Molecular Information Delivery in Porous Media

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Abstract—Information delivery via molecular signals is abundant in nature and potentially useful for industry sensing. Many propagation channels (e.g., tissue membranes and catalyst beds) contain porous medium materials and the impact this has on communication performance is not well understood. Here, communication through realistic porous channels is analyzed for the first time via statistical breakthrough curves. Assuming that the number of arrived molecules can be approximated as a Gaussian random variable, analytical results for the throughput, mutual information, error probability, and information diversity gain are presented. Using numerical results, the unique characteristics of the porous medium channel are investigated.

I. INTRODUCTION

For decades, conveying information over a distance has been an important component of organized behavior. The conventional electromagnetic signals are not appropriate in many biological and chemical engineering environments since electromagnetic signals quickly decay in such environments. In nature, molecular signals are used for many microorganisms to signal each other and share information, e.g., quorum sensing and excitation-contraction coupling [1]. Inspired by nature, molecular communication (MC) has been proposed.

Significant research has been done to investigate molecular signal propagation in both free space (FS) and simple bounded environments, e.g., [2], [3]. These papers have been suitable for establishing tractable limits on communication performance by assuming that molecules propagate in environments without obstacles. However, in many biological (e.g., tissue membrane [4] and chemical engineering (e.g., catalyst bed [5]) environments, the channel consists of porous medium (PM) materials. The PM is a solid with pores (i.e., voids) distributed more or less uniformly throughout the bulk of the body [6]. Many natural and man made substances, e.g., rocks, soils, and ceramics, can also be classified as PM materials [7].

PM channels are fundamentally different from FS channels due to the intricate network of pores. The molecules undergo complex trajectories and experience heterogeneous advection as they propagate through pores of different sizes and lengths, causing so-called mechanical dispersion [8], [9], which is an augmented effective diffusion caused by velocity fluctuations. More importantly, particles may become trapped in immobile or re-circulation zones in the vicinity or the wake of solid grains [9], [10], therefore taking some time to exit, and causing non-trivial anomalous transport phenomena, such as long tails in the arrival time distributions. Hence, it is of fundamental importance to investigate what impact these PM flow and transport properties have on the MC performance.

This work is the first to consider a PM channel in MC. We consider a binary sequence transmitted between a transmitter (TX) and a receiver (RX) located at the ends of the PM channel. The main contributions are summarized as follows:

1) Assuming that the number of molecules arrived can be approximated as a Gaussian random variable (RV), we present closed-form expressions for different performance metrics, i.e., throughput, mutual information, and error probability, for the channel. We also numerically evaluate the diversity gain that is defined (as in [11]) as the exponential decrease rate of the probability of error as the number of released molecules increases.

2) Using numerical results, we investigate the differences in channel characteristics and performance metrics between a PM and diffusive FS channel with flow. In particular, we show that the PM channel response tail is wider than the FS channel and the wider PM channel response significantly affects the communication performance due to larger inter-symbol-interference (ISI).

The rest of this paper is organized as follows. The system model is presented in Section II. The performance metrics are derived in Section III. Numerical results are presented in Section IV. The paper is concluded in Section V.

II. SYSTEM MODEL

We consider an MC system via the PM in a three-dimensional (3D) environment where the TX and the RX are located at the inlet and the outlet of the PM, respectively. A two-dimensional (2D) sketch of the considered system is given in Fig. 1(a) and a 3D sample of a PM is shown in Fig. 1(b). In a PM, pores and grains refer to its void and solid components, respectively. Grain size distribution and porosity (i.e., the ratio of the volume of voids over the total volume) affect the transport behavior in the PM. In the following, we detail the key steps of the considered system.

Modulation and Emission: A sequence of binary symbols is transmitted with Pr(Xn = 1) = P1, where Xn is the nth transmitted symbol. We consider the on-off keying modulation scheme with a fixed symbol slot length T, which is commonly adopted in MC literature, i.e., at the beginning of the nth symbol slot, the TX releases N molecules if Xn = 1; otherwise, no molecule is released. The TX uniformly releases the molecules over the cross section at the inlet of the PM.

