CmpE 49G - Project 3 - Report
Emre Girgin - 2016400099

1. Introduction

Communication in computer networks is a widely studied and grown area for several decades. Although endless improvements have been achieved in both wired and wireless communication, the nanoscale level remains a new and relatively less studied area even today. The application of molecular communication can be utilized in various fields, such as healthcare, agriculture, and industry. However, there are limitations in both hardware capabilities and application channels. For instance, developing a device that can both fit into the blood vessel and send proper signals to a receiver efficiently, is an extremely hard problem. Besides, testing the solutions brought to such problems may have ethical issues because it may require the use of a living creature as an environment. At this point designing a simulation to test this solution gains critical importance. By exploiting the simulations, we may come up with a really promising solution before we test it in a real environment. As a result, simulations for this kind of problems allow us to have flexibility, reproducibility, and safety. Thus, simulation techniques used in molecular communication have to be studied and examined in detail.

One fundamental phenomenon of the nanoscale dynamics is Brownian Motion or in other words propagating via diffusion. According to this model, the particles in a liquid or gas environment move around randomly depending on some properties of the environment such as the diffusion coefficient. This property allows particles released from a point in the space to reach another point in the same space with some ratio. By defining such rules of environment, one can define the release point of the particles as transmitter and the target point as the receiver. Using this analogy we may measure the ratio of the molecules received by the receiver at a certain time. Furthermore, by recording the number of molecules received in each unit of time, we may simulate a pulse, which may correspond to the logical one in computer networks. However, like every pulse, such pulses also have the tail causing Intersymbol Interference (ISI) problem. Sending consecutive signals without waiting a sufficient amount of cooldown period leads to this problem. On the other hand, waiting between signals will slow down the communication process. This problem is a fundamental problem of molecular level communication.

The properties of the environment are not limited to the Brownian Motion. If we are looking from the biological perspective, enzymes are very common in such

environments and they may affect the lifetime of the particles that have been being tracked. The systems developed for communication should be robust to degrading factors like enzymes. However, enzymes may help us to develop systems encountering ISI problems. Since we want to reset the particles which are not absorbed by the receiver in our environment after the peak point, enzymes may conduct this by degrading the molecules in the environment.

To conclude, molecular level communication is an essential field of study in both today and the future. As humankind, we are going to need such devices eventually. However, recent studies still have some fundamental problems that have been overcome decades ago in computer networks. The reason is the techniques we applied to traditional communication are not designed for such an environment. This is why molecular communication needs a brand new point of view.

2. System Model

a. Topology

During the following experiments, I have examined two main cases: Communication via diffusion with and without enzymes.

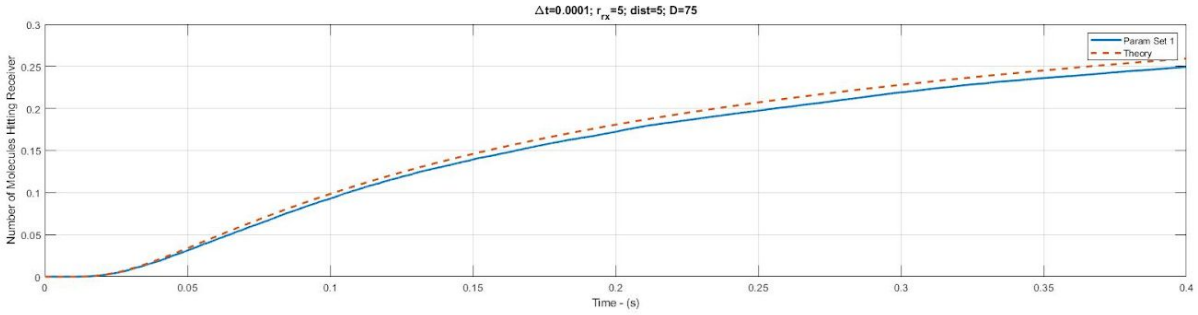
For the cases without enzymes, there is a point transmitter and a spherical receiver. The particles released from the point transmitter, diffuse through the environment with Brownian Motion. This motion is simulated using a Gaussian Distribution depending on the diffusion coefficient of the environment. At each step, the L2 distance between each molecule and receiver's center is calculated and if it is less than the radius of the sphere, then it is counted as a hit. These steps are continued until a certain amount of time which is sufficient for neatly all particles to be absorbed. The step that it is hit is stored for each particle. Using this statistics to graphs are plotted: The first one is the total number of particles that hit the receiver up to a given time. This graph corresponds to a function and from now on this function will be called as F(t). The other graph shows the number of molecules hit to the receiver for a certain timestep. However, for illustrative purposes each 10 timestep is merged. The function of this graph will be called as f(t), from now on.

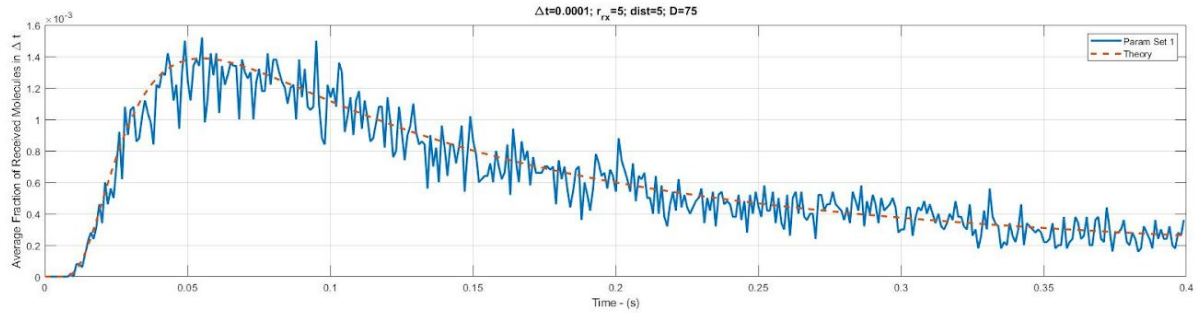
The second case, which is the one with enzymes, very resembles the first case except some additions. At each step, before checking for absorption, we generate a uniform random number for each particle. If the generated number is less than a number obtained by combination delta t (unit time length) and degrading rate (related with the nature of the enzymes), then we count that particle to be not degraded. This calculation comes from the half life property of the particles that can be degraded by the enzymes. Similar to the shelf-life of the products in the market, the half-life of the particles in an environment with enzymes follows an exponential distribution. The rest of the experiment is the same with the one without enzymes.

