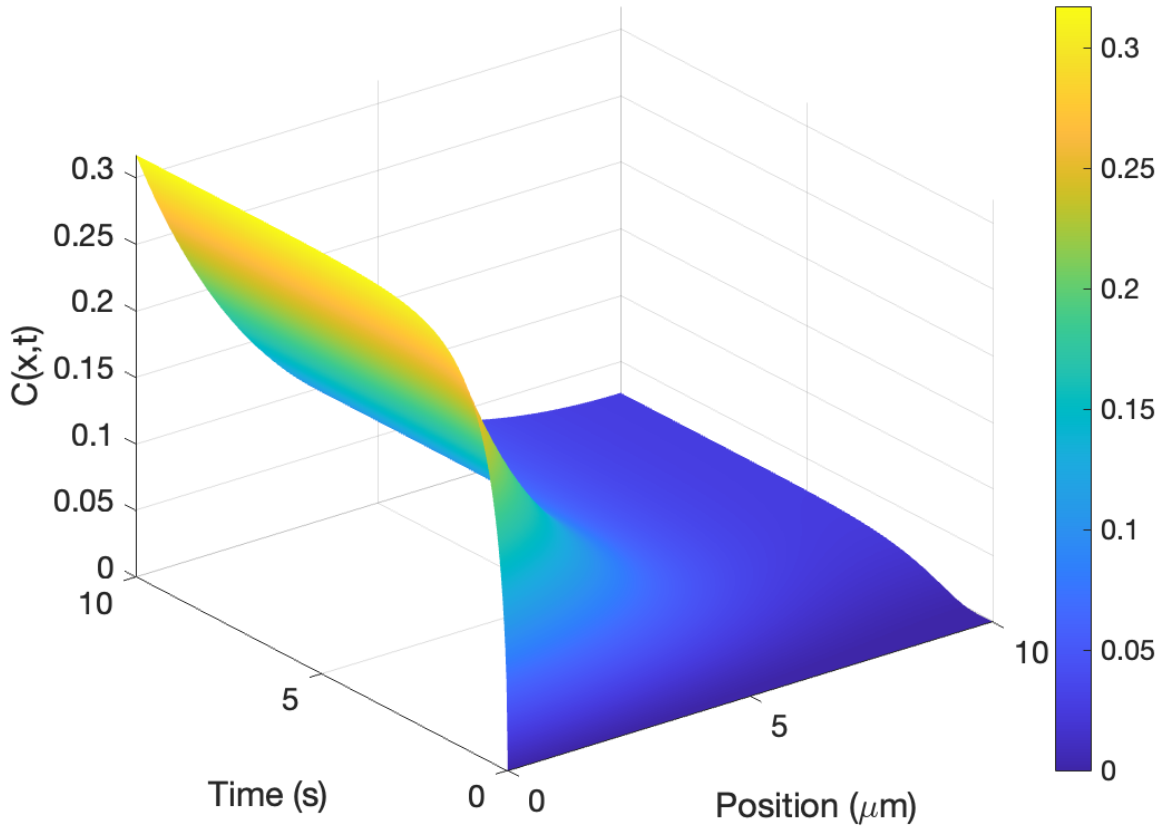
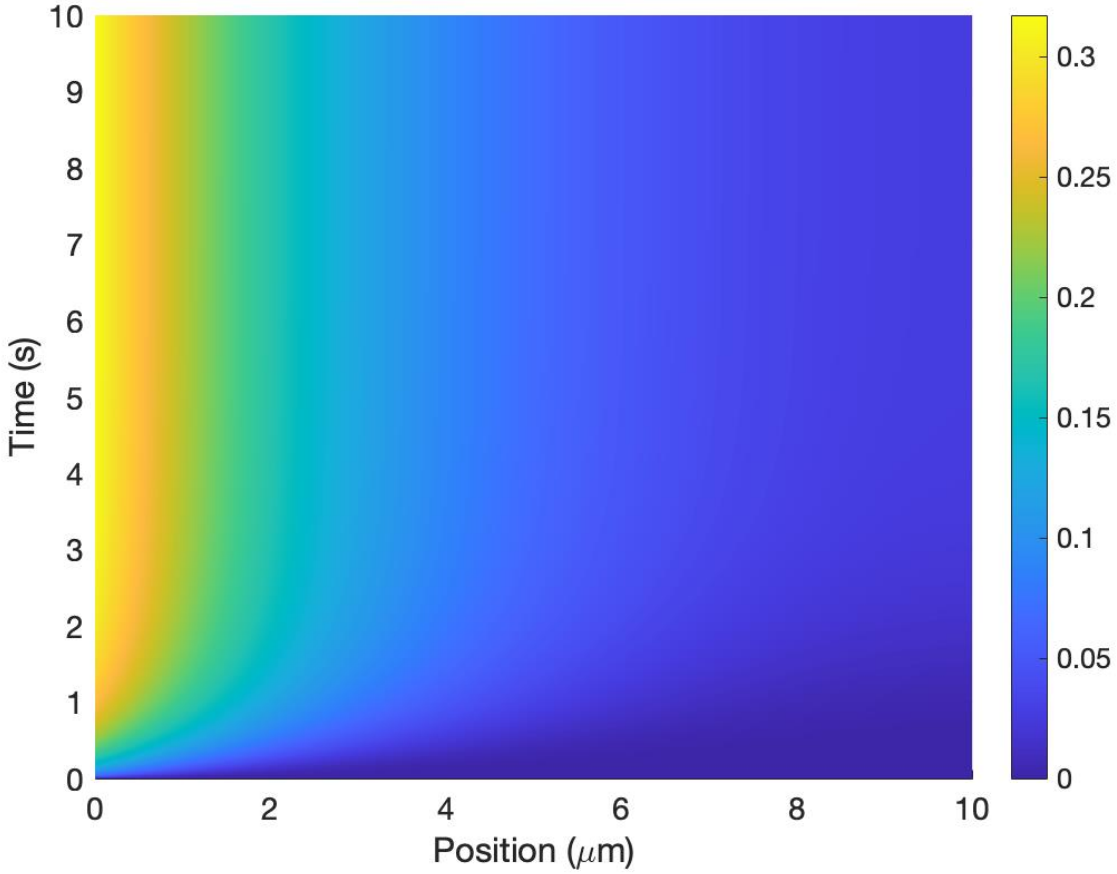
Dynamic Models in Biology
HW 10
Jonathan Levine
Fall 2023

