Molecular Communication Using Acids and Bases

Nariman Farsad, *Member, IEEE*, and Andrea Goldsmith, *Fellow, IEEE*, Department of Electrical Engineering, Stanford University, CA, USA.

Abstract—Concentration modulation, whereby information is encoded in the concentration level of chemicals, is considered. One of the main challenges with such systems is the limited control the transmitter has on the concentration level at the receiver. For example, concentration cannot be directly decreased by the transmitter, and the decrease in concentration over time occurs solely due to transport mechanisms such as diffusion. This can result in inter-symbol interference (ISI), which can have degrading effects on performance. In this work, a new and novel scheme is proposed that uses the transmission of acids, bases, and the concentration of hydrogen ions for carrying information. By employing this technique, the concentration of hydrogen ions at the receiver can be both increased and decreased through the sender's transmissions. This enables novel ISI mitigation schemes as well as the ability to form a wider array of signal patterns for control, high-level modulation and multiple access.

I. Introduction

Molecular communication is a new and emerging field, where information is conveyed through chemical signals [1]. In this paradigm, the transmitter releases tiny particles, where information is modulated onto the chemical properties of these particles. The particles then propagate through the medium until they arrive at the receiver, where the chemical signal is demodulated and the information is decoded. Although there are many different forms of transport in molecular communication, the most common propagation mechanism considered in the literature is diffusion-based transport with and without flow between the transmitter and receiver [1].

Different modulation schemes have been proposed for molecular communication including: concentration modulation, type-based modulation, and timing of release modulation. Between these modulation schemes, concentration modulation has received the most attention in the literature, since it can be detected with relative ease. One of the issues with concentration-modulated diffusion-based molecular communication is that the concentration at the receiver increases with consecutive transmissions and only decreases as the particles diffuse away. Since diffusion can be a slow process, this will result in significant inter-symbol interference (ISI) [1], and limits the types of signal patterns that could be formed.

In this work, a new and novel signaling scheme using acids, bases, and the concentration of hydrogen ions is proposed. In this scheme, the transmitter can release either a strong acid or a strong base. The strong acids and bases dissociate almost completely in aqueous solutions (i.e. solutions where water is the solvent) to form hydrogen ions and hydroxide ions, respectively [2]. Moreover, if used in low concentrations, strong acids and bases are not corrosive or destructive to the transmitter and receiver. Because of the water autoionization reaction [2], the

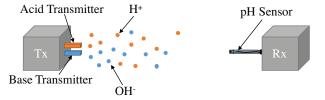


Fig. 1: Depiction of the proposed communication system.

concentration of hydrogen ions and hydroxide ions are almost always non-zero, and the product of concentration of both ions is a constant. Therefore, an increase in the concentration of one species results in a proportional decrease in the concentration of the other species. The received signal at the destination is obtained by measuring the pH level, where pH is the negative log of the concentration of hydrogen ions.

There are multiple benefits to using this scheme. First, for detection at the receiver, pH sensors are available at microscales and macro-scales, which makes this technique practical. Second, the concentration of hydrogen ions at the receiver can be directly increased *and decreased* by the transmitter. Third, a wider array of signal patterns can be formed using this extra degree of freedom, which could then be used in different applications such as to generate control signals for synthetic biological devices, or as non-binary modulation schemes. For example, it was recently shown that pH signals could be used to control the motion direction of bacteria [3]. In this work we focus on ISI mitigation, and show that the proposed system could significantly reduce the ISI.

II. SYSTEM MODEL

The system that is considered in this paper consists of a molecular communication transmitter that can release two different types of chemicals: a strong acid or a strong base. 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. Figure 1 depicts the proposed communication system. It is assumed that the transmitter can transmit both chemicals simultaneously in any concentration. It is also assumed that the distance between the "nozzles" that release the acid and base is small enough such that we can assume both chemicals are released from a single nozzle. The coordinate system that is used to study this communication channel is assumed to be centered at the tip of the nozzle, and the transmitter is a point source at this location.

The strong acids and bases almost completely dissociate in water to form hydrogen (H⁺) or hydroxide (OH⁻) ions [2].

This process happens very rapidly within a few microseconds [4]. Therefore, in this work it is assumed that transmitting a strong acid is equivalent to releasing hydrogen ions and transmitting a strong base is equivalent to releasing hydroxide ions. The released ions propagate through convection-diffusion (or potentially pure diffusion) until they arrive at the receiver. The receiver would then use a pH meter to measure the pH level and detect the concentration of hydrogen ions.

