# A Mutual Information Estimate for a Redox-based Molecular-Electrical Communication Channel

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## ABSTRACT

Redox-based molecular communication has been demonstrated to facilitate information flow between biology and electronics. In this paper, an estimate Mutual Information (MI) is provided using differential entropy and Doane's binning method for a molecular channel based on redox reactions. Though preliminary, the obtained MI will shed further light on the inherent potential of this novel communication technology.

## CCS CONCEPTS

• **Mathematics of computing** → **Information theory**; • **Computing methodologies** → **Modeling and simulation**.

## KEYWORDS

Molecular Communication, Redox-based Communication Channel, Mutual information

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## 1 INTRODUCTION

With the current advances in the field of implantable and wearable devices, there is need for a robust technology to realize communication between biology and electronics, *i.e.,* the molecular/biological domain and electrical/electronics domain. A tool that can be used to achieve this is Molecular Communication (MC). MC deals with the molecular/biological domain where particles exist at molecular scale (micro and below) while employing metrics used in generic electrical communication domain to analyze information in molecular/biological domain. Creating an interface that can convert the information freely between the molecular and electrical domain can be achieved via many modalities and one such modality is based on redox reactions [4]. In [3], we built a simulation tool based on the experimental proof of concept introduced in [4]. In this paper, we discuss our latest advancements and take it a step further to provide a preliminary estimate for the performance of such a communication channel in terms of Mutual Information (MI).


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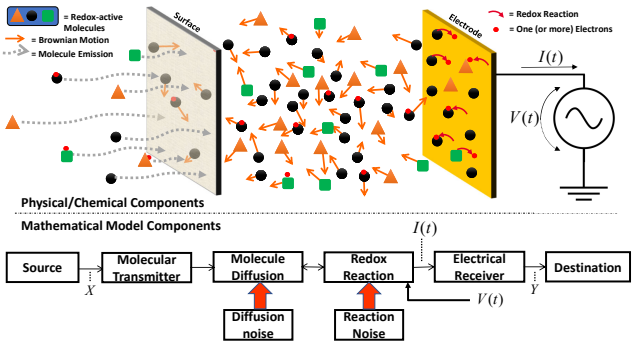


**Figure 1: System model with noise.**

## 2 SYSTEM MODEL AND IMPLEMENTATION

Let us briefly discuss about the system model and implementation based on Fig. 1. Considering a single redox active species and assuming an initial homogeneous concentration as input, *i.e.,* a Dirac delta input signal, the complete process at the basis of the redox channel between a molecular input and an electrical output can be expressed in terms of an inhomogeneous Fick's law as

$$\left\{\frac{\partial C_S(\bar{x},t)}{\partial t} = -\nabla(-D_S \nabla C_S(\bar{x},t) \pm \frac{I(t)}{nFA}\right\}_{S=O,R}, \quad (1)$$

$$I(t) = nFA[k_f(t)C_O(\bar{x},t) - k_b(t)C_R(\bar{x},t)]\mathbb{I}_{\bar{x}\in\text{electrode}}, \quad (2)$$

where $C_S$ is the concentration of a redox-active species in a redox state $S$ at time $t$ in space $\bar{x}$, $D_S$ is the diffusion coefficient of the species in a redox state $S$, $I(t)$ is the current at time $t$, $n$ is number of electrons transferred, $F$ is the Faraday constant, $A$ is the cross-sectional area of the reacting surface of the electrode, $k_f(t)$ is the forward reaction rate constant at time $t$, and $k_b(t)$ is the backward reaction rate constant at time $t$. As opposed to the system model equations in [3], here we use redox-state-based diffusion coefficients.

The equations above do not account for the noise involved. The noise sources as seen in Fig. 1 are the diffusion noise and the reaction noise. Both sources follow Poisson probability densities. As their name suggests, the diffusion noise is caused by the random

Brownian motion that dictates the diffusion process while the reaction noise is generated by the stochastic behaviour exhibited by a chemical reaction. It should be noted that the diffusion noise is considered only at the region next to the electrode since the noise in the rest of the space is negligible as it balances out in the diffusion process. A more robust and generalized system model along with corresponding equations has been discussed at length in [3].

