-----------|-------|-----------|-----------|
| 1 | $\{(0,0,0,0),(1,0,1,0),\ (0,1,0,1),(1,1,1,1)\}$ | $B_{R_{1,k}}c_{PNC}$ | $B_{R_{2,k}}c_{PNC}$ |
| 2 | $\{(0,0,1,0),(0,1,1,1)\}$ | max\{$(B_{1,k} - B_{2,k} - \nu_3^{T_1R})c_{PNC}$\} | max\{$(B_{2,k} - B_{1,k} + \nu_3^{T_1R})c_{PNC}$\} |
| 3 | $\{(0,1,0,0),(1,1,1,0)\}$ | max\{$(B_{1,k} - B_{2,k} - \nu_3^{T_1R})c_{PNC}$\} | max\{$(B_{2,k} - B_{1,k} + \nu_3^{T_1R})c_{PNC}$\} |
| 4 | $\{(0,0,0,1),(1,0,1,1)\}$ | max\{$(B_{1,k} - B_{2,k} + \nu_3^{T_2R})c_{PNC}$\} | max\{$(B_{2,k} - B_{1,k} - \nu_3^{T_2R})c_{PNC}$\} |
| 5 | $\{(1,0,0,0),(1,0,1,0)\}$ | max\{$(B_{1,k} - B_{2,k} + \nu_3^{T_3R})c_{PNC}$\} | max\{$(B_{2,k} - B_{1,k} - \nu_3^{T_3R})c_{PNC}$\} |
| 6 | $\{(0,0,1,1)\}$ | max\{$(B_{1,k} - B_{2,k} - \nu_\pm)c_{PNC}$\} | max\{$(B_{2,k} - B_{1,k} + \nu_\pm)c_{PNC}$\} |
| 7 | $\{(1,1,0,0)\}$ | max\{$(B_{1,k} - B_{2,k} + \nu_\pm)c_{PNC}$\} | max\{$(B_{2,k} - B_{1,k} - \nu_\pm)c_{PNC}$\} |
| 8 | $\{(0,1,1,0)\}$ | max\{$(B_{1,k} - B_{2,k} - \nu_\pm)c_{PNC}$\} | max\{$(B_{2,k} - B_{1,k} + \nu_\pm)c_{PNC}$\} |
| 9 | $\{(1,1,0,1)\}$ | max\{$(B_{1,k} - B_{2,k} + \nu_\pm)c_{PNC}$\} | max\{$(B_{2,k} - B_{1,k} - \nu_\pm)c_{PNC}$\} |

$B_{R_{i,k}} = B_{i,k}(B_{1,k} \oplus B_{2,k})$, $i \in \{1,2\}$, \(\nu_+ = \nu_3^{T_1R} + \nu_3^{T_2R}\), \(\nu_- = \nu_3^{T_1R} - \nu_3^{T_2R}\).

TABLE V: Probability of error at the relay for the PNC scheme in the presence of ISI