Transport through the PM: We consider the PM filled with an incompressible fluid of viscosity µ, moving with a mean velocity \( \vec{v}_m \) oriented from the TX to the RX. Due to the small pore sizes, the flow is laminar (Reynolds number of the flow is negligible) and governed by the Stokes equation

\[
\mu \frac{\nabla^2 \vec{v}(a)}{p(a)} = \nabla p(a) + \frac{\nabla \vec{v}(a)}{\rho(a)} = 0,
\]

where \( \nabla \) is the nabla operator, \( \vec{v} \) is the velocity, and \( p(a) \) is the pressure. The boundary conditions are

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of zero velocity (no-slip) on the surface of the solid grains, and periodic on the external boundaries, with a fixed pressure gradient along the mean flow direction. The resulting velocity field $\vec{v}$ is characterized by a chaotic heterogeneous structure.

The molecular transport in the pores is due to molecular diffusion and the complex heterogeneous advection around solid grains, as shown in Fig. 1(c). The molecular concentration $c(a, t)$ is modeled by an advection-diffusion equation:

$$\frac{\partial c(a, t)}{\partial t} + \vec{v}(a) \nabla c(a, t) - D \nabla^2 c(a, t) = 0, \quad (1)$$

where $D$ is the constant diffusion coefficient, with a constant flux of molecules on the inlet and zero diffusive flux on all other boundaries. Although these equations are linear and relatively easy to solve, the complexity of the geometry makes the discretization and solution particularly cumbersome [8].

The Péclet number (Pe), which combines advective and diffusive transport over the whole PM length $L$, is given by $\text{Pe} = |\vec{v}|L/D$. Thanks to the interplay of these two phenomena, molecules not only are transported along the streamlines but also travel across streamlines, experiencing therefore a wide range of velocities, and possibly reaching stagnant zones in the wake of the solid grains. Molecules that enter these zones can remain there for some time before they escape and return into the mobile portion of the medium.

Reception and Demodulation: We consider a RX that is mounted on the cross section at the outlet of the PM and is able to count the number of molecules that arrive. To decrease the complexity, we consider a fixed threshold-based demodulation rule at the RX: $Y_n = 1$ if $N_n^\text{ob} \geq \xi$; otherwise, $Y_n = 0$, where $Y_n$ is the $n$th received symbol, $N_n^\text{ob}$ is the number of molecules that arrive during the $n$th slot, and $\xi$ is a fixed threshold.

III. PERFORMANCE METRICS

In this section, we present the analytical results of system performance metrics. To this end, we first analyze the (cumulative) breakthrough curve, i.e., the cumulative density function (CDF) of the first arrival time at the outlet of any molecule released from the inlet, which is used for characterizing molecular transport in the PM. This is given by [10]

$$F(t) = \frac{\int \! \! \int \mathbb{1}(a_1 = L, a_2, a_3, t) |\vec{v}(a_1 = L, a_2, a_3)| \, da_2 \, da_3}{\int \! \! \int |\vec{v}(a_1 = L, a_2, a_3)| \, da_2 \, da_3} \quad (2)$$

where $a = \{a_1, a_2, a_3\}$ denotes location in Cartesian coordinates. The analytical expression for $F(t)$ is mathematically intractable, so we will rely on a numerical solution obtained by the full discretization of (1) and (2). For more details about numerical solvers, we refer the readers to [8].

Remark 1: Assuming that the number of molecules arrived can be approximated as a Gaussian RV, we derive the mutual information $I$, throughput $C$, and error probability $Q$. Using particle-based simulation methods, [13], [14] have verified the accuracy of Gaussian approximation. According to the central limit theorem, the accuracy of this approximation improves as $N$ increases. Due to the space limitation, we present the derivation of statistical distributions of molecules arrived and system performance metrics in Appendix A.

We next discuss the diversity gain. Each molecule behaves independently and experiences different propagation paths. Thus, the channel can be seen as a multiple-input and multiple-output channel and the RX achieves diversity when $N$ molecules are released. Also, there is an optimal $\xi$ that minimizes error probability $Q$, i.e., $Q^* = \min_{\xi} Q$. Since an explicit expression for $\alpha$ is mathematically intractable, we use a data-fitting method to obtain $\alpha$. The method will be detailed in Sec. IV. We note that a similar definition of $\alpha$ was studied in [11] for timing channels, but our method for evaluating $\alpha$ is different from [11].

For $P_1 = \frac{1}{2}$, we have the following corollaries on $Q$ and $I$:

Corollary 1: The optimal error probability converges to zero when the released number of molecules for symbol “1” tends to infinity, i.e., $\lim_{N \to \infty} Q^* = 0$.

