Physical Channel Characterization for Medium-Range Nanonetworks using Catalytic Nanomotors

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Abstract

Molecular communication is a promising paradigm to implement nanonetworks, the interconnection of nanomachines. Catalytic nanomotors constitute one of the techniques that have been proposed for medium-range molecular communications. This paper presents a physical channel characterization that shows how nanomachines communicate using catalytic nanomotors as information carriers. Quantitative results of the packet transmission delay and loss probability are then obtained through simulation. Finally, some trade-offs that will arise when designing these networks are outlined.

Keywords: Nanonetworks, Molecular Communication, Catalytic Nanomotors, Nanorods, DNA Packet

1. Introduction

Nanotechnology, the study of nanometer-scale systems, is a multidisciplinary field comprising diverse scientific areas and with potential applications in the biomedical, environmental and industrial fields [1][2][3]. A

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nanomachine is the most basic functional unit able to perform very simple tasks at the nano-scale. These tasks include computing, data storage, sensing and actuation [4].

There are currently several approaches proposed to build nanomachines [4]. First, the *top-down* approach is based on downscaling current micro-electronic and micro-electro-mechanical devices to the nano-level [5]. This approach is still at a very early stage. Second, in the *bottom-up* approach, nanomachines are assembled by using individual molecules as building blocks [6]. Manufacturing technologies which are able to assemble nanomachines molecule by molecule do not exist to date, but once they do, nanomachines could be efficiently created by the precise and controlled arrangement of molecules. This process is called molecular manufacturing [6][7] and may be developed from current technologies in a couple of decades, if adequate research efforts are devoted. Finally, the *bio-inspired* approach takes advantage of existing biological nanomachines (such as molecular motors or cell receptors). Molecular machines are assembled by means of molecular engineering [8] in order to develop new nanomachines, or they are used as building blocks of more complex systems. This approach offers promising solutions in the short term.

Nanonetworks, the interconnection of nanomachines, provide means for cooperation and information sharing among them, allowing nanomachines to fulfill more complex tasks. Several techniques have been proposed to interconnect nanomachines [4]. Among the most promising ones is molecular communications, which is based on the use of molecules to encode the desired information and transmit it by mimicking biological systems found in nature. This communication paradigm is particularly well suited for bio-inspired nanomachines.

Different communication techniques must be used depending on the distance between emitters and receivers. They can be classified in three approaches: short-range (nm to μm), medium-range (μm to mm) and long-range (mm to m). For the *short range*, two methods have been proposed [4]. The first one is molecular signaling, based on encoding the information in the concentration rate of molecules which diffuse in the medium, and the second is based on molecular motors, protein complexes that are able to transport molecules through microtubules. We introduced two mechanisms intended for *medium-range* molecular communication in a previous work: flagellated bacteria and catalytic nanomotors [9]. Both methods are based on encoding the information in DNA sequences (a DNA packet) and carrying it from transmitter to receiver using bacteria or nanomotors, respectively. Finally, several techniques have been proposed for the *long range* [10]. The most promising among them appears to be light transduction, i.e., converting the molecular signals into the optical domain. The envisaged network architecture is composed of a cluster of nanomachines that communicate among them using short-range mechanisms, and gateways, which, taking advantage of medium and long-range techniques, inter-connect clusters.

The main contributions of our work are: (i) a description of the physical channel of a point-to-point molecular communication using catalytic nanomotors as information carriers, and (ii) quantitative results, in terms of propagation delay and packet loss probability, for the previous scenario.

The rest of this paper is organized as follows. In Section 2, we outline the process of molecular communication using catalytic nanomotors. Section 3 contains the description of the physical channel. In Section 4, we present quantitative results obtained from simulation. Finally, Section 5 concludes the paper.

2. Molecular communication using Catalytic Nanomotors

Catalytic nanomotors are synthetic particles that are able to propel themselves and small objects, by means of self-generated gradients that are produced by catalyzing the free chemical energy present in the environment. One of the most common types of catalytic nanomotors is platinum (Pt) and gold (Au) nanorods, which are 370 nm in diameter and 2 μm long (1 μm of gold and 1 μm of platinum). These nanorods are able to propel themselves, approximately in a unidirectional way, in an aqueous hydrogen peroxide (H_2O_2) solution by catalyzing the formation of oxygen at the Pt end (see Fig. 1(A)) [11].