b. Diffusion Simulations (wo/Enzymes)

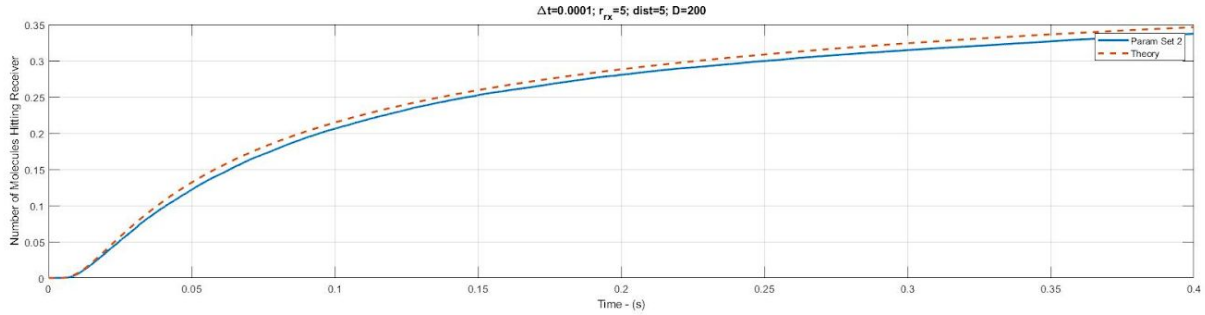
For the graphs below, for each figure, the upper one represents the F(t) and the lower one represents the f(t).

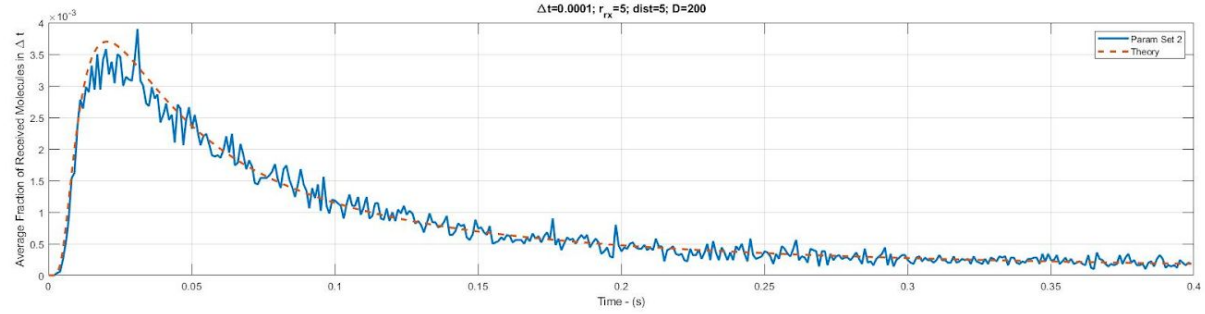
i. Parameter Set 1





ii. Parameter Set 2



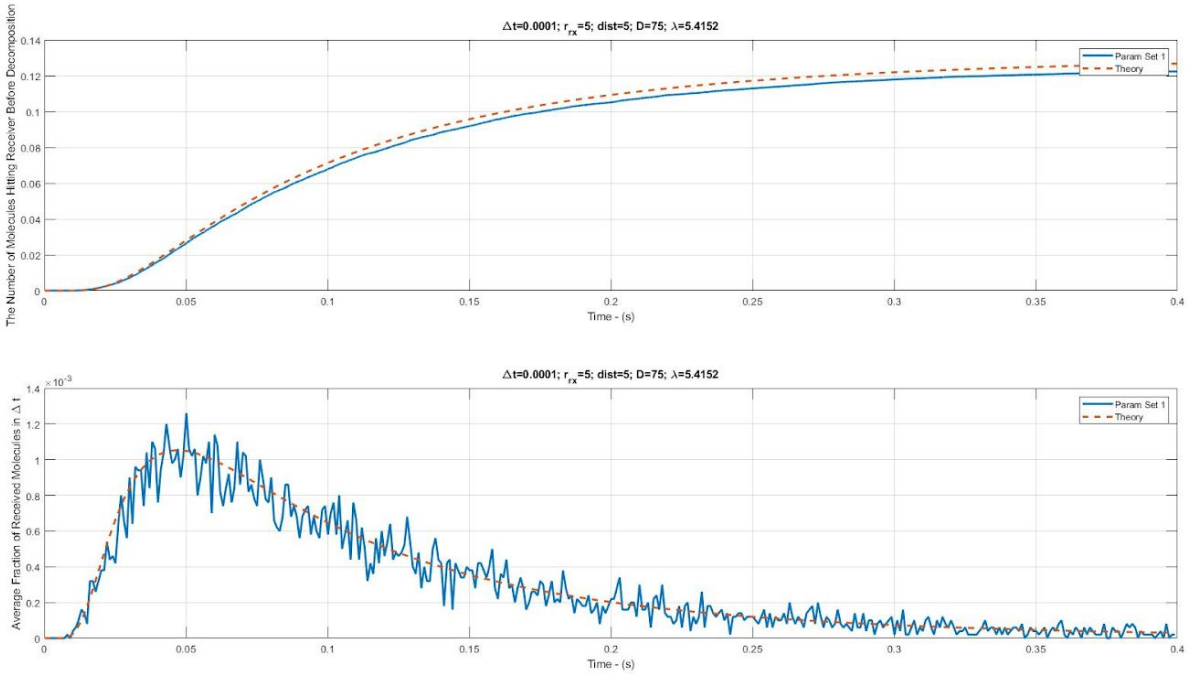


The difference between the experiments above is the diffusion coefficient. Both experiments are consistent with the theoretical calculation. They show that, the higher the diffusion coefficient, the higher the rate of received molecules.