Corollary 2: The mutual information is bounded by $I \leq 1$ bits/slot and $I = 1$ bits/slot is obtained if and only if $Q \to 0$.

Proof: The proofs of Corollaries 1 and 2 are given in Appendices B and C, respectively.

IV. NUMERICAL RESULTS

In this section, we present numerical results to investigate the channel response and communication performance of MC
TABLE I
ENVIRONMENTAL PARAMETERS

| Parameter              | Symbol | Value          |
|------------------------|--------|----------------|
| Length of PM           | $L$    | 2 mm           |
| Number of grains       | $\phi$ | $2 \times 10^4$ |
| Average grain diameter | $d$    | 0.277 mm       |
| Characteristic pore length (estimated) | $\ell_0$ | 0.277 mm |
| Mean velocity          | $|\bar{v}_m|$ | $5.73 \times 10^{-6}$ m/s |

Fig. 2. The CDF and PDF $f(t)$ of the arrival time of the molecule versus time $t$ in the PM channel for different Pe.

via the PM. We consider the 3D sand-like PM described in [8]. The medium was generated according to the characteristics of standard sand samples. Specifically, the PM is a cube of size $L = 2$ mm with a porosity of 35%. The grain size distribution follows a Weibull distribution with Weibull parameter $k = 7$. We also consider $n = 10$ symbols are transmitted with $P_1 = \frac{1}{2}$. The other parameters are given in Table I. With these parameters, numerically solving (1) and (2), obtaining the values of $F(t)$ for $P_e = 3, 30, 300, 1000$. The results in the following figures are obtained based on this simulation data.

In order to provide more insights, we compare with a one-dimensional (1D) diffusive FS channel with a flow oriented from the TX to the RX, which is referred to as the “FS channel” in the following for brevity. This is because the PM channel is effectively a 1D channel due to the TX and RX covering the entire inlet and outlet. The probability density function (PDF) of the first arrival time at $a_1 = L$ in the FS channel is given by

$$f(t) = \frac{L}{\sqrt{4\pi D t}} \exp\left(-\frac{(|\bar{v}_m| t-L)^2}{4Dt}\right)$$

For this FS channel, we consider the same parameter values as those for the PM channel for the fairness of our comparison.

A. Channel Response

In Fig. 3 we show the arrival time distribution in the PM channel. The PDF curves are obtained by numerically evaluating the derivative of $F(t)$. Firstly, for all $P_e$, $F(t) \rightarrow 1$ as $t \rightarrow \infty$, which means that all molecules released will eventually arrive at the RX. This is because no flow is going out of the lateral directions and no molecule can escape from the lateral directions by advection nor by diffusion. Secondly, when $P_e$ is smaller, the CDF converges more quickly to 1, meaning that less molecules stay trapped in the PM.

In Fig. 3 we compare the arrival time PDF in the PM channel with that in the FS channel. Interestingly, when $P_e$ is 3, the PDF curve for the PM is similar to that for FS. This is because the fact that molecular diffusion is fairly large, causing particles to uniformly sample the velocity space, and resulting in an overall transport that can be conveniently described as a single advection-diffusion channel. Secondly, PM channel behavior is much less sensitive to $P_e$ than in the FS channel. This is due to molecules entering dead-end pores or stagnant regions, and taking a long time to escape in the PM. For FS, when $P_e$ is larger, since there are no such regions, the only effect is a more dominant advection than the diffusion, thus FS channel behavior is more sensitive to larger $P_e$. Importantly, as $P_e$ increases (e.g., larger molecules with smaller diffusion coefficient), the peak value of the PDF curve for the FS channel increases, while that for the PM model decreases, i.e., the PDF curve for the FS channel becomes narrower but the PDF curve for the PM becomes wider. This is because for the PM, the particles travel in all directions through the complex network of pores, thus generating a much larger longitudinal dispersivity, i.e., a higher equivalent diffusion in the longitudinal direction, proportional to $P_e$ [8]. This means that, as $P_e$ increases, the ISI of the PM channel increases but ISI of the FS channel decreases. Based on this, for the PM channel we expect the error performance and mutual information would become worse when $P_e$ increases, which will be verified by the observations in Fig. 4.