One of the main drawbacks of Pt/Au nanorods is the lack of a complete control over the direction of the movement, although they show an important improvement in comparison with the movement of particles in the nanoscale, which follows Brownian diffusion laws [12]. Their directionality can be improved by adding nickel (Ni) segments, with a length shorter than the diameter of the rod. The Au/Ni/Au/Ni/Pt striped nanorods are 1.3 μm long (with respective segment sizes of 350, 100, 200, 100 and 550 nm) and 400 nm on diameter, and can be externally directed by applying magnetic fields, as shown in Fig. 1(B). This behavior is caused by the nickel segments introduced in the nanorods, which cause them to align in the perpendicular

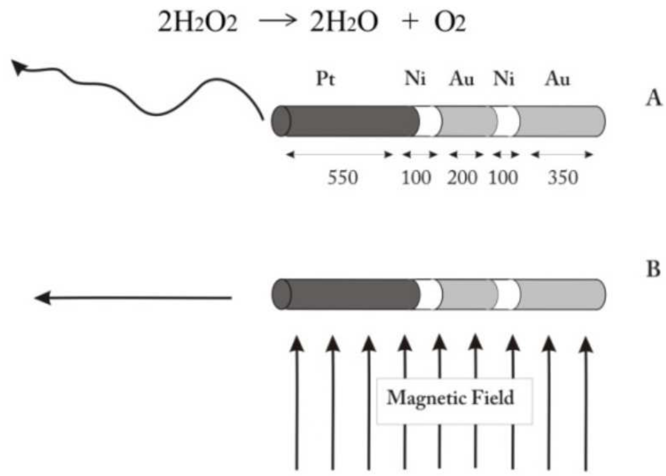

Figure 1: The movement of Au/Ni/Au/Ni/Pt rods in aqueous hydrogen peroxide solution without a magnetic field applied (A), and with an applied field (B)

direction of the magnetic field. Various techniques to increase the nanomotor speed, such as the use of Ag/Au alloy segments [13] or the incorporation of Carbon Nanotubes into the Pt segments [14], have been recently proposed as well.

We propose the use of catalytic nanomotors for the exchange of information among nanomachines. The communication process is composed of the following steps: encoding, transmission, propagation, reception and decoding [9]. It can be summarized as follows:

- The transmitter nanomachine encodes the desired information in the catalytic nanomotor, by means of loading DNA plasmids in the nanorod, which is used as a gene delivery system [15]. After that, the transmitter releases the nanorod to the environment.

- There exist several alternatives to guide the nanorod across the medium. In this paper, we consider that there exists a pre-established magnetic path from the emitter to the receiver. Due to the presence of this magnetic field, the catalytic nanomotor aligns and moves in the perpendicular direction of the field, which leads the nanorod towards the receiver.

- Finally, the nanorod arrives at the receiver, where it binds to one of its transferrin receptors. Once the DNA packet is extracted from the plasmid, the receiver is able to process its information.

3. Physical Channel for Catalytic Nanomotors

In this section, we describe the physical channel of a point-to-point molecular communication using catalytic nanomotors as information carriers. Both transmitter and receiver are assumed to be in a fixed position in the space. The channel medium is composed of a solution of hydrogen peroxide (H_2O_2) in water. There exist certain paths created by means of magnetic fields that will lead the nanorod from the transmitter towards the receiver. Taking into account that currently there is no general agreement about the physics that govern the rod movement, we model the propagation of the information based on experimental observations of the directionality of the nanorod [11][12].

3.1. Magnetic field

We propose two alternatives for the creation of the magnetic field. The first one, shown in Fig. 2, is to create the magnetic field (represented by dashed lines) by means of a solenoid or a small magnet placed in each of the nodes of the network. As shown by the solid lines, the nanorods have a set of predefined paths that join the transmitter with the receiver. The other alternative is shown in Fig. 3, in which the magnetic field is created by means of injecting an electrical current into a small dipole placed at the receiver node. This dipole can be implemented with a carbon nanotube, as presented in [16]. As shown in Fig. 3, the magnetic field produced in a certain point is always perpendicular to the radial direction, exactly the direction in which the nanorods will align.