c. Diffusion Simulations (w/Enzymes)

For the graphs below, for each figure, the upper one represents the F(t) and the lower one represents the f(t).

i. Parameter Set 1



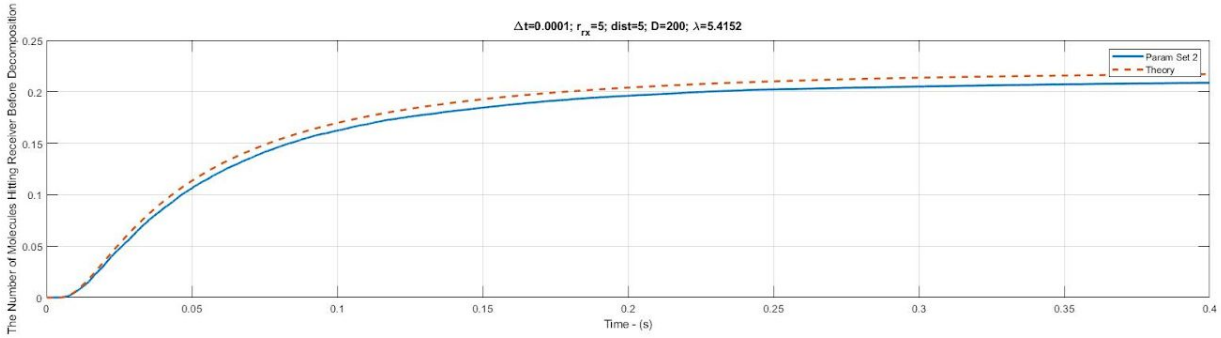
This experiment can be compared with **b.i, c.ii**, and **c.iii**.

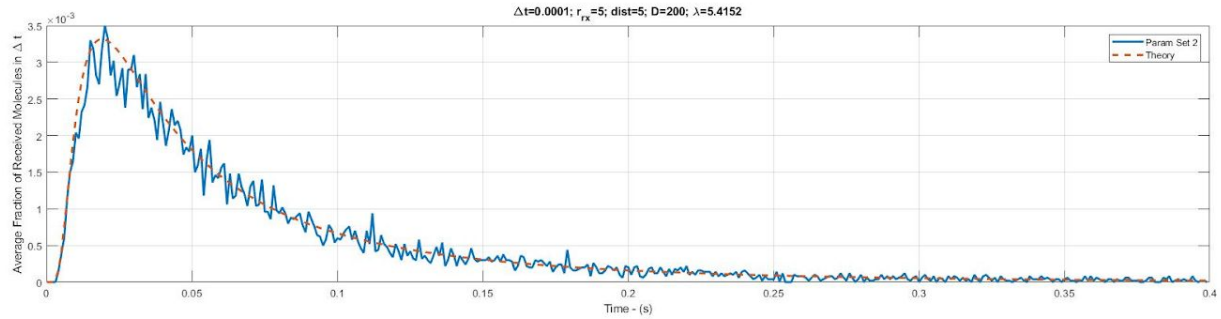
Compared to **b.i** the only difference is the presence of the enzymes. As a result of that the ratio of the total number of absorbed molecules decreases. (0.35 vs 0.12) On the other hand, the number of received molecules per timestep reaches its peak at the same time but with different ratios. However, the peak values are not that different (1.4x10^(-3) vs 1.0x10^(-3)) and we don't see the heavy tail that we saw in **b.i** in this setup, which may help us to overcome the ISI problem.

Compared to **c.ii**, the only difference is the diffusion coefficient. We see the exact difference we saw between **b.i** and **b.ii**. The higher the diffusion coefficient, the higher the rate of the absorbed molecules.

Compared to **c.iii**, the only difference is the degrading rate of the enzymes. As the degrading rate of the enzymes increases, the total number of particles reaching to the receiver increases. Besides, the amplitude at the peak gets lower and the tail is less heavy now. Although the amplitude of the peak is less, the pulse is still observable.

ii. Parameter Set 2





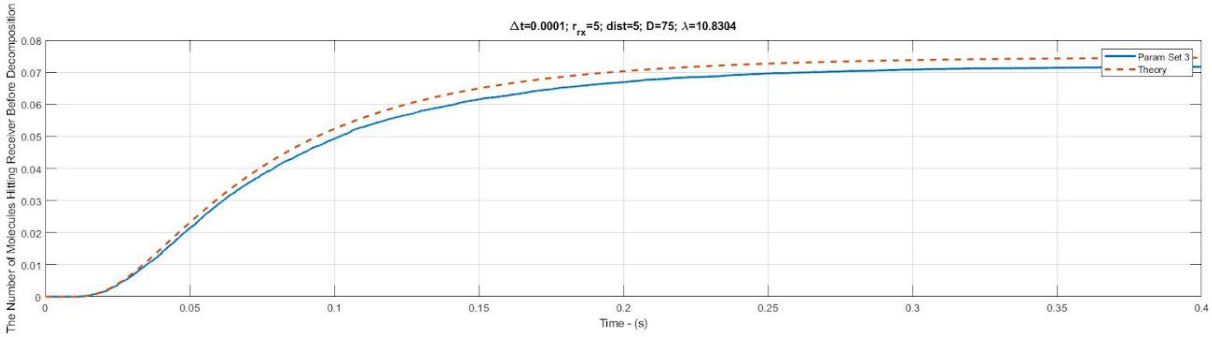
This experiment can be compared with **b.ii**, **c.i**, **c.iv**.

