Capacity of a Diffusion-Based Molecular Communication System With Channel Memory and Molecular Noise

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***Abstract*—Molecular Communication (MC) is a communication paradigm based on the exchange of molecules. The implicit biocompatibility and nanoscale feasibility of MC make it a promising communication technology for nanonetworks. This paper provides a closed-form expression for the information capacity of an MC system based on the free diffusion of molecules, which is of primary importance to understand the performance of the MC paradigm. Unlike previous contributions, the provided capacity expression is independent from any coding scheme and takes into account the two main effects of the diffusion channel: the memory and the molecular noise. For this, the diffusion is decomposed into two processes, namely, the Fick's diffusion and the particle location displacement, which are analyzed as a cascade of two separate systems. The Fick's diffusion captures solely the channel memory, while the particle location displacement isolates the molecular noise. The MC capacity expression is obtained by combining the two systems as function of the diffusion coefficient, the temperature, the transmitter–receiver distance, the bandwidth of the transmitted signal, and the average transmitted power. Numerical results show that a few kilobits per second can be reached within a distance range of tenth of micrometer and for an average transmitted power around 1 pW.**

***Index Terms*—Channel memory, information capacity, molecular communication (MC), molecular noise, molecule diffusion, nanonetworks.**

I. Introduction

MOLECULAR communication (MC) is a promising paradigm for communication in nanonetworks [1], where the applicability of classical communication technologies is limited by several constraints. In particular, the very restricted size of the nanodevices and the peculiarities of the environments in which they are envisioned to operate (e.g., biological scenarios) demand for novel solutions from the perspective of both the choice of the communication medium and the study of suitable communication techniques. While a possible solution to the problem of communication in nanonetworks is suggested by recent studies [2] on nanostructures and on the properties of carbon nanoelectronics, a bioinspired approach suggests MC [3] as a new paradigm.

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MC is based on the exchange of molecules, through which information is transmitted, propagated, and received. This approach is studied in biology since it is successfully adopted by cells for intra- and intercellular communication [28], where message-carrying molecules are synthesized, emitted, collected, and converted to cellular responses through biochemical processes. Given the tight integration of MC within the biological environment and its feasibility at the cellular scale (nm), we study MC not only as a candidate for nanonetwork communication, but also as a possible tool for the future nanonetworks to interact with the living organisms and their biological processes. Disease control and infectious agent detection [38], smart drug delivery systems [18], bacterial biofilm monitoring and control [12], and automated surveillance systems against biological and chemical attacks [39] are among the potential practical applications of MC-enabled nanonetworks.

MC relies on mass transport phenomena for the propagation of information between a sender and a receiver, since information-bearing molecules have to physically cover the distance from one location to the other. Amongst others, molecular motors [26], bacteria chemotaxis, pheromone diffusion [11], [30], and ion (e.g., calcium) diffusion [27] have been taken into account as mass transport phenomena options for MC. Among those, the free molecule diffusion in a fluid is the most basic and widespread mass transport phenomenon, where molecules, due to the Brownian motion, are subject to a random walk which tends to spread their concentration throughout the available space. In this paper, we focus on MC systems based on the free molecule diffusion (diffusion-based MC systems). This allows the maximum possible generality for the obtained results, which will be tailored in the future to address special cases where the transport phenomena, such as turbulent diffusion [35] for the pheromones or electro-diffusion [36] for the ions, stem from the free molecule diffusion.

The theoretical analysis and the modeling of the information capacity in MC are of primary importance to understand the performance of an MC system from an information theoretical perspective. Up to date, some contributions from the literature have attempted to study the information capacity in diffusion-based MC systems, but often these are focused on specific modulation and coding schemes or do not take into account the two main effects of the molecule diffusion channel, namely, the memory and the molecular noise. The work in [4] addresses for the first time the capacity of MC systems by emphasizing the need for its mathematical analysis, but no concrete solutions are proposed. In [6] and [7], the MC capacity is computed for

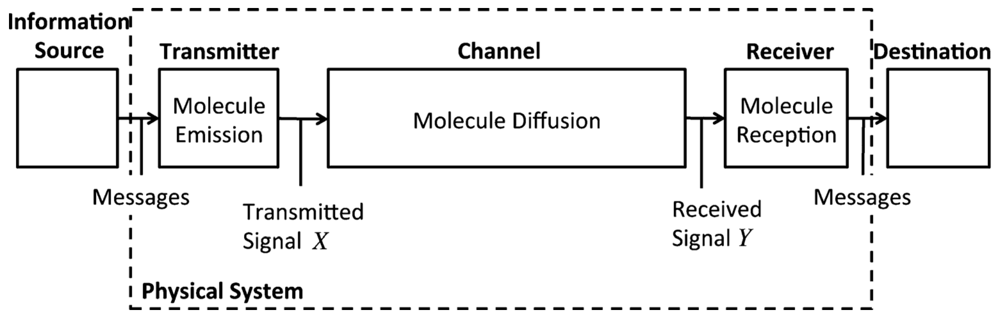

Fig. 1. Information-theoretic diagram of a diffusion-based MC system.

a specific binary coding scheme and by taking into account the molecular receiver model, but without modeling the molecule diffusion propagation. An analysis of the molecular achievable rate is conducted in [8] by assuming a single instantaneous emission of molecules from the transmitter, a deterministic diffusion channel, and a detailed chemical model of the receiver, but the effects of an emission of molecules over time is not considered. In [16], the capacity of an MC system in case of binary coding is properly analyzed on the basis of the effects of the channel memory, but without accounting for molecular noise sources. Two different coding techniques are analyzed in [22] in terms of achievable rates, while the diffusion channel models are reduced to a binary or a quadruple channel. Similarly, discrete memoryless approximations are applied to the molecule diffusion channel in [5], where the MC capacity is computed for a binary coding scheme.

The objective of this paper is to provide a closed-form mathematical expression for the information capacity of a MC system based on free molecule diffusion. In [33], we used solutions from statistical mechanics and equilibrium thermodynamics to derive an MC capacity expression, but by taking a system in equilibrium as a model, we did not account for the dynamic effects of diffusion, in particular the channel memory. Differently, and unlike previous contributions, we provide here a capacity expression that takes into account the two main effects of the diffusion channel, namely, the memory and the molecular noise. For this, we decompose the molecule diffusion into two main processes: 1) the Fick's diffusion, which captures solely the effects of the channel memory; and 2) the particle location displacement, which isolates the molecular noise. The properties of these two processes allow to analyze them as a cascade of two separate communication systems. We compute the information capacity by assuming that the transmitter can modulate the emission of molecules in the space according to any possible time continuous input message, differently from previous contributions where the transmitter is assumed to modulate (e.g., binary coding) impulses according to discrete input messages (e.g., binary digital messages). As a consequence, our information capacity is proposed as the theoretical upper bound of the performance of an MC system, independent from any specific coding scheme.

The final expression for the MC capacity is a function of the medium diffusion coefficient, the system temperature, the distance between the transmitter and the receiver, and the bandwidth of the transmitted signal. The MC capacity is also expressed as a function of the average transmitted power, which corresponds to the thermodynamic power spent at the transmitter for molecule emission. We provide numerical results to evaluate the obtained closed-form formula for the MC capacity in relation to several different values of its parameters.

The remainder of this paper is organized as follows. In Section II, the schematic diagram of a diffusion-based MC system is detailed and its components are modeled in relation to the physical system, which defines the underlying physical laws and parameters at the basis of the molecule diffusion propagation. The capacity of the diffusion-based MC system is treated in Section III. The decomposition of the molecule diffusion into two processes is detailed in Section III-A, while the analyses of the Fick's diffusion system and the particle location displacement system are performed in Sections III-B and III-C, respectively. In Section III-D, we obtain the closed-form expression of the MC capacity. Numerical results are provided in Section IV. Finally, in Section V, we conclude this paper.