Comparing both schemes, it is easy to notice that the paths created with the dipole are much more effective because they connect the actual position of the nanorod with the receiver in the shortest possible direction. However, this scheme has some shortcomings. Note that if, for some reason —such as the rotational diffusion or a lack of directionality— the rod rotates more than 90 degrees, it will start moving away from the receiver. Moreover, when the nanorod reaches the receiver, the rod may overtake it by some micrometers due to the rotational diffusion; in that case, the rod will keep the same orientation moving away from the receiver.

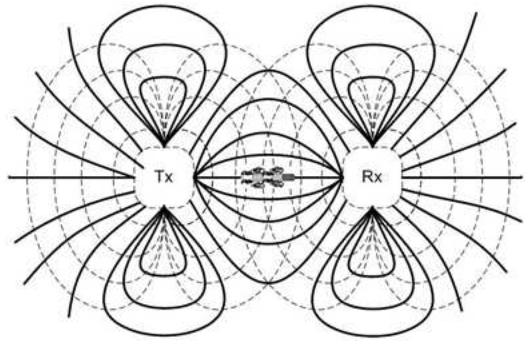

Figure 2: Communication scheme using a solenoid to create the magnetic field

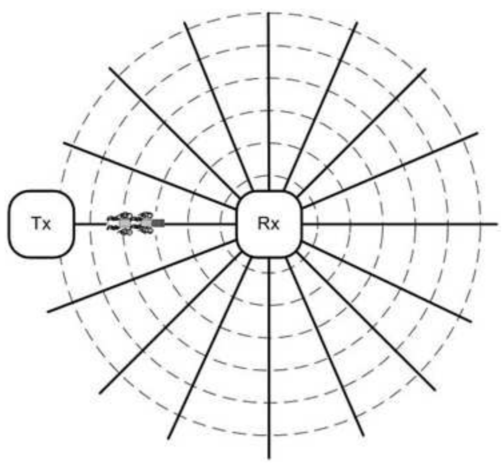

Figure 3: Communication scheme using a dipole to create the magnetic field

These issues do not arise when magnetic fields are created with solenoids. In that case, if the nanorod is deviated more than 90 degrees by the rotational diffusion, it will go back to the transmitter, which will retransmit the packet. If the nanorod passes by the receiver, it will be reoriented by the magnetic field towards the receiver again.

Power consumption is another issue that must be taken into consideration, since nanomachines will only have a small amount of power available. In order to minimize power requirements, we propose that the nanomachines generate the magnetic field intermittently. Therefore, while there is no magnetic field, the nanorod will move freely in an approximately unidirectional way. At some point, the nodes will generate the magnetic field, which will align the rods with the correct path. Once aligned, the rods will continue moving again in a free manner, and so forth, recurrently.

We can see that there is a tradeoff between propagation delay and power consumption: the smaller the interval without magnetic field, the smaller the propagation delay becomes, but the larger the power consumption (quantitative results are given in Section 4). Also, the scheme involving solenoids will have a higher power consumption than the one using dipoles, since the magnetic field must be created both in the emitter and the receiver. Moreover, in the solenoid case there must be a perfect synchronization between transmitter and receiver in order to generate the magnetic field in the exact same instant. Global time synchronization may be obtained by transmitting a signal from a macro-node.

3.2. Directionality

Catalytic nanomotors are objects in the micro-scale and their motion is governed by viscous forces rather than by inertial forces, due to their low Reynolds number [17]. Furthermore, they are affected by rotational diffusion (collisions with water molecules cause the nanorod to slightly drift following a Brownian motion model) as well as by other factors that produce small changes in the direction of the rod. As stated in the previous section, if the nanorod deviates significantly from its original direction, it will realign in the wrong direction when the magnetic field is applied.

The directionality is used to analyze the center-to-center displacement of the nanorod after a certain period of time Δt. Directionality is defined as the cosine of the angle between the rod axis $\hat{z}$ and the direction of movement $\vec{D}$ [18], as shown in Fig. 4.

