Influence of inter-nanoparticle interaction on nanonetworks-based molecular communications

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With the rapid penetration of nanonetworks-based molecular communication (MC), many studies potentially investigated the influence of nanoparticles on the performance of transmission/delivering nanoscale information. In this study, we analytically investigate a new collision/adhesion-based MC framework by considering the inter-nanoparticles near field interaction such as van der Waals forces and the electronic structure of the nanoparticles in terms of hardness coefficient. In this context, we derive a closed-form expression of the required velocity for two nanoparticles to physically contact in terms of near field forces and hardness coefficient of the nanoparticles. In consequence, we study the performance of the proposed MC framework in intra-body nervous system nanonetwork. Then, we evaluate the performance of the proposed nanonetwork-based mobile ad hoc molecular nanonetwork metrics of interest such as average packet delay, network throughput and sustained traffic rate. The numerical results reveal that when the mutual interaction between molecules is attractive force, it generally provides a better performance; more specifically, it can deliver information with lower delay than repulsive force although the hardness coefficient of nanoparticles is small.

1. Introduction

With the rapid penetration of nanonetworks-based molecular communication (MC), there are many works that investigated the influence of nanoparticles (molecules) on the performance of transmission/delivering nanoscale information [1–6]. More recently, a mobile ad hoc molecular nanonetwork (MAMNET) paradigm based on collision process has been proposed in [7]. A molecular neurospike communication that is analogous to electrochemical impulses among neuron cells [15] has been adopted for transmission of nanoscale information in MAMNET. Neurotransmitter (information molecule) can be envisioned as a mobile nanomachine in MAMNET, which has the characteristic and behavior of nanoparticle Brownian motion, with a collision and adhesion basis, it transmits its nanoscale information to another nanomachine by means of neurospike communication. In addition, neurotransmitters are involved in broad aspects of physiological and cognitive processes, such as memory, learning, depression and Alzheimer’s disease, which is controlled by neuron’s brain-based CORNU AMMONIS (CA) area [8].

In intra-body nervous system nanonetworks, communication between neurons occurs through a process called neurotransmission. Neurotransmission takes place through substances termed as neurotransmitters. At least 100 substances are known to act as neurotransmitters; about 18 are of major importance. The most important neurotransmitters are serotonin, adrenaline, noradrenaline, dopamine, acetylcholine and amino butyric acid (GABA) [9]. From the list of neurotransmitters released by a neuron, the type of transmitter released by a neuron determines the action on the postsynaptic neuron. This can be either excitatory, e.g., glutamate and acetylcholine or inhibitory, e.g., GABA and glycine [9]. Kobayashi and Terao [10] have calculated the hardness, H, and electronegativity forces, Ea, parameters and they applied this foundation to neurotransmitter in order to identify or characterize different types of neurotransmitters and receptors involved in neurospike molecular communication. As consequence, the electronic structure of neurotransmitters can be defined by using H and Ea parameters [10] and [11]. Moreover, they pioneered this research and showed that there is a direct relationship between H and biological activity of neurotransmitters.

On the other hand, neurotransmitters are considered as biological molecules that collide together by various reversible and
non-covalent interactions. Consequently, they play an essential mechanism in the folding of proteins, the recognition of neurotransmitter and the interactions between receptor and ligand [12]. The ability of a protein to bind selectively and with high affinity to a ligand depends on the formation of a set of weak, noncovalent bonds—hydrogen bonds, ionic bonds and van der Waals attractions plus favorable hydrophobic interactions. Even the weak forces such as electrostatic interactions, van der Waals forces, hydrogen bonding and hydrophobic interactions are responsible for the correct structure and functioning of the biological molecules [13]. The process of constructing and deconstructing of hydrogen bonds permits functional proteins to change from one form to another. For instance, Alzheimer’s disease (due to acetylcholine deficiency) might damage the electrical charges routes which travel within neuron cells and the activity of neurotransmitters, wherein the neurotransmitters are able to form hydrogen bonds and to interact through van der Waals, thus result in conformational changes by breaking hydrogen bonds in proteins [14].

As molecular neurospike communication, formulated on the foundation of an electrochemical communication among biological neurons, is proposed in [15], also widely used in many literatures. Although neurospike molecular communication has been extensively studied in [7] and [16–19], the influence on performance of nervous communication applied in nanonetworks in conjunction with neurotransmitters electronic structure and the mutual interaction forces of the nanomachines (nanoparticles) have not been successfully addressed and examined. Specifically, the major objectives of this study is to investigate the influence of electronic structure and intermolecular forces on the performance of nanonetwork-based MC. To the best of our knowledge, in this paper, we illuminate the aspect of neurotransmitters electronic structure and interacting molecules that are not explored in previous literatures. We especially focus on determining the critical velocity, which is required for two molecules to adhere after collision process.

In addition, due to the random mobility of nanoparticles, it initiates nanoparticle’s fluctuating electrical charge; hence, we will take into account the interactions between molecules, in terms of interaction near-field forces such as van der Waals force. As a consequence, we derive a closed-form expression of critical velocity required for physically to be in contact, as a function of molecule’s size, hardness, density and inter-molecule near-field interaction. After that, we fine-tuned the theory of neural communication, in order to obtain the relationship between signal-to-noise ratio (SNR) and optimal threshold at the receptor. Then, we determine neurospike channel capacity and probability of error according to SNR. Moreover, we consider a single-input–single-output (SISO) molecular communication channel-based MAMNET specification in order to evaluate the performance of the proposed nanonetwork in terms of average packet delay, network throughput and sustained traffic rate. The numerical results reveal that when the mutual interaction between molecules is attractive force, it generally provides a better performance. More specifically, average packet delay improvement in the nanonetwork under van der Waals attractive force is better enhanced than when under repulsive experience.

