U2151556 (Assignment-2)

Task-1

Part - (a)

For 10000 events, **T** is observed to be 63 seconds.

Below chart is plotted for 10 events to make the simulation readable, where green and red bars represent that the channel is open and closed respectively. And the length of the bars represent the **Tau** of each event. Transition is shown using dashed lines, C → O -- , O → C --

Code : A function is written to simulate the problem using truncated Gillespie's algorithm, which takes all the parameters as an input along with the number of events for which the simulation has to run. It returns the cumulative time array along with corresponding state(O-1,C-0) in an array. Then these two arrays are used to plot the chart below. It also returns two additional arrays for Tau-close and Tau-open computed at every alternate event.

```
Intial State is considered to be closed
Time interval covered : 113.82
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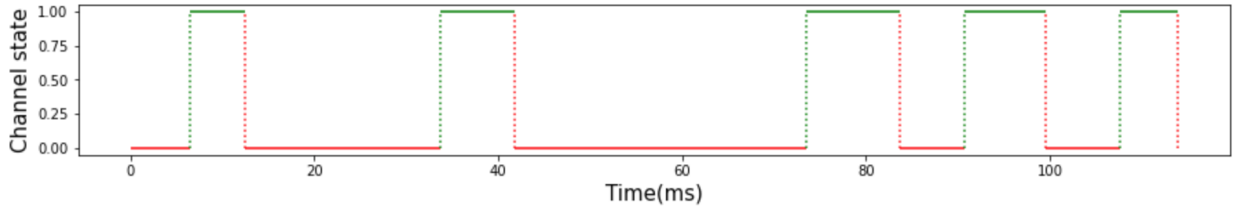


Part - (b)

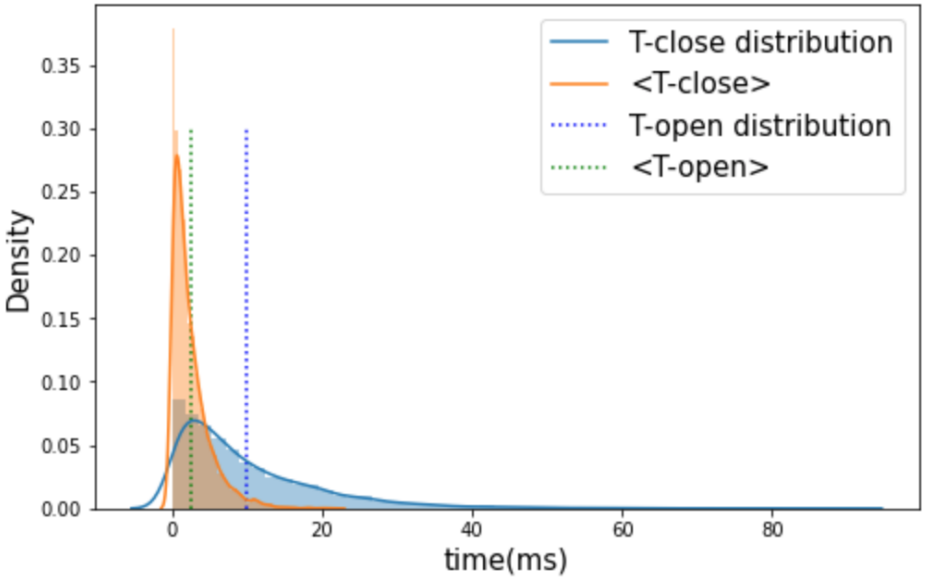
Simulation has run for 10000 events, for ~ 63 seconds.

Average closed dwell time = 10.02, and the Expected Value is 10.0

Average open dwell time = 2.49, and the Expected Value is 2.5

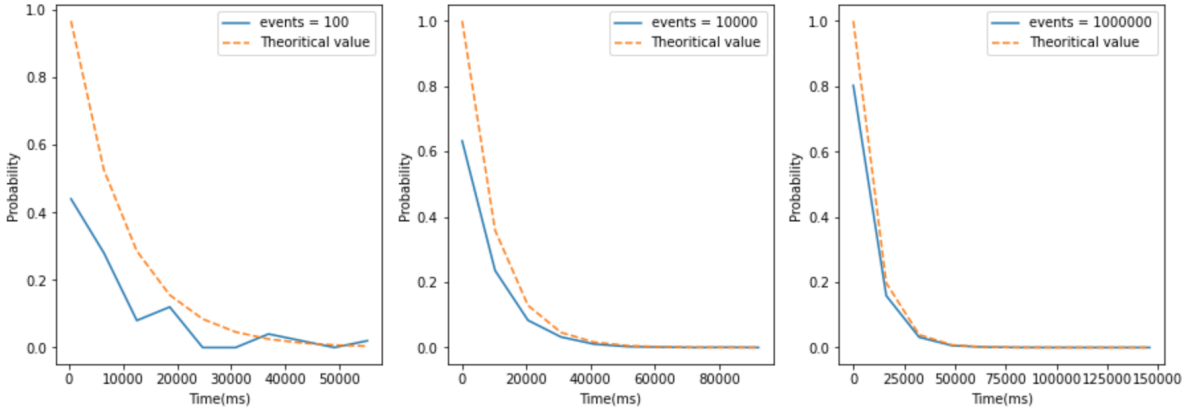
Below is the distribution of open and closed dwell times, where the dashed lines represent the expected values $1/K^{+}$ & $1/K^{-}$.