| group $g$ | $p_0(0,0) = p_0(1,1)$ | $p_2(1,0)$ | $p_2(0,1)$ |
|-----------|------------------------|------------|------------|
| 1 | 0 | $\left(\frac{K_{D,2}}{\nu_3^{T_1R}c_{PNC} + K_{D,2}}\right)^{\gamma_2}$ | $\left(\frac{K_{D,1}}{(1 - \nu_3^{T_1R})c_{PNC} + K_{D,1}}\right)^{\gamma_1}$, $\nu_+ < 1$ |
| 2 | $1 - \left(\frac{K_{D,2}}{\nu_3^{T_1R}c_{PNC} + K_{D,2}}\right)^{\gamma_2}$ | $\left(\frac{K_{D,1}}{(1 - \nu_3^{T_1R})c_{PNC} + K_{D,1}}\right)^{\gamma_1}$, $\nu_+ < 1$ |
| 3 | $1 - \left(\frac{K_{D,1}}{\nu_3^{T_1R}c_{PNC} + K_{D,1}}\right)^{\gamma_1}$ | $\left(\frac{K_{D,2}}{(1 - \nu_3^{T_1R})c_{PNC} + K_{D,2}}\right)^{\gamma_2}$, $\nu_+ < 1$ |
| 4 | $1 - \left(\frac{K_{D,2}}{\nu_3^{T_1R}c_{PNC} + K_{D,2}}\right)^{\gamma_2}$ | $\left(\frac{K_{D,1}}{(1 - \nu_3^{T_1R})c_{PNC} + K_{D,1}}\right)^{\gamma_1}$, $\nu_+ < 1$ |
| 5 | $1 - \left(\frac{K_{D,1}}{\nu_3^{T_1R}c_{PNC} + K_{D,1}}\right)^{\gamma_1}$ | $\left(\frac{K_{D,2}}{(1 - \nu_3^{T_1R})c_{PNC} + K_{D,2}}\right)^{\gamma_2}$, $\nu_+ < 1$ |
| 6 | $1 - \left(\frac{K_{D,1}}{\nu_3^{T_1R}c_{PNC} + K_{D,1}}\right)^{\gamma_1}$ | $\left(\frac{K_{D,1}}{(1 - \nu_3^{T_1R})c_{PNC} + K_{D,1}}\right)^{\gamma_1}$, $\nu_+ < 1$ |
| 7 | $1 - \left(\frac{K_{D,2}}{\nu_3^{T_1R}c_{PNC} + K_{D,2}}\right)^{\gamma_2}$ | $\left(\frac{K_{D,1}}{(1 - \nu_3^{T_1R})c_{PNC} + K_{D,1}}\right)^{\gamma_1}$, $\nu_+ < 1$ |
| 8 | $1 - \left(\frac{K_{D,1}}{\nu_3^{T_1R}c_{PNC} + K_{D,1}}\right)^{\gamma_1}$ | $\left(\frac{K_{D,2}}{(1 - \nu_3^{T_1R})c_{PNC} + K_{D,2}}\right)^{\gamma_2}$, $\nu_+ < 1$ |
| 9 | $1 - \left(\frac{K_{D,2}}{\nu_3^{T_1R}c_{PNC} + K_{D,2}}\right)^{\gamma_2}$ | $\left(\frac{K_{D,1}}{(1 - \nu_3^{T_1R})c_{PNC} + K_{D,1}}\right)^{\gamma_1}$, $\nu_+ < 1$ |

\(\nu_+ = \nu_3^{T_1R} + \nu_3^{T_2R}\), \(\nu_- = \nu_3^{T_1R} - \nu_3^{T_2R}\) (without loss of generality, we assume \(\nu_- \geq 0\)).

(assuming that \(\nu_3^{T_1R} < 1\)), we have $C_{1,k} = (1 - \nu_3^{T_1R})c_{PNC}$ and $C_{2,k} = 0$, and thus, $\mathbb{P}(E_{R_{2,k}}) = 0$. When $B_{1,k} = 0, B_{2,k} = 1$, we get $C_{1,k} = 0$ and $C_{2,k} = (1 + \nu_3^{T_1R})c_{PNC}$, and hence, $\mathbb{P}(E_{R_{2,k}}) = 0$. Therefore,

$\begin{align*}
p_2(0,0) &= p_2(1,1) = 1 - \left(\frac{K_{D,2}}{\nu_3^{T_1R}c_{PNC} + K_{D,2}}\right)^{\gamma_2}, \\
p_2(1,0) &= \left(\frac{K_{D,2}}{(1 - \nu_3^{T_1R})c_{PNC} + K_{D,1}}\right)^{\gamma_1}, \\
p_2(0,1) &= \left(\frac{K_{D,2}}{(1 + \nu_3^{T_1R})c_{PNC} + K_{D,2}}\right)^{\gamma_2}.
\end{align*}$

$p_2(b_{1,k}, b_{2,k})$ for the other groups can be obtained similarly (Table V), which can be used along with (58) to obtain a recursive equation for the error probability at the relay.

DRAFT