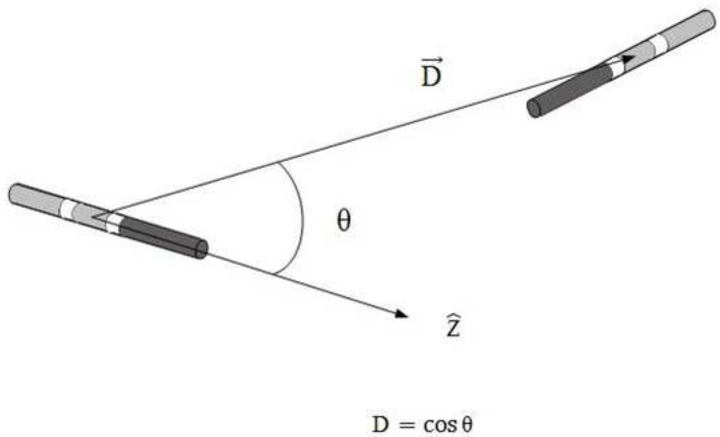

Figure 4: Directionality of the catalytic nanomotor

Irregularities in the direction of the rod have been observed and modeled in terms of directionality in [12]. Under a 5% concentration of H_2O_2 in water, the nanorods move with a directionality of 0.6 when there is no magnetic field applied. However, with the effect of the magnetic field, the directionality increases to 0.85. These data are used in the following section in order to characterize the movement of the nanorods in the medium.

4. Simulation results

In this section, we aim to obtain quantitative results in terms of propagation delay and packet loss probability in the scenario described in the previous section. We have developed a tool that simulates a point-to-point link using catalytic nanomotors as information carriers, taking into account both the directionality factor of the nanorod and the magnetic field. With this tool, we are not only able to obtain the path that a certain nanorod follows but also the required time to reach the receiver, i.e., the packet propagation delay. In case that the nanorod does not reach the receiver after a given time t_{max}, we assume that the transmitted packet is lost.

The main parameters used in the simulation are described next. The simulation space is assumed to be a 2-dimensional square with a side length of 2 mm. The magnetic field is generated by a dipole in the receiver, as shown in Fig. 3. The directionality factor of the nanorod is set to 0.6, as observed in [12]. We assume the propagation speed of the nanomotors to be

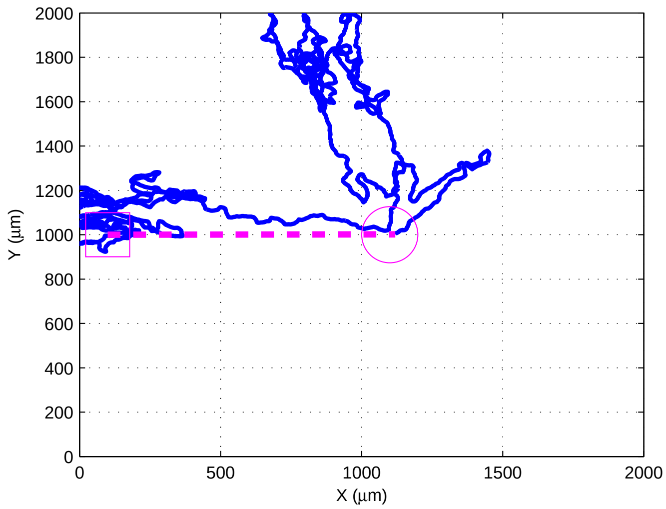

Figure 5: Trace of the catalytic nanomotor from the transmitter (square) to the receiver (circle)

20 $\mu m/s$, as it was reported in [19]. We did not consider recently proposed techniques which could increase the velocity of catalytic nanomotors up to 200 $\mu m/s$ [13][14] and therefore greatly reduce the propagation delay. The maximum simulation time is $t_{max} = 3000\ s$.

The trace of a single catalytic nanomotor from the transmitter (square) to the receiver (circle) is shown in Fig. 5. We observe that the nanorod moves in an approximately radial direction to the receiver, and that the action of the magnetic field might cause the rod to orient in the wrong direction. Moreover, we can see that the nanorod meanders because of its lack of directionality. Fig. 5 also shows that the catalytic nanomotor may go past the receiver. This causes the motor to move away from the receiver for an extended period of time before returning to its destination, and thus a long propagation delay.