Code : Function written is part(a) is used to run the simulation for 10000 events. And Tau-close and Tau-open arrays are used to create the results and the charts.



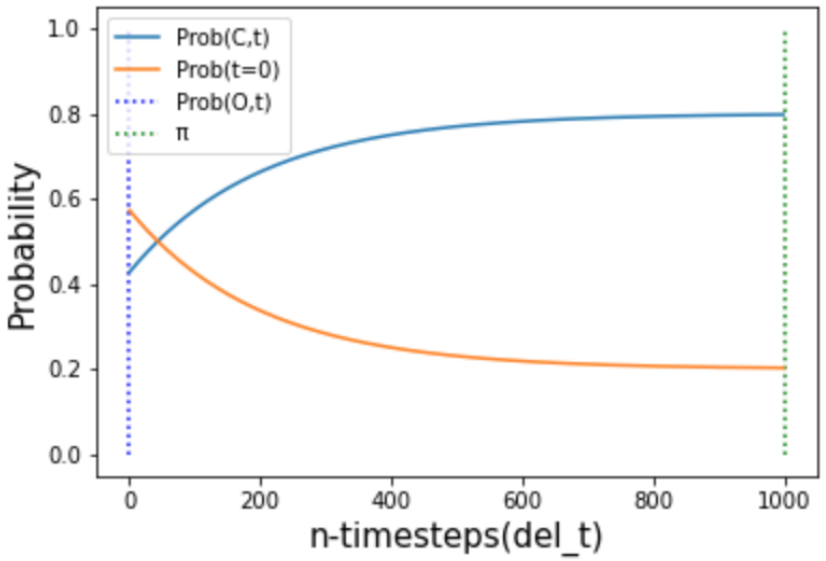
Part - (c)

Code : Used the function written in part(a) to pull the array of **Tau-close** and the array is discretized for a given value of Δt. Then the normalised densities of discretized Tau-close is plotted with its theoretical expected value: $e^{-K^{+}*Tau}$ for different values of events. It can be seen from the below chart that as the value of number of events increases the curve overlaps the theoretical value curve.



Part - (d)

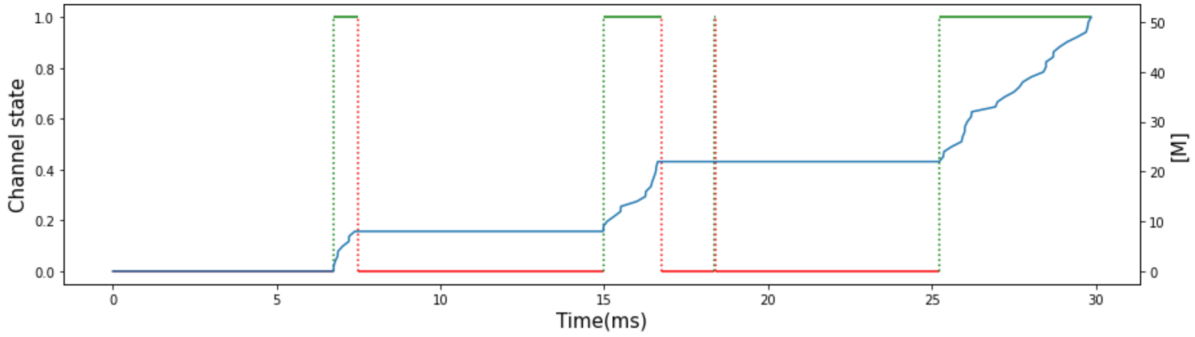
Code : A state is simulated using random numbers at any given time t as $P(t)$ = [Prob(C,t) ; Prob(O,t)] Formulated the transition matrix **Q** using rates and assumed value of Δt=0.01. Computed the state at any time "**t + n**Δt" iteratively for 1000 value of **n** using expression$P(t + n\Delta t) = Q^{n} * P(t)$. It seems to converge at a particular state as plotted below, which we call π. where π = Qπ is found to be validated post convergence.



Task-2

Part - (a)

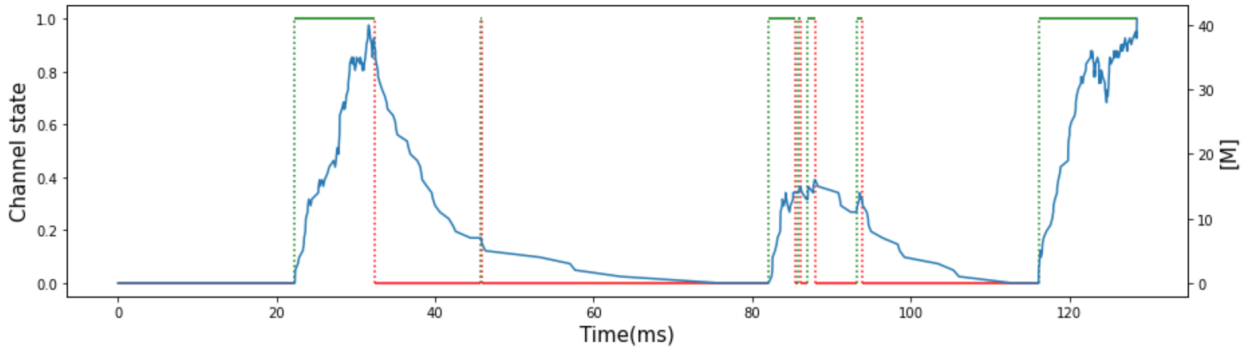
Code : Gillespie's algorithm is implemented for the "N = 3" number of reactions with all the parameters mentioned in the question. Iteratively updating the reactants for the products until the intracellular strength of the molecules attains a certain value. Below chart is plotted for M = 50, and it validates that the number of intracellular molecules increases only when the channel is open.