II. Information Theoretical Scheme of a Diffusion-Based MC System

The schematic diagram of a diffusion-based MC system is shown in Fig. 1, and it is composed by the classical [13] cascade of information source, transmitter, channel, receiver, and destination. The *information source* produces *messages* to be communicated to the destination. The type of message depends on the particular application in which the diffusion-based MC system is deployed. In case of intelligent drug delivery applications [19], the message can be a time sequence of ON/OFF values that trigger/stop the release of the drug molecules. In nanomachine communication [4], the message can be any function of the time carrying data such as nanomachine states [1] or sensory measurements [2]. The *Transmitter*, the *Channel* and the *Receiver*, which are based on the molecule emission, molecule diffusion and molecule reception, respectively, are within a *Physical System*, whose underlying laws and parameters affect how these components are physically realized. The *Destination* is the recipient of the *messages* coming from the receiver. Upon reception of a message, the destination reacts according to the meaning and to the particular application.

The *Physical System* considered in this paper is sketched in Fig. 2 and it is based on the following considerations.

1) The diffusion-based MC channel is in a three-dimensional space indexed by the three axes X, Y, Z and it has infinite extent in all three dimensions. This space is filled with a

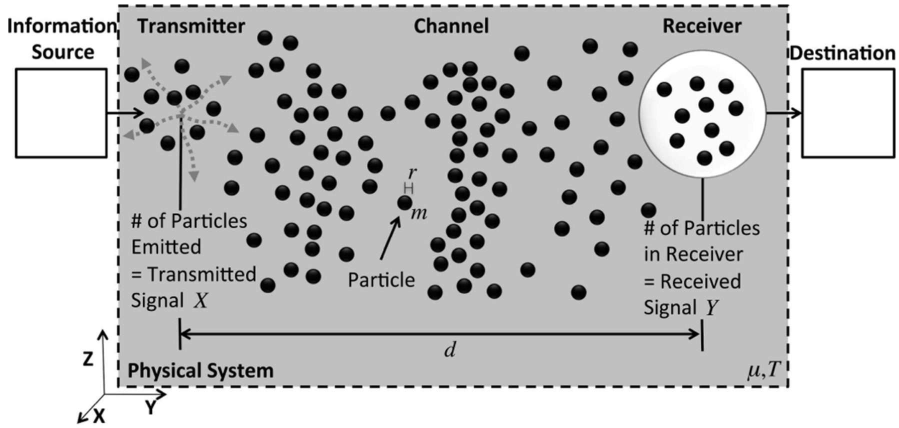

Fig. 2. Sketch of the physical realization of the diffusion-based MC system.

fluidic medium having viscosity μ. The fluidic medium does not have flow currents or turbulence; therefore, the propagation of the molecules between the transmitter and the receiver is solely realized by the Brownian motion.

2) All the molecules in the system, which are emitted by the transmitter, are indistinguishable and equivalent to spherical *particles* of radius r and mass m, where $r \ll d$, d being the distance between the transmitter and the receiver in the diffusion-based MC system. As a consequence, from now on we will refer to particles when talking about molecules in the physical system.
3) The transmitter is considered point-wise (size equal to zero) and at location $\mathbf{T} = (T_X, T_Y, T_Z)$ in the 3-D space.
4) Once emitted from the transmitter, every particle moves independently from the others and according to its Brownian motion in the fluidic medium. The Brownian motion of a molecule is referred to as the random motion of the particles suspended in a fluid and its formulation according to the Langevin equation [23] states that the location $p_i^n(t)$ of the particle n at time t along any i of the 3-D axes X, Y, Z obeys the following stochastic differential equation:
$$m\frac{\partial^2 p_i^n(t)}{\partial t^2} = -6\pi\mu r\frac{\partial p_i^n(t)}{\partial t} + f_i(t), \quad i \in \{X, Y, Z\} \quad (1)$$
where m is the particle mass, $\partial^2(\cdot)/\partial t^2$ and $\partial(\cdot)/\partial t$ are the second and first time derivative operators, respectively, μ is the viscosity of the fluid, r the radius of the particle, and $f_i(t)$ is a random process whose probability density function is Gaussian and has correlation function $< f_i(t)f_j(t') >$ given by
$$< f_i(t)f_j(t') >= 12\pi\mu r k_B T \delta_{i,j}\delta(t-t'), \quad i,j \in \{X, Y, Z\} \quad (2)$$
where $< \cdot >$ is the average operator, k_B is the Boltzmann constant, T is the absolute temperature of the fluid, considered homogeneous throughout the space, and $\delta_{i,j}$ is equal to 1 if $i = j$ and zero otherwise; $\delta(t-t')$ is the Dirac delta function.
5) The receiver detects a signal which is proportional to the concentration of the incoming particles. The receiver location is at a distance d from the transmitter.

In the following, the components included in the physical system are described in light of the aforementioned considerations.

The *Transmitter* processes the messages from the information source and produces a signal suitable for the transmission over the channel. The *transmitted signal*, denoted by X,[1] is here defined as the number of particles $n_T(t)$ emitted into the space as a function of the time t:
$$X := n_T(t),\ t > 0 \quad (3)$$
At the time t of emission of a particle, denoted by $\bar{n}$, its location $\mathbf{p}^{\bar{n}}(t) = (p_X^{\bar{n}}(t), p_Y^{\bar{n}}(t), p_Z^{\bar{n}}(t))$ corresponds to the location of the transmitter $\mathbf{T} = (T_X, T_Y, T_Z)$:
$$\mathbf{p}^{\bar{n}}(t) = \mathbf{T},\ \bar{n} = \int_0^t n_T(\tau)d\tau,\ t > 0 \quad (4)$$
where $\mathbf{T}$ is the vector of the 3-D coordinates (T_X, T_Y, T_Z) of the transmitter. $\bar{n}$ is here an index assigned to each particle on the basis of the order in which they are emitted. This index serves only for the mathematical formulation of their propagation through the Langevin equation in (1), while, as mentioned above, particles are identical and indistinguishable in the physical system.

The *Channel* propagates the signal from the transmitter to the receiver by means of molecule diffusion, which is the result of the collective translation by Brownian motion of many particles from an area in which they are more dense to an area of lower density. This results in the propagation of the particles emitted by the transmitter throughout the 3-D space. This propagation can be expressed as the translation of the 3-D coordinates from the location $\mathbf{T}$ of the transmitter to a location $\mathbf{p}^n(t)$ at time t computed by applying (1) to each particle n from the set $\mathcal{N}_T(t)$:
$$\mathbf{T} \rightarrow \mathbf{p}^n(t), \quad \forall n \in \mathcal{N}_T(t) \quad (5)$$

[1]For the information capacity analysis of this communication system, the transmitted signal X is considered as a band-limited random process whose value at every time instant t is a realization of the random variable $n_T(t)$. As a consequence, the entropy of X is found by decomposing X into a band-limited ensemble of functions, as detailed in Section III-B.

where $\mathcal{N}_T(t)$ is the set containing all the indexes of the particles emitted by the transmitter from time 0 to time t:

$$\mathcal{N}_T(t) = \left\{ \int_0^{t'} n_T(\tau)d\tau \middle| 0 < t' < t \right\}. \quad (6)$$

The *Receiver* reconstructs the messages (sent by the transmitter) from the received signal Y, which is proportional to the concentration of incoming particles. In this paper, we assume an ideal receiver where the received signal Y is defined as the time-varying number of particles that are present inside a spherical volume V_R centered at the receiver location and with radius $R_{V_R} \ll d$, where d is the distance between the transmitter and the receiver. This choice makes the results of this paper independent from any specific techniques for the reception (e.g., chemical ligand-binding reception [34]). As a consequence, the received signal Y is expressed as the number of particles emitted by the transmitter from time instant 0 to time instant t whose location $\mathbf{p}^n(t)$ is inside the volume V_R:

$$Y := \#\left\{n \in \mathcal{N}_T(t) : \mathbf{p}^n(t) \in V_R\right\}, \quad t > 0 \quad (7)$$

where $\#\{\cdot\}$ stands for the cardinality (number of elements) of the set enclosed in the brackets.