B. Performance Evaluation

In Fig. 4 we show the average mutual information $I$ and the average error probability $Q$ of the MC system via the PM versus the threshold $\xi$ for different $P_e$: $P_e = 3, 30, 300, 1000$. $N = 100$ and $T = 1000$ s.
TABLE II

| Diversity Gain | Pe = 3 | Pe = 30 | Pe = 300 | Pe = 1000 |
|----------------|--------|--------|---------|-----------|
| T = 300 s      | PM     | 0.0009 | 0.0014  | 0.0001    | 0.0001    |
| FS             | 0.0014 | 0.0049 | 0.0010  | 0.0007    |
| T = 350 s      | FS     | 0.0093 | 0.0034  | 0.0053    | 0.0097    |
| PM             | 0.0189 | 0.0112 | 0.0147  | 0.0186    |
| T = 400 s      | FS     | 0.0851 | 0.2573  | 0.3423    | 0.3422    |
| PM             | 0.0823 | 0.0654 | 0.0570  | 0.0585    |

which numerically validates Corollary 2. Secondly, the average mutual information is smaller and the error probability is higher as Pe increases. This is because when Pe is higher, the tail of the channel response of the PM is longer, i.e., larger ISI, as we observed in Figs. 2 and 3.

In Fig. 5 we show the throughput of the PM and FS channels. Firstly, for both channels and all Pe, C increases as T increases and C = 1 bits/slot is achieved when T ≥ 400 s. This is because of a very small probability that a molecule arrives at t ≥ 400 s, as observed in Fig. 3. Secondly, the difference of C between the PM and FS channels when T ≤ 300 s becomes larger as Pe increases. This is because in Fig. 5 when Pe increases, the PM and FS channels diverge.

In Fig. 6 we plot the optimal average error probability versus the number of molecules released for bit “1” for different symbol slots. The considered symbol slots are around the detection time that maximizes the PM and FS channel responses based on Fig. 3. Firstly, Q* decreases when N increases. We then see that error probability curves can be well approximated by the fitted curves, Q* ≈ exp(−αN + β), where α and β are obtained by solving Q*|N=10 = exp(−α10 + β) and Q*|N=100 = exp(−α100 + β). Thus, we can use the diversity gain α to quantify the decrease rate of Q* as N increases. We present α for different T and Pe in Table II. We find that the PM achieves higher α than the FS channel for any Pe with T = 300 s, 350 s and Pe = 3 with T = 400 s. This is because the decrease rate of Q* is affected by ISI. The PM has less ISI than the FS channel for these parameter values, based on the tails of the PDF curves of arrival time shown in Fig. 3.

V. CONCLUSION

We for the first time considered MC via a realistic PM channel, modeled as a 3D complex pore structure. Using Gaussian approximations for the number of molecules arrived, we analyzed the throughput, mutual information, error probability, and diversity gain of the considered system. Using fully resolved computational fluid dynamics results for the arrival time distribution, we explored the differences in channel characteristics between PM and FS channels and their impact on communication performances in both channels. Our results suggest that the reliability of a PM channel can be improved by decreasing Pe, while that of a FS channel can be improved by increasing Pe. In our future work, we could derive an analytical expression for the arrival time distribution of a simplified, yet realistic, PM channel.

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SUPPLEMENTARY INFORMATION

APPENDIX A
DERIVATION OF PERFORMANCE METRICS

Due to the transport delay experienced by the molecules that arrive at the RX, the RX may receive the molecules released from the current and all previous symbol slots. Based on (2), we obtain the probability that the molecule being released in the \(k\)th symbol slot arrives during the \(n\)th symbol slot, i.e., \(F((n - k + 1)T) - F((n - k)T)\). We denote \(N_{n,k}^{\text{rob}}\) as the number of molecules that arrive during the \(n\)th slot that were released at the beginning of the \(k\)th symbol slot. We then have \(N_{n,k}^{\text{rob}} = \sum_{k=1}^{n} X_{n,k}^{\text{rob}} = \sum_{k=1}^{n-1} N_{n,k}^{\text{rob}} + N_{n,n}^{\text{rob}}\), where \(\sum_{k=1}^{n-1} N_{n,k}^{\text{rob}}\) is the ISI and \(N_{n,n}^{\text{rob}}\) is from the intended molecular signal. Since the molecules released in a given slot are transported independently and have the same probability to arrive during the \(n\)th slot, \(N_{n,k}^{\text{rob}}\) follows a binomial distribution, i.e.,

\[
N_{n,k}^{\text{rob}} \sim X_k B(N, F((n - k + 1)T) - F((n - k)T)).
\]

