

Information Capacity of Diffusion-based Molecular Communication in Nanonetworks

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Abstract—Molecular Communication (MC) is a promising bio-inspired paradigm in which molecules are transmitted, propagated and received between nanoscale machines. One of the main challenges is the theoretical study of the maximum achievable information rate (capacity). The objective of this paper is to provide a mathematical expression for the capacity in MC nanonetworks when the propagation of the information relies on the free diffusion of molecules. Solutions from statistical mechanics and thermodynamics are used to derive a closed-form expression for the capacity as function of physical parameters, such as the size of the system, the temperature and the number of molecules as well as of the bandwidth of the system and the transmitted power. An extremely high order of magnitude of the capacity numerical values demonstrates the enormous potential of the diffusion-based MC systems.

I. INTRODUCTION

Molecular Communication (MC) is a promising paradigm for communication in nanonetworks [1], where molecules are used to encode, transmit and receive information. Nanonetworks are interconnections of nanomachines, i.e., devices consisting of nanoscale-precise components and able to sense, compute, actuate and communicate. Unlike classical communication techniques, we believe that the integration process of MC transceivers in nanomachines is more feasible due to their size and natural domain. Amongst others [10], we focus on the diffusion-based architecture, as it represents the most general and simple MC architecture.

Up to date, very limited research has addressed the problem of modeling and analyzing the information capacity in diffusion-based MC in nanonetworks. While in [2] some open questions about nanoscale information theory are outlined, concrete mathematical solutions for diffusion-based MC channel modeling are not provided. In [3], a MC receiver model is developed, but without taking into account the molecule diffusion-based propagation theory. A more recent approach to information theory applied to a specific case of molecular communication, namely, calcium signaling, can be found in [9]. In [11], a physical model of the diffusion-based MC is developed in terms of end-to-end information delivery.

The objective of this paper is to provide a mathematical expression of capacity in MC when the propagation of information relies on the free diffusion of molecules. The diffusion-

based molecular environment is based on radically different mechanisms than the mechanisms underlying classical EM-based communication. For this, some assumptions used by Shannon [12] for expressing the capacity of an EM channel are no longer valid, such as the assumption of having an additive white gaussian noise source. As a consequence, there is a need to rethink the basis of information theory from the perspective of the diffusion-based MC scenario. For this, we study the relationship between thermodynamic entropy and information entropy and derive a closed-form expression for the capacity in diffusion-based MC in nanonetworks. We define a physical reference model as the most basic realization of a nanonetwork with molecular communication and we express the capacity as function of physical parameters, such as the size of the system, the temperature and the number of molecules as well as of the bandwidth of the system and the transmitted power. We provide numerical results to evaluate the capacity of MC.

The remainder of the paper is organized as follows. In Sec. II, we detail the schematic diagram of a diffusion-based MC system and we define the physical reference model. The closed-form expression of the capacity is derived in Sec. III, together with the relation between thermodynamic entropy and information entropy, the input signal entropy and the equivocation. Numerical results are provided in Sec. IV. Finally, in Sec. V, we conclude the paper.

II. A DIFFUSION-BASED MOLECULAR COMMUNICATION SYSTEM AND THE PHYSICAL REFERENCE MODEL

The schematic diagram of a diffusion-based MC system is shown in Fig. 1, where the system is depicted as a cascade of different parts, namely, the information source, the transmitter, the channel, the noise source, the receiver and the destination. The schematic diagram in Fig. 1 specializes the scheme presented in [12] in light of the diffusion-based MC paradigm. In the following, we detail each different part.

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 channel is deployed. In nanomachine communication [2] the message can be any function of the time which carries data such as nanomachine states or sensory measurements [1].

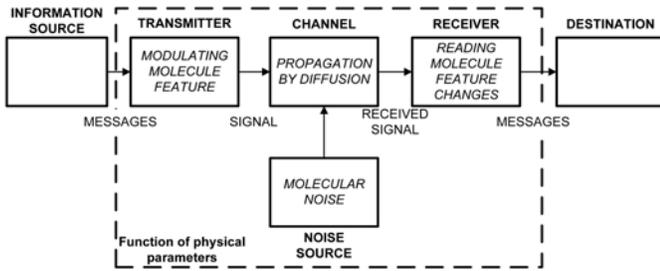


Fig. 1. Schematic diagram of a diffusion-based MC system.