III. Information Capacity of a Diffusion-Based MC System

The *capacity* C of a communication system in bits per second is defined as the maximum rate of transmission between the information source and the destination, where this maximum is with respect to all possible signals produced by the transmitter [37]. This is expressed by the general formula from Shannon [13], which defines the capacity as the maximum mutual information $I(X;Y)$ between the transmitted signal X and the received signal Y with respect to the probability density function $f_X(x)$ in all the possible values of the transmitted signal:

$$C = \max_{f_X(x)} \left\{I(X;Y)\right\}. \quad (8)$$

The *mutual information* $I(X;Y)$ in bits per second is defined as

$$\begin{aligned} I(X;Y) &= H(X) - H(X|Y) = H(Y) - H(Y|X) \\ &= H(X) + H(Y) - H(X,Y) \end{aligned} \quad (9)$$

where $H(X)$ is the entropy per second of the transmitted signal X, defined in Section III-B, $H(X|Y)$ is the entropy per second of the transmitted signal X given the received signal Y, $H(Y|X)$ is the entropy per second of the received signal Y given the transmitted signal X, and $H(X,Y)$ is the joint entropy per second of the transmitted signal X and the received signal Y.

In the following, we analytically compute the mutual information of an MC system, as expressed by (8), by considering the transmitter, the channel, and the receiver, defined through (3), (5), and (7), when evaluating (9). From the physical system defined in Section II, two phenomena play an important role in the quantification of the mutual information, namely, the channel memory and the molecular noise, as we highlight in Section III-A. For this, we propose to divide the computation of the mutual information into two processes, namely, the Fick's diffusion, treated in Section III-B, which captures solely the effects of the channel memory, and the particle location displacement, treated in Section III-C, which isolates the effects of the molecular noise.

A. Molecule Diffusion as Fick's Diffusion and Particle Location Displacement

The Langevin equation in (1) is the most general expression of the molecule diffusion due to the Brownian motion. In an MC system, it impacts on the communication performance (mutual information and capacity) through the following two phenomena.

1) *Channel memory*: It is the effect of the persistent presence in the 3-D space of the particles from the moment they are emitted by the transmitter until infinite time. This is a consequence of the fact that in the physical system considered in this paper each emitted particle is subject to the Brownian motion. For this, each particle wanders randomly in the 3-D space without being destroyed. This is expressed through a positive probability of having any of the emitted particles at any time after the emission instant inside the receiver volume:

$$\begin{aligned} &P\left(n \in \mathcal{N}_T(t) : \mathbf{p}^n(t) \in V_R\right) > 0 \\ &\forall n,\ t > 0 \end{aligned} \quad (10)$$

where $\mathcal{N}_T(t)$ is given by (6), $\mathbf{p}^n(t)$ is the vector with the location coordinates for the particle n at time t, and V_R is the set containing all the space coordinates included in the receiver volume.

2) *Molecular noise*: It is the effect of the randomness of the particle locations in the 3-D space, which results in random fluctuations of the received signal. This is a consequence of the random process $f_i(t)$ of the particle locations expressed in (1). This is expressed by considering the received signal Y as a random variable with a generic distribution F. Its expected value $E[Y]$ is the integral of the expected particle distribution, denoted by $\rho(\mathbf{p},t)$, integrated in the receiver volume V_R:

$$Y \sim F,\ E[Y] = \int_{V_R} \rho(\mathbf{p},t)d\mathbf{p},\ t > 0 \quad (11)$$

where $\rho(\mathbf{p},t)$ is the particle distribution at location $\mathbf{p} = (p_X, p_Y, p_Z)$ and time t, whose equation will be defined in the following.

In this paper, we propose to analyze the impact of the aforementioned phenomena on the mutual information (9) by separating the molecule diffusion from the Langevin equation (1) into two processes, namely, the *Fick's diffusion* and the *particle location displacement*, as shown in Fig. 3. This is possible since the molecule diffusion expressed by the stochastic differential equation in (1) and having X (3) as input and Y (7) as output can be equivalently expressed by the deterministic Fick's equation [14] followed by a stochastic process which results in the assignment of the particle locations in the 3-D space.

The Fick's equation is a parabolic partial differential equation [14] in the variable $\rho(\mathbf{p},t)$, which is the particle distribution at location $\mathbf{p} = (p_X, p_Y, p_Z)$ and time t. The expression of this equation for the diffusion-based MC system accounts for the transmitter as a source of particles at location $\mathbf{T}$. This translates

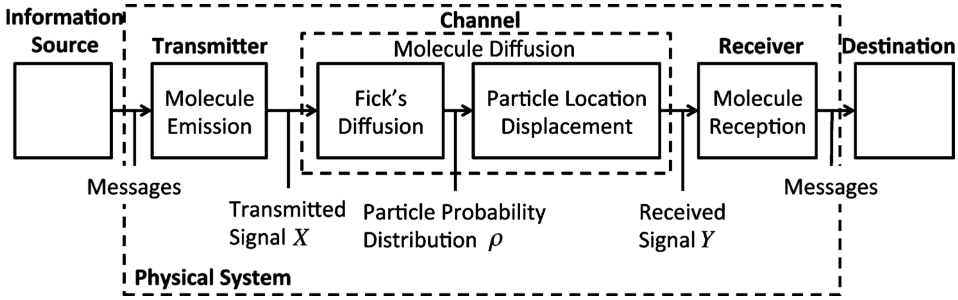

Fig. 3. Diagram of the diffusion-based MC system with the Fick's diffusion and the particle location displacement contributions to the molecule diffusion.

into an additional term, namely, $n_T(t)\delta(|\mathbf{p}-\mathbf{T}|)$, which corresponds to the number of particles $n_T(t)$ emitted into the space as a function of the time t at the location $\mathbf{T}$, where the Dirac delta $\delta(|\mathbf{p}-\mathbf{T}|)$ is nonzero. We express the Fick's equation as follows:

$$\frac{\partial \rho(\mathbf{p},t)}{\partial t} = D\nabla^2\rho(\mathbf{p},t) + n_T(t)\delta(|\mathbf{p}-\mathbf{T}|), \quad t>0 \quad (12)$$

where $\partial./\partial t$ is the time derivative operator of the particle distribution $\rho(\mathbf{p},t)$, which corresponds to the expected number of particles at location $\mathbf{p}$ and time t, and ∇^2 is the Laplacian operator. D is the particle diffusion coefficient, whose expression is as follows:

$$D = \frac{K_b T}{6\pi\mu r} \quad (13)$$

where K_b is the Boltzmann constant, T is the absolute temperature of the system, μ is the viscosity of the fluid, and r is the particle radius.

The particle location displacement is expressed through the stochastic process that randomly assigns the location to each transmitted particle according to the particle distribution $\rho(\mathbf{p},t)$ at each time instant t:

$$\mathbf{p}^n(t) \sim \rho(\mathbf{p},t), \forall n \in \mathcal{N}_T(t) \quad (14)$$

where $\mathcal{N}_T(t)$ is given by (6).

The channel memory phenomenon of the molecule diffusion introduced above is fully captured by the Fick's diffusion contribution. This is expressed by stating that the probability that the location of a particle is inside the receiver volume is never zero from the time instant of the particle emission until infinite time. This is detailed through the following relation:

$$\int_{V_R} \rho_{t'}(\mathbf{v},t)d\mathbf{v} > 0,\ \forall t,t' :\ t > t' > 0 \quad (15)$$

where the integral is performed by spanning the set V_R containing all the space coordinates included in the receiver volume. $\rho_{t'}(\mathbf{v},t)$ is the particle distribution. This is the solution of the Fick's equation in case the particles are emitted only at the time instant t':

$$\frac{\partial \rho_{t'}(\mathbf{p},t)}{\partial t} = D\nabla^2\rho_{t'}(\mathbf{p},t) + n_T(t')\delta(|\mathbf{p}-\mathbf{T}|)\delta(t-t'), \quad t>0. \quad (16)$$

The molecular noise phenomenon is isolated into the particle location displacement contribution, since it contains the stochastic process which contributes to the Langevin equation (1). This is expressed by noting that the number of the particles whose location $\mathbf{p}^n(t)$ is within the receiver volume at time t is a realization of the particle location displacement, as expressed in (14).

