

CmpE49G - Project 3

Effect of Enzyme Region on Diffusion

Due Date: 2021.01.04 (Monday) @ 23:59

A time dependent function $F(t)$ that is defining the mean fraction of received molecules until time t defines the Molecular Communication channel, since you can estimate the channel response by evaluating the channel coefficients for a given communication symbol duration (please refer to the slides week06a).

Enzymes in the environment affect $F(t)$, hence the received molecular signals. When there are enzymes in the environment molecules degrade in the environment with a **degradation rate** that is denoted by λ or the half-life $\Lambda_{1/2}$ (slides week06a, Eqn. 5).

Simulation Task 1- No Enzymes:

First, you need to simulate the diffusion process when there is a spherical absorber. You need to record the number of received molecules at each simulation time step Δt (you may utilize the codes provided in week03). The cumulative number of received molecules with respect to time should obey the following formula:

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

where r_{rx} is the radius of the receiver/absorber, d is the distance between emission point and the closest point on the surface of the receiver, and D is the diffusion coefficient.

Run the simulation with the following parameters and plot the analytical formula of $N^{Rx}(t)$ and the cumulative number of received/absorbed molecules that is recorded in the simulations. Please note that the provided codes in the lecture plot different thing (non-cumulative signal), it is easier to plot cumulative signal since it does not require merging with respect to time. You may watch the recordings of week3 for the details of the diffusion simulator.

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  = [sim_params.rx_tx_distance+sim_params.rx_r_inMicroMeters, 0, 0];
sim_params.D_inMicroMeterSqrPerSecond = 75;

sim_params.tend           = 0.4;
sim_params.delta_t        = 0.0001;
sim_params.num_molecules  = 50000;
```

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  = [sim_params.rx_tx_distance+sim_params.rx_r_inMicroMeters, 0, 0];
sim_params.D_inMicroMeterSqrPerSecond = 200;

sim_params.tend           = 0.4;
sim_params.delta_t        = 0.0001;
sim_params.num_molecules  = 50000;
```

Simulation Task 2- With Enzymes:

In this case, there will be enzymes in the environment and you need to incorporate not degrading probability at each simulation time step. The cumulative number of received molecules with respect to time should obey the following formula:

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

where λ is the degradation rate.

Run the simulation with the following parameters and plot the analytical formula of $N^{Rx}(t)$ and the cumulative number of received/absorbed molecules that is recorded in the simulations. Please note that the provided codes in the lecture plot different thing (non-cumulative signal), it is easier to plot cumulative signal since it does not require merging with respect to time. You may watch the recordings of week6 for the details of the diffusion simulation with enzymes in the environment. For evaluating the probability of not-degrading at each step, please refer to Eqn. 10 in slides of the 6th week.

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  = [sim_params.rx_tx_distance+sim_params.rx_r_inMicroMeters, 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;
```

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  = [sim_params.rx_tx_distance+sim_params.rx_r_inMicroMeters, 0, 0];
sim_params.D_inMicroMeterSqrPerSecond = 200;
sim_params.lambda_degRate   = 5.4152

sim_params.tend            = 0.4;
sim_params.delta_t         = 0.0001;
sim_params.num_molecules   = 50000;
```

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  = [sim_params.rx_tx_distance+sim_params.rx_r_inMicroMeters, 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;
```

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  = [sim_params.rx_tx_distance+sim_params.rx_r_inMicroMeters, 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;
```

Submission:

- You need to run 6 simulations and compare them with the analytical formulations
- You should plot cumulative and non-cumulative signal to compare the effect of λ on the received signal. When you increase the degradation rate, you need to answer the following questions: i) Does it affect the received signal amplitude? ii) Does it have a heavier tail or not?
- You need to submit **two pdf files** with the name <stuID_prj3_name_surname_report.pdf> and <stuID_prj3_name_surname_codes.pdf>. Report should have
 - An introduction section (between 1 and 2 pages),
 - System model section including the following subsections:
 - Topology
 - Diffusion simulations (without enzymes)
 - Diffusion simulations (with enzymes)
 - Analytical formulations (with and without enzymes)
 - Numerical Results (for each plot you should give the system parameters in the caption)
- You may use **any** programming language, but I strongly suggest Matlab or Python.

Important:

- You need write the report with your own words. You may read and get inspired from articles and/or internet, but you have to write your report with your own words.
- You have to cite your sources.
- For turnitin assignments, you will be able to see similarity score for your submission few minutes after you submit it. You may submit 3 times, if you are not happy with the similarity score. If you use your own words, the similarity score would be less than 20%. I will be checking your similarity scores; they should be less than 35%, otherwise you will get penalty on your scores.