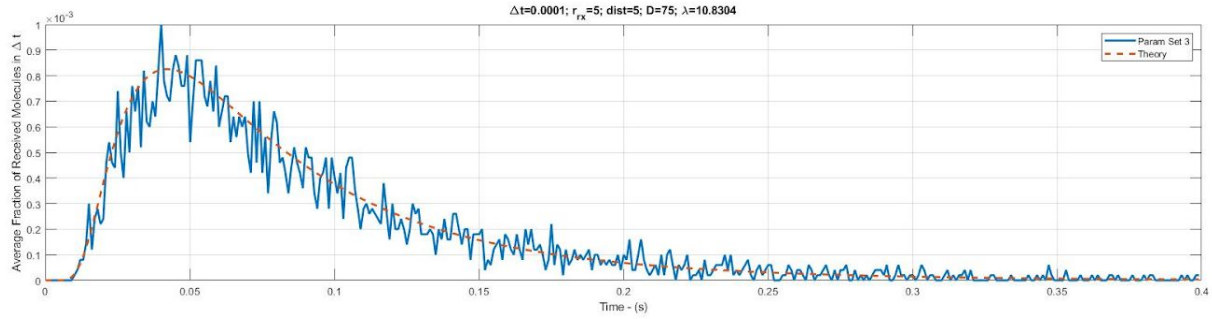
Compared to **b.ii**, the only difference is the enzymes. We see a similar relation that we saw between **c.i** and **b.i**. The total number of absorbed molecules decreases but peak amplitude stays as it is. In addition, the tail we saw in **b.ii** is heavier. If ve compare the number of absorbed molecules at time 0.1, in **b.ii** the value is around whereas in here (**c.ii**) the value is below the 1.

Compared to **c.iv**, the only difference is the degrading rate of the enzymes. The amplitudes at peaks are the same but **c.iv** has a more steep peak compared to **c.ii**. This property allows us to get rid of the heavy tail more accurately.

The comparison between **c.ii** and **c.i** has been done in the part of **c.i**.

iii. Parameter Set 3





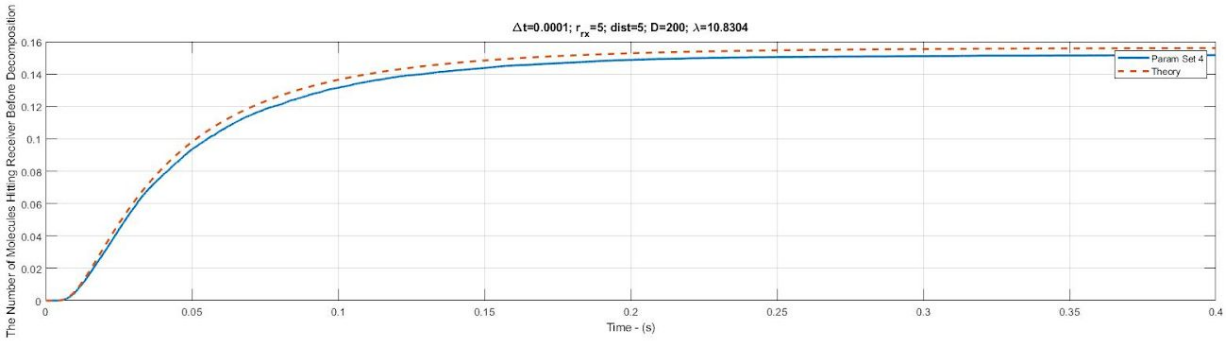
This experiment can be compared with **b.i**, **c.i**, and **c.iv**.

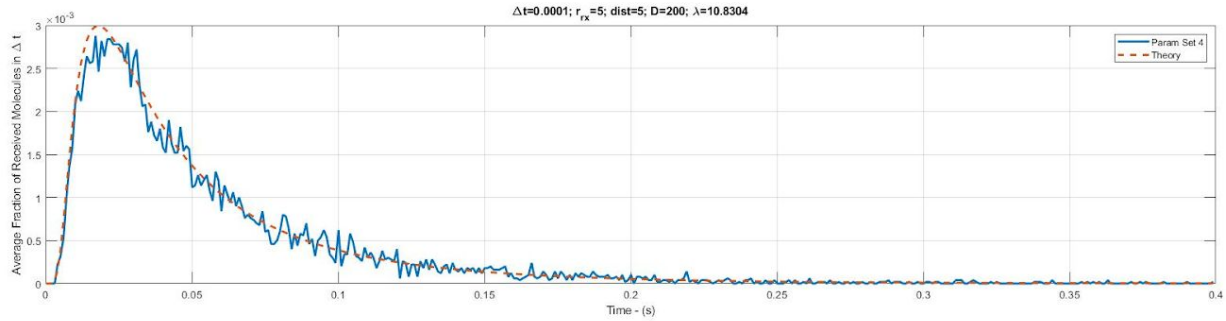
Compared to **c.iv** the only difference is the diffusion coefficient. This allows us to have a more steep and apparent peak. In addition, the total number of molecules being absorbed is more than **c.iv**.

Comparison to **c.i** is done in the section of **c.i**.

Comparison to **b.i** is very similar to done in **c.i**.

iv. Parameter Set 4





This experiment can be compared with **b.ii**, **c.ii**, and **c.iii**.

