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# A New Modulation Method for Diffusion Molecular Communication

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***Abstract:*** *Molecular communication is becoming an important approach for nanoscale communication. More and more researchers come into this field to promote the development of molecular communication. In molecular communication, as an important modulation technique, concentration modulation can largely introduce the inter symbol interference(ISI), especially applied to macroscale molecular communication. In this paper, we combine concentration modulation with molecular shift keying(MoSK) techniques, and the attributes of acid, bases and salts to propose a more effective methods to immigrate the ISI of molecular communication, which can be used to design a better macroscale molecular communication test bed.*

***Keywords:*** *Concentration Modulation, ISI, Molecular Communication, MoSK, Acid*

## 1. Introduction

With the rapid development of nanotechnology and molecular communication, more and more researchers are shifting their research to molecular communication. For example, the Horizon 2020 CIRCLE project, funded by the European Commission, aims to coordinate research on molecular communication across Europe by providing a structured research agenda to accelerate convergence and breakthroughs in this field. On April 2, 2013, the Obama administration announced the “Brain Project”, which is mainly used to study the work mechanism of the human brain, and ultimately to develop specific treatments for brain diseases. As for China's “brain program”, which mainly focuses on brain science and brain-like research, which is called “one body and two wings”. “One body” refers to the interpretation of the neural basis of human cognition as the main body. “Two wings” includes the research of major brain diseases and the research of artificial intelligence through calculation and system simulation. In addition, the “brain plan” has been identified as one of the major scientific and technological innovation projects by the national 13th five year plan, and has entered the implementation stage of the preparation project as one of the 2030 major project. This project is to explore the work mechanism of the human brain on the basis of the existing biological research. Regarding the working mechanism of the human brain, a large part of it is to study how the human brain transmits information, and this process is the core content of our nanonetwork and molecular communication.

At present, the main goal in the field of molecular communication is to enable nanomachines to communicate in a biological environment. In this new mode of communication, information can be encoded as a carrier such as molecules or ions for transmission. Examples of using molecular communication to solve problems have been studied including calcium ion signal[1], molecular diffusion[2], bacterial communication[3] and so on. Therefore, it can be applied to various fields. Such as military field, industrial field, environmental field[4], biomedicine field[5-8]. In the military field, it can be applied to nuclear, biological, chemical (NBC) monitoring and defense. In the industrial field, molecular communication systems can produce new molecular layouts and structures together with chemical processes. In addition, when nanomachines communicate with each other through molecular communication, advanced nanomaterials can be mixed into these nanomachines to make antibacterial, antifouling, and mosquito repellent textiles. In the environmental field, it can be used to identify and monitor some specific molecules that can cause polluted environmental problems, such as illegal pollution and radioactive leakage. In the field of biomedicine, it can be used for biological hybrid transplantation, drug delivery system, disease treatment, health supervision, etc.

The communication process of molecular communication generally includes the following five processes: (1) the Transmitter(Tx) encodes information into information molecules; (2) the Tx sends the encoded information molecules to the environment; (3) the information molecules are in the environment to transmission; (4) The Receiver(Rx) receives information molecules; (5) The Rx decodes the information molecules to obtain the original information. The flow chart is shown in Fig. 1.

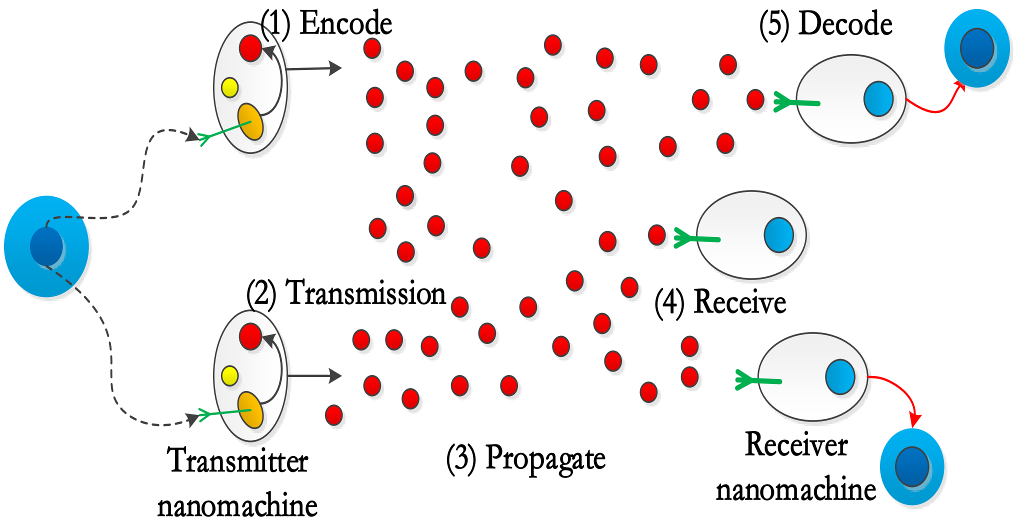


*Fig.1 An outline of a molecular communication system incorporating bio-nanomachines*