The **transmitter** receives the messages from the information source and produces a *signal* suitable for the transmission over the channel. The signal is produced by modulating one or more molecular features. Molecular features are properties of the molecules that the transmitter can vary and whose value is propagated by the channel towards the receiver. The molecular features considered in this paper are the local particle number and the particle type.

The **channel** is the medium that propagates the signal from the transmitter to the receiver. In diffusion-based MC, the channel propagates the signal by means of the molecule diffusion process. Molecule diffusion is defined as the movement of molecules from an area of higher concentration to an area of lower concentration by means of Brownian motion [5].

The **noise source** operates a random unwanted perturbation on the signal while it propagates from the transmitter to the receiver. In diffusion-based MC the noise is related to the randomness present in the particle propagation and it is due to Brownian motion of the particles.

The **receiver** reconstructs the *messages* sent by the transmitter from the *received signal* coming from the channel and the noise source. It reads the changes that the transmitter operated on the molecule features during their modulation.

The **destination** is the recipient of the *messages* coming from the receiver. Upon reception of a message, it reacts according to the meaning and to the particular application.

The transmitter, the channel, the noise source and the receiver are functions of physical parameters, such as the temperature or the chemical composition of the environment, and depend on how the diffusion-based MC system is physically realized. We define a **physical reference model** as the most basic realization of a diffusion-based MC system as follows:

- The physical reference model is contained in the *space* S , whose shape is spherical with radius r_S .
- All the molecules are considered as mono-atomic and with negligible spatial dimension (zero-dimensional point *particles*) when compared to the size of the space S . Each particle is randomly-moving in the space following the Brownian motion random process and we assume the same particle diffusion coefficient D for all the particles.
- Each particle i is characterized by two quantities, namely, the location \bar{x}_i and the momentum $\bar{\rho}_i$. The location of a particle is a vector $\bar{x}_i = [x_i, y_i, z_i]$ containing the values of the three space coordinates where the particle is located. The momentum $\bar{\rho}_i$ of a particle is the product of the velocity \bar{v}_i , which is a vector containing all the velocity components $\bar{v}_i = [v_i^x, v_i^y, v_i^z]$, by the particle mass m . The set containing

the locations and momenta of all the particles in the system define the Phase Space Φ of the system.

- The transmitter has a spherical shape of radius r_T , where $r_T \ll r_S$, while the receiver is point-wise. The location of the transmitter corresponds to the center $[x_T, y_T, z_T]$ of the spherical space S and the receiver is at a distance d from the transmitter, where $r_T < d < r_S$.

Given the above statements, the particles of the physical reference model behave according to the theory of the ideal gases [6]. The ideal gas concept allows us to define the following **physical parameters** for the physical reference model when it is in a state of thermodynamic equilibrium [5]: the temperature T , the pressure P , the volume V and the number of particles N_p . The physical parameters define the state of the system and they are bound by the Ideal Gas Law.

The information capacity of a communication system is defined as the maximum rate of transmission at the information source that allows the reception of all the sent information at the destination. *The goal of the research work detailed in this paper is the study of the information capacity as a function of the physical parameters that control the diffusion-based MC systems in the physical reference model.*

III. INFORMATION CAPACITY OF A DIFFUSION-BASED MOLECULAR COMMUNICATION SYSTEM

The information **capacity** of a communication system is expressed by the general formula from Shannon [12]. The general formula defines the information capacity as the maximum difference between the entropy $H(x)$ of the signal x in input to the channel and the equivocation $H_Y(x)$:

$$C = \max_{f_X(x)} \{H(x) - H_Y(x)\} \quad (1)$$

where the maximum is found with respect to the probability density function $f_X(x)$ in the values of the input signal x .

Definition 3.1: The **entropy** $H(x)$ of the input signal x is defined [12] as the opposite of the integral of the probability density function $f_X(x)$ multiplied by its base 2 logarithm in the space of all the possible values of the input signal x :

$$H(x) = - \int f_X(x) \log_2(f_X(x)) dx \quad (2)$$

where $H(x)$ is the entropy expressed in bits per transmitted sample [12] [*bit/sample*]. If we assume that the system has a bandwidth W , the entropy $H'(x)$ of the input signal [12] expressed in bits per second [*bit/sec*] is the entropy in [*bit/sample*] multiplied by the maximum rate of samples per second, which is equal to $2W$. The formula is [12]:

$$H'(x) = 2WH(x) \quad (3)$$

Definition 3.2: The **equivocation** $H_Y(x)$ is defined as the entropy of the signal x in input given the output signal y . The equivocation $H_Y(x)$ is computed as the opposite of the integral of the joint input-output distribution $f_{X,Y}(x,y)$ multiplied by the base 2 logarithm of the probability density function $f_{X|Y}(x|y)$ of the input signal x given the output signal y . The integral is computed over all the possible values

of the input signal x and the output signal y :

$$H_Y(x) = - \int \int f_{X,Y}(x,y) \log_2(f_{X|Y}(x|y)) dx dy \quad (4)$$

A. Information Entropy from Thermodynamic Entropy

The thermodynamic entropy is defined by Gibbs [7] as a measure of the disorder in a thermodynamic system. For the physical reference model introduced in Sec. II, the thermodynamic entropy S_r is expressed as follows:

$$S_r = -K_b \int_{\phi \in \Psi} f_{\Phi}(\phi) \ln(f_{\Phi}(\phi)) d\phi \quad (5)$$

where ϕ is a particular value for the phase space Φ of the system, $f_{\Phi}(\phi)$ is the distribution of phase space values for a specific set of values for the physical parameters and Ψ is the set of all the possible phase space values.

As stated in Sec. II, the physical reference model behaves according to the ideal gas theory. According to the Sackur-Tetrode equation [4], the entropy of an ideal gas in thermodynamic equilibrium has a closed-form expression as function of the physical parameters. Therefore, the entropy S_r of the physical reference model is [4]:

$$S_r = N_p K_b \left[\ln \left(\frac{V}{N_p} \left(\frac{2\pi m K_b T}{h^2} \right)^{\frac{3}{2}} \right) + \frac{5}{2} \right] \quad (6)$$

where N_p is the number of particles present in the system, K_b is the Boltzmann constant [7], V and T are the volume and the absolute temperature of the system, respectively, m is the particle mass and h is the Planck's constant [4].

The thermodynamic entropy formula in (5) can be reduced to the information entropy formula in (2) if the Boltzmann constant K_b is removed and the logarithm \ln is set to \log_2 . In the case of a diffusion-based MC system, we can interpret the thermodynamic entropy as an information entropy where the input signal values are the phase space values ϕ of the physical reference model. The Boltzmann constant K_b relates only to the conventional units of the temperature and it has meaning only in thermodynamics [7]. The logarithm \ln is converted into the \log_2 because [12] the units of the information entropy are $[bit/sample]$ or $[bit/sec]$. Thus, the information entropy H_{ref} of the physical reference model can be expressed as follows:

$$H_{ref} = N_p \left[\log_2 \left(\frac{V}{N_p} \left(\frac{2\pi m K_b T}{h^2} \right)^{\frac{3}{2}} \right) + \frac{5}{2} \right] \quad (7)$$

B. Input Signal Entropy

The input signal in the physical reference model introduced in Sec. II corresponds to the modulation of the **molecular features** (the local particle number and the particle type) operated by the **transmitter**.

A local entropy can be defined for the transmitter when it modulates the molecular features. The local information entropy depends on the molecular features and it can be computed from (7). The local entropy H_T at the transmitter is a function of the set M of all possible particle types, the number N_m for each particle type m from the set M ,

the absolute temperature T of the system and the transmitter volume V_T :

$$H_T = \sum_{m \in M} N_m \left[\log_2 \left(\frac{V_T}{N_m} \left(\frac{2\pi m K_b T}{h^2} \right)^{\frac{3}{2}} \right) + \frac{5}{2} \right] \quad (8)$$

where the transmitter volume V_T is equal to $(4/3)\pi r_T^3$. Due to the Gibbs theorem [7], (8) is the sum of each contribution coming from the application of (7) to each particle type at the transmitter, considered as independent contributions.