We note that modeling \(N_{n,k}^{\text{rob}}\) with the binomial distribution makes the analysis of \(N_{n,k}^{\text{rob}}\) cumbersome, since a sum of Binomial random variables (RVs) is not in general a Binomial RV. Fortunately, \(N_{n,k}^{\text{rob}}\) can be accurately approximated by a Poisson distribution, i.e.,

\[
N_{n,k}^{\text{rob}} \sim X_k P(N(F((n - k + 1)T) - F((n - k)T))).
\]

The sum of Poisson RVs is also a Poisson RV whose mean is the sum of the means of the individual Poisson RVs. As such, we have

\[
N_{n,k}^{\text{rob}} \sim P \left( N \sum_{k=1}^{n} X_k (F((n - k + 1)T) - F((n - k)T)) \right).
\]

In the following, we aim to derive \(\Pr(N_{n}^{\text{rob}} < \xi)\), but the evaluation of the CDF of the Poisson RV \(N_{n}^{\text{rob}}\) has high computational complexity when \(\xi\) is large. To facilitate the evaluation, we further approximate \(N_{n}^{\text{rob}}\) as a Gaussian RV as follows:

\[
N_{n}^{\text{rob}} \sim N(\gamma, \gamma),
\]

where \(\gamma = N \sum_{k=1}^{n} X_k (F((n - k + 1)T) - F((n - k)T))\). We define \(X_{1:n} = \{X_1, X_2, \ldots, X_n\}\) as the subsequence of the symbols transmitted by the TX. Based on (6), we obtain the conditional CDF of the Gaussian RV \(N_{n}^{\text{rob}}\) for the given \(X_{1:n}\) as

\[
\Pr(N_{n}^{\text{rob}} < \xi) = \frac{1}{2} \left( 1 + \text{erf} \left( \frac{\xi - 0.5 - \gamma}{\sqrt{2}\gamma} \right) \right),
\]

where 0.5 is a continuity correction. Using (7), we obtain the following conditional probabilities for the given \(X_{1:n-1}\) as

\[
\Pr(Y_n = 0|X_n = 0) = \Pr(N_{n}^{\text{rob}} < \xi|X_n = 0),
\]

\[
\Pr(Y_n = 1|X_n = 0) = 1 - \Pr(N_{n}^{\text{rob}} < \xi|X_n = 0),
\]

\[
\Pr(Y_n = 0|X_n = 1) = \Pr(N_{n}^{\text{rob}} < \xi|X_n = 1),
\]

and

\[
\Pr(Y_n = 1|X_n = 1) = 1 - \Pr(N_{n}^{\text{rob}} < \xi|X_n = 1).
\]

Using (8)-(11), we now derive the mutual information between channel input and output, the channel throughput, the error probability, and the diversity gain of the system for the fixed threshold detector.

Mutual Information: We derive the conditional mutual information between \(X_n\) and \(Y_n\) for the given \(X_{1:n-1}\) as

\[
H(X_n; Y_n) = H(Y_n) - H(Y_n|X_n) \text{ bits/slot.}
\]

where \(H(\cdot)\) is the entropy. We derive \(H(Y_n)\) as

\[
H(Y_n) = - \Pr(Y_n = 0) \log_2 \Pr(Y_n = 0) - \Pr(Y_n = 1) \log_2 \Pr(Y_n = 1),
\]

where \(\Pr(Y_n = 0)\) and \(\Pr(Y_n = 1)\) are written as

\[
\Pr(Y_n = 0) = (1 - P_1) \Pr(Y_n = 0|X_n = 0) + P_1 \Pr(Y_n = 0|X_n = 1)
\]

and

\[
\Pr(Y_n = 1) = (1 - P_1) \Pr(Y_n = 1|X_n = 0) + P_1 \Pr(Y_n = 1|X_n = 1),
\]

respectively. We derive \(H(Y_n|X_n)\) as

\[
H(Y_n|X_n) = (1 - P_1) H(Y_n|X_n = 0) + P_1 H(Y_n|X_n = 1),
\]

where \(H(Y_n|X_n = 0)\) and \(H(Y_n|X_n = 1)\) are given by

\[
H(Y_n|X_n = 0) = - \Pr(Y_n = 0|X_n = 0) \log_2 \Pr(Y_n = 0|X_n = 0)
- \Pr(Y_n = 1|X_n = 0) \log_2 \Pr(Y_n = 1|X_n = 0),
\]