The reminder of the paper is organized as follows. In Section 2, we give a brief summary of molecular theory-based collision. Section 3 introduces the near-field interaction theory, wherein the collision and adhesion rates are derived in terms of critical velocity and mutual interaction forces. In Section 4, we illustrate the theory of neurospike communication in intra-body nervous system. In Section 5, we evaluate the performance of nanonetwork-based MC in terms of MAMNET metrics. The numerical results of the proposed network are presented in Section 6. Finally, Section 7 concludes the paper. For the remainder of this paper, the terms molecule, nanomachine and nanoparticle are used interchangeably.

2. Molecular communication (MC) theory

Molecular communication (MC) mechanism defined as the transfer of nanoscale information as carrier-based molecules. Recently, MC is considered a promising technique for realizing the communication between nanomachines [1,21]. In MC, transmitter nanomachine (TN) utilizes molecules for encoding and transmitting nanoscale information unlike traditional electromagnetic waves. For instance, nanoscale information can be encoded into the number, level of concentration or type of the nanoparticles released. Irrespective to encoding scheme, information is transmitted through mass transfer (i.e., transfer of particles). The theory and concept of MC has presented in [1], wherein two MC techniques are presented, namely MC-based molecular motors and MC-based calcium signaling. Furthermore, inspired by biophysical, MC is performed by the chemical interaction among different molecules, it is essential based on diffusion and collision procedure. With the potential impact of MC on various applications, numerous research efforts have motivated to apply the principle and theory of conventional communication system into MC [1]. Drug delivery is the most recent application of MC in nanomedical field by allowing groups of nanomachines to cooperate in order to maximize the therapeutic effect of drug molecules [4].

Similar to traditional mobile ad hoc network (MANET), in MC, due to the random motion or freely diffuse of molecules in aqueous medium, the mobile molecules (nanomachines) collide with each other and the molecular adhesion-based chemical reaction occurs between the collided molecules [22], a MAMNET paradigm is proposed in [7]. In MAMNET, as illustrated in Fig. 1, when transmitter nanomachines have information, collide and adhere to other nanomachines, they transmit their message to those nanomachines. A typical reception mechanism observed among living cells is based on a ligand–receptor binding process [23], in which, arriving molecules at the receiver nanomachine collide and bind to the unbound receptor of the receiver. Molecules adhesion are accomplished by the ligand–receptor binding process. Therefore, after collision procedure, the adhesion should occur in order to allow for transmitting nanoscale information and the communication between molecules happen as illustrated in Fig. 1. As shown in this figure, the nanoscale information is communicated from transmitter nanomachines (TNs) to receiver nanomachines (RNs) after the diffusion, collision and adhesion and hence reaction process.

3. Near-fields interaction

The desired nanoscale information at the location of the receptor may vary from one individual to the other, depending on the interactions between the receptor and ligand, which in fact depends on the amino acids binding of nanoparticles to the receptors. The
amino acid-based chemical properties are classified according to the type of binding that may occur. There are two well-known non-polar amino acids, namely aliphatic and aromatic [13]. They can mainly interact via hydrophobic interactions and van der Waals forces. In this study, we focus on van der Waals forces, which occurred as a result of an nanoparticle’s fluctuating electrical charge. Further, due to the random mobility of nanoparticles, it initiates an electrical dipole; this induces a temporary charge in a neighboring nanoparticles by attracting or repelling the electrons associated with it, resulting in a momentary attractive force between the two nanoparticles [24,25].

In the following section, we derive a closed-form expression of the required velocity for two nanoparticles to be in a physical contact while taking into account the van der Waals forces. The objective of this study aims to shed light on various fundamental aspects of molecule collision and adhesion phenomena. With an emphasis on realistic adhesion procedure, the biophysical process for molecules interaction is similar to nanoparticles interactions; it should be studied under the influence of near-field forces. In particular, we isolate and focus on a single aspect of molecule adhesion, targeting the determination of the impact velocity needed for two nanoscale molecules to adhere as a function of molecule size, hardness coefficient, density and inter-molecule near-fields interaction.

### 3.1. Critical velocity-based nanoparticles interaction

After the collision of any two nanoparticles, the occurrence of adhesion may happen or not, depending on the coefficient of restitution, e. More specifically, e \(\equiv 1\) is perfectly elastic impact and e \(\equiv 0\) is a perfectly plastic, i.e., full adhesion impact [26]. Let us consider an illuminating scenario. We consider two nanoparticles having spherical shape and with different diameters are in contact with each other and relative velocity is \(v_{kj}\) as illustrated in Fig. 2. The radii of the left and right nanoparticle are \(b_k\) and \(b_j\), respectively.

During collision process, the van der Waals force is taken into account. From Fig. 2, we can obtain the following equations. The collision between two nanoparticles, k and j depends upon the coefficient of restitution, e as follows:

\[
e = \frac{\text{Relative speed after collision}}{\text{Relative speed before collision}}
\]