The results in terms of propagation time of the catalytic nanomotor are shown in Fig. 6. The mean propagation time t_{prop} is plotted as a function of the distance from transmitter to receiver, for three different alignment intervals (3, 6 and 9 seconds), and averaged over 500 simulation runs. The solid lines are the second-order polynomials which approximate t_{prop}, obtained by polynomial fitting. Note that for alignment intervals larger than 3 seconds the propagation delay is very high; this will certainly degrade the channel

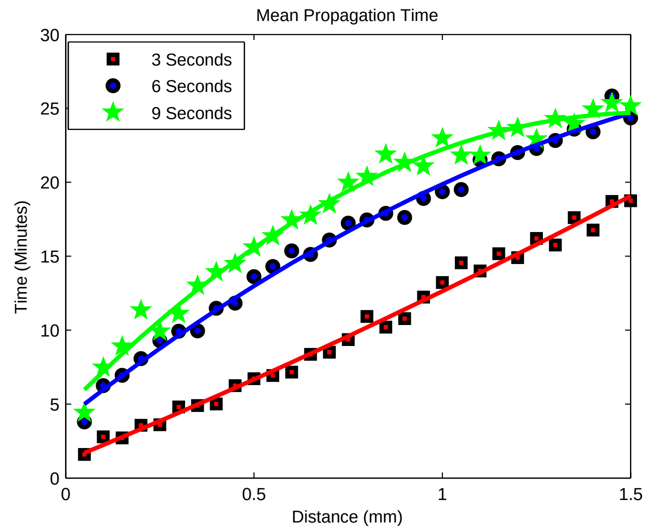

Figure 6: Mean propagation time for different alignment intervals (from 3 to 9 s)

capacity.

The packet loss probability for alignment intervals of 3, 6 and 9 seconds is shown in Fig. 7. We observe that, with an alignment interval of 6 seconds and a transmission distance of 1 mm, more than 40% of the packets do not reach the receiver. Reducing the alignment interval to 3 seconds notably improves the loss probability to below 10%.

Due to the observed long delays and high error rates, we run new simulations using smaller values of the alignment interval (from 0.6 to 2.4 seconds). In this case, the propagation delay is significantly smaller, as it can be seen in Fig. 8. Moreover, we observe that the loss probability drops to zero when the alignment interval is less than 3 seconds.

An open research issue is the optimum alignment interval of catalytic nanomotors. There clearly exists a tradeoff between the propagation delay and the energy required by the nano-machine to create the magnetic field: the smaller the alignment interval, the smaller the propagation time and the higher the required energy. The previous results indicate that, in order to achieve reasonable values of the propagation delay, nano-machines will be required to have enough battery to generate a magnetic field at least every few seconds.

For a given transmission distance, it is possible to analyze the probability

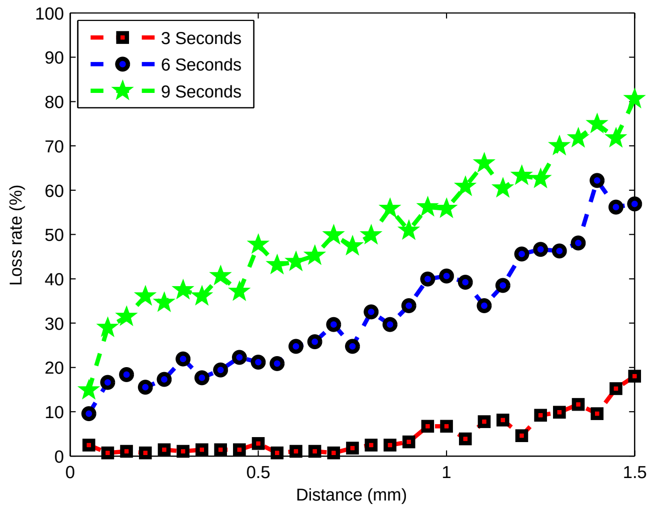

Figure 7: Packet loss rates for different alignment intervals, for $t_{max} = 3000\ s$

