Interference Reduction via Enzyme Deployment for Molecular Communication

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In a molecular communication via diffusion (MCvD) system, enzymes are known to reduce interference molecules. In this letter, we consider an MCvD system with a fixed amount of enzymes around the spherical receiver. Since the enzyme amount is fixed, increasing the size of the enzyme region increases the probability of entering the enzyme region while it decreases the effectiveness of the enzymes. Therefore, the size of the enzyme region needs to be optimized. We thus analyze the effect of system parameters on the optimal enzyme region radius.

Introduction: Molecular communication via diffusion (MCvD) has been proposed for communication between nanonetworking-enabled nodes that are within a short range of one another [1]. In an MCvD system, molecules are emitted by a transmitter and propagate through the medium until they arrive at the receiver. The received molecules constitute the received signal and this is of prime importance for modeling and analyzing the MCvD channel. In [2], the authors derived the mean number of received molecules when the receiver was an absorbing sphere in a 3-dimensional (3-D) medium. In [3], the authors modeled the arrival process utilizing the formulation in a 3-D medium. One of the main challenges in MCvD is the heavy tail nature and the long propagation time of the received signal. The heavy tail of the received signal causes inter-symbol-interference (ISI). ISI must be carefully handled.

The literature has proposed using enzymes to cope with the deteriorating effects of ISI [4, 5, 6]. In [4], Noel *et al.* presented an analysis for the enzymatic degradation by modeling enzymatic reactions according to the Michaelis-Menten mechanism. In their model, the receiver node does not absorb or manipulate the messenger molecules, instead the molecules are able to pass through the receiver boundary with no resistance. In [5], Heren *et al.* provided a detailed analysis for the enzymatic degradation of messenger molecules. They derived the analytical formulation for the received fraction of molecules with respect to time when the receiver was an absorbing sphere in a 3-D environment. With the derived formulation, the authors analyzed the characteristics of the received molecular signal and realized that propagation time was improved at a cost of higher path loss. In [6], Wang *et al.* introduced secondary molecules to cancel the effect of the primary molecules, that is, to shape the transmit signal. They used the first hitting (absorption) formulation of a 1-D environment.

Analytical solutions for the differential equations of the diffusion and absorption processes require symmetry and an infinite environment for tractability. All the studies that consider enzymes, for tractability, assume that enzymes exist everywhere, which is unrealistic and requires an infinite amount of enzymes.

In this letter, we consider the case where a fixed amount of enzymes is deployed around the spherical receiver node in a 3-D environment. When the enzyme region around the receiver is enlarged, then the degradation effect is reduced due to a lowered enzyme concentration. Hence, we investigate the optimum radius for the enzyme region with our findings suggesting that such a radius exists. *To the best of our knowledge, this is the first attempt to optimize the enzyme deployment with a finite amount of the enzymes depending on the system parameters.*

System Topology and Processes: An MCvD system model is depicted in Fig. 1, where the information is modulated via emitted molecules. Following the emission, molecules diffuse in the fluid environment and arrive in a probabilistic manner at the receiver (with a radius of r_{rx}). Around the receiver an enzyme region is shown with an extending radius of r_{enz}. Two cases are depicted in the figure: one corresponds to a successful arrival at the receiver and the other corresponds to coinciding to an enzyme and degradation. The receiver node counts the number of received molecules and demodulates the information. Signal detection can be done via thresholding the number of received molecules.

The main processes of an MCvD system are the emission, propagation, and reception. For the reception we consider the first-hitting process, where the received molecules are removed from the 3-D environment (i.e., each molecule contributes to the received signal only once). Also, we consider a scenario where a fixed amount of enzymes is deployed around the receiver

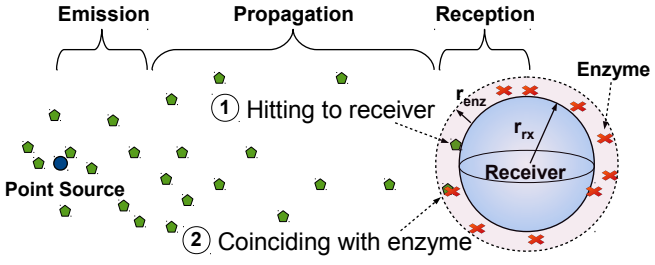

Fig. 1. MCvD system model with enzymes deployed around the receiver node.

in a spherical region with an extending radius of r_{enz} as depicted in Fig. 1. The enzyme region helps reduce the number of interference molecules.