All of the comparisons made above but to talk especially for this experiment, we need to state this setup helps us most when we consider the objectives of our simulation. We see the pulse characteristics more apparent and the tail is not as heavy as the previous ones.

d. Analytical Formulations

The formulations are adopted from the project description.

i. w/Enzymes

$$N^{Rx}(t) = N^{Tx} F(t|\lambda) = N^{Tx} \frac{1}{2} \frac{r_{rx}}{r_{rx}+d} \left\{ e^{-d\sqrt{\lambda/D}} \, erfc\left(\frac{d}{\sqrt{4Dt}} - \sqrt{\lambda t}\right) + e^{d\sqrt{\lambda/D}} \, erfc\left(\frac{d}{\sqrt{4Dt}} + \sqrt{\lambda t}\right) \right\}$$

The parameters changed are lambda and D, corresponding to degrading rate and diffusion coefficient, respectively. Generally, lambda is inverse proportioned to the number of absorbed molecules. However, since it is multiplied with time t in the erfc function, for the earlier period of time of the experiment, it's effect is not that observable. This is why we don't see so much difference in the amplitude of the peak, in the graphs.

ii. wo/Enzymes

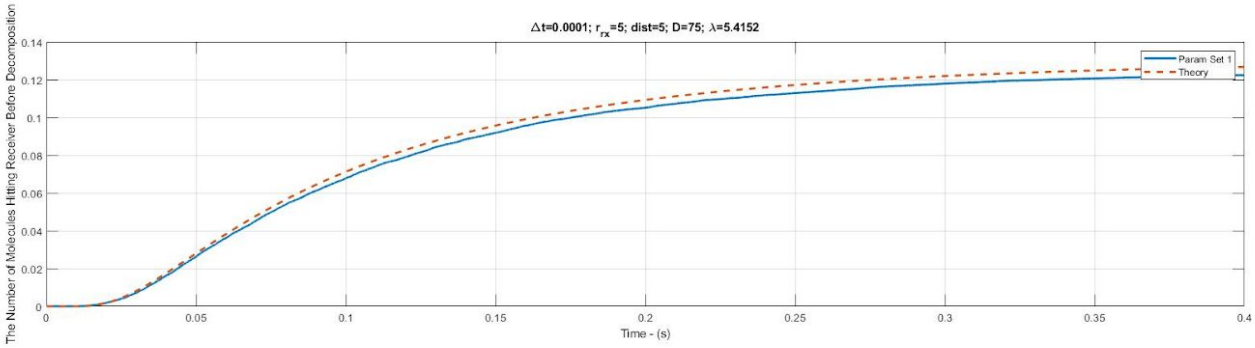
$$N^{Rx}(t) = N^{Tx} F(t) = N^{Tx} \frac{r_{rx}}{r_{rx}+d} \, erfc\left(\frac{d}{\sqrt{4\,D\,t}}\right)$$

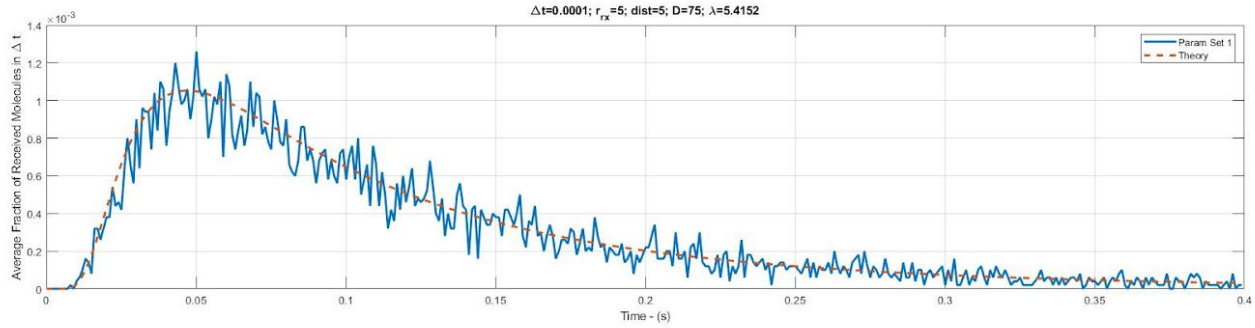
The only parameter we changed during our experiments was the diffusion coefficient in the formula. The output of the complementary error function decreases as its input increases.[1] Thus, we can see, by comparing the results of **b.i** and **b.ii**, when we increase the diffusion coefficient, we see a higher number of absorbed molecules.