MC as a promising approach for nanoscale communication, which can be applied to many areas, such as information and communication technology(ICT), biomedical, environment, industrial and military applications. To be best our knowledge, there have been many advancements in theoretical MC. MC channel is typically a memory channel, therefore, many researchers focus on investigating how to decrease the Inter symbol Interference(ISI) and meanwhile improve the performance of MC channel. Different modulation methods have been proposed for molecular communication. In [9], authors proposed a method based on concentration shift keying (CSK), which is simple but easyily caused error under information transmission. In [10], authors introduced a molecular type based modulation technique to encode information for transmission, which information can be encoded as different molecules to transmission. While all of these modulation schemes have no ability to mitigate ISI thus cannot achieve the optimal system performance. Based on the above analysis, although existing modulation methods have been proposed to reduce ISI and improve communication reliability, the ISI interference in the channel still exists. Therefore, the existing methods still have some limitations.

The motivation of this paper is to reduce the impact of ISI on the accuracy of information transmission. Based on this goal, we proposed a new modulation method to encode information. Moreover, the new modulation method using ion reaction is easier to implement on nanomachine.

The main novelties and contributions of this paper are:

● A new modulation method is proposed to reduce ISI of MC using acids, bases and salts ions concentration.

● Through simulation analysis, we also find that our proposed method will largely reduce ISI and improve the accuracy of the information transfer.

The rest of this paper is organized as follows. In Section 2, we introduce the system model. In Section 3, we develop the novel modulation scheme using acids, bases and salt. In Section 4, we provide numerical results and discussions. Finally, we summarize this paper in Section 5.

## 2. System Model

The system that is considered in this paper, we consider that the transmitter of molecular communication system can release three different types of chemicals: a strong acid, a strong base or salt. Note that a strong acid or base does not necessarily result in a very low or high pH value that could be destructive. If they are used in low concentrations, the pH levels could be kept closer to the neutral pH. Fig. 2 depicts the proposed communication system. It is assumed that the Tx can transmit three chemicals simultaneously in any concentration. It is also assumed that the distance between the "nozzles" that release the acid, base and salts is small enough such that we can assume three chemicals are released from a single nozzle. The coordinate system that is used to study this communication channel is assumed to be centered on the tip of the nozzle, and the Tx is a point source of this location.