Moreover, the author at [26] has presented a detailed study for the coefficient of restitution \(e\) and the dependence of this coefficient on severity of influence velocity and, implicitly, the pressure in the contact area. Therefore, for any two nanoparticles, moving with critical relative velocity \(v_c\) in opposite direction each other, the parameter \(e\) can be approximated by a linear scaling with pressure-to-hardness ratio. Consequently, for an individual nanoparticle \(k\), the parameter \(e_k\) depends upon the critical impact velocity \(v_c(0)\), size of the nanoparticle and the contact area between the nanoparticles as follows:

\[
e_k = \max \left(1 - \frac{m_k v_c(T_c) - v_c(0)}{2H_k T_c A_k}, 0\right)
\]

where, \(T_c \equiv k b_k / m_k\) denotes the collision time and \(k_2\) is a dimensionless constant. \(A_k\) is the contact area between two nanoparticles, \(m_k \equiv (4/3)\rho_k \pi (b_k)^3\) is the mass of nanoparticle with density of \(\rho_k\) and radius of \(b_k\). \(H_k\) is the hardness coefficient of nanoparticle. In particular, we isolate and focus on a single aspect of nanoparticle adhesion, namely the determination of the impact velocity needed for two nanoscale molecules to adhere as a function of molecule size, hardness and density. As a consequence, after the collision of any two molecules, the occurrence of adhesion may happen or not, that is, it depends on the coefficient of restitution, \(e_k\) (where, \(e_k \equiv 1\) is fully elastic impact and \(e_k \equiv 0\) is an entirely plastic, i.e., fully adhesion impact).

By setting \(e_k \equiv 0\) and \(v_c(T_c) \equiv 0\) in Eq. (1) for fully adhesion condition, we can obtain the critical velocity \(v_c(0)\) for collided molecules to adhere as follows [26]:

\[
v_c^2 \geq \frac{2H_k T_k A_k}{m_k} = \frac{3H_k A_k k_2}{2\pi \rho_k b_k^5}
\]

In simpler terms, the critical velocity for two molecules to adhere, based solely on contact area, is directly proportional to the molecule’s hardness and inversely proportional to its density [26]. By taking into account the effect of inter-nanoparticles near-field’s interaction such as van der Waals forces, electrostatic, etc. As a type of forces between the nanoparticles, an excellent theoretical study of van der Waals forces and its applications has been studied in [27]. The van der Waals force is important and may be affected by the type of chemical drug or biological bonds. The adhesion condition takes the following form [26]:

\[
v_{kj}^2 \geq \frac{2H_k A_k + E_{kj}(d_{kj})}{m_k} T_k
\]

where, \(E_{kj}(d_{kj})\) denote the average impulse acting between the nanoparticles due to the inter-nanoparticles near-field interactions and, may be considered as a function distance, where, \(d_{kj}\) is the distance between the centers of the molecules and is expressed as \(d_{kj} = |\mathbf{r}_k - \mathbf{r}_j|\). Both \(\mathbf{r}_k\) and \(\mathbf{r}_j\) are the position vectors of the centers of nanoparticles, and the minimum distance between the centers of nanoparticles is the sum of radii \(b_k + b_j\) (at the moment of collision contact). By substituting \(T_c\) and \(m_k\) into Eq. (3), we obtain:

\[
v_{kj}^2 \geq \frac{2H_k A_k + E_{kj}(d_{kj})}{m_k} \frac{3k_2}{4\pi \rho_k b_k^5}
\]

A simplified expression of \(E_{kj}(d_{kj})\) can be given as [26]

\[
E_{kj}(d_{kj}) = \frac{m_k m_j}{d_{kj}} \left(\frac{4\pi}{3}\right)^{2} \rho_k \rho_j b_k^5 b_j^5 |\mathbf{r}_k - \mathbf{r}_j|^{-\beta} \times \alpha
\]

The parameters \(\alpha\) and \(\beta\) in Eq. (5) play a significant role in the strength and the type of the inter-nanoparticles force. As a consequence, \(\beta\) refers to the strength of the inter-nanoparticles force, such that \(0 < \beta < \infty\), while \(\alpha\) expresses the type of inter-nanoparticles interaction. If \(\alpha < 0\), then the interaction between the nanoparticles is repulsive force, otherwise when \(\alpha > 0\), the interaction between the nanoparticles is attractive force. At the moment of contact and the occurrence of adhesion of any two nanoparticles substituting \(|\mathbf{r}_k - \mathbf{r}_j| = (b_k + b_j)\) into Eq. (5), we obtain

\[
E_{kj}(d_{kj}) = \left(\frac{4\pi}{3}\right)^{2} \rho_k \rho_j b_k^5 b_j^5 (b_k + b_j)^{-\beta} \times \alpha
\]
On the other hand, if the two nanoparticles have the same properties \((\rho_k \equiv \rho_1\) and \(b_k \equiv b_1)\), we obtain
\[
E_{ki} = \frac{2^4}{9} \pi^2 \rho^2 b^6 \beta \times \alpha
\]  
(7)

By substituting of \(E_{ki}(d_{ki})\) into Eq. (4), we obtain
\[
v_{ki} \geq 3Hb_{ki}k_2 \left[ \frac{3Hb_{ki}k_2}{2\rho b^3} + 4 \frac{2^2}{3} k_2 \rho b^2 \beta (b_1 + b_1)^2 \alpha \right]
\]  
(8)

There are two types of mobile nanoparticles in nanonetwork called nanomachine and infostation. Without any loss of generality, we have two types of collision between mobile nanoparticles as follows:

1. When the nanoparticles are the same and considered as nanomachines then the critical velocity is given by
\[
v_{cm} \geq \sqrt{\frac{3Hb_{ki}k_2}{2\rho b^3} + 4 \frac{2^2}{3} k_2 \rho b^2 \beta (b_1 + b_1)^2 \alpha}
\]  
(9)

When the nanoparticles are different, considered as nanomachine and infostation or vice versa then the critical velocity is
\[
v_{cm} \geq \sqrt{\frac{3Hb_{ki}k_2}{2\rho b^3} + 4 \frac{2^2}{3} k_2 \rho b^2 \beta (b_1 + b_1)^2 \alpha}
\]  
(10)