and

\[
H(Y_n|X_n = 1) = - \Pr(Y_n = 0|X_n = 1) \log_2 \Pr(Y_n = 0|X_n = 1)
- \Pr(Y_n = 1|X_n = 1) \log_2 \Pr(Y_n = 1|X_n = 1),
\]

respectively. We finally derive the average mutual information over all realizations of \(X_{1:n-1}\) and all symbol slots from 1 to \(n\) as

\[
I = \frac{1}{n} \sum_{k=1}^{n} \sum_{k=1}^{n} \frac{X_{k} (X_{k-1} + \Psi_k)}{2^{k-1}} \text{ bits/slot},
\]

where \(\Psi_k\) is a set that includes all realizations of \(X_{1:k-1}\).

Throughput: We derive the throughput, i.e., the maximal average mutual information, as

\[
C = \max_{\xi} \frac{1}{n} \sum_{k=1}^{n} \sum_{k=1}^{n} \frac{X_{k} (X_{k-1} + \Psi_k)}{2^{k-1}} \text{ bits/slot}.
\]
Error Probability: We derive the symbol error probability in the \(n\)th slot for the given \(X_{1:n-1}\) as

\[
Q[n|X_{1:n-1}] = (1 - P_1)\Pr(Y_n = 1|X_n = 0, X_{1:n-1}) + P_1\Pr(Y_n = 0|X_n = 1, X_{1:n-1}). \tag{21}
\]

We derive the average symbol error probability over all realizations of \(X_{1:n-1}\) and all symbol slots from 1 to \(n\) as

\[
Q = \frac{1}{n} \sum_{k=1}^{n} \sum_{X_{1:k-1} \in \Psi_k} Q[n|X_{1:n-1}] 2^{k-1}. \tag{22}
\]

APPENDIX B

PROOF OF COROLLARY \([1]\)

Since \(Q\) is the sum of \(Q[n|X_{1:n-1}]\) based on (22), we need to prove that \(Q^*[n|X_{1:n-1}]\) where \(Q^*[n|X_{1:n-1}] = \min_{\xi} Q[n|X_{1:n-1}]\). Assuming \(P_1 = \frac{1}{2}\), we first rewrite (21) as

\[
Q[n|X_{1:n-1}] = \frac{1}{2} + \frac{1}{4} \left[ \text{erf} \left( \frac{\xi - 0.5 - (N(Y_1 + Y_2))}{\sqrt{2N(Y_1 + Y_2)}} \right) - \text{erf} \left( \frac{\xi - 0.5 - NY_2}{\sqrt{2NY_2}} \right) \right], \tag{23}
\]

where \(Y_1 = (F(T) - F(0))\) and \(Y_2 = \sum_{k=1}^{n-1} X_k(F((n-k+1)T) - F((n-k)T)).\) We then obtain the optimal \(\xi\) that minimizes \(Q[n|X_{1:n-1}]\). To this end, we take the first derivative of (23) with respect to \(\xi\) and solve the resultant equation to derive the optimal \(\xi\) that minimizes \(Q[n|X_{1:n-1}]\) as

\[
\xi^*[n|X_{1:n-1}] = \frac{NY_1}{\ln((Y_1 + Y_2)/Y_2)}. \tag{24}
\]

Substituting (24) into (23), we write the optimal error probability \(Q^*[n|X_{1:n-1}]\) as

\[
Q^*[n|X_{1:n-1}] = \frac{1}{2} + \frac{1}{4} \left[ \text{erf} \left( \frac{\sqrt{NA}}{\sqrt{2(Y_1 + Y_2)}} \right) - \text{erf} \left( \frac{\sqrt{NB}}{\sqrt{2Y_2}} \right) \right], \tag{25}
\]

where

\[
A = \left( \frac{Y_1}{\ln((Y_1 + Y_2)/Y_2)} - (Y_1 + Y_2) \right) \tag{26}
\]

and

\[
B = \left( \frac{Y_1}{\ln((Y_1 + Y_2)/Y_2)} - Y_2 \right). \tag{27}
\]

If we can prove \(A < 0\) and \(B > 0\), then we have

\[
\lim_{N \to \infty} Q^*[n|X_{1:n-1}] = \frac{1}{2} + \frac{1}{4} [\text{erf}(-\infty) - \text{erf}(\infty)] = 0. \tag{28}
\]