The only reaction involving the hydrogen and hydroxide ions in the channel is the water autoionization reaction [2]. Because the communication environment is inside a fluid, where the main solution is water, it can be assumed that there are always water molecules everywhere ready to dissociate. The reaction between the two ions can be written as

$$H^{+}(aq) + OH^{-}(aq) \stackrel{k_f}{\rightleftharpoons} \varnothing$$
 (1)

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

Let $C_H(\mathbf{x},t)$ and $C_{OH}(\mathbf{x},t)$ 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

$$\frac{\partial C_H}{\partial t} = D_H \nabla^2 C_H - \nabla \cdot (\mathbf{v}C_H) - k_f C_H C_{OH} + k_r \qquad (2)$$

$$\frac{\partial C_{OH}}{\partial t} = D_{OH} \nabla^2 C_{OH} - \nabla \cdot (\mathbf{v}C_{OH}) - k_f C_H C_{OH} + k_r, \qquad (3)$$

where D_H and D_{OH} are the diffusion coefficients of H^+ and OH^- ions in water, and \mathbf{v} is the velocity field. For pure diffusion the velocity field is assumed to be zero everywhere in the channel. It is assumed that dimensions of the channel environment are much larger than the separation distance between the transmitter and receiver. Therefore, infinite boundary conditions are assumed.

III. ISI MITIGATION

One of the main benefits of the proposed scheme is the ability of the transmitter to control the increase and decrease of hydrogen ions at the receiver through transmitting acids and bases. Although all concentration-encoded molecular communication techniques can control the increase of concentration at the receiver, there have been no previous works that have reported a transmission technique for decreasing the concentration at the receiver. Therefore, one of the most important benefits of the proposed system could be in reducing ISI.

One strategy for removing the tail is to transmit hydroxide ions (i.e. a strong base) after the acid transmission. Note that since the model presented in the previous section cannot be solved analytically, only numerical evaluation is possible. Therefore, we rely on the finite difference method (FDM) to find a solution [5], and will further study this system in the future using particle based simulators, where the motions and reaction of individual ions are simulated.

Consider the case when an acid impulse is transmitted followed by a base impulse. Figure 2 shows the results when

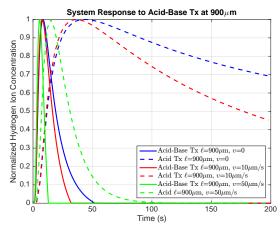


Fig. 2: The system response at 900 μ m when the transmitter releases a strong acid only (dashed lines), and when the transmitter releases a strong acid followed by base 0.5 second later (solid lines).

the separation distance between the transmitter and the receiver is $900\mu m$. It is assumed that the time between the two impulses is 0.5 seconds, where 0.001 moles of strong acid is released followed by 0.001005 moles of strong base. The number of hydroxide ions (i.e. moles of strong base) released is larger to compensate for the smaller diffusion coefficient, which results in a flatter concentration curve. The plots are normalized by the peak's maximum for easy comparison. As can be seen, the width of the response is decreased significantly and the tails drop quickly toward zero when an acid impulse is followed by a base impulse, which reduces the ISI significantly.

IV. CONCLUSIONS AND FUTURE WORK

A new and novel concentration-modulated molecular communication scheme using acids, bases and hydrogen ion concentration has been presented. This system enables new inter-symbol interference mitigation techniques as well as the possibility to form a wide array of signal patterns which may be beneficial for control, high-level modulation and multiple access. Another important benefit of this work is the availability of pH sensors at micro-scale and macro-scale for detection, which makes low-cost receivers readily available.

In the future, we will further demonstrate the feasibility of this system by building an experimental platform. Moreover, we will explore the possibility of forming different signal patterns such as orthogonal signals.

REFERENCES

- N. Farsard, A. Yilmaz, H. B.and Eckford, C.-B. Chae, and W. Guo, "A comprehensive survey of recent advancements in molecular communication," arXiv:1410.4258v2, Oct. 2014.
- [2] N. J. Tro, Principles of Chemistry: A Molecular Approach, 1st ed. Upper Saddle River, NJ: Prentice Hall, Jan. 2009.
- [3] J. Zhuang, R. Wright Carlsen, and M. Sitti, "pH-Taxis of Biohybrid Microsystems," *Scientific Reports*, vol. 5, p. 11403, Jun. 2015.
- [4] M. L. Donten, J. VandeVondele, and P. Hamm, "Speed limits for acid-base chemistry in aqueous solutions," CHIMIA International Journal for Chemistry, vol. 66, no. 4, pp. 182–186, 2012.
- [5] R. LeVeque, Finite Difference Methods for Ordinary and Partial Differential Equations: Steady-State and Time-Dependent Problems. Philadelphia, PA: SIAM, Jul. 2007.