Therefore, the average relative velocity between any two nanoparticles can be determined while the mutual interaction force between nanoparticles is taken into account. Let us assume that \(f_i[v_{in}]\) is the average relative velocity for nanomachines and \(f_i[v_{in}]\) is average relative velocity for nanomachine and infostation. Thus, according to Eqs. (10) and (11), \(f_i[v_{in}]\) and \(f_i[v_{in}]\) can be determined as follows:

\[
f_i[v_{in}] = \frac{1}{2}(v_{in} + v_{ni})
\]  
(11)

3.2. Collision and adhesion rate

Due to the stochastic nature of mobile nanoparticles in the aqueous medium in nanonetwork, the collision rate is governed by not only the mobility of the nanoparticles but also by the near-field interactions of the nanoparticles each to other, or in other words, there is a mutual effect generates from the inter-nanoparticle near fields. Therefore, the collision rate between two nanomachines, is denoted as \(R_{nm}\) and the collision rate between nanomachine and infostation is \(R_{ni}\); both \(R_{nm}\) and \(R_{ni}\) can be approximated respectively as follows [7]:

\[
R_{nm} \approx \frac{\pi(2b_n)^2 f_i[v_{in}]}{V}
\]  
and

\[
R_{ni} \approx \frac{\pi(b_n + b_i)^2 f_i[v_{in}]}{V}
\]  
(13)

where, \(b_n\) and \(b_i\) are the radii of nanomachine and infostation, respectively, and all of these nanoparticles are considered to be contained in the volume \(V\) since \(V \times b_n\) and \(b_1 > b_n\).

The adhesion is assumed to happen via binding nanoparticles on the surface of two nanomachine and depends on the contact area [26]. The full adhesion is happened when the velocity of nanomachine reached to its critical value as derived in Eq. (3), hence, we can obtain the contact area \(A_c\) as follows:

\[
A_c = \frac{v_{ni}m_1}{2H_{ki}} - E_{ki}(d_{ki}) \leq 2\pi b^2
\]  
(14)

The probability of \(n\) bonds at time \(t\), \(P_n(t)\) can be given by [23]:

\[
P_n(t) = \left(\frac{c_{m_{\min}}}{n}\right)^n[1 - P_1(1)]
\]  
(15)

where, \(m_{\min}(m_{\max})\) is the minimum (maximum) surface density of bonding molecules and \(P_1(1)\) is the probability of forming one bond given by

\[
P_1(1) = \frac{1 - e^{-K_t}}{1 + (m_{\max}K_t)}
\]  
(16)

Here, \(K_t = k_f/k_i\) is the equivalent constant. \(K_t = m_{\max}k_f/k_i\) is the total rate of reaction [23], \(k_f\) and \(k_i\) denote the forward and reverse binding reactions.

A simplified expression of adhesion rate provided that the kinetic probability rates are constants [23]. If the adhesion of nanomachines needs minimum of \(n\) bonds, then the rate of adhesion at contact time \(T\) is:

\[
R_{ad}(t) = 1 - \sum_{i=0}^{n-1} P_i(t)
\]  
(17)

4. Intra-body nervous system nanonetworks

A simplified block diagram of nervous system-based nanonetworks is illustrated at Fig. 3. In nervous system, the communication between different neurons can be enabled based on spike or action potential. The arrival of arriving spike yields an influx of calcium (Ca2+) ions through voltage-dependent calcium ion channels [16]. Generally, spike signals are propagated and transmitted, from the axon of input (presynaptic) neuron to a dendrite of that neuron, then axon can transmit an output signal to an output (postsynaptic) neuron, and a dendrite receives an input signal from a presynaptic neuron as illustrated in Fig. 3. Calcium ions then bind to the proteins found within the membranes of the synaptic vesicles. The vesicles then release their contents, neurotransmitters, i.e., information molecules, to the synaptic cleft. There are two known types of neurotransmitter, namely, chemical and electrical. The chemical neurotransmitters enable nervous nanonetwork to communicate and control other network in the body and they are based on biological computations [28].

In human nervous system, the neurotransmitters are the main information carrier and a precise control of their action at their
specific presynaptic and/or postsynaptic receptors. A neuron can recognize many different types of receptors, each sensitive to a specific neurotransmitter. The two main types of neurotransmitter receptors are called ionotropic and metabotropic receptors [8]; the main difference between them is the ionotropic receptors are considered faster and generate shorter responses than metabotropic receptors. Thus, the action on the postsynaptic neuron is determined by the neurotransmitter released by presynaptic neuron. This can be either excitatory (common: glutamate, acetylcholine) or inhibitory (common: GABA, glycine) [8–10].

Furthermore, as illustrated at Fig. 3, the intra-body nervous system is experienced of noise, n(t), effect on the response of receptor [16]. There are two different sources of noise in the intra-body nervous nanonetwork, due to thermal noise and channel noise. This type of noise represents the synaptic noise at the membrane receptor. In the presence of such noise, the mechanism of receptor/detector to optimally detect the absence or presence of a single spike-based knowledge of membrane voltage. In this paper, we fine-tuned the principles of neural communication in order to accomplish the relationship between signal-to-noise ratio (SNR) and optimal threshold at the receptor.

