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 molecular signal interference caused by eliminating unwanted chemicals that persist in the system. An MCvD system with a fixed amount of enzymes around the spherical receiver is considered. 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 optimised. Thus, the effect of system parameters on the optimal enzyme region radius is analysed.

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, 2]. 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 modelling and analysing the MCvD channel. In [3], the authors derived the mean number of received molecules when the receiver was an absorbing sphere in a 3D medium. In [4], the authors modelled the arrival process utilising the formulation in a 3D 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). The ISI must be carefully handled.

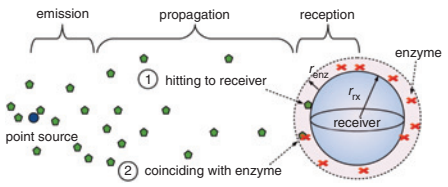

Fig. 1 *MCvD system model with enzymes deployed around receiver node*

The literatures have proposed using enzymes to cope with the deteriorating effects of ISI [5–7]. In [5], Noel *et al.* presented an analysis for the enzymatic degradation by modelling 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 [6], 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 3D environment. With the derived formulation, the authors analysed the characteristics of the received molecular signal and realised that propagation time was improved at a cost of higher path loss. In [7], 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 1D 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 3D 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.

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 3D 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 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.

Received molecular signal for absorbing receiver: First hitting probability function, when there is no enzyme effect, is formulated for an absorbing spherical receiver in a 3D environment as

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

where d and D stand for the distance and the diffusion coefficient, respectively [3]. The expected fraction of molecules hitting the receiver (i.e. the molecular received signal) until time t is formulated as

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

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

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

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 [6]. 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 can be expressed as

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

The expected amount of received molecules from time 0 to t is

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

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 3D 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 [6]. Therefore, if $\Lambda_{1/2}^{r_1}$ is known for $r_{enz} = r_1$, then $\Lambda_{1/2}^{r_2}$ for $r_{enz} = r_2$ can be evaluated as

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

where V_i denotes the volume of the enzyme region for $r_{enz} = r_i$. 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 $\Lambda_{1/2}^{r_{enz}}$ from (6) by utilising $\Lambda_{1/2}^1$ and r_{enz}. The value of $\Lambda_{1/2}^{r_{enz}}$ with (3) determines the probability of not degrading at each simulation step (Δt) for a molecule in the enzyme region as follows

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

First, we analysed 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_{enz} = 6 μm has a higher peak value compared with other cases with enzymes. However, its interference with symbols that follow is also higher for a range of symbol duration.

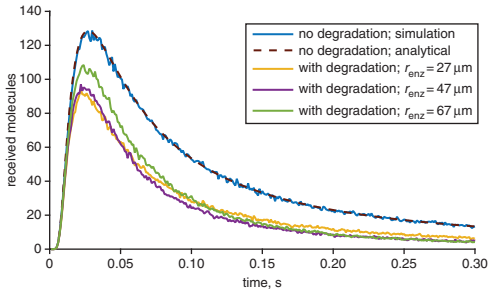

Fig. 2 *Time against received signal for time resolution of 1 ms, d = 4 μm, r_{rx} = 5 μm, D = 100 μm²/s, and $\Lambda^1_{1/2} = 5$ ms*

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

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

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 $\Lambda^{r_{enz}}_{1/2}$ (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 optimise 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 behaviour in which $r_{enz} \to \infty$ 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.

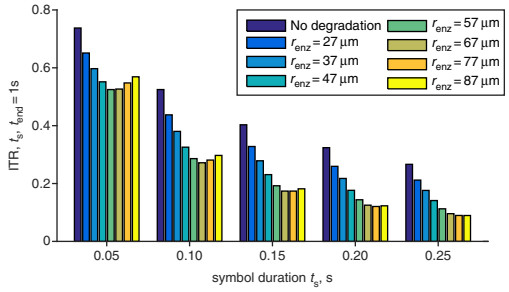

Fig. 3 *Symbol duration against ITR (t_s, t_{end} = 1 s) values for d = 4 μm, r_{rx} = 5 μm, D = 100 μm²/s, and $\Lambda^1_{1/2} = 5$ ms*

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 choose $t_s = 0.1$ 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 behaviour is observed for all $\Lambda^1_{1/2}$ values. Moreover, $r_{enz} = 6$ μm 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.

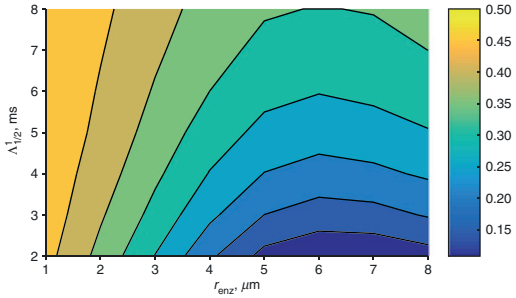

Fig. 4 *Heatmap of ITR ($t_s = 0.1$ s, $t_{end} = 1$ s) for d = 4 μm, r_{rx} = 5 μm, and D = 100 μm²/s*

Conclusion: In this Letter, we analysed an MCvD system with a fixed amount of enzymes around the receiver node in a 3D 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. First, we formulated $\Lambda^{r_{enz}}_{1/2}$ 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 analysed 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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One or more of the Figures in this Letter are available in colour online.

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