Part - (b - i)

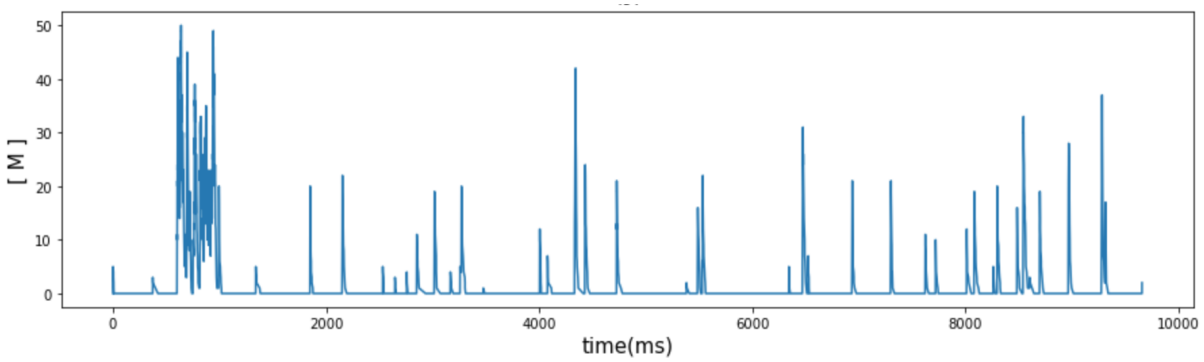
Code : Added one more reaction for diffusion to the Task-2 | part-(a), with propensity function = M(t)*K^d. which updates the molecule strength by "M(t) - 1" if this reaction is found to be happening.

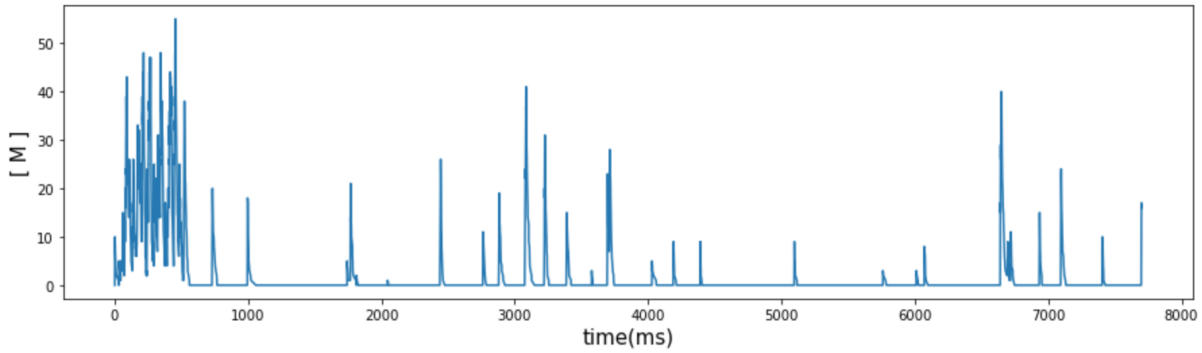
Below chart validates both the things that the number of molecules is increasing only when the channel is open but decreasing irrespective of the channel state.



Part - (b - ii)

Code : The activation function is added in the logic of "Task-2 | Part(b-i)" which triggers the K^+(i.e. U = -15 mV) for a random interval of time. And in the charts below it can be seen that activities(change in [M]) are happening within that time interval only





Task-3

Code : The system of equations are solved using “RK- 45” method and the concentration of all the forms of Kai-C and Kai-A are plotted wrt time using the solution of the ODE solver.
Then the period of oscillation is calculated by locating the troughs in the concentration trends, by finding the indexes where the sign of slope is changing and where every alternate index will give the troughs in the trend.

The mean period of oscillation is calculated to be **~21 hrs**, which can be seen in the graph as well.