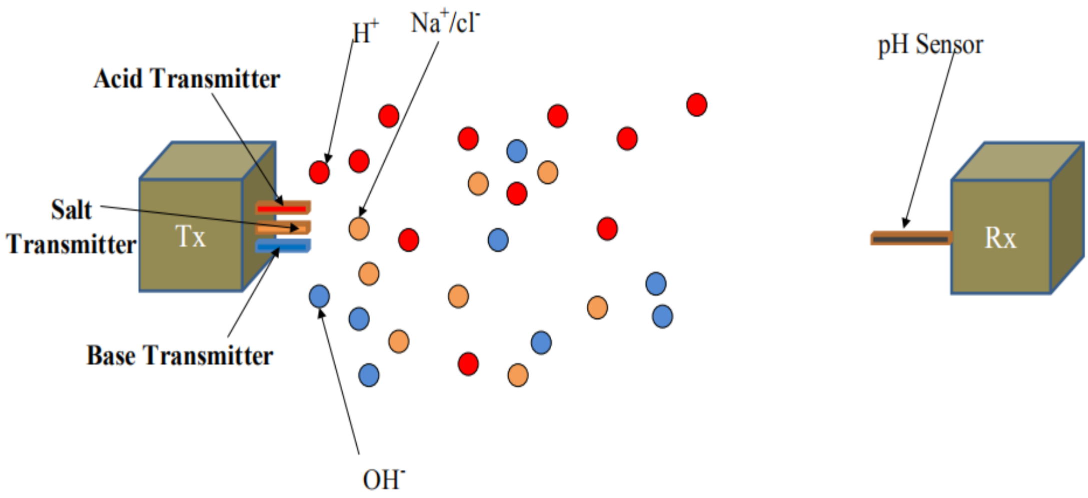


*Figure 2: The new communication system.*

As shown in Fig.2, the Tx consists of three nozzles, which can emitting strong acid($H^+$), strong base($OH^-$) and the salt(NaCl). The Rx is made of a pH sensor which can detect the pH value and decode the information according to the pH value. The acid or base should not have a very low or high pH value which could be destructive. The $OH^-$ can react with $H^+$ which will decrease the concentration of $H^+$ and ISI. The salt in this system has three advantages. Firstly, the salt is neutral, it almost cannot affect the pH of the solution. Secondly, due to the reaction of $H^+$ and $OH^-$ can product the water, after a long time, the concentration of the solution will be lower and have a negative effect on the detection of the pH sensor. Thirdly, the salt can be a kind of information, as we know when we use MoSK modulation technique, the ISI will be immigrated.

The only ion in the reaction channel involving hydrogen and hydroxide is water auto ionization reaction. Because the communication environment is internal fluid, the main solution are water and it can be assumed that there are always water molecules ready to free everywhere. Therefore, water auto ionization reaction can be written as follows equation(1):

$$\mathrm{H^+(aq) + OH^-(aq)} \underset{k_r}{\overset{k_f}{\rightleftharpoons}} \emptyset \tag{1}$$

where $k_f$ and $k_r$ are the forward and reverse reaction rates, respectively.

Here, we assume that $C_{H+}(x, t)$ and $C_{OH^-}(x, t)$ represent the average spatiotemporal concentration of H+ and $OH^-$ ions, respectively. The average behavior of the transport system can be represented using a system of partial differential equations as follows equation(2):

$$\begin{aligned} \frac{\partial C_H}{\partial t} &= D_H \nabla^2 C_H - \nabla \cdot (\mathbf{v} C_H) - k_f C_H C_{OH} + k_r \\ \frac{\partial C_{OH}}{\partial t} &= D_{OH} \nabla^2 C_{OH} - \nabla \cdot (\mathbf{v} C_{OH}) - k_f C_H C_{OH} + k_r \end{aligned} \tag{2}$$

where $D_{H+}$ and $D_{OH-}$ are the diffusion coefficients of $H^+$ and $OH^-$ ions in water, and v is the velocity. For free diffusion the velocity is assumed to be zero everywhere in the channel.

The information encode can be adjusting the release of hydrogen ions only(i.e. strong acids), the release of hydroxide ions only (i.e. strong bases) or release of salts only(i.e. Nacl). Note that if both hydrogen and hydroxide ions are released (i.e. strong acid and strong base), they will immediately combine and neutralize to form water molecules due to the very high forward reaction rate $k_f$. Therefore, the current concentration of hydrogen ions and hydroxide ions in the solution is calculated as follows:

$$\text{Tx releases } \mathrm{H^+} \begin{cases} C_{\mathrm{H^+}}(\mathbf{x}, t=0) = N_{\mathrm{H^+}} \delta(\mathbf{x}) + C_{\mathrm{H^+}}^{\mathrm{init}}(\mathbf{x}) \\ C_{\mathrm{OH^-}}(\mathbf{x}, t=0) = C_{\mathrm{OH^-}}^{\mathrm{init}}(\mathbf{x}) \end{cases} \tag{3}$$

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$$\text{Tx releases OH}^- \begin{cases} C_{\mathrm{H}^+}(\mathbf{x}, t=0) = C_{\mathrm{H}^+}^{\mathrm{init}}(\mathbf{x}) \\ C_{\mathrm{OH}^-}(\mathbf{x}, t=0) = N_{\mathrm{OH}^-}\delta(\mathbf{x}) + C_{\mathrm{OH}^-}^{\mathrm{init}}(\mathbf{x}) \end{cases} \quad (4)$$

Where $N_{\mathrm{H}^+}\delta(\mathbf{x})$ and $N_{\mathrm{OH}^-}\delta(\mathbf{x})$ represent the moles of hydrogen ions and hydroxide ions released by the transmitter, $C_{\mathrm{H}^+}^{\mathrm{init}}(\mathbf{x})$ and $C_{\mathrm{OH}^-}^{\mathrm{init}}(\mathbf{x})$ represent the initial concentration distribution of hydrogen ions and hydroxide ions in the channel, and δ(.) is the vector form of the Dirac δ function. For the first transmission, we assume $C_{\mathrm{H}^+}^{\mathrm{init}} = C_{\mathrm{OH}^-}^{\mathrm{init}} = 10^{-7}$ .Base this assumption, we can simplify our numerical analysis.