Reaction Diffusion system

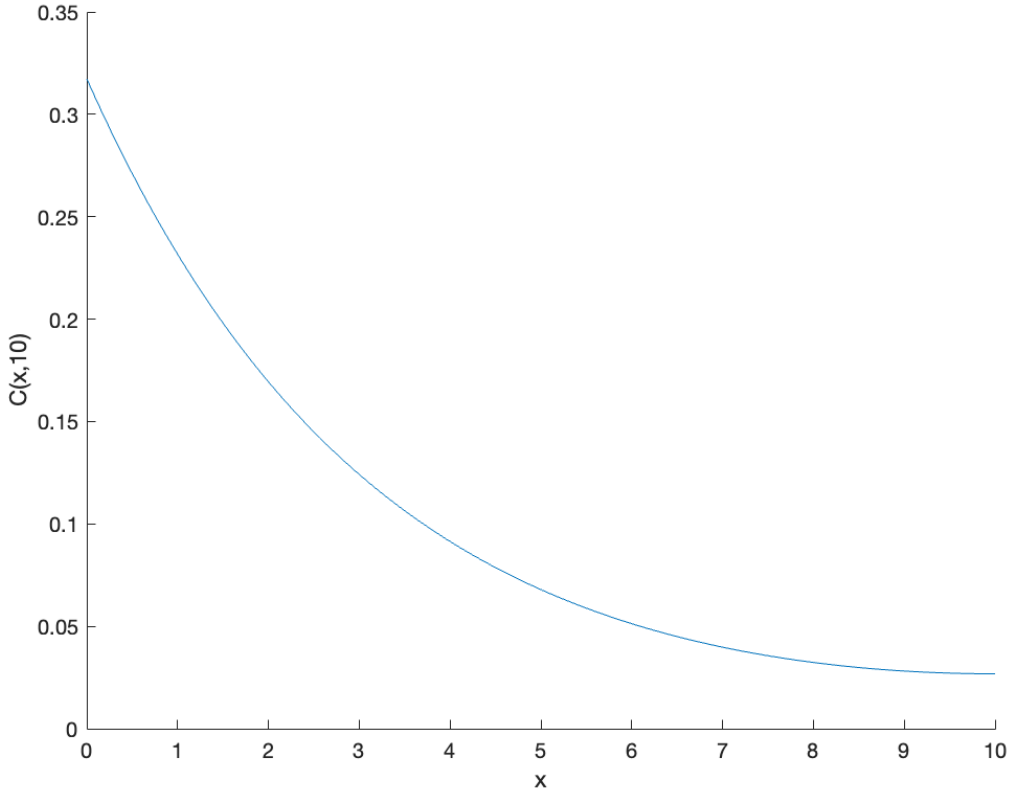
(a)