The total entropy H_{ref}^{mod} of the physical reference model when the transmitter is modulating the particle features can be written as the sum of H_T from (8) and H_{ref} from (7):

$$H_{ref}^{mod} = H_T + H_{ref} \quad (9)$$

While the transmitter modulates, it inserts information in the system. This information, according to the Second Law of Thermodynamics [6], eventually will fade out when the physical reference model will reach a new thermodynamic equilibrium state, characterized by a higher entropy H_{ref}^{new} , which is expressed as follows:

$$H_{ref}^{new} = N_{tot} \left[\log_2 \left(\frac{V}{N_{tot}} \left(\frac{2\pi m K_b T}{h^2} \right)^{\frac{3}{2}} \right) + \frac{5}{2} \right] \quad (10)$$

where $N_{tot} = N_p + \sum_{m \in M} N_m$ is the total number of particles in the system and N_p is the number of particles before modulation. In order to quantify the input signal entropy, we subtract the total entropy H_{ref}^{mod} from the entropy H_{ref}^{new} :

$$H(x) = H_{ref}^{new} - H_{ref}^{mod} \quad (11)$$

where $H(x)$ is the input signal entropy in $[bit/sample]$

If we consider a bandwidth W for the system, we can transmit $2W$ samples per second without equivocation. According to (3) the input signal entropy in $[bit/sec]$ becomes:

$$H'(x, W) = 2W (H_{ref}^{new} - H_{ref}^{mod}) \quad (12)$$

C. Equivocation

The received signal in the physical reference model introduced in Sec. II corresponds to the reading of the changes in the **molecular features** operated by the **receiver**.

The propagation of the signal from the transmitter to the receiver affects the value of the local entropy at the receiver. The variation in the local entropy at the receiver H_R at instant t and distance d corresponds to the variation in the entropy of the spherical surface at instant t and distance d , divided by the spherical surface area $4\pi d^2$:

$$H_R(d, t) = \frac{H_R^{sph}(d, t)}{4\pi d^2} \quad (13)$$

The variation in the entropy in the spherical surface can be computed from (7) with a number of particles N_{eq}^m and a volume V_{eq} . The variation in the entropy $H_R^{sph}(d, t)$ in the spherical surface is:

$$H_R^{sph}(d, t) = \sum_{m \in M} N_{eq}^m \left[\log_2 \left(\frac{V_{eq}}{N_{eq}^m(d, t)} \left(\frac{2\pi m K_b T}{h^2} \right)^{\frac{3}{2}} \right) + \frac{5}{2} \right] \quad (14)$$

The equivalent number of particles $N_{eq}^m(d, t)$ of the ideal gas corresponds to the number of particles that diffuse from the

transmitter to the receiver located at a distance d , expressed as the number N_m of transmitter particles (of type m) multiplied by the probability for each particle of shifting by a distance d at a time instant t , according to the Brownian motion [5]:

$$N_{eq}^m(d, t) = N_m \frac{1}{\sqrt{4\pi Dt}} e^{-\frac{d^2}{4Dt}} \quad (15)$$

The value of the equivalent volume V_{eq} divided by the equivalent number of particles $N_{eq}^m(d, t)$ the inverse of the concentration of type m particles at the spherical surface at instant t and distance d . This is expressed as follows:

$$\frac{N_{eq}^m(d, t)}{V_{eq}} = \frac{N_m}{V_T} \frac{1}{\sqrt{4\pi Dt}} e^{-\frac{d^2}{4Dt}} = \frac{N_{eq}^m(d, t)}{V_T} \quad (16)$$

The equivocation formula in (4) corresponds to the increase in entropy of the signal as it propagates in the channel, and it depends on the number of particles that reach the receiver location in a certain time t . The equivocation $H_Y(x)$ is expressed as follows:

$$H_Y(x) = H_R(d, t) - \frac{H_T}{V_T} \quad (17)$$

where $\frac{H_T}{V_T}$ is the entropy of the transmitted signal per unit volume and $H_R(d, t)$ is the entropy of the received signal, (13).

If we consider a bandwidth W for the system, we can receive up to $2W$ samples per second without equivocation. The variation in the entropy $H_{R,W}^{sph}$ in a spherical surface with bandwidth W at distance d is computed through:

$$H_{R,W}^{sph} = \sum_{m \in M} N_{eq,W}^m \left[\log_2 \left(\frac{V_{eq}}{N_{eq,W}^m} \left(\frac{2\pi m K_b T}{h^2} \right)^{\frac{3}{2}} \right) + \frac{5}{2} \right] \quad (18)$$

where $N_{eq,W}^m$ is equal to the number of particles that diffuse from the transmitter to the receiver located at a distance d and for a bandwidth W , under the hypothesis of not having influences between the diffusion of two different samples. This will result in an overestimation of the capacity. $N_{eq,W}^m$ is expressed as follows:

$$N_{eq,W}^m = N_m \sqrt{\frac{2W}{4\pi D}} e^{-\frac{2Wd^2}{4D}} \quad (19)$$

As a consequence, the variation in the local entropy at the receiver $H_R(W)$ with bandwidth W and distance d is:

$$H_R(W) = \frac{H_{R,W}^{sph}}{4\pi d^2} \quad (20)$$

The equivocation formula in [bit/sec] becomes:

$$H_Y(x, W) = 2W \left(H_R(W) - \frac{H_T}{V_T} \right) \quad (21)$$

where $H_R(W)$ is computed through (20), H_T through (8) and V_T is defined in Sec. (III-B).