4.1. Error probability in neuronal communication

The neuronal communication is analogues of traditional communication system, involved by synaptic encoding, transmission, propagation, reception and decoding, respectively, as depicted in Fig. 4. Thereby, the performance of synaptic transmission depends on SNR ratio and hence is negatively affected by the error probability of spike detection. At the presynaptic side, we utilized a stochastic Poisson process in order to modulate a spike rate, as a convolution between the stimulus m(t) and a phenomenological filter k(t) as follows: ±(t) ≡ k(t) × m(t) [15]. The stimulus is drawn from a Gaussian probability distribution. Without loss of generality, we assume a fully synchronization between the neurons and hence the channel state information (CSI) at the postsynaptic is available. Then, we consider a symmetric binary channel as the approach to model the channel for synaptic transmission. Let p0 denote the a priori probability of spike release at presynaptic neuron, while at the postsynaptic, the response to release of a single packet neurotransmitter is modeled by the synaptic transient function h(t) [35] and [19]:

\[ h(t) = h_p(t / τ_p) e^{-t / τ_p} \]  

(18)

where, \( h_p \) is the maximum excitatory postsynaptic potential (EPSP) magnitude and \( τ_p \) is the equivalent time-to-maximum.

Subsequently, we model synaptic variability by multiplying the response h(t) by a random variable q of probability distribution \( P(q) \) [35]. Moreover, q represents the variability in the amplitude of the postsynaptic responses neurons. We model \( P(q) \) by Gamma distribution as expressed in [19]:

\[ P(q) = \frac{a^q e^{-aq}}{\Gamma(j - 1)} \]  

(19)

where, a and j are, respectively, the shape and rate of Gamma distribution.

Inspired by information theory, the performance of synaptic transmission depends on SNR, which relies nature random process of additive white Gaussian noise (AWGN). Therefore, for the postsynaptic neuron voltage v(t) coexisting with noise, n(t) should be estimated. The power spectral density (PSD) for a band limited n(t) is denoted by \( P_{\text{in}}(f) \) and is given by

\[ P_{\text{in}}(f) = \begin{cases} \frac{σ^2}{2πf^n} & -B_n ≤ f ≤ B_n \\ 0 & \text{otherwise} \end{cases} \]  

(20)

Where, \( σ^2 \) is the variance of n(t) over a bandwidth \( B_n \). The SNR ratio for the synapse defined as

\[ \text{SNR} = \frac{1}{P_{\text{in}}(f)} \int_0^\infty h^2(t)dt = \frac{2B_n}{σ^2} \int_0^\infty h^2(t)dt \]  

(21)

The corresponding postsynaptic voltage waveform v(t), measured over a time slot, corresponds to either the noise process n(t) (denoted by hypothesis \( Ω_0 \)) or to a noisy version of the EPSP h(t) gatened by stochastic vesicle release W (denoted by hypothesis \( Ω_1 \)) [35]. Thereby, the detection of binary signal can be properly expressed by binary hypothesis \( \Omega_k \) testing problem as follows:

\[ \Omega_0 : v(t) = n(t) \]  

(22)

\[ \Omega_1 : v(t) = q × W + h(t) + n(t) \]  

where, q is the random EPSP amplitude and W is a binary variable representing the spike-conditioned vesicle release process (W \( \equiv 1 \)).

Let X and Y represent the binary variables of presynaptic spike and decision occurrence, respectively. Hence, X \( \equiv 1 \) if a spike is emitted, otherwise X \( \equiv 0 \). Similarly, Y \( \equiv 1 \) expresses the decision that a spike is delivered. At postsynaptic side, the optimal decision rule minimizes the error probability in detecting binary presynaptic spike from postsynaptic membrane voltage. However, in practice, the binary channel depends on cross-over error probabilities and more specifically false alarm and miss detection errors [15]. Let \( P_f \) and \( P_m \) denote the false alarm and miss detection probabilities that are defined as \( P_f = \text{Prob}(Y \equiv 1 | X \equiv 0) \) and \( P_m = \text{Prob}(Y \equiv 0 | X \equiv 1) \), respectively. Then, if TN emits spike bit 1 with a priori probability, \( p_0 \) and spike bit 0 with probability, \( p_1 = (1 - p_0) \), the probability of detection error, \( P_e \) can given by

\[ P_e = p_0 P_m + p_1 P_f \]  

(23)

The probability for detecting error at postsynaptic neuron depends formerly on SNR and latterly on the threshold utilized by the decision rule [29]. Let \( θ_\text{in} \) and \( θ \) denote the threshold and comparing correlation parameter for optimal decision rule, respectively. Thereby, \( P_f \equiv \text{Prob}(\theta ≥ θ_\text{in} | X \equiv 0) \) and \( P_m = \text{Prob}(θ < θ_\text{in} | X \equiv 1) \). \( p_0 \) and \( p_1 \) can be derived in terms of SNR and \( θ \). A closed-form expression for \( P_f \) and \( P_m \) is derived in [15] and [35] as follows:

\[ P_f = \frac{1}{2} \left[ 1 - \text{Erf} (\theta) \right] \]  

(24)

\[ P_m = \frac{1}{2} \left[ 1 + \int_{0}^{∞} \text{Erf} (\theta - q √ \text{SNR}) \cdot P(q) dq \right] \]

where, \( \text{Erf}(z) \) is the error function, given by \( \frac{2}{\sqrt{π}} \int_{0}^{z} e^{-x^2} dx \). In a consequence, the communication between different neurons is enabled based on spike transmission. The successful transmission rate of l bits of spike (\( R_s \)), can be expressed as follows:

\[ R_s = (1 - P_e)^l \]  

(25)
4.2. Neurospike channel capacity

The performance of SISO molecular neurospike communication is measured in terms of the mutual information and neurospike channel capacity [29]. The transition matrix of the molecular neurospike channel, \( P(X/Y) \), can be written, in terms of \( p_0, P_t \) and \( P_m \), as follows:

\[
P(X/Y) = \begin{pmatrix}
p_0(1 - P_m) & (1 - p_0)P_t \\
p_0P_m & (1 - p_0)(1 - P_t)
\end{pmatrix}
\] (26)

By using Eq. (26), we can obtain the mutual information \( I(X,Y) \) between \( X \) and \( Y \) as follows [30]:

\[
I(X, Y) = H(Y) - H(Y/X)
\]

\[
= H(p_0P_m + (1 - p_0)(1 - P_t)) - p_0H(p_0) - (1 - p_0)H(P_t)
\] (27)

where, \( H(z) \) is the binary entropy function, \( H(z) \equiv -z\log_2(z) - (1 - z)\log_2(1 - z) \). Further, we can obtain the capacity of neurospike channel as follows:

\[
C = \frac{I(X,Y)}{t_s} \text{ bits/sec}
\] (28)

where, \( t_s \) denotes the required time for transmitting one spike. It is usually composed of the time required for spike release (action potential) and recovery (\( t_s \) is typically 3 ms).