The cascade of the Fick's diffusion and the particle location displacement contributions, as shown in Fig. 3, define a Markov chain [13] in the variables X, ρ, and Y following the order $X \rightarrow \rho \rightarrow Y$. This is justified by the property that X and Y are conditionally independent given ρ, which is expressed as follows:

$$f_{X,Y|\rho}(x,y) = f_{X|\rho}(x)\ f_{Y|\rho}(y) \quad (17)$$

since ρ is function of X from (3) and (12), and the distribution of Y is a function of ρ from (7) and (14). The chain rule applied to the joint entropy of X, ρ and Y states the following [13]:

$$\begin{aligned} H(X,\rho,Y) &= H(X,Y|\rho) + H(\rho) \\ &= H(X|\rho) + H(Y|\rho) + H(\rho). \quad (18) \end{aligned}$$

Since ρ is a deterministic function of X through the Fick's equation from (12), the joint entropy per second of X, ρ and Y is equal to the joint entropy per second of X and Y:

$$H(X,\rho,Y) = H(X,Y). \quad (19)$$

By applying (18) and (19) to the third expression in (9), we obtain that the mutual information $I(X;Y)$ of the transmitted signal X and the received signal Y as the sum of the mutual information of a communication system which includes only the Fick's diffusion (mutual information $I(X;\rho)$ of the transmitted signal and the particle distribution) and the mutual information of a system which includes only the particle location displacement (mutual information $I(Y;\rho)$ of the received signal and the particle distribution), respectively, with the subtraction of the entropy per second $H(\rho)$ of the particle distribution:

$$\begin{aligned} I(X;Y) &= H(X) + H(Y) - H(X|\rho) - H(Y|\rho) - H(\rho) \\ &= I(X;\rho) + I(Y;\rho) - H(\rho) \quad (20) \end{aligned}$$

where we applied the first two definitions of mutual information from (9) to obtain the last expression.

We provide closed-form solutions to the mutual information of the Fick's diffusion and to the mutual information of the particle location displacement in Sections III-B and III-C, respectively. In Section III-D, we apply (8) and (20) to the results of the previous sections to obtain a closed-form expression of the mutual information of the diffusion-based MC system and, ultimately, to obtain its capacity.

B. Fick's Diffusion Mutual Information

The closed-form expression for the mutual information $I(X;\rho)$ in bits per second of the Fick's diffusion is computed by applying the following relation:

$$I(X;\rho) = H(X) - H(X|\rho) \tag{21}$$

where $H(X)$ is the entropy per second of the transmitted signal X and $H(X|\rho)$ is the conditional entropy per second of the transmitted signal X given the particle distribution ρ.

The entropy per second $H(X)$ of the transmitted signal is computed as the entropy measured in bits per symbol, multiplied by twice the bandwidth W, which corresponds here to the rate of the symbol transmission in symbols per second. This results from considering the transmitted signal X defined in (3) as a band-limited ensemble of functions [37] within a bandwidth W. The ensemble has the following expression:

$$X = \sum_{k=0}^{\infty} n_T\left(\frac{k}{2W}\right)\frac{\sin\left[\pi(2Wt-k)\right]}{\pi(2Wt-k)}, \quad k \in \mathbb{N} \tag{22}$$

where the bandwidth W is here defined as the maximum frequency contained in the time-continuous signal $n_T(t)$ (3), which corresponds to the number of emitted particles as function of the time t. The Shannon–Hartley theorem [13] assures the equivalence of the expressions in (22) and (3), respectively. As proven in [37], we can express the entropy per second $H(X)$ of the transmitted signal X as the entropy of the ensemble per degree of freedom in bits per sample multiplied by twice the bandwidth W in samples per second. The entropy of the ensemble per degree of freedom corresponds to the entropy $H(\hat{n}_T)$ of a sample $n_T(k/2W)$ of the time-continuous signal $n_T(t)$:

$$H(X) = 2W\, H(\hat{n}_T). \tag{23}$$

The distribution of the stochastic process model for the sampled signal $\hat{n}_T$, which allows to compute the capacity C through (8), is assigned in Section III-D as the distribution leading to the maximum possible mutual information for the MC system constrained by the average power consumption for particle emission at the transmitter.

The conditional entropy per second $H(X|\rho)$ of the transmitted signal X given the particle distribution ρ is computed as a result of the two following properties of the Fick's diffusion from (12).

1) Its linearity, which allows to interpret the Fick's diffusion block in Fig. 3 as a linear filter having the transmitted signal X as input and the particle distribution ρ as output. As a consequence, the formula of the entropy loss in linear filters [9] can be applied to compute the entropy per second $H(\rho)$ of the particle distribution as the sum of the entropy per second $H(X)$ of the transmitted signal and the integral of the transfer function Fourier transform [15] of the Green's function [24] of the Fick's diffusion in the portion W of its frequency spectrum that is excited by the transmitted signal X:

$$H(\rho) = H(X) + \frac{1}{W}\int_W \log_2 |G_d(f)|^2\, df. \tag{24}$$

2) Its deterministic nature, since (12), in contrast to the expression in (1), does not contain any stochastic term. For this, given the transmitted signal X as the input of the Fick's diffusion, the output particle distribution ρ is completely known. As a consequence, the conditional entropy per second $H(\rho|X)$ of the particle distribution given the transmitted signal is equal to zero:

$$H(\rho|X) = 0. \tag{25}$$

Given the aforementioned properties, the conditional entropy per second $H(X|\rho)$ of the transmitted signal X given the particle distribution ρ is computed by applying (24) and (25) to the following relation [13]:

$$H(\rho) = H(X) + H(\rho|X) - H(X|\rho) \tag{26}$$

which results in the following expression:

$$H(X|\rho) = -\frac{1}{W}\int_W \log_2 |G_d(f)|^2\, df \tag{27}$$

where $G_d(f)$ is the transfer function Fourier transform [15] as function of the frequency f of the Green's function [24] of the Fick's diffusion, expressed by (12). W is the bandwidth of the transmitted signal X, which corresponds to the portion of the frequency spectrum of the transfer function $G_d(f)$ that is excited by the transmitted signal X.

The transfer function Fourier transform [15] as function of the frequency f of the Green's function [24] of the Fick's diffusion from (12) has the following expression:

$$G_d(f) = \frac{e^{-(1+j)\sqrt{\frac{2\pi f}{2D}}d}}{\pi D d} \tag{28}$$

where d is the distance between the transmitter and the receiver and D is the diffusion coefficient expressed by (13). By applying (28) to (27), we obtain the closed-form expression of the conditional entropy per second $H(X|\rho)$ of the transmitted signal X given the particle distribution ρ:

$$H(X|\rho) = 2\log_2(\pi D d) + \frac{4d}{3\ln 2}\sqrt{\frac{\pi W}{D}}. \tag{29}$$

The closed-form expression for the mutual information $I(X;\rho)$ of the Fick's diffusion is finally computed by subtracting the conditional entropy per second $H(X|\rho)$ of the transmitted signal X (29) given the particle distribution ρ from the entropy per second $H(X)$ (23) of the transmitted signal X. This results in the following expression:

$$I(X;\rho) = 2WH\left(\hat{n}_T\right) - 2\log_2\left(\pi D d\right) - \frac{4d}{3\ln 2}\sqrt{\frac{\pi W}{D}} \tag{30}$$

where $H\left(\hat{n}_T\right)$ is the entropy of a time sample of $n_T(t)$.

C. Particle Location Displacement Mutual Information

The mutual information $I(Y;\rho)$ in bits per second of the particle location displacement is computed from the following expression:

$$I(Y;\rho) = H(\rho) - H(\rho|Y) \tag{31}$$

where $H(\rho)$ is the entropy per second of the particle distribution ρ and $H(\rho|Y)$ is the conditional entropy per second of the particle distribution ρ given the received signal Y.