Molecular Received Signal for Absorbing Receiver: First hitting probability function, when there is no enzyme effect, is formulated for an absorbing spherical receiver in a 3-D environment as

$$h(t) = \frac{r_{\text{rx}}}{d+r_{\text{rx}}} \frac{d}{\sqrt{4\pi D t^3}} e^{-\frac{d^2}{4Dt}} \tag{1}$$

where d and D stand for the distance and the diffusion coefficient, respectively [2]. The expected fraction of molecules hitting the receiver (i.e., the molecular received signal) until time t is formulated as

$$F(t) = \int_0^t h(t')dt' = \frac{r_{\text{rx}}}{d+r_{\text{rx}}} \operatorname{erfc}\left[\frac{d}{\sqrt{4Dt}}\right] \tag{2}$$

which determines the expected number of received molecules when multiplied by the number of emitted molecules. For each symbol duration, we can formulate the expected amount of received molecules.

To incorporate molecular degradation into MCvD, we consider the generic exponential decay function that is appropriate for MCvD

$$C(t) = C_0\, e^{-t\lambda} = C_0 \left(\frac{1}{2}\right)^{t/\Lambda_{1/2}} \tag{3}$$

where C_0, $C(t)$, λ, and $\Lambda_{1/2}$ are the initial concentration, the concentration at time t, the rate of degradation, and the half-life of the molecules [5]. Generally, λ is calculated from the corresponding half-life $\Lambda_{1/2}$ value, i.e., $\lambda = \ln(2)/\Lambda_{1/2}$. The probability of degrading at each step is determined by (3). For the enzyme everywhere case, the channel response function becomes

$$h(t|\lambda) = \frac{r_{\text{rx}}}{d+r_{\text{rx}}} \frac{d}{\sqrt{4\pi D t^3}} e^{-\frac{d^2}{4Dt} - \lambda t}. \tag{4}$$

The expected fraction of received molecules until time t becomes

$$F(t|\lambda) = \frac{1}{2} \frac{r_{\text{rx}}}{d+r_{\text{rx}}} \left\{ e^{-d\sqrt{\frac{\lambda}{D}}} \operatorname{erfc}\left[\frac{d}{\sqrt{4Dt}} - \sqrt{\lambda t}\right] + e^{d\sqrt{\frac{\lambda}{D}}} \operatorname{erfc}\left[\frac{d}{\sqrt{4Dt}} + \sqrt{\lambda t}\right] \right\}. \tag{5}$$

In our case, enzymes are not spread all around, hence we are not able to use (4) and (5) directly. We simulate the MCvD system extensively in a 3-D environment that is shown in Fig. 1 using (3). Note that, depending on r_{enz}, $\Lambda_{1/2}$ changes (i.e., the probability of degradation changes in the enzyme region). If a fixed amount of enzymes is used, then λ is inversely proportional to the volume of the enzyme region [5]. Therefore, if $\Lambda_{1/2}^{r_1}$ is known for $r_{\text{enz}} = r_1$, then $\Lambda_{1/2}^{r_2}$ for $r_{\text{enz}} = r_2$ can be evaluated as

$$\Lambda_{1/2}^{r_2} = \Lambda_{1/2}^{r_1} \frac{V_2}{V_1} = \Lambda_{1/2}^{r_1} \frac{(r_{\text{rx}}+r_2)^3 - r_{\text{rx}}^3}{(r_{\text{rx}}+r_1)^3 - r_{\text{rx}}^3} \tag{6}$$

where V_i denotes the volume of the enzyme region for $r_{\text{enz}} = r_i$. Note that it does not include the volume of the receiver; only the volume of the fluid environment with enzymes is considered. In our study, we use $\Lambda_{1/2}$ at 1 µm (namely $\Lambda_{1/2}^1$) for specifying the cases, and for different r_{enz} values we evaluate effective $\Lambda_{1/2}^{r_{\text{enz}}}$ from (6) by utilizing $\Lambda_{1/2}^1$ and r_{enz}. The value of $\Lambda_{1/2}^{r_{\text{enz}}}$ with (3) determines the probability of not degrading at each