D. Capacity

The information capacity of the diffusion-based MC system, given the physical reference model detailed in Sec. II, is expressed by the formula in (1), where the input signal entropy $H(x)$ is given by (11) and the equivocation is given by (17).

The final expression of the capacity becomes:

$$C = \max_{f_X(x)} \left\{ H_{ref}^{new} - H_{ref}^{mod} - \left(H_R - \frac{H_T}{V_T} \right) \right\} \quad (22)$$

with reference to (10), (9), (13) and (8).

If we consider a bandwidth W for the system, the information capacity $C(W)$ of the diffusion-based MC system is expressed as a function of W by the formula in (1), where the input signal entropy $H(x, W)$ is given by (12) and the equivocation $H_Y(x, W)$ is given by (21).

$$C(W) = \max_{f_X(x)} 2W \left\{ H_{ref}^{new} - H_{ref}^{mod} - \left(H_R(W) - \frac{H_T}{V_T} \right) \right\} \quad (23)$$

with reference to (10), (9), (20) and (8).

A closed form expression for the capacity of the diffusion-based MC system is given by the input signal probability density function $f_X(x)$ that maximizes (1). Such a value for $f_X(x)$ can be found by setting a constraint on the total transmitted power, namely, the transmitter enthalpy power $P_{\mathcal{H}}$:

$$P_{\mathcal{H}} = 2\mathcal{H}W \quad (24)$$

where \mathcal{H} is the transmitter enthalpy and W is the bandwidth.

Definition 3.3: The **transmitter enthalpy** is defined as the energy necessary to insert N particles in the system and to heat these particles up to a temperature T when the system has the pressure P and the volume V [6]. In our case, the transmitter enthalpy can be computed from:

$$\mathcal{H} = PV + \frac{3}{2} K_b T \sum_{m \in M} N_m \quad (25)$$

where P and V are the pressure and the volume of the physical reference model, respectively. M is the set of all possible particle types that the transmitter can emit, N_m is the number of particles of type m , K_b is the Boltzmann constant and T is the absolute temperature of the system.

The entropy H_{ref}^{mod} from (9) can be written as function of the transmitter power by expressing N_m as a function of $P_{\mathcal{H}}^m$:

$$N_m^P = \frac{P_{\mathcal{H}}^m - 2WPV}{3WK_bT} \quad (26)$$

where $P_{\mathcal{H}}^m$ is the fraction of the power assigned to each particle type m and P and V are the pressure and the volume of the physical reference model, respectively. The maximum of the input signal entropy $H(x, W)$ corresponds to the distribution of the power that results in the minimum H_T^{min} of H_T from (8), which is the even distribution of the power $P_{\mathcal{H}}^m$ among all the M types of particles that the transmitter can send:

$$P_{\mathcal{H}}^m = \frac{P_{\mathcal{H}}}{M} \rightarrow H_T = H_T^{min} \quad (27)$$

The equivocation $H_Y(x)$ as function of the transmitter enthalpy power is computed through (21) where both H_T and $H_R(W)$ can be expressed as function of the fraction of power $P_{\mathcal{H}}^m$ assigned to each particle type m . The optimal distribution of power in (27) minimizes $\frac{H_T}{V_T}$, and it minimizes also $H_{R,W}^{sph}$ and, consequently, $H_R(W)$ from (20). We can logically assume that if d is sufficiently large, the entropy $\frac{H_T}{V_T}$