3. Numerical Results

a. w/Enzymes

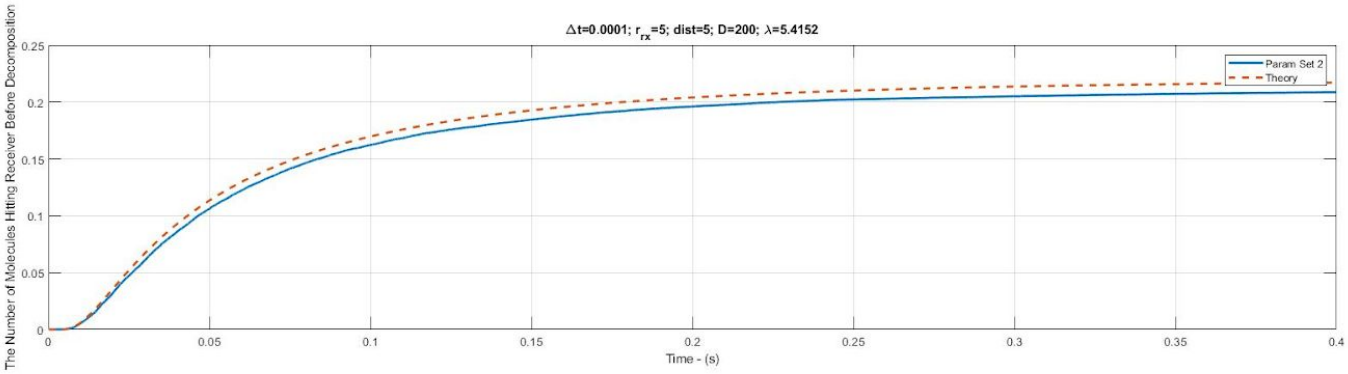
i. Parameter Set 1

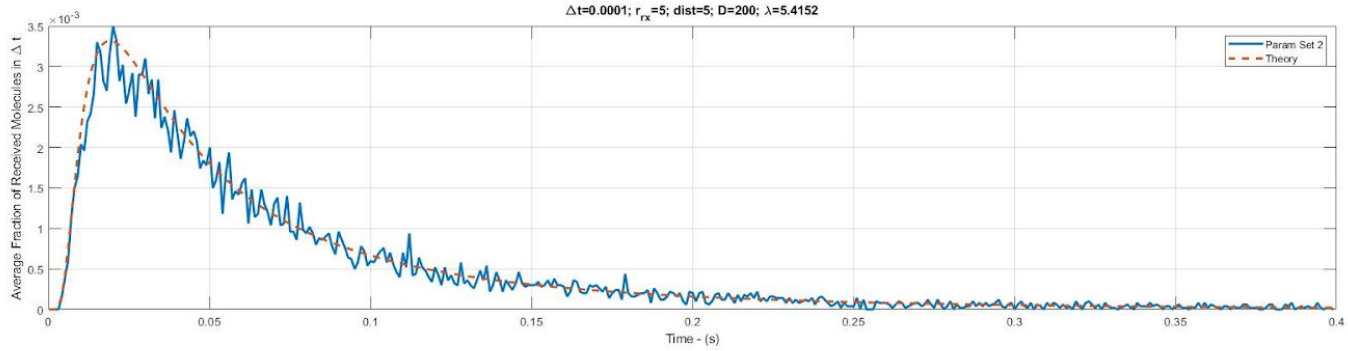




sim_params.rx_center	[0, 0, 0]
sim_params.rx_r_inMicroMeters	5
sim_params.rx_tx_distance	5
sim_params.tx_emission_pt	[10, 0, 0]
sim_params.D_inMicroMeterSqrPerSecond	75
sim_params.lambda_degRate	5.4152
sim_params.tend	0.4
sim_params.delta_t	0.0001
sim_params.num_molecules	50000

ii. Parameter Set 2





sim_params.rx_center	[0, 0, 0]
sim_params.rx_r_inMicroMeters	5
sim_params.rx_tx_distance	5
sim_params.tx_emission_pt	[10, 0, 0]
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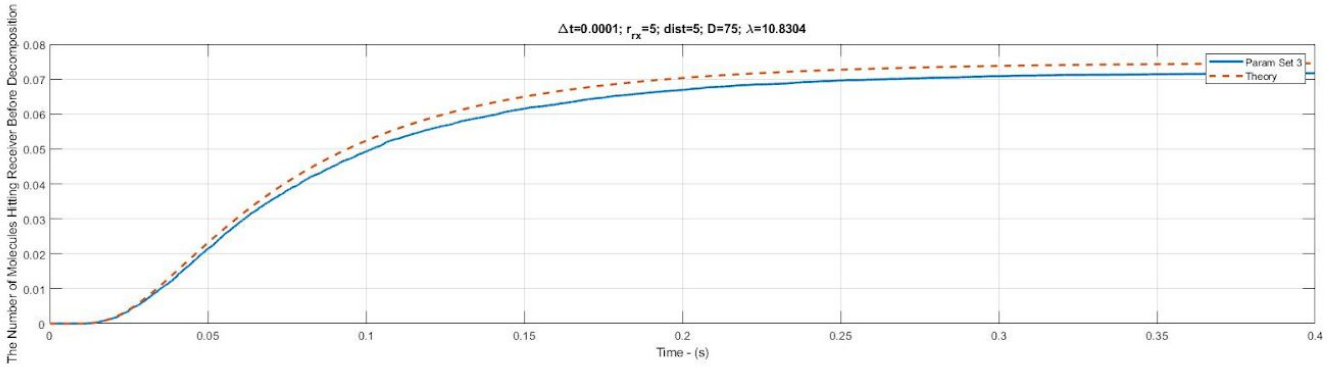
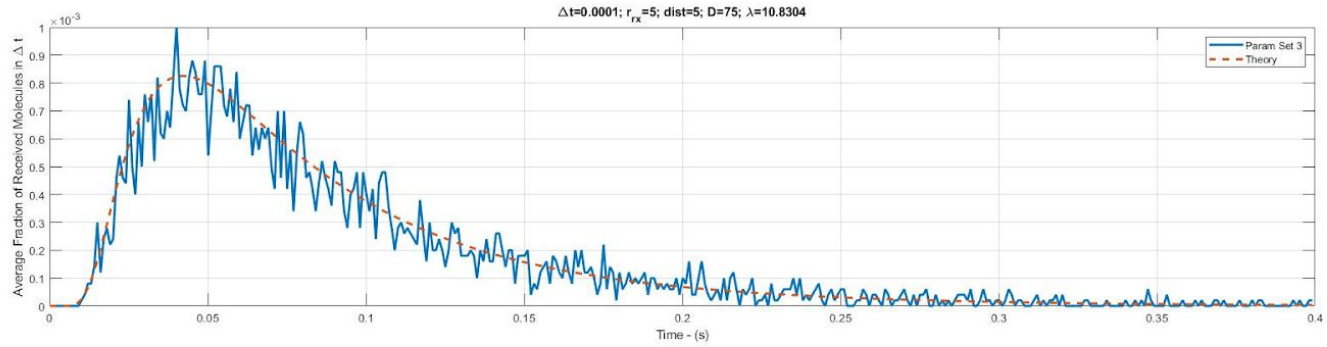
sim_params.lambda_degRate	5.4152
sim_params.tend	0.4
sim_params.delta_t	0.0001
sim_params.num_molecules	50000