Simulating the Reaction-Diffusion system with baseline parameters. With constant influx from the x=0 boundary, it reaches steady state quickly in time, and concentration decays in space:



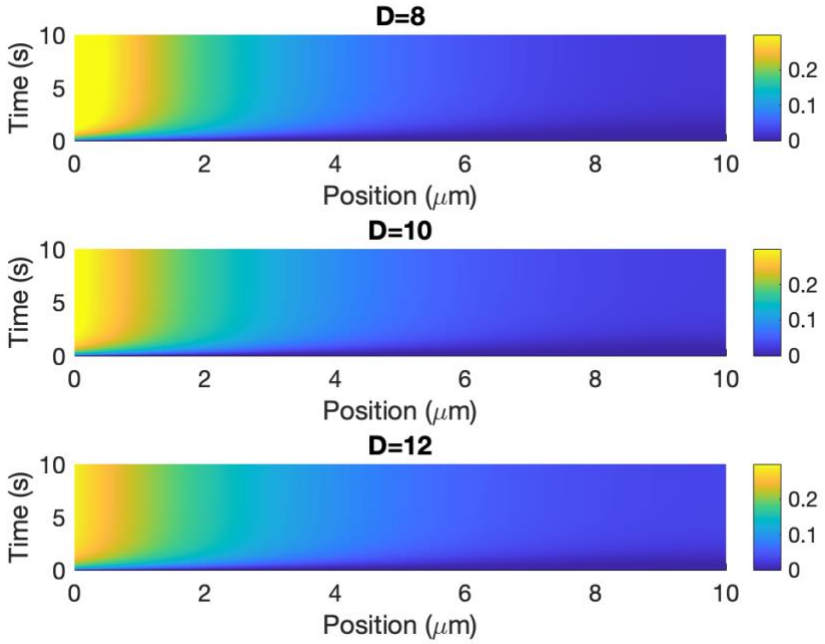


Looking at the distribution of concentration, *C*, over the position, *x*, at t=10:

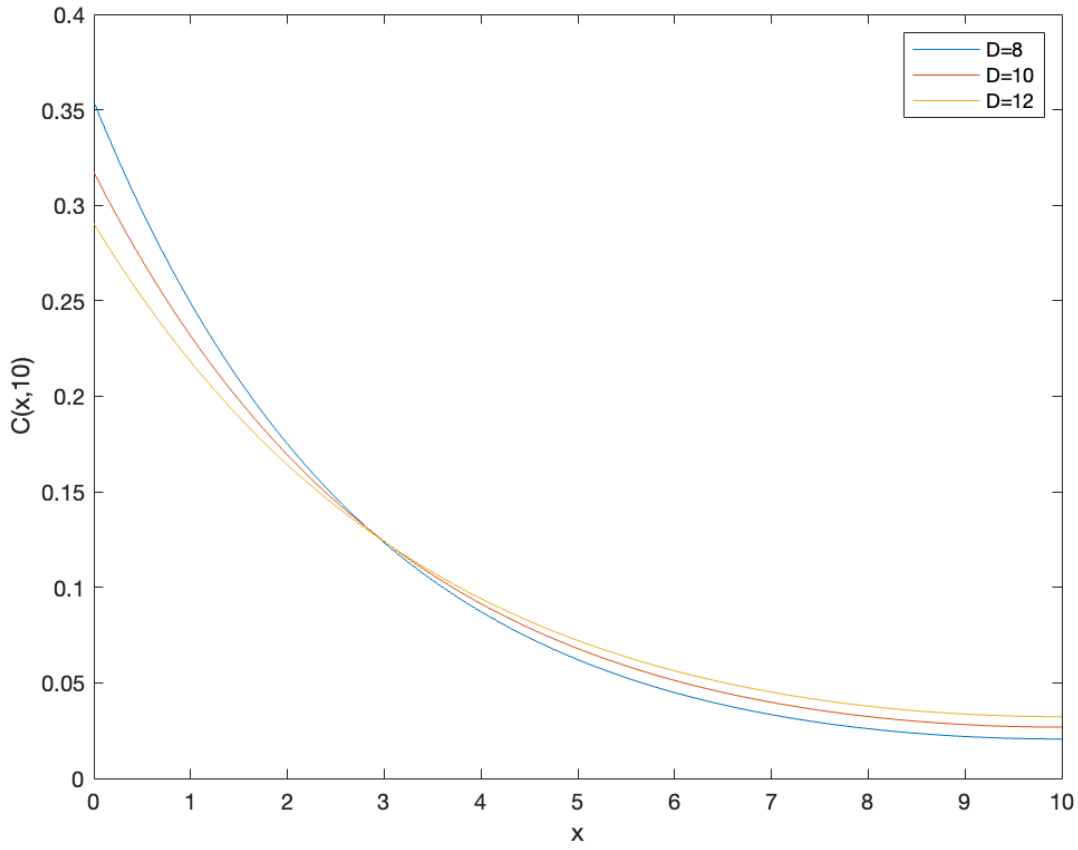


(b)