5. Metrics performance of nanonetwork

In this section, we present the performance analysis of synaptic transmission in SISO nanonetwork based on the proposed realistic molecular communication. Furthermore, we evaluate the performance of SISO nanonetwork in terms of average packet delay, throughput and sustained traffic rate.

In this analysis, we model the propagation of a single neurotransmitter packet that is generated by TN as a spread of one infectious disease [31]. In epidemiological schemes such as classical susceptible-infected-recovery (SIR) model, a single packet is propagated according to the store-carry-forward discipline [31]. This type of communication is called intermittent connectivity and it is comparable to the epidemic routing scheme. Many routing schemes in different systems are similar to epidemic disease spreading and have been studied in [31] and [32].

In nanonetworks, as inspired by epidemic disease spreading, nanomachines can be traced in three various states, i.e., infected, susceptible and recovered. Thereby, within a nanomachine, when a packet (i.e., infected in state \( I \)) collides and adheres with another nanomachine that does not have a copy of the packet information (i.e., susceptible in state \( S \)), it is forwarded to this nanomachine. A nanomachine is considered to be recovered (i.e., recover in state \( R \)) after it has offloaded the packet to infostation. The classical epidemic SIR model is analyzed by a Markov model. As illustrated in Fig. 5, \( S(t) \) represents the number of suspected nanomachine in state \( S \) at time \( t \), \( I(t) \) represents the number of infected nanomachine in state \( I \) at time \( t \) and \( R(t) \) represents the number of nanomachine in state \( R \) for time \( t \). Hence, the transition into state \( I \) rate can be derived as \( \lambda \times S \times I \) and transition out of state \( I \) yields to rate \( \mu \times I \).

We can deduce the differential equation that represents the SIR system as follows [33]:

\[
\frac{dI(t)}{dt} = \lambda \times S(t) \times I(t) - \mu \times I(t)
\] (29)

For the purposes of representation of accurate collision, adhesion and transmission procedures based on the above description for molecular neurospike communication and as a refining in [7], let \( \lambda \) represents the rate of packet spreading among nanomachines. As a consequence, \( \lambda \) can be evaluated as

\[
\lambda = R_{in} \times R_s \times R_s
\] (30)

Additionally, let \( \mu \) represent the rate at which infected nanomachines become recovered. Notably, \( \mu \) contains infostation and nanomachine collision, adhesion and transmission rates. As a result, \( \mu \) can be given by the following formula [7]:

\[
\mu = R_{in} \times R_s \times R_s
\] (31)

Let \( N_a \) denote the overall nanomachines in the nanonetwork. In addition, \( T_d \) is defined as a random variable, it corresponds to the time elapsed from first generation of information packet by a nanomachine to the time that packet is first offloaded to an infostation. Initially, we consider an SISO, i.e., single packet in the system. At \( t = 0 \), only one nanomachine is infected, i.e., \( I(0) = 1 \), \( S(0) = N_a - 1 \) and \( R(t) = 0 \) for \( t < T_d \). At the time of offloading, \( R(T_d) = 1 \). Thereby, Eq. (29) can be rewritten as follows:

\[
\frac{dI(t)}{dt} = \lambda \times S(t) \times I(t) \text{ and } I(t) = N_a - S(t)
\] (32)

For \( I(0) = 1 \), the solution of this equation can give the analytical form of \( I(t) \) as follows:

\[
I(t) = \frac{N_a}{1 + (N_a - 1) \times e^{-\lambda I(t)}}
\] (33)

The cumulative distribution function (CDF) of the nanoscale packet delay, \( F(t) = \text{Prob}(T_d < t) \), represents the probability that the packet is offloaded by time \( T_d \) to an infostation and thus the probability density function (pdf) of delivering nanoscale packet can be determined [33]. An analogue to ad hoc networks, the connectivity probability between two nodes depends on the transmission range. In SISO nanonetwork-based molecular system, the nanoscale packet depends on collision and adhesion rates along with the rate of nanoscale packet spreading (\( \lambda \)) and recovering (\( \mu \)) between nanomachine and infostation. The cumulative distribution function (CDF), \( F(t) \) is derived in [34] as follows:

\[
F(t) = 1 - \left( \frac{N_a - 1}{N_a} \right)^\frac{\mu}{\lambda} \left[ 1 - \frac{4\pi(b_3^3 - b_2^3)}{3V} \right] \left( \frac{N_a - 1}{N_a - 1 + e^{-\lambda N_a t}} \right)^\frac{\mu}{\lambda}
\] (34)