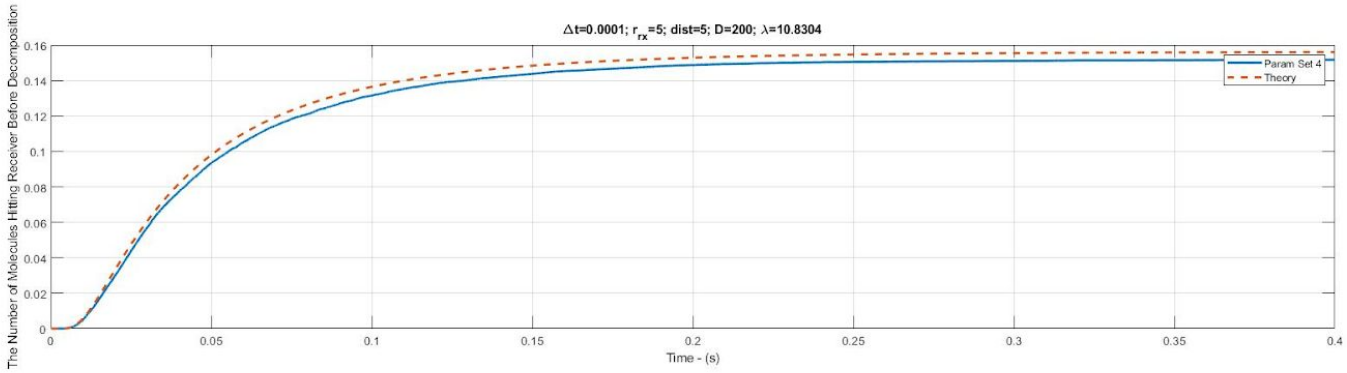
iii. Parameter Set 3

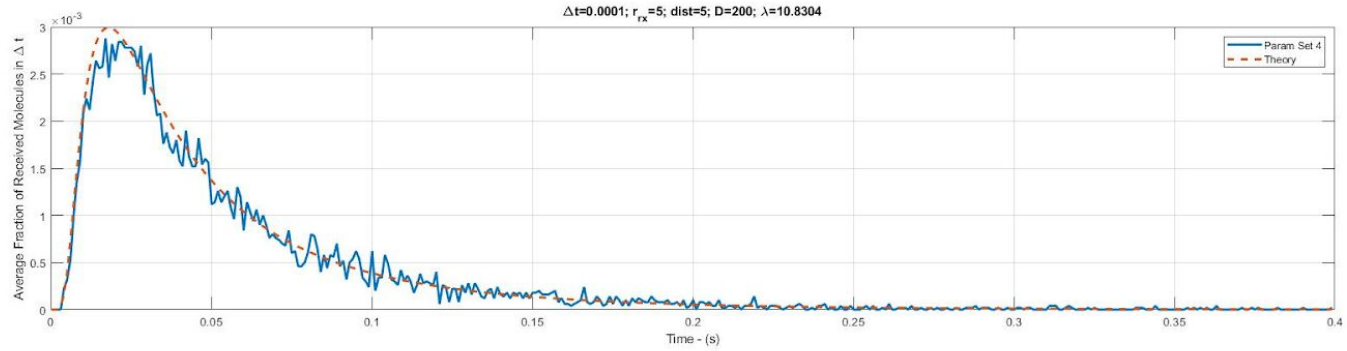




sim_params.rx_center	[0, 0, 0]
sim_params.rx_r_inMicroMeters	5
sim_params.rx_tx_distance	5
sim_params.tx_emission_pt	[10, 0, 0]
sim_params.D_inMicroMeterSqrPerSecond	75
sim_params.lambda_degRate	10.8304
sim_params.tend	0.4
sim_params.delta_t	0.0001
sim_params.num_molecules	50000