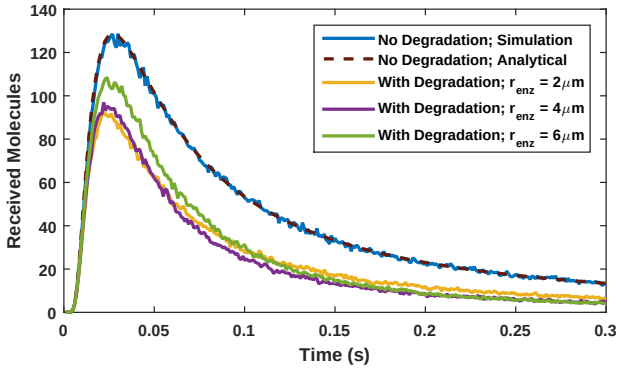

Fig. 2 *Time versus received signal for time resolution of* 1 ms, $d = 4\,\mu$m, $r_{rx} = 5\,\mu$m, $D = 100\,\mu\text{m}^2$/s, *and* $\Lambda^1_{1/2} = 5$ ms.

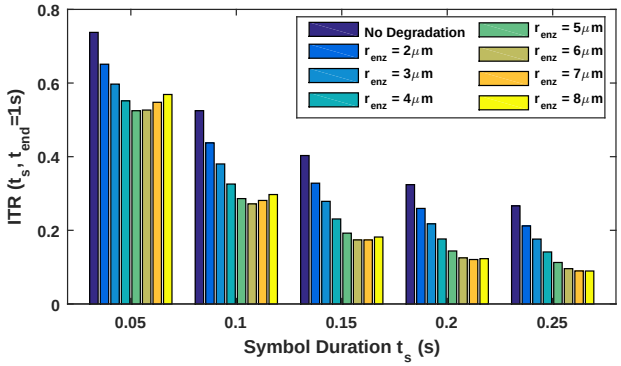

Fig. 3 *Symbol duration versus ITR* (t_s, t_{end}=1 s) *values for* $d = 4\,\mu$m, $r_{rx} = 5\,\mu$m, $D = 100\,\mu\text{m}^2$/s, *and* $\Lambda^1_{1/2} = 5$ ms.

simulation step (Δt) for a molecule in the enzyme region as follows:

$$\mathbf{P}(\text{not degrading}\,|\Lambda^{r_{\text{enz}}}_{1/2}) = e^{-\ln(2)\Delta t/\Lambda^{r_{\text{enz}}}_{1/2}} = \frac{1}{2^{\Delta t/\Lambda^{r_{\text{enz}}}_{1/2}}} \tag{7}$$

First, we analyzed the number of received molecules with respect to time. In Fig. 2, we see the effect of the enzyme region for the cases with degradation. It is clearly seen that the received signal structure is changed when the degrading enzymes are used. For example, the peak amplitude decreases when enzymes are deployed. Moreover, the peak times differ depending on r_{enz}. The curve that corresponds to $r_{\text{enz}} = 6\,\mu$m has a higher peak value compared to other cases with enzymes. However, its interference with symbols that follow also higher for a range of symbol durations.

ITR Formulation: After seeing the difference in the received signal structures, we needed a metric that focuses on the interference so as to compare the enzyme deployment scenarios. We evaluate the interference-to-total-received-molecules ratio (ITR) for a given symbol duration (t_s) and the end time (t_{end}) as follows

$$\text{ITR}(t_s, t_{\text{end}}) = \frac{F^{\text{sim}}(t_{\text{end}}|\lambda) - F^{\text{sim}}(t_s|\lambda)}{F^{\text{sim}}(t_{\text{end}}|\lambda)}\,. \tag{8}$$

In other words, ITR is the ratio of the interference molecules to the total received molecules. For example, having an ITR of 0.1 means that the number of interference molecules after t_s is 1/10 of the total received molecules. Therefore, the smaller the ITR values the better.