The average delay time, \( E(T_d) \), required to deliver a nanoscale packet information to an infostation can be determined as follows [34]:

\[
E(T_d) = \int_0^\infty 1 - F(t) dt = \int_0^\infty \frac{\mu}{\lambda} \left[ 1 - \frac{4\pi(b_3^3 - b_2^3)}{3V} \right] \left( \frac{N_a - 1}{N_a - 1 + e^{\lambda N_a t}} \right) dt
\] (35)
Table 1
Parameters for numerical results.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of nanomachines, $N_n$</td>
<td>10–100</td>
</tr>
<tr>
<td>Prior probability of spike release, $p_0$</td>
<td>0.5</td>
</tr>
<tr>
<td>Signal to noise ratio, SNR</td>
<td>10dB</td>
</tr>
<tr>
<td>Comparable decision threshold of spike, $\theta$</td>
<td>1.1</td>
</tr>
<tr>
<td>The shape of Gamma distribution, $\alpha$</td>
<td>1</td>
</tr>
<tr>
<td>The rate of Gamma distribution, $J$</td>
<td>1</td>
</tr>
<tr>
<td>Number of bonds, $e$</td>
<td>40</td>
</tr>
<tr>
<td>The contact area, $A_c$</td>
<td>3</td>
</tr>
<tr>
<td>Radius of nanomachine, $b_n$</td>
<td>7.5 $\mu$m</td>
</tr>
<tr>
<td>Radius of nanomachine, $b_i$</td>
<td>15 $\mu$m</td>
</tr>
<tr>
<td>Volume, $V$</td>
<td>$1 \times 10^6 \mu$m$^3$</td>
</tr>
<tr>
<td>Forward binding rate, $k_1$</td>
<td>0.003 $\text{m}^3$/s</td>
</tr>
<tr>
<td>Reverse binding rate, $k_2$</td>
<td>0.03 s$^{-1}$</td>
</tr>
<tr>
<td>Maximum surface density, $m_{\text{max}}$</td>
<td>100 $\mu$m$^{-2}$</td>
</tr>
<tr>
<td>Minimum surface density, $m_{\text{min}}$</td>
<td>75 $\mu$m$^{-2}$</td>
</tr>
<tr>
<td>Contact time, $\tau$</td>
<td>1 s</td>
</tr>
<tr>
<td>Length of message, $L$</td>
<td>8 bits</td>
</tr>
<tr>
<td>The strength of the intermolecular force, $\beta$</td>
<td>6</td>
</tr>
<tr>
<td>Vicker’s hardness for nanomachine, $H_n$</td>
<td>10–90 kg/mm$^2$</td>
</tr>
<tr>
<td>Vicker’s hardness for infostation, $H_i$</td>
<td>29 kg/mm$^2$</td>
</tr>
<tr>
<td>Density of nanomachine, $\rho_n$</td>
<td>1 gm/cm$^3$</td>
</tr>
<tr>
<td>Density of infostation, $\rho_i$</td>
<td>1.61 gm/cm$^3$</td>
</tr>
</tbody>
</table>

$E(T_d)$ can be numerically evaluated for any value of $\lambda$ and $\mu$ by using hypergeometric function [36] as follows:

$$E(T_d) = \frac{(N_n)^{i-1}}{2\mu} \times \frac{4\pi(k_1^2 - k_2^2)}{3V} \text{Hyper}\left(\frac{\mu}{\lambda}, \frac{\mu}{\lambda}, 1 + \frac{\mu}{\lambda}, 1 - N_n\right). \tag{36}$$

The average network throughput, $\psi(T_d)$ for transmission $L$ spike bits in the proposed nanonetwork is given by

$$\psi(T_d) = \frac{L}{E(T_d)} \tag{37}$$

Furthermore, the sustained traffic rate, $\rho_{\text{sat}}$ for transmitting $L$ spike bits to infostation is given by [7]

$$\rho_{\text{sat}} = \frac{N_n \times \psi}{1 + (N_n - 1)e^{-\lambda T_d}} \tag{38}$$

6. Numerical results

In this section, we evaluate the performance of nanonetwork based on the proposed molecular communication system. We adopt typical parameters in [7] and [20,36] for this scenario, as it naturally occurs in a biochemical neural system. Numerical equations are generated and solved with the use of Matlab. Default parameters for the proposed nanonetwork are illustrated in Table 1. In this experiment, we set the radius of nanomachine to 7.5 $\mu$m, while the radius of the infostation is set to 15 $\mu$m. We utilize the optimal threshold for decision at the receiver that we proved in the neuronal communication to $\theta = 1.1$ at SNR = 10 dB. The spike release probability (a priori probability), $p_0$ is assigned the value of 0.5 for the estimation of spike detection, error probability. Hence, we evaluate the metrics performance such as average packet delay, throughput and sustained traffic rate.

6.1. Performance analysis for neurospike communication

The objective of this section is to study the effect of neurospike communication parameters in the proposed nanonetwork performance. Consequently, we evaluate the performance of molecular neurospike communication in terms of successful probability for spike transmission, $R_s$, spike average delay time, $E(T_d)$, as well as average throughput, $\psi(T_d)$, and average sustained traffic rate, $\rho_{\text{sat}}$, with varying a priori probability, $p_0$, and the detection threshold, $\theta$, for different values of SNR, by adopting network default parameters as typified inside Fig. 6 (a – h).

Fig. 6(a) and (b) show successful probability for spike transmission, $R_s$ against the decision threshold, $\theta$ and the a priori probability, $p_0$, respectively, for different values of SNR. We observe that the successful spike transmission increases as the decision threshold $\theta$ increases under all SNR values, while obviously the spike with higher SNR has better performance, until reaching an optimal value of $\theta$. Further increase in $\theta$ above the optimal value will significantly lessen the successful spike transmission as shown in Fig. 6(a). On the other hand, the probability of successful spike transmission quickly decreases as the a priori probability, $p_0$, increases for any value of SNR as illustrated in Fig. 6(b).