We now prove \(A < 0\) and \(B > 0\). Since \(Y_1 > 0\) and \(Y_2 > 0\), it is reasonably to assume \(Y_1 = xY_2, x > 0\). Using \(Y_1 = xY_2\), we simplify the conditions \(A < 0\) and \(B > 0\) to \(x/(1+x) - \ln(1+x) < 0\) and \(x - \ln(1+x) > 0\), respectively. We find that \(g(x) = x/(1+x) - \ln(1+x)\) is a decreasing function and \(f(x) = x - \ln(1+x)\) is an increasing function with respect to \(x\) since \(g'(x) = -x/(1+x)^2 < 0\) and \(f'(x) = 1-1/(1+x) > 0\) if \(x > 0\). By inspection, we also find \(g(x) = 0\) and \(f(x) = 0\) at \(x = 0\). Thus, we have \(g(x) < 0\) and \(f(x) > 0\) for \(x > 0\), which means \(A < 0\) and \(B > 0\). Thus, we verify that \(Q^*[n|X_{1:n-1}] \to 0\) when \(N \to \infty\), which completes the proof.

APPENDIX C

PROOF OF COROLLARY \([2]\)

We first prove \(I(X_n; Y_n) \leq 1\) bits/slot. As per the Shannon entropy of probability distributions for single parties, we have \(I(X_n; Y_n) \leq \min\{H(X_n), H(Y_n)\}\). Based on definition of entropy, the maximal \(H(X_n)\) and \(H(Y_n)\) is 1 bits/slot when \(\Pr(X_1 = 0) = P_1 = \frac{1}{2}\) and \(\Pr(Y_1 = 0) = \frac{1}{2}\). Thus, the mutual information is bounded by \(I(X_n; Y_n) \leq 1\) bits/slot.

We then prove that \(Q \to 0\) is a sufficient condition for \(I(X_n; Y_n) = 1\) bits/slot. Based on (21), \(Q[n|X_{1:n-1}] \to 0\) means \(\Pr(Y_n = 1|X_n = 0) \to 0\) and \(\Pr(Y_n = 0|X_n = 1) \to 0\). Applying these two expressions to \(\text{(13)}\) and \(\text{(16)}\), we obtain \(I(X_n;Y_n) = 1\) bits/slot, which proves \(Q \to 0\) is a sufficient condition. We finally prove that \(Q \to 0\) is a necessary condition for \(I(X_n; Y_n) = 1\) bits/slot. Since \(H(Y_n) \leq 1\) and \(H(Y_n|X_n) \geq 0\), thus \(I(X_n; Y_n) = 1\) bits/slot is achieved only when \(H(Y_n) = 1\) and \(H(Y_n|X_n) = 0\). \(H(Y_n|X_n) = 0\) means \(H(Y_n|X_n = 0) = 0\) and \(H(Y_n|X_n = 1) = 0\) based on (16). There are four cases leading to \(H(Y_n|X_n = 0) = 0\) and \(H(Y_n|X_n = 1) = 0\) including:

1. \(\Pr(Y_n = 0|X_n = 1) = 0\) and \(\Pr(Y_n = 1|X_n = 0) = 0\);  
2. \(\Pr(Y_n = 0|X_n = 1) = 0\) and \(\Pr(Y_n = 1|X_n = 0) = 0\);  
3. \(\Pr(Y_n = 0|X_n = 1) = 0\) and \(\Pr(Y_n = 1|X_n = 0) = 0\);  
4. \(\Pr(Y_n = 0|X_n = 1) = 0\) and \(\Pr(Y_n = 1|X_n = 0) = 0\).

Since case 4) does not satisfy \(\Pr(Y_n = 0|X_n = 1) + \Pr(Y_n = 1|X_n = 0) \leq 1\), case 4) is not valid. Moreover, cases 2) and 3) result in \(\Pr(Y_n = 0) = 1\) and \(\Pr(Y_n = 1) = 1\), respectively, which leads to \(H(Y_n) = 0\). Thus, they are not valid either. We note that only case 1) satisfies both \(H(Y_n) = 1\) and \(H(Y_n|X_n = 0)\) and case 1) leads to \(Q \to 0\). Thus, \(Q \to 0\) is a necessary condition. Therefore, we prove \(Q \to 0\) is a sufficient and necessary condition for \(I(X_n; Y_n) = 1\) bits/slot.