Using a finite difference methodology, we converted the above analytical equations into computational expressions for their implementation into the code [2][1]. The equations are described as follows

$$\left\{C_S(t+1,x) = C_S(t,x) + DM_S[C_S(t,x-1) - 2 * C_S(t,x) + C_S(t,x+1)]\right\}_{S=O,R}, \tag{3}$$

$$\left\{DM_S = \frac{D_S \Delta t}{(\Delta x)^2}\right\}_{S=O,R}, \tag{4}$$

$$I(t) = nFA\frac{k_f(t)C_O(1,t) - k_b(t)C_R(1,t)}{1 + \Delta x(\frac{k_f(t)}{D_O} + \frac{k_b(t)}{D_R})}, \tag{5}$$

where $C_S$ is the concentration of a redox-active species in redox state $S$ ($O$ or $R$) at time $t$ and distance $x$ from the electrode, $DM_S$ is the model diffusion coefficient of the species in redox state $S$, $D_S$ is the diffusion coefficient of the species in redox state $S$, $\Delta t$ is the sampling time, $\Delta x$ is the sampling space used in the finite difference method, $I(t)$ is the output current at time $t$, $k_f(t)$ is the forward reaction rate constant at time $t$, $k_b(t)$ is the backward reaction rate constant at time $t$, and $C_O(1,t)$ and $C_R(1,t)$ are the concentrations of the species in oxidized and reduced states respectively in the region next to electrode at time $t$.

## 3 RESULTS

Using the simulation code detailed in [3] as basis, we updated the model to consider the use of different diffusion coefficients based on the molecule's current redox state, *i.e.,* oxidized or reduced. In the scope of this paper, we run the simulation for lower concentration where it is more likely to produce a significantly lower SNR leading to possible error at the electrical receiver, as shown in Fig. 1. For the calculation of MI, we used an input concentration range from 1fM to 1.9fM with increments of 0.1fM, resulting in a total of 10 inputs. We simulated the channel for each input value for 1000 runs with our code in Matlab, and we used the peak anodic current as the channel output to calculate entropy and MI. Doane's method has been employed to estimate a reasonable bin size for the data [5]. Figure 2 shows the probability distribution function (pdf) for each input concentration. Notice that the pdf for higher concentrations is actually on the farther left, this is attributed to the fact that the output anodic peak current is negative. For this range-limited input, we achieved an output entropy of 3.5643 bits, a conditional entropy of the output given input of 2.6614 bits, and a MI of 0.9029 bits.

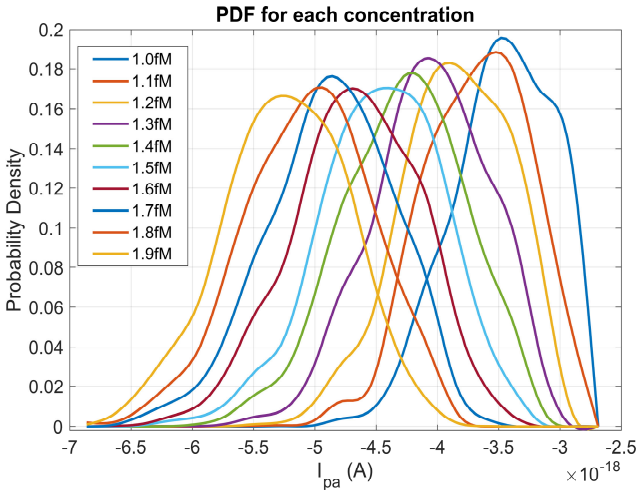


**Figure 2: PDF for each input concentration within the range 1fM - 1.9fM.**

## 4 CONCLUSION

In this paper, we shared our latest results in the analysis of a redox-based MC channel. We also used information theoretic and statistical analysis methods to provide a preliminary estimate of the redox channel communication performance in terms of MI. We believe this framework will enable us to better understand and analyze the information flow in a redox-based molecular-electrical interface and further optimize such an interface by further investigation in the direction of estimating information capacity bounds as a function of physical and biochemical parameters.

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