As noted above, increasing r_{enz} increases $\Lambda^{r_{\text{enz}}}_{1/2}$ (i.e., decreases the probability of degradation). On the other hand, it increases the probability of entering to the enzyme region. Hence there is a tradeoff between these two probabilities, giving rise to a need to optimize r_{enz}. In Fig. 3, ITR values are presented for different symbol durations and r_{enz}. We observe that there is an optimal r_{enz} and a worse ITR is produced after that specific value; i.e., nothing gained by increasing the enzyme region size. This is reasonable, since the enzyme effect diminishes if you consider the asymptotic behavior in which $r_{\text{enz}} \to \infty$. For $t_s = 0.1$ s, the optimal r_{enz} is 6 μm and the ITR is reduced to nearly the half of the no degradation case.

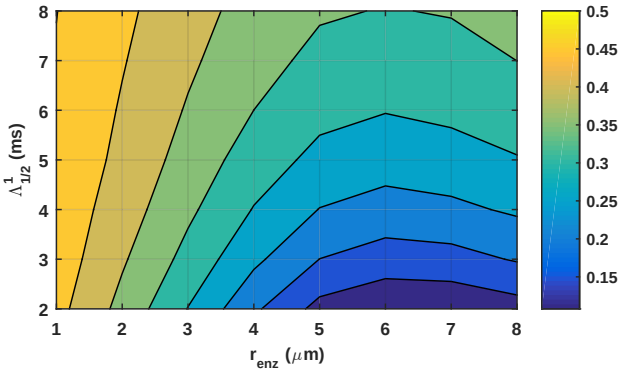

Fig. 4 *Heatmap of ITR* (t_s=0.1 s, t_{end}=1 s) *for* $d = 4\,\mu$m, $r_{rx} = 5\,\mu$m, *and* $D = 100\,\mu\text{m}^2$/s.

The next eventual question is whether the optimal r_{enz} depends on $\Lambda^1_{1/2}$ or not. From Fig. 3, we can understand that it depends on t_s but are offered no clue as to its dependence on $\Lambda^1_{1/2}$ since it is fixed for this analysis. Hence, we also varied $\Lambda^1_{1/2}$ to understand the dynamics of r_{enz}. We chose t_s=0.1 s for the more detailed analysis from Fig. 3 and varied $\Lambda^1_{1/2}$ and r_{enz}. In Fig. 4, a heatmap of ITR (t_s=0.1 s, t_{end}=1 s) is depicted for varied parameters. First of all, decreasing $\Lambda^1_{1/2}$ improves ITR; i.e., it reduces the interference molecules with the given parameters. Secondly, increasing r_{enz} improves ITR up to a point after which it deteriorates. Similar behavior is observed for all $\Lambda^1_{1/2}$ values. Moreover, $r_{\text{enz}} = 6\,\mu$m is the optimum enzyme deployment scenario for all $\Lambda^1_{1/2}$ values with given parameters. For some cases with the optimal r_{enz} there is five-fold improvement (in terms of ITR), which means five times fewer interference molecules.

Conclusion: In this letter, we analyzed an MCvD system with a fixed amount of enzymes around the receiver node in a 3-D environment. Enzymes improve the system performance in terms of ITR since the lingering molecules are degraded. There is an important system parameter to decide for a system designer: r_{enz} determines the enzyme effectiveness. Increasing r_{enz} increases the probability of entering to the enzyme region for the diffusing molecule. On the other hand, having a fixed amount of enzyme in a bigger volume decreases the enzyme concentration, hence the probability of degradation. Firstly, we formulated $\Lambda^{r_{\text{enz}}}_{1/2}$ depending on $\Lambda^1_{1/2}$. Then, we presented the effect of r_{enz} on the signal shape and ITR. Results showed that the minimum ITR is achieved with specific r_{enz} values for different t_s options. We also analyzed the ITR while varying r_{enz} and $\Lambda^1_{1/2}$. Results suggest that the optimal r_{enz} does not change with $\Lambda^1_{1/2}$ but depends on t_s when the distance is fixed.

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