The entropy $H(\rho)$ per second of the particle distribution ρ is computed from (24) by substituting the expression for the entropy per second $H(X)$ of the transmitted signal X from (23) and by applying (27) and (29) as the solution of the integral in (24). As a result, the entropy per second $H(\rho)$ of the particle distribution ρ has the following expression:

$$H(\rho) = 2WH(\hat{n}_T) - \log_2\left[(\pi Dd)^2\right] - \frac{4d}{3\ln 2}\sqrt{\frac{\pi W}{D}}. \tag{32}$$

The conditional entropy per second $H(\rho|Y)$ of the particle distribution ρ given the received signal Y is computed similarly to (23) in Section III-B. Under the assumption that the realizations of the stochastic process $\rho|Y$ are independent [29] for different time instants, and band limited within a bandwidth W, we express the entropy per second $H(\rho|Y)$ as the entropy of $H(\rho|\mathcal{Y})$ in bits, where $\mathcal{Y}$ is the received signal per time sample, multiplied by the maximum time sample rate $2W$ in 1/sec given by the Shannon–Hartley theorem [15]:

$$H(\rho|Y) = 2WH(\rho|\mathcal{Y}). \tag{33}$$

The received signal $\mathcal{Y}$ per time sample is defined as

$$\mathcal{Y} = \sum_{i=1}^{1/(2W\tau_p)} y_i \tag{34}$$

where $1/(2W\tau_p)$ is the number of independent measures of the number of particles inside the receiver volume that can be performed within a time sample, for which we consider a quasi-constant particle distribution. W is the bandwidth of the transmitted signal X. We assume independent measures when they are taken at time instants spaced by an interval τ_p, as we considered in [32]. The time interval τ_p is equal to the squared linear dimension of the receiver volume R_{V_R} divided by the diffusion coefficient D [32]:

$$\tau_p = \frac{R_{V_R}^2}{D}. \tag{35}$$

The conditional entropy $H(\rho|\mathcal{Y})$ of the particle distribution ρ given the received signal $\mathcal{Y}$ per time sample is defined as

$$H(\rho|\mathcal{Y}) = \int H(\rho|\mathcal{Y}=y)p_{\mathcal{Y}}(y)dy = E_y\left[H(\rho|\mathcal{Y}=y)\right] \tag{36}$$

where $H(\rho|\mathcal{Y}=y)$ is the entropy of the particle distribution ρ given a value y for the received signal per time sample $\mathcal{Y}$, $p_{\mathcal{Y}}(y)$ is the probability density of the received signal $\mathcal{Y}$ per time sample and $E_y[\cdot]$ is the average value operator with respect to the probability density of the value y.

The entropy $H(\rho|\mathcal{Y}=y)$ is based on the probability density $p_{\rho|\mathcal{Y}}(r|y)$ of the possible values y of the particle distribution ρ at the receiver given a value y for the received signal per time sample $\mathcal{Y}$ through the formula:

$$H(\rho|\mathcal{Y}=y) = -\int p_{\rho|\mathcal{Y}}(r|y)\log_2 p_{\rho|\mathcal{Y}}(r|y)dr. \tag{37}$$

With the goal of having a closed-form expression for this probability density, we use the following assumptions, with reference to our previous work on the diffusion noise in MC systems [32].

1) The actual number of particles y_i inside the receiver volume for every measurement is a random process whose average value is the average particle distribution at the receiver $\bar{\rho}$ within a time sample multiplied by the size $size(V_R)$ of the receiver volume:

$$E[y_i] = \bar{\rho}\,\mathrm{size}(V_R). \tag{38}$$

Since the particle distribution ρ is the output of the Fick's diffusion, whose input is the stationary stochastic process of the number of the emitted particles $\hat{n}_T$ for every time sample, by applying the theory of the random processes through linear filters [29], we obtain

$$\bar{\rho} = E\left[\hat{n}_T\right]G_d(f)|_{f=0} = \frac{E\left[\hat{n}_T\right]}{\pi Dd} \tag{39}$$

where $G_d(f)$ is from (28) and $E[\cdot]$ is the average operator.

2) It is unlikely to have two particles occupying the same location in space at the same time instant. In other words, the probability of having a distance equal to zero between two particles is zero:

$$Pr\left[\|P_p(t) - P_q(t)\| = 0\right] = 0, \;\; p \neq q,\, p, q \in \mathcal{N}_T(t) \tag{40}$$

where $\mathcal{N}_T(t)$ is given by (6), $\|\cdot\|$ is the Euclidian distance operator, and p and q are two particles previously emitted by the transmitter, which are subject to the Brownian motion. This assumption is justified by the independence of the Brownian components in the movement of different particles in the space.

3) An event concerning a particle which occupies a location in space is independent from any event of the same kind occurring at any other space location. This assumption is justified by the property of the Wiener process [14] underlying the particle Brownian motion of having independent realizations. This implies that the location of a particle is independent from the location of any other particle. As a consequence, the events concerning the location of particles in the space have the property of *memorylessness*.

4) The occurrence rate of particle locations in the space is proportional to the particle distribution at the receiver location ρ.

Under these assumptions, the resulting single measurement y_i, which corresponds to the number of particles inside the receiver volume, is a volumetric Poisson counting process [29], whose rate of occurrence corresponds to the average value of the particle distribution $\bar{\rho}$ within a time sample:

$$y_i \sim \mathrm{Poiss}(\bar{\rho}). \tag{41}$$

According to the theory of Bayesian inference [20], the estimator of the rate of occurrence $\hat{\rho}$ of a Poisson counting process given a series of measurements of the output of the process, which corresponds to a value y of the received signal per time sample $\mathcal{Y}$ defined in (34), follows a Gamma distribution with parameters y and $1/(2W\tau_p)$:

$$\hat{\rho} \sim \text{Gamma}(y, 1/(2W\tau_p)) \quad (42)$$

where W is the bandwidth of the transmitted signal X and τ_p is the time interval in which we consider a quasi-constant particle distribution. The probability density of the estimator $\hat{\rho}$ corresponds to the probability density $p_{\rho|\mathcal{Y}}(r|y)$ of the possible values r of the particle distribution ρ at the receiver given a value y for the received signal in a time sample $\mathcal{Y}$ [20]:

$$p_{\rho|\mathcal{Y}}(r|y) = r^{y-1}\frac{e^{-rW\tau_p}}{(W\tau_p)^y\Gamma(y)}, \quad r \geq 0,\ y > 0 \quad (43)$$

where $\Gamma(y)$ is the gamma function [25], defined as follows:

$$\Gamma(y) = (y-1)! \quad (44)$$

The entropy $H(\rho|\mathcal{Y}=y)$ of the particle distribution ρ given a value y for the received signal per time sample $\mathcal{Y}$ corresponds to the computation of the formula in (37) by using the expression of the probability density $p_{\rho|\mathcal{Y}}(r|y)$ from (43), thus obtaining the following expression [20]:

$$H(\rho|\mathcal{Y}=y) = y + \ln(2W\tau_p) + \ln(\Gamma(y)) + (1-y)\psi(y) \quad (45)$$

where $\psi(y)$ is the digamma function.

For the final computation of the conditional entropy $H(\rho|\mathcal{Y})$, expressed in (36), we apply a formulation of the Jensen's inequality [29], which is based on the consideration that $H(\rho|\mathcal{Y}=y)$ is a concave function of y, since its expression in (45) is a sum of concave or linear components.

1) The first term y is linear.
2) The second term $\ln(\Gamma(y))$ is concave in y since the gamma function $\Gamma(y)$ has the property of being log-concave [25].
3) The third term $(1-y)\psi(y)$ is concave in y when the value of y is sufficiently high ($y \gg 1$). This can be proven from the decomposition of the digamma function as follows [10]:

$$\psi(y) = \ln y - \frac{1}{2y} - \frac{1}{12y^2} + \frac{1}{120y^4} - \frac{1}{252y^6} + O\left(\frac{1}{y^8}\right). \quad (46)$$

By taking the limit of $(1-y)\psi(y)$ as $y \to \infty$, we obtain

$$(1-y)\psi(y) \to -y\ln y \quad (47)$$

which is a concave function of y.

For the aforementioned considerations, the Jensen's inequality [29] applied to (36) states that the average value $E_y[H(\rho|\mathcal{Y}=y)]$ of the entropy $H(\rho|\mathcal{Y}=y)$ as function of the value y for the received signal per time sample $\mathcal{Y}$ is less or equal than the entropy $H(\rho|E[\mathcal{Y}])$ as function of the average value $E[\mathcal{Y}]$ of the received signal per time sample $\mathcal{Y}$:

$$H(\rho|\mathcal{Y}) = E_y[H(\rho|\mathcal{Y}=y)] \leq H(\rho|E[\mathcal{Y}]). \quad (48)$$

As a consequence, by substituting the left-hand side of (48) for the computation (36) of the conditional entropy $H(\rho|\mathcal{Y})$ of the particle distribution ρ given the received signal Y per time sample with the right-hand side of (48), we provide a higher bound to the real value of $H(\rho|\mathcal{Y})$. This results in a higher bound to the conditional entropy $H(\rho|Y)$ of the particle distribution ρ given the received signal Y in (33) and, consequently, in a lower bound to the mutual information $I(\rho;Y)$ of the transmitted signal and the particle distribution in (31). Since the capacity is the maximum mutual information $I(X;Y)$ between the transmitted signal X and the received signal Y, as expressed in (8), the substitution of $I(\rho;Y)$ with its lower bound in the computation of the mutual information $I(X;Y)$ expressed in (20) results in a lower bound to the capacity C of an MC system. We consider this in agreement with the purpose of this paper, since it allows expressing achievable performance of an MC system with a closed-form mathematical expression, even if it is an underestimate of the theoretical capacity C.