As illustrated in Fig. 6(c), the effect of SNR on the average packet delay, $E(T_d)$, decreased observable level when decision threshold, $\theta$, increases until it reaches a certain point, after that point, $E(T_d)$ begins to increase. Also, as we saw in Fig. 6(a), with decreasing SNR, the successful spike transmission decreases and hence yields higher delays. On the other hand, the average packet delay increases as a priori probability, $p_0$, increases as illustrated in Fig. 6(d). The same interpretation for the average throughput, $\psi(T_d)$, and average sustained traffic rate, $\rho_{\text{sat}}$, can be illustrated in Fig. 6(e) and Fig. 6(g) with respect to decision threshold, $\theta$, wherein the $\psi(T_d)$ and $\rho_{\text{sat}}$ are increased until they reach an optimal point, after that point, they are going to decrease. Additionally, $\psi(T_d)$ and $\rho_{\text{sat}}$ significantly decreased as a priori probability, $p_0$, increases as depicted in Fig. 6(f) and Fig. 6(h).

We can conclude (from the observations in all plots at Fig. 6) that, there are optimal or critical parameters that effect on the performance of neurospike transmission such as detection threshold, $\theta$, a priori probability, $p_0$, and SNR. Those parameters should be carefully selected when we study the performance of the proposed molecular communication-based nanonetworks. According to the above discussion, we considered the following parameters, $\theta = 1.1$, $p_0 = 0.5$ and SNR = 10 dB, in order to evaluate the performance nanonetwork-based MC as illustrated in the following subsection.

6.2. Performance analysis for nanonetwork-based MC

6.2.1. Average delay performance

In Fig. 7(a) and (b), the average packet delay, $E(T_d)$, for packet transmission in the proposed nanonetwork-based MC decreases as the hardiness coefficient ($H_n$) of nanomachine increases. We also can observe that the average packet delay is significantly reduced when $T_i$ increases and similarly when the number of nanomachines is large. From this it can be concluded that the lower delay in message delivery can be achieved when the time of collision is high and the number of nanomachine in the network is large.

On the other hand, the impact of a change in the inter-nanoparticles interaction behaved according to the adoption $\alpha$ value. In this scenario, we set the value of $\alpha$ to 30, 0 and $30$ to express the attractive, vanish and repulsive van der Waals force between the nanoparticles. As we can see in Fig. 7(a) and (b), the average packet delay is greatly affected by the value of $\alpha$, since the average packet delay is dramatically decreased when $\alpha = 30$ compared to $\alpha = 30$ and $\alpha = 0$. This is because when the binding between nanoparticles is associated with attractive force, the average delay of message delivery is significantly reduced although the hardness is low. The average packet delay at $\alpha = 30$ is higher than the average packet delay at $\alpha = 0$, which is due the repulsive force between nanoparticles. Meanwhile, in Fig. 7(c) and (d), the average packet delay, $E(T_d)$, is plotted with varying the number of nanomachines, $N_n$. For this plot, nanomachine hardness is set to $H_n = 20$ for different values of nanomachine’s size and SNR, respectively.
per plot analysis, the average packet delay dramatically decreases as the nanomachine size increases and SNR value remains high.

Finally, we observe in overall plots that the average packet delay of nanoscale information delivery is varied from one hundred to several hundreds. These results are better than the results in [7] under the same condition in the nanonetwork dimensions; this is because we are taking into account the electronic structure and interaction near-field forces of nanomachines.

6.2.2. Throughput performance

Fig. 8(a) and (b) show the average throughput ($\psi(T_d)$) of nanoscale information transmission in the proposed nanonetwork-based MC as the hardness coefficient of neurotransmitter increases for different values of $\alpha$ and $T_c$. Obviously, the average throughput improves when the hardness parameter increases and when the collision time, $T_c$, increases and the number of nanomachines is large. Moreover, throughput have better performance when inter-nanoparticles binding is associated attractive force rather than repulsive force.

On the other hand, the network’s throughput is high as the number of nanomachines, $N_n$, increases and the achievable SNR value is high as illustrated in Fig. 8(c) and (d), respectively. Also, we can observe that the effect of interaction near field force between nanoparticles is neglected when the signal to noise ratio is the
Fig. 7. Average packet delay performance of proposed nanonetwork-based MC.

6.2.3. Sustained traffic rate performance

Finally, we sketch in Fig. 8(a) and (b) the average sustained traffic rate ($\rho_{tr}$) in the proposed nanonetwork-based MC as the number of nanomachines increase at different value of nanomachine size and SNR value, respectively. As we can observe, the performance of the proposed nanonetwork-based MC can be improved by increasing the number of nanomachines which carry the message in nanonetwork. Also, we can see the sustained traffic rate enhanced when the nanomachine size is large and when the SNR value is high.

To summarize, our performance analysis for the proposed nanonetwork-based MC shows that the high value of hardness coefficient for the neurotransmitter increases the interaction between nanomachines and infostation; also, when the binding at
receptor is accompanied with attractive van der Waals force, the delay performance is enhanced and larger throughput in the overall nanonetwork is achieved.

7. Conclusion

In this paper, we investigated the influence of nanoparticles in the performance of nanonetwork-based MC. We derived a closed-form expression of the nanoparticle's critical velocity for physically contact in the collision/adhesion process. We studied the effects of the electronic structure and the near-field interaction of nanoparticles on the nanonetworks-based MC. The numerical results demonstrate the necessity of taking into account the electronic structure (hardness) of neurotransmitters and mutual interaction forces during the communication of nanomachines in nanonetworks. We can envision that the nanonetwork based on the proposed MC scheme will enable a novel intelligent drug delivery system in the intra-body nanonetwork.

References