Varying D we get slightly different dynamics:



Again, looking at steady state C(x) (at t=10), gives us distinct shaped decay patterns:

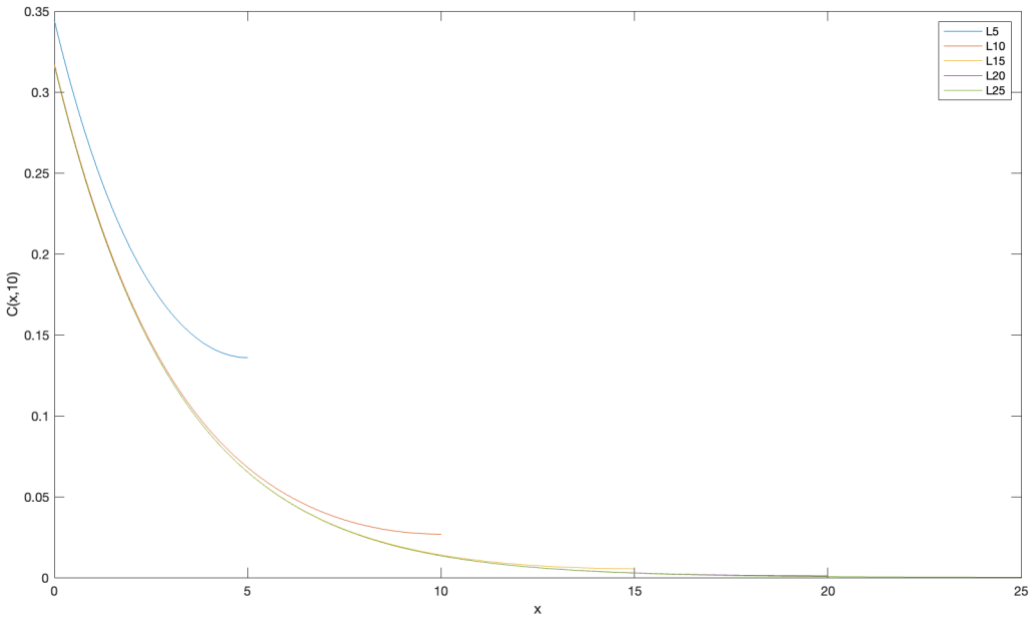


At the left boundary (at x=0): the steady-state concentration is larger for smaller values of D, since there is less diffusion away from the source influx.

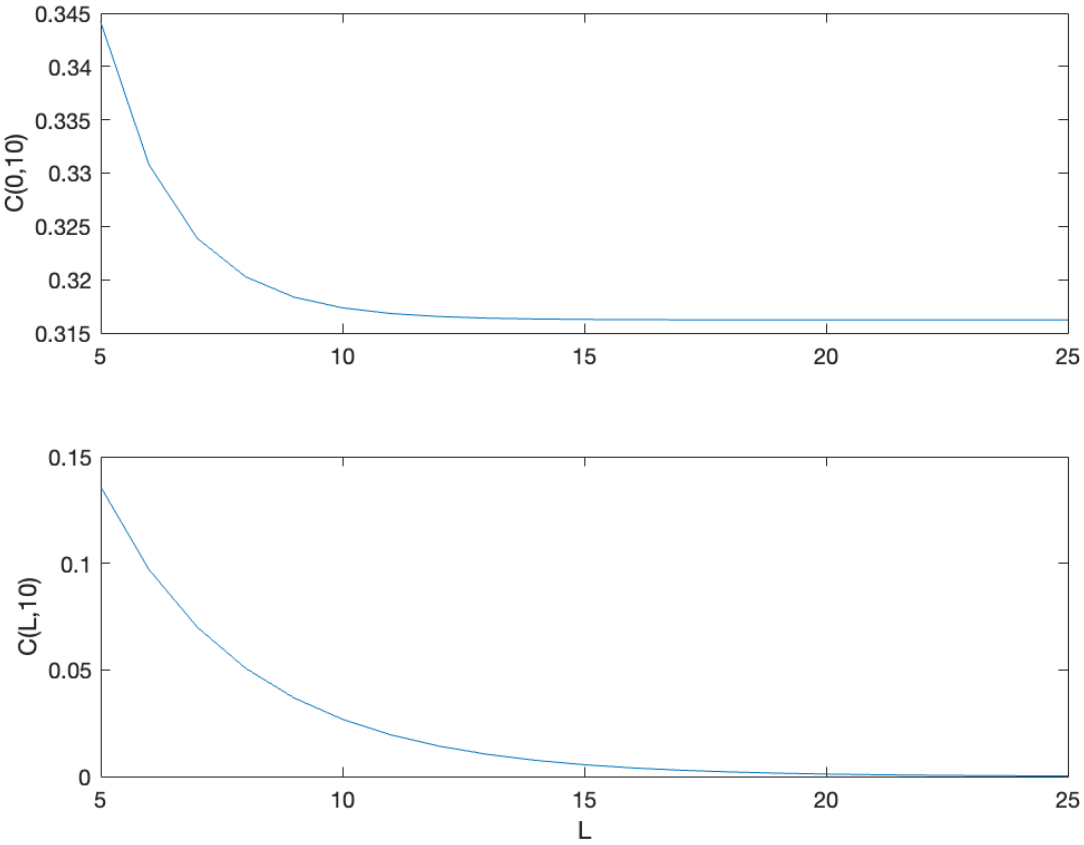
At the right boundary (x=L=10), the steady-state concentration is larger for larger values of D, since there is more diffusion towards from the influx to the far end of the system in x.