iv. Parameter Set 4

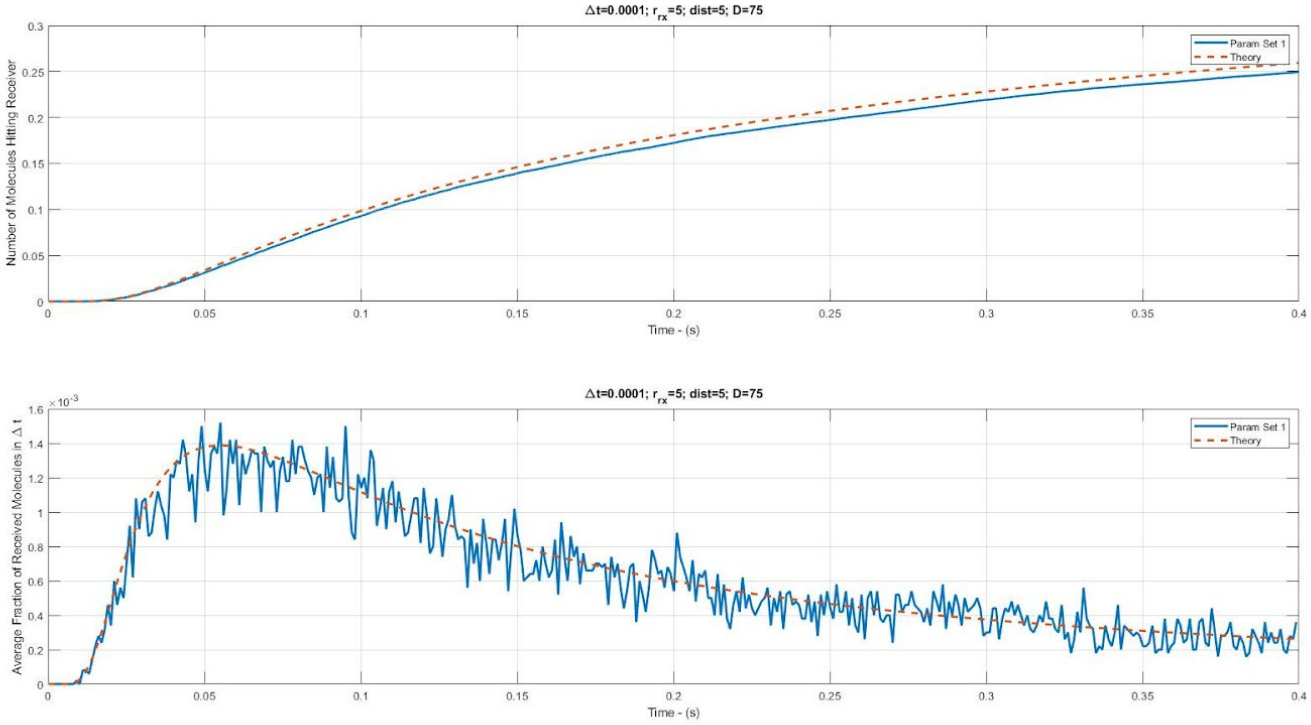




sim_params.rx_center	[0, 0, 0]
sim_params.rx_r_inMicroMeters	5
sim_params.rx_tx_distance	5
sim_params.tx_emission_pt	[10, 0, 0]
sim_params.D_inMicroMeterSqrPerSecond	200
sim_params.lambda_degRate	10.8304
sim_params.tend	0.4
sim_params.delta_t	0.0001
sim_params.num_molecules	50000

b. wo/Enzymes

i. Parameter Set 1



Parameter Set 1:

sim_params.rx_center	[0, 0, 0]
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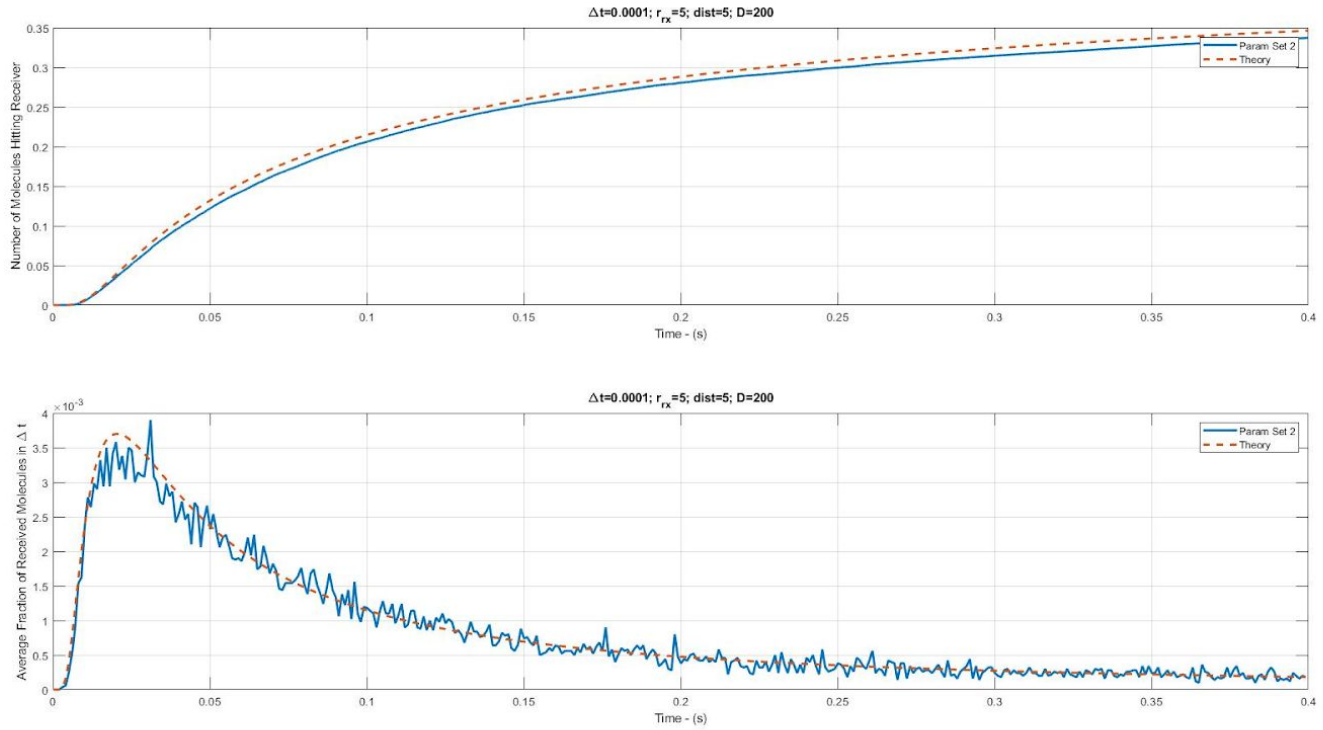
sim_params.D_inMicroMeterSqrPerSecond	75
sim_params.tend	0.4
sim_params.delta_t	0.0001
sim_params.num_molecules	50000

ii. Parameter Set 2



Parameter Set 2:

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sim_params.rx_tx_distance	5
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sim_params.D_inMicroMeterSqrPerSecond	200
sim_params.tend	0.4
sim_params.delta_t	0.0001
sim_params.num_molecules	50000

Statistics:

Setup	Fraction of Total Number Absorbed Molecules at Time T_end	Amplitude at Peak	Fraction of Absorbed Molecules at Time 0.1
wo/E - D:75	~0.25	~1.4*10^(-3)	~1.1*10^(-3)
wo/E - D:200	~0.35	~3.5*10^(-3)	~1.2*10^(-3)
w/E - D:75 - λ: 5.4152	~0.12	~1.0*10^(-3)	~0.7*10^(-3)
w/E - D:200 - λ: 5.4152	~0.21	~3.2*10^(-3)	~0.7*10^(-3)
w/E - D:75 - λ: 10.8304	~0.07	~0.8*10^(-3)	~0.4*10^(-3)
w/E - D:200 - λ: 10.8304	~0.15	~3.0*10^(-3)	~0.4*10^(-3)

As it can be seen from the table the experiment at the last row has the least heavy tail, despite to its amplitude at peak is competitive with the best (ranked at three).

References:

1. https://www.mathworks.com/help/matlab/ref/erfc.html#bupp9aq-4