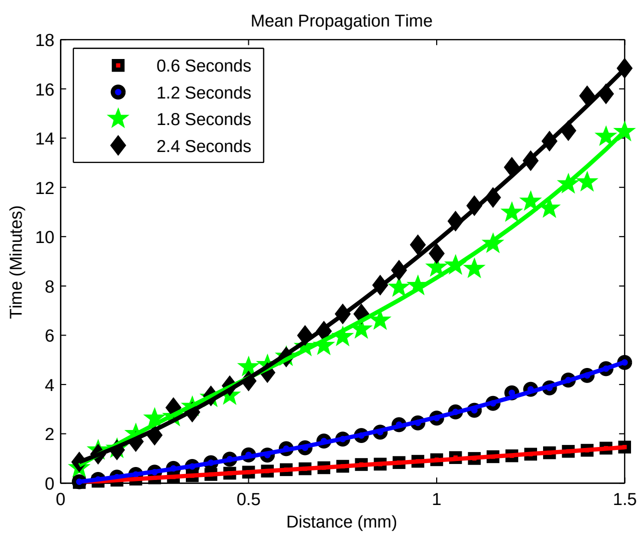

Figure 8: Mean propagation time for different alignment intervals (from 0.6 to 2.4 s)

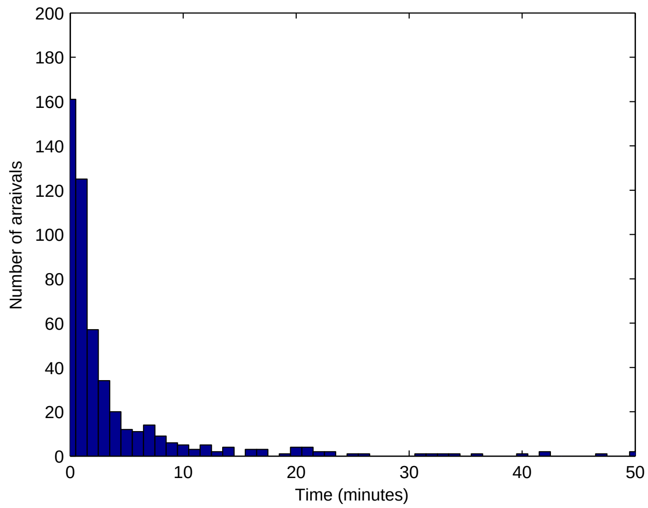

Figure 9: Number of arrivals as a function of time for a distance of 200 μm

distribution of the packet propagation delay. Simulation results indicate that it closely matches a Poisson distribution. This behavior can be seen in Fig. 9 and Fig. 10, which show the number of arrivals as a function of propagation time for transmission distances of 200 μm and 700 μm, respectively. As expected, the mean propagation time rises as the distance increases.

5. Conclusion

In this paper, we have presented a physical channel characterization for nano communication networks using catalytic nanomotors. We believe that catalytic nanomotors, synthetic particles that are able to propel themselves by means of catalysis, will serve as information carriers in medium-range molecular communications.

We have focused our characterization on two key performance metrics: the transmission delay and the packet loss probability. We have defined them and obtained quantitative results through simulation. The results clearly indicate that there is a tradeoff between transmission delay and energy consumption. Finally, the distribution of the packet propagation delay is found to match a Poisson distribution.

Researchers may consider these results as a guideline when designing complex nanonetworks based on molecular communications.

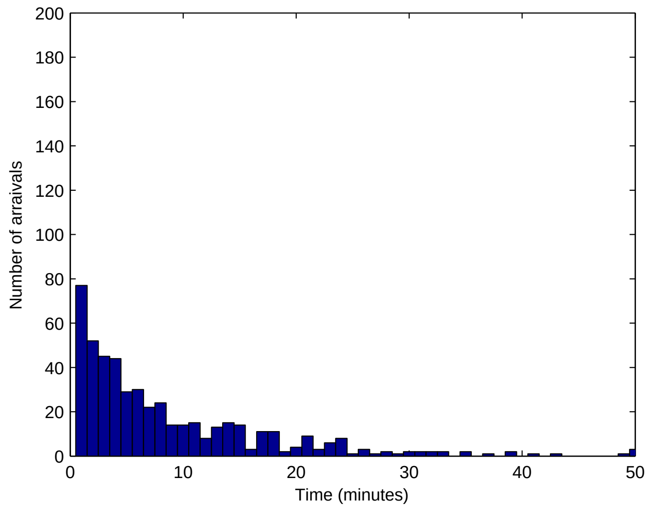

Figure 10: Number of arrivals as a function of time for a distance of 700 μm

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