The average value $E[\mathcal{Y}]$ of the received signal per time sample $\mathcal{Y}$ is given by (38) and (39). Since the distribution of particles ρ is a deterministic function of the transmitted signal X, whose average value per time sample is $E[\hat{n}_T]$, the value of $E[\mathcal{Y}]$ becomes

$$\begin{aligned} E[\mathcal{Y}] &= \sum_{i=1}^{1/(2W\tau_p)} E[y_i] = \frac{1}{2W\tau_p}\bar{\rho}size(V_R) \\ &= \frac{D}{2WR_{V_R}^2}\frac{E[\hat{n}_T]}{\pi D d}\frac{4}{3}\pi R_{V_R}^3 = \frac{2}{3}\frac{E[\hat{n}_T]R_{V_R}}{Wd}. \end{aligned} \quad (49)$$

As stated previously, the expression for the conditional entropy $H(\rho|\mathcal{Y})$ can be approximated with the right-hand side of (48), whose expression is found by applying the average value $E[\mathcal{Y}]$ of the received signal per time sample $\mathcal{Y}$ to (45):

$$\begin{aligned} H(\rho|\mathcal{Y}) \cong H(\rho|E[\mathcal{Y}]) &= E[\mathcal{Y}] + \ln(2W\tau_p) + \ln(\Gamma(E[\mathcal{Y}])) + \\ &+ (1-E[\mathcal{Y}])\psi(E[\mathcal{Y}]). \end{aligned} \quad (50)$$

The final approximated expression for the conditional entropy $H(\rho|\mathcal{Y})$ is found by substituting the expression in (49). This becomes

$$\begin{aligned} H(\rho|\mathcal{Y}) \cong & \frac{2}{3}\frac{E[\hat{n}_T]R_{V_R}}{Wd} + \ln(2W\tau_p) + \\ &+ \ln\left(\Gamma\left(\frac{2}{3}\frac{E[\hat{n}_T]R_{V_R}}{Wd}\right)\right) + \\ &+ \left(1 - \frac{2}{3}\frac{E[\hat{n}_T]R_{V_R}}{Wd}\right)\psi\left(\frac{2}{3}\frac{E[\hat{n}_T]R_{V_R}}{Wd}\right) \end{aligned} \quad (51)$$

where W is the bandwidth of the transmitted signal X, τ_p is the time interval in which we consider a quasi-constant particle distribution, $\psi(\cdot)$ is the digamma function, D is the diffusion coefficient, d is the distance between the transmitter and the receiver, and R_{V_R} is the radius of the spherical receiver volume V_R.

The closed-form expression for the mutual information $I(Y;\rho)$ of the particle location displacement is finally computed by subtracting the conditional entropy $H(\rho|\mathcal{Y})$ of the particle distribution ρ given the received signal $\mathcal{Y}$ per time sample from (51) multiplied by two times the bandwidth W of the transmitted signal X from the entropy $H(\rho)$ (32) of the particle distribution ρ. This results in the following expression:

$$I(Y;\rho) = 2WH(\hat{n}_T) - \log_2\left[(\pi Dd)^2\right] - \frac{4d}{3\ln 2}\sqrt{\frac{\pi W}{D}} + \\ - 2W\frac{2}{3}\frac{E[\hat{n}_T]R_{V_R}}{Wd} - 2W\ln(2W\tau_p) + \\ - 2W\ln\left(\Gamma\left(\frac{2}{3}\frac{E[\hat{n}_T]R_{V_R}}{Wd}\right)\right) + \\ - 2W\left(1 - \frac{2}{3}\frac{E[\hat{n}_T]R_{V_R}}{Wd}\right)\psi\left(\frac{2}{3}\frac{E[\hat{n}_T]R_{V_R}}{Wd}\right). \quad (52)$$

D. Capacity of the Diffusion-Based MC System

The capacity of the diffusion-based MC system is computed from (8), by maximizing the mutual information $I(X;Y)$, expressed in Section III-D1 with respect to the probability density function $f_X(x)$ of the transmitted signal X. It is common in information theory [37] to compute the maximum probability density function $f_X(x)$ subject to a constraint on the average power of the transmitted signal X defined in (3). As explained in Section III-D2, the expression for this average power is here related to the thermodynamic energy spent for the emission of particles in the MC signal transmission. Finally, in Section III-D3, we obtain the closed-form capacity expression.

1) Mutual Information: The expression for the mutual information $I(X;Y)$ of the diffusion-based MC system is obtained by applying the expression of the mutual information $I(X;\rho)$ of the Fick's diffusion from (30), the mutual information $I(Y;\rho)$ of the particle location displacement from (52) and the entropy $H(\rho)$ of the particle distribution ρ from (32) to the formula in (20). We obtain the following expression:

$$I(X;Y) = 2WH(\hat{n}_T(t)) - \log_2\left[(\pi Dd)^2\right] - \frac{4d}{3\ln 2}\sqrt{\frac{\pi W}{D}} + \\ - 2W\frac{2}{3}\frac{E[\hat{n}_T]R_{V_R}}{Wd} - 2W\ln(W\tau_p) + \\ - 2W\ln\left(\Gamma\left(\frac{2}{3}\frac{E[\hat{n}_T]R_{V_R}}{Wd}\right)\right) + \\ - 2W\left(1 - \frac{2}{3}\frac{E[\hat{n}_T]R_{V_R}}{Wd}\right)\psi\left(\frac{2}{3}\frac{E[\hat{n}_T]R_{V_R}}{Wd}\right) \quad (53)$$

where W is the bandwidth of the transmitted signal X, τ_p is the time interval in which we consider a quasi-constant particle distribution, $\psi(\cdot)$ is the digamma function, D is the diffusion coefficient, d is the distance between the transmitter and the receiver, and R_{V_R} is the radius of the spherical receiver volume V_R.

2) Average Thermodynamic Power: Given the physical system from Section II considered in this paper, the average power necessary for signal transmission corresponds to the energy necessary to emit the average number $E[\hat{n}_T]$ of particles per time sample, divided by the duration of a time sample. In thermodynamics, this energy is defined as enthalpy.

Definition 3.1: The enthalpy $\mathcal{H}$ [40] is the energy necessary to emit N particles in the physical system and to heat these particles up to a temperature T when the system has the pressure P and the volume V. The considerations detailed in Section II of having spherical particles with radius $r \ll d$ independently and randomly moving in the space are in agreement with the approximation of the system as an ideal gas. According to the ideal gas theory [17], the enthalpy is expressed through the following formula:

$$\mathcal{H} = PV + \frac{3}{2}K_bTN \quad (54)$$

where P and V are the pressure and the volume, and T is the absolute temperature of the physical system, K_b is the Boltzmann constant.

When associated with the transmitter of the MC system, the enthalpy is the energy necessary for communication if N particles are emitted into the space.

In this paper, we define the *average thermodynamic power* $\bar{P}_{\mathcal{H}}$ as the enthalpy variation $\Delta\mathcal{H}$ in a time sample divided by the time sample duration $1/2W$. As a consequence, the average thermodynamic power $\bar{P}_{\mathcal{H}}$ quantifies the energy necessary to emit $E[\hat{n}_T]$ particles per time sample divided by the time sample duration $1/2W$, at a temperature T. This is given by the following expression:

$$\bar{P}_{\mathcal{H}} = \frac{\Delta\mathcal{H}}{1/2W} = \frac{3}{2}K_bTE[\hat{n}_T]2W \quad (55)$$

where the enthalpy variation $\Delta\mathcal{H}$ is computed from (55) by taking into account that no variations in the pressure P and the volume V occur in the physical system, and the absolute temperature T is considered a constant parameter with respect to the time t.