(c)

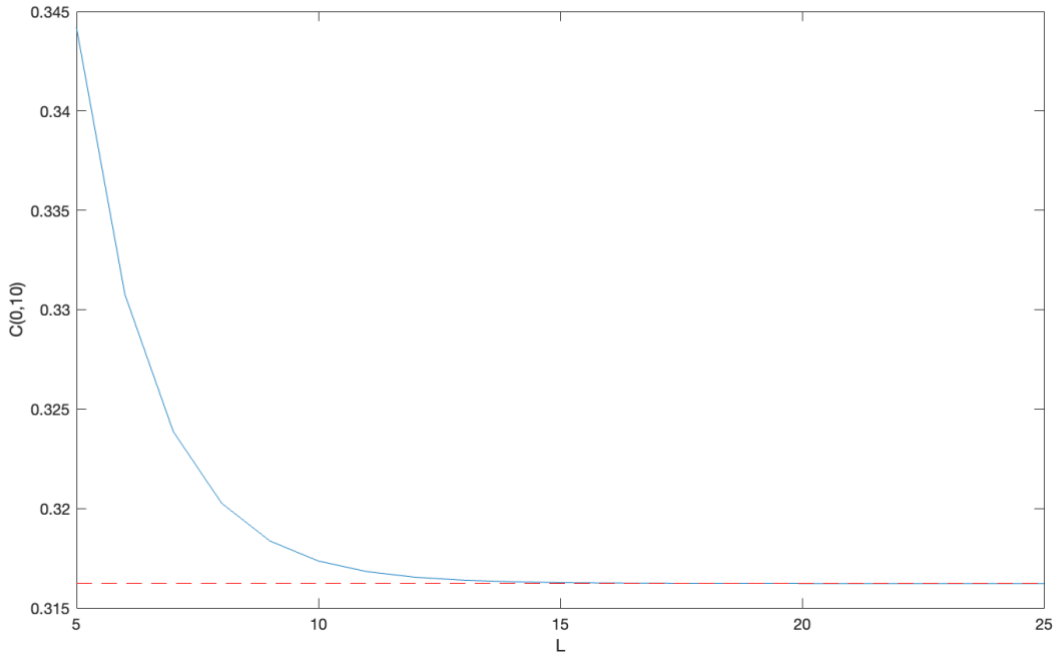
Varying the length scale L:



At first, when L increases, the space spread at steady state changes significantly. After a certain threshold though, additional increases in L doesn't change the spread C(x,t=end) much. Specifically, looking at the C(0,10) and C(L,10) for each trace:



You can see that increasing L has diminishing effects on the boundary concentrations at steady state. At the left boundary (source influx boundary), the concentration never dips below a/sqrt(kD), plotted below with the dotted red line:



Problem 2: Spatial model

In the spirit of reaction diffusion models, I decided to add a diffusion component to the reactions studied in HW4 for glycolysis. In that model, we had concentrations of F6P and ADP as the state variables S and P respectively. The model, based on mass action kinetics of the underlying chemical reactions was:

$$\dot{S} = V_0 - cSP^2$$
$$\dot{P} = cSP^2 - kP$$

Let's say we want to also model this cytoplasmic reaction in space, introducing 3 spatial variables x,y,z representing location in the cell. While the above equation relies on the approximation of