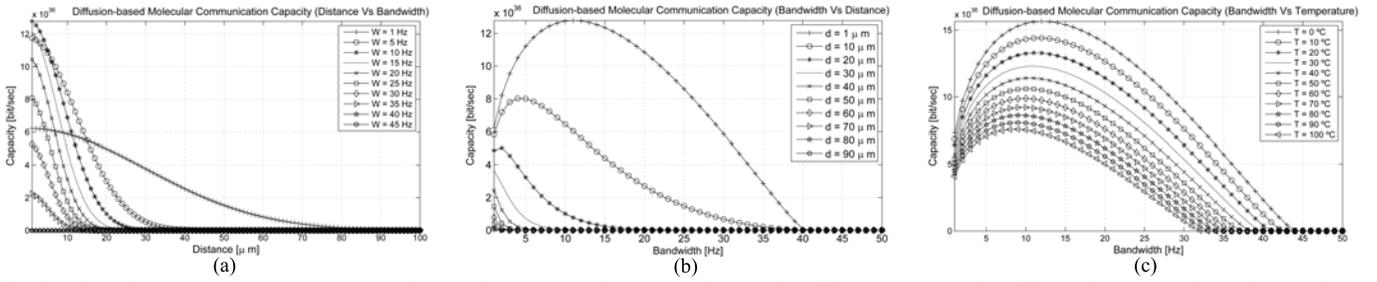


Fig. 2. Capacity in relation to: (a) the transmitter-receiver distance for values of bandwidth W , (b) the bandwidth W and for values of the distance d , (c) the bandwidth W and values of the system temperature T .

is negligible with respect to the contribution of $H_R(W)$:

$$H_R(W) \gg \frac{H_T}{V_T} \quad (28)$$

Therefore, the minimum of the equivocation $H_Y(x)$ corresponds roughly to the minimum of $H_R(W)$, denoted as $H_R^{\min}(W)$, given by the even power distribution in (27).

A closed form expression for the capacity of the diffusion-based MC system is:

$$C(W) = 2W \left[H_{ref}^{new} - H_{ref}^{mod,min} - \left(H_R^{\min}(W) - \frac{H_T^{\min}}{V_T} \right) \right] \quad (29)$$

with reference to (10), (9), (20), (8), evaluated with (27). The transmitter volume V_T is defined in Sec. (III-B) and $H_{ref}^{mod,min}$ is equal to (9) where H_T is substituted with H_T^{\min} .

IV. NUMERICAL RESULTS

In this section, we provide numerical results for the capacity in MC nanonetworks. All the results are computed for a common set of parameters, whose values are assigned as follows: the total transmitter enthalpy power $P_{\mathcal{H}} = 1\mu\text{W}$ (arbitrary value), the radius of the space $r_S = 1\text{cm}$, while the radius of the transmitter $r_T = 1\mu\text{m}$, the mass of the particles $m = 1.66053878283 \times 10^{-27}\text{kg}$ (standard atomic mass unit [8]), the number of particles N_p is set equal to one mole [6] $6.0221417930 \times 10^{23}$, the number $M = 5$. The diffusion coefficient D is set [11] to $10^{-9}[\text{m}^2/\text{sec}]$ for a temperature of 25°C as a reference, and it is varied according to the actual temperature values by following the Einstein-Stokes equation [5].

All the results come from the evaluation of (29), (20), (10) and (8), given the condition of having an even distribution of the transmitted power among all the types of particles, (27).

The results in Fig. 2 (a), (b) and (c), show extremely high values for the capacity which are on the order of magnitude of $10^{36}[\text{bit}/\text{sec}]$. They can be physically explained as follows: we consider a transmitted sample as any combination of the number of particles of any possible type out of M , bounded by the transmitter power using (26). We achieve a maximum number of molecules N_m^P (Eq. (27) and (26)) on the order of magnitude of 10^{12} per each type m . Therefore, the number of combinations we can achieve using the optimal modulation scheme is extremely high and, consequently, also the capacity.

In Fig. 2 (a) and (b) we show the capacity of a diffusion-based Molecular Communication nanonetwork in relation to the transmitter-receiver distance from 1 μm to 100 μm and

different values of the bandwidth W , from 1 Hz to 45 Hz. In Fig. 2 (c) we show the capacity dependent on the bandwidth W ranging from 1 Hz to 45 Hz and the temperature T . Different lines refer to different system temperature T values, from 0°C to 100°C .

V. CONCLUSION

Molecular Communication (MC) is a promising paradigm for communication in nanonetworks. The objective of this paper is to provide a mathematical expression for capacity in MC when the propagation of information relies on the free diffusion of molecules. Molecular communication capacity is derived as a function of the physical parameters as well as the bandwidth of the system and the transmitter power. Numerical results have an extremely high order of magnitude if compared to capacity values in classical EM-communication systems. Further investigation will be focused in the future on finding more stringent upper bounds to the performance (e.g., using a given modulation scheme at the transmitter).

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