As a consequence, a constraint on the average thermodynamic power $\bar{P}_{\mathcal{H}}$ spent by the transmitter corresponds to a constraint in the average number $E[\hat{n}_T]$ of emitted particles according to the following expression:

$$E[\hat{n}_T] = \frac{\bar{P}_{\mathcal{H}}}{3WK_bT}. \quad (56)$$

3) Capacity: In the expression of $I(X;Y)$ (53), only the term $H(\hat{n}_T(t))$ depends on the probability density function $f_{\hat{n}_T}(n)$. Therefore, the capacity C is achieved (8) for a probability density function $f_{\hat{n}_T}(n)$ leading to the maximum entropy $H(\hat{n}_T(t))$.

The distribution $f_{\hat{n}_T}(n)$ with the maximum possible entropy $H(\hat{n}_T)$ in the number of emitted particles per time sample constrained on its average value $E[\hat{n}_T]$, as expressed in (56), is the exponential distribution [13] whose rate corresponds to $E[\hat{n}_T]$:

$$f_{H(\hat{n}_T)}(n) = \frac{e^{-\frac{n}{E[\hat{n}_T]}}}{E[\hat{n}_T]}. \quad (57)$$

The entropy of the number $H(\hat{n}_T)$ of emitted particles per time sample is, therefore, [13]

$$H(\hat{n}_T) = 1 + \log_2 E[\hat{n}_T]. \quad (58)$$

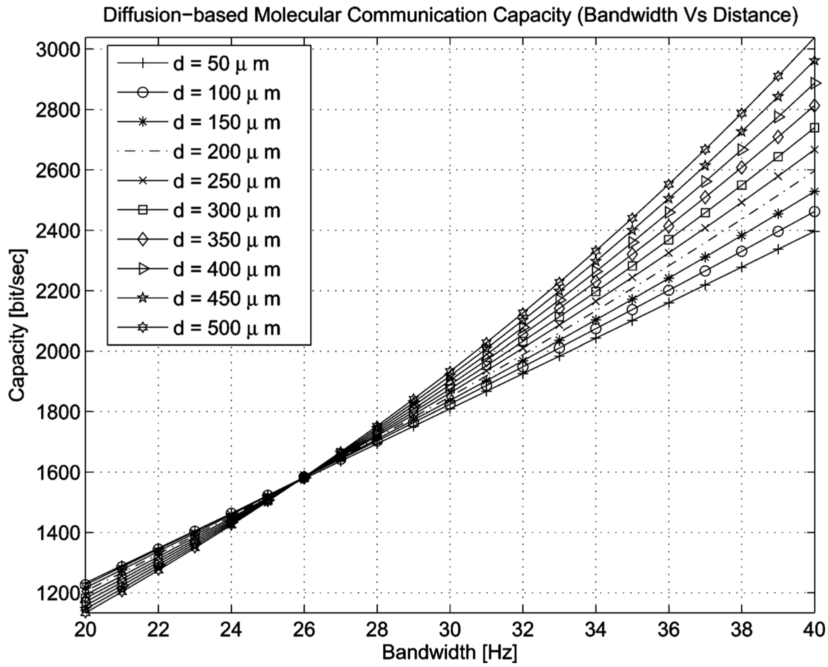

Fig. 4. Capacity in relation to the bandwidth and for different values of the transmitter–receiver distance d.

By applying (56) and (58) to the expression of the mutual information $I(X;Y)$ from (53), we obtain the expression of the capacity C of the diffusion-based MC system:

$$\begin{aligned} C = & 2W\left(1+\log_2\frac{\bar{P}_{\mathcal{H}}}{3WK_bT}\right) - 2\log_2(\pi D d) - \frac{4d}{3\ln 2}\sqrt{\frac{\pi W}{D}} + \\ & - 2W\frac{2\bar{P}_{\mathcal{H}}R_{V_R}}{9W^2 dK_bT} - 2W\ln(W\tau_p) + \\ & - 2W\ln\left(\Gamma\left(\frac{2\bar{P}_{\mathcal{H}}R_{V_R}}{9W^2 dK_bT}\right)\right) + \\ & - 2W\left(1-\frac{2\bar{P}_{\mathcal{H}}R_{V_R}}{9W^2 dK_bT}\right)\psi\left(\frac{2\bar{P}_{\mathcal{H}}R_{V_R}}{9W^2 dK_bT}\right) \end{aligned} \quad (59)$$

where $\bar{P}_{\mathcal{H}}$ is the average thermodynamic power spent by the transmitter, K_b is the Boltzmann constant, T is the absolute temperature of the system, W is the bandwidth of the transmitted signal X, τ_p is the time interval in which we consider a quasi-constant particle distribution, $\psi(\cdot)$ is the digamma function, D is the diffusion coefficient, d is the distance between the transmitter and the receiver, and R_{V_R} is the radius of the spherical receiver volume V_R.

IV. Numerical Results

In this section, we provide a numerical evaluation of the closed-form expression for the diffusion-based MC capacity obtained in Section III-D. All the results are computed for a common set of parameters, whose values are assigned as follows. The radius R_{V_R} of the receiver volume V_R, which we assume to be spherical, is set to 10 nm. The temperature T of the system is set to a standard room temperature of 25 °C and the diffusion coefficient D is set [31] to $10^{-9}\ \mathrm{m^2/s}$. The Boltzmann constant [21] is $K_b = 1.380650424 \times 10^{-23}\ \mathrm{J/K}$.

A. Capacity Versus Bandwidth

The capacity of a diffusion-based MC system is shown in Fig. 4 in relation to the bandwidth W and different values of the transmitter–receiver distance d. We evaluate the capacity in bits per second for a bandwidth W ranging from 20 to 40 Hz and different lines refer to different distance values, from 50 to 500 $\mu\mathrm{m}$. The choice of the values for the bandwidth can be justified from a biological viewpoint, since, according to biochemical studies [28], the neurons in our brain communicate through the exchange of molecules (and their diffusion between the synapses) at a frequency of around 20 Hz for the processing of general information and around 60 Hz for the processing of visual images. We restricted our range to a maximum of 40 Hz in order to visualize better the intersection of the curves around 26 Hz. The average transmitter power $P_{\mathcal{H}}$ is set to 10^{-12} W, equivalent to 1 pW. This value should not be compared to the transmitted power values used for electrical devices, since the average transmitted power is a thermodynamic quantity. Note also that this is only a reference value, since so far we do not know how much average thermodynamic power a transmitter nanomachine will be able to provide. According to the obtained results, the capacity of an MC system with the chosen parameters can achieve a value close to 3 kilobits per second at a distance of 500 $\mu\mathrm{m}$ and for a bandwidth of 40 Hz. This is a theoretically achievable maximum value, which reveals the maximum potential of MC. Further investigation on information coding schemes is required in order to provide achievable bit rates related to specific MC implementations.

Fig. 4 shows the trend of the MC capacity, which is monotonically increasing as the bandwidth increases from 20 to 40 Hz for all the given values of the transmitter–receiver distance d. The capacity values range from 1.2 to 2.4 kilobits per second for a distance of 50 $\mu\mathrm{m}$ and between a few bits per second and 3 kilobits per second for a distance of 500 $\mu\mathrm{m}$. For a

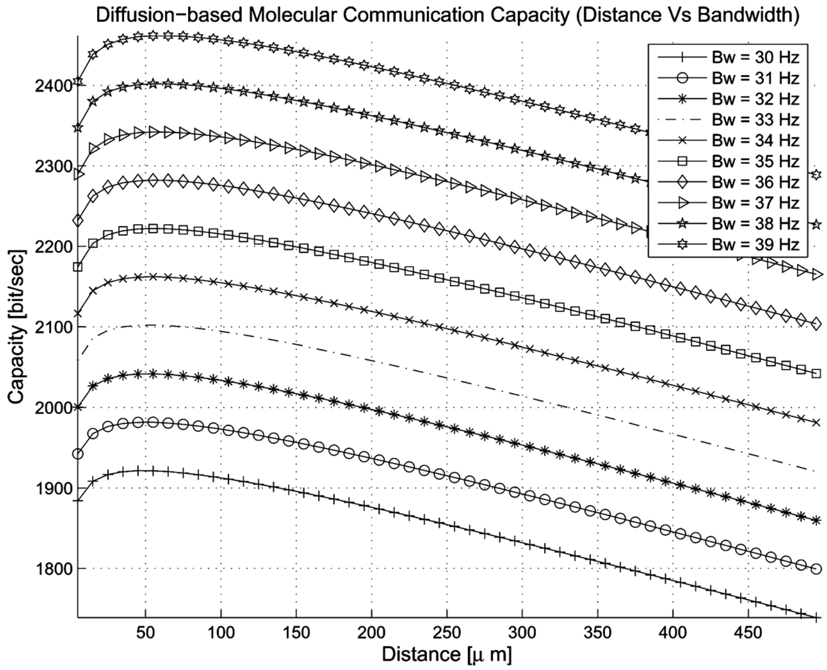

Fig. 5. Capacity in relation to the transmitter–receiver distance and for different values of the bandwidth W.