Here, we assume that the Tx and the Rx maintain a high degree of synchronization at all times, and the information molecules only collide with the surface of the Rx in a freely diffused channel. At this time, the diffusion motion of the information molecules released by the Tx in the channel can be attributed to the one-dimensional Brownian motion in the horizontal direction, thereby simplifying the analysis process.

When the sending nanomachine releases information molecules into the channel, after a period of time, these information molecules reach the Rx through diffusion and are absorbed by it. At the same time, the Rx will decode the received information molecules to obtain the original Information, and finally these information molecules received are removed from the channel.

We first consider an acid pulse in which the number of acid molecules released is much greater than the concentration of ions in the channel. An approximate pulse response is obtained if it is assumed that there are no chemical interactions in the channel. If the velocity is constant and in the direction from the Tx to the Rx and there is a sudden pulse response of *M* molar particles at time *t=0*, then the function of the ion concentration received by the Rx over time is as follows:

$$C(x,t) = \frac{M}{\sqrt{4\pi Dt}} \exp(-\frac{(x-vt)^2}{4Dt}) \quad (5)$$

where *D* is the diffusion coefficient of the particle, *x* is the diffusion distance between the transmitter and receiver, and v is the constant velocity.

## 3. Proposed new modulation scheme

In order to decrease the ISI, we need to arrange the sequence of each information molecule properly. When we utilize hydrogen ions($H^+$) to encode the bit information “1”, release salt(NaCl) to encode the bit information “0”. The information transmitted each time slot is represented by an array, and the encode of the information by the TN can be formally defined as follows:

$$\mathrm{a[i]} = \begin{cases} 1, TN \rightarrow H^+ \\ 0, TN \rightarrow NaCl \end{cases}$$

When the current time slot transmits bit information “1”, the Tx releases strong acid (that is, hydrogen ions). At the same time, when the next time slot transmits bit information “0”, because there is a residual hydrogen ion concentration in the channel, it will cause a interference with transmitting bit information "0" under current time slot. In order to solve this problem, we can add a strong base (i.e hydroxide ion) and ensure that the concentration of hydroxide ions is less than or equal to the concentration of hydrogen ions. Too much hydroxide ions will eliminate hydrogen ions, but it will affect the transmission of hydrogen ions under the next slot. Moreover, If the amount of hydroxide ions remains the same as the amount of hydrogen ions, because the release time of hydroxide ions and $H^+$ are different, a certain period of time is needed to ensure that hydroxide ions and hydrogen ions are fully neutralized. Then, we need to add NaCl instead of water. The reason for not adding water to the solution is that adding water will reduce the concentration of the solution, causing some errors in information transmission and affect the accuracy of experimental results. If the amount of hydroxide ions is less than the amount of hydrogen ions, ISI will be reduced, but cannot be eliminated. Therefore, we need to add salt to replenish the easy concentration.

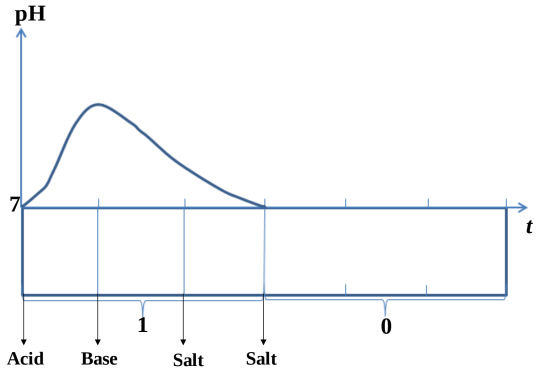


*Figure 3:time mechanism of releasing different ions when transmitting bit information "1" or "0"*

As shown in Fig. 3, two bits of information “1” and “0” are transmitted, due to the time slot for sending “0” or “1” is equal, which can be denoted as $\tau$ , and we divide the slot of sending “1” into three small time slots $\tau_1$, $\tau_2$, $\tau_3$, making $\tau_1+\tau_2+\tau_3= \tau$ . Therefore, when we can transmit bit “1”, at the start of the $\tau_1$, Tx emits strong acid(i.e hydrogen ions) a moles, after a while($\tau_1$), then Tx emits strong base(i.e hydroxide ions)a moles at the beginning of $\tau_3$ emits salt, to make sure the hydroxide ions and hydrogen ions can react completely in this period. Finally, The concentration of the solution is $10^{-7}$, (i.e the pH of the solution is 7), which is neutral and indicates that the ISI is well removed from the channel. When the bit information “0” was transmitted, in order to make the solution is neutral, the Tx can emit a little salt in the beginning of the time slot $\tau$ .

## 4. Simulation Experiment and Result Analysis

In this paper, the main merits of the proposed new modulation scheme is the ability of the Tx to control the increase and decrease of hydrogen ions at the Rx through transmitting acids, bases or salts, which can remove the tail is to transmit hydroxide ions (*i.e. a strong base*) after the hydrogen ions transmission(*i.e. a strong acid*). In order to verify the superiority over our proposed scheme, we analyze it through experimental simulation. The experiment runs on a Windows 10 (64-bit) operating system, with a memory size of 16 GB and a CPU of i5-8500, using MATLAB software for simulation experiments.

We assume that the diffusion coefficient $D=0.005um^2/s$, *diffusion distance* $d=50um$, and velocity $v=0.02um/s$. Then, we analyzed the impact of no ion reaction, adding strong acid(*i.e. hydrogen ions*), strong base(*i.e. hydroxide ions*) and salt(*i.e. NaCl* ) successively on the pulse response of the system.

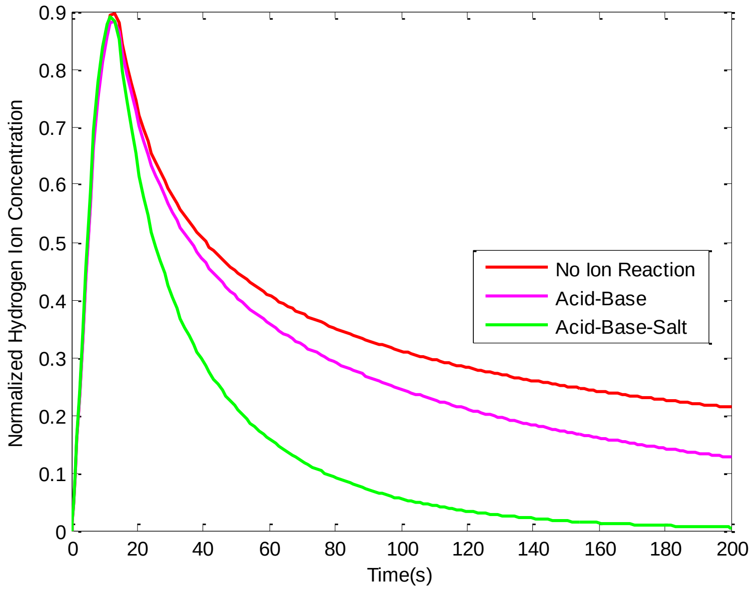


*Fig. 4. The system response when the Tx releases a strong acid(i.e. hydrogen ions)、Base and Salt*

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As shown in Fig. 4, when we did not add other ions to eliminate the residual ISI molecules in the solution after transmitting the bit information, we found that the system response has a longer tail, and the hydrogen ion concentration needs a longer time to recover to the previous state. time. When adding 0.05 moles of strong acid (i.e. hydrogen ions) to the solution to transmit bit information “1”, and at the same time we added 0.05008 moles of strong base (i.e. hydroxide ions), we found that the tail of the system response curve became shorter compared to not adding other ion methods. Finally, when we add a little salt (i.e. NaCl) after adding 0.05008 moles strong base, we can see that adding a little salt after adding strong acid and strong base can effectively reduce the channel ISI, and the width of the system response and the tailing of the curve have been rapidly reduced, and its value is close to “0” under the acceptable delay of the system, which effectively reduces the interference with ISI in the channel to information transmission.

## 5. Conclusion

In this paper, a new modulation method is proposed to reduce ISI of MC using acids, bases and salts. In addition, we divide the time slot for transmitting the bit information “1” into three parts. Since the strong acid (hydrogen ions) in the current time slot may affect the next time slot, we introduce a strong base (hydroxide ions) to react with hydrogen ions and ensure that hydroxide ions can fully react with hydrogen ions, and add a little salt to the solution to ensure that the next time slot transmits another bit of information, the solution remains neutral. Through simulation analysis, we find that our proposed method will largely reduce ISI and improve the accuracy of the information transfer, which can be used to design a better macroscale molecular communication test bed.

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