bandwidth value within 20 and 26 Hz, the MC capacity values corresponding to the lowest transmitter–receiver distance d are higher than the values corresponding to other transmitter–receiver distances and, as this distance increases, the MC capacity values decrease monotonically. For a bandwidth value higher than 26 Hz, higher MC capacity values correspond to higher transmitter–receiver distances d. This behavior, which is apparently counterintuitive, can be explained as a consequence of the interactions between the channel memory and the molecular noise contributions in the second and third term of the first line and in the second, third, and fourth lines of (59), respectively. For low bandwidth values (lower than 26 Hz), the channel memory terms tend to outperform the molecular noise terms and the MC capacity values tend to be proportional to the transmitter–receiver distance (higher MC capacity when lower transmitter–receiver distance). For high bandwidth values (higher than 26 Hz), the molecular noise terms outperform the channel memory terms and the MC capacity values become inversely proportional to the transmitter–receiver distance (higher MC capacity when higher transmitter–receiver distance).

B. Capacity Versus Distance

In Fig. 5, we show the capacity in relation to the distance d between the transmitter and the receiver locations and different values of the bandwidth W. We evaluate the capacity in bits per second for a distance ranging from 1 to 500 μm. The different lines refer to different bandwidth W values, from 30 to 39 Hz. We restricted these numerical results to this narrow bandwidth interval in order to better visualize the differences in the MC capacity for the considered values of the distance between the transmitter and the receiver. The average transmitted power $P_{\mathcal{H}}$ is set to 1 pW.

The curves in Fig. 5 show a monotonically increasing trend of the capacity as function of the transmitter–receiver distance ranging from 1 to 50 μm, while they show a monotonically decreasing value for a distance ranging from 50 to 500 μm. The capacity values range from a value around 1.9 kilobits per second and a 1.85 bits/s for a bandwidth of 30 Hz and between 2.45 and 2.3 kilobits per second for a bandwidth of 39 Hz. The different behavior when the distance ranges from 1 to 50 μm with respect to when the distance ranges from 50 to 500 μm can be explained as a consequence of the interactions between the channel memory and the molecular noise contributions, similarly to Fig. 4: as the distance increases from 1 to 50 μm, the contribution coming from the channel memory gets lower and the capacity values tend to increase, until reaching a distance of 50 μm, where the contribution coming from the molecular noise becomes relevant and decreases the capacity values as the distance is further increased.

C. Capacity and Average Transmitted Power

In Fig. 6, we show the capacity as a function of the bandwidth W ranging from 30 to 40 Hz and the average transmitted power $P_{\mathcal{H}}$. Similarly to Fig. 5, we restricted these numerical results to this narrow bandwidth interval in order to better visualize the differences in the MC capacity for the values of the average transmitter power. Different lines refer to different average transmitted power $P_{\mathcal{H}}$ values, from 1 to 10 pW. The transmitter–receiver distance d is here set to 50 μm.

Fig. 6 shows for all the curves a monotonic increasing trend as the bandwidth increases from 30 to 40 Hz. The capacity values range from a value between 1.92 and around 2.5 kilobits per second for an average transmitted power of 1 pW and between 2.05 and 3.7 kilobits per second for an average transmitted power of 10 pW. The MC capacity values are higher for higher values of the average transmitted power. Even if the average transmitted power is applied with constant increments of 1 pW from a value of 1 to 10 pW, the increment in the values of

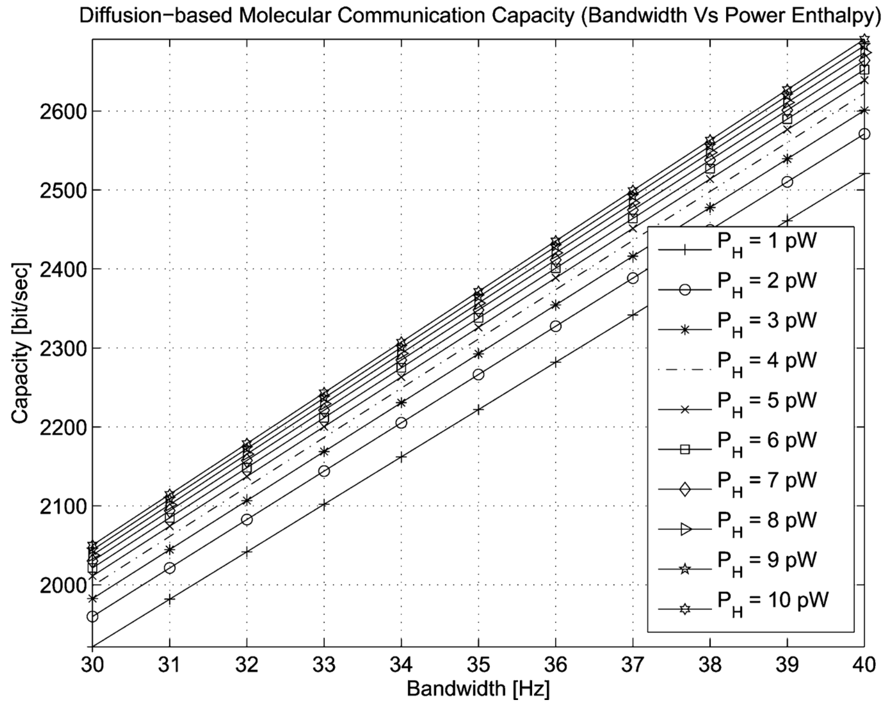

Fig. 6. Capacity in relation to the bandwidth and for different values of the average transmitted power $P_{\mathcal{H}}$.

the capacity is not constant and it is higher for lower values of the average transmitted power. This behavior can be explained through the dependency of the molecular noise terms in the second, third, and fourth lines of (59) with respect to the average transmitted power. As the average transmitted power increases, we have an increase in the first positive term in the first line of (59), but, at the same time, we have an increase in the aforementioned molecular noise terms.

V. Conclusion

MC is a promising paradigm for communication in nanonetworks [1], where the applicability of classical communication technologies is limited by the constraints posed by the nanodomain. The objective of this paper is to provide a closed-form mathematical expression for the information capacity of an MC system based on free molecule diffusion (diffusion-based MC). Unlike previous contributions from the literature, the provided information capacity expression takes into account the two main effects of the molecule diffusion channel, namely, the memory and the molecular noise. The capacity analysis in this paper is also independent from any specific coding scheme by assuming that the transmitter can send in general any continuous time signal which complies to a constraint on the average transmitted power.

The closed-form diffusion-based MC capacity is obtained here by combining two separate contributions, namely, the Fick's diffusion and the particle location displacement, which separately capture the effects of the channel memory and the molecular noise, respectively. The obtained capacity expression is a function of the medium diffusion coefficient, the system temperature, the distance between the transmitter and the receiver, and the bandwidth of the transmitted signal. The MC capacity is also expressed as a function of the average transmitted power, which corresponds to the thermodynamic power spent at the transmitter for molecule emission. Numerical results show interesting properties of the relationship between diffusion-based MC capacity and parameters such as the distance, the bandwidth, and the average thermodynamic power.

The numerical results have the validity of an upper bound to the communication performance of a diffusion-based MC system. Further investigation will be carried out in the future on finding more stringent upper bounds to the performance (e.g., using a given coding scheme at the transmitter). According to the provided results, capacity values of a few kilobits per second can be reached within a distance of tenth of micrometer between the transmitter and the receiver and for an average transmitted power around 1 pW (Note that this power value should not be compared to the transmitted power values used for electrical devices, since the transmitted power in an MC system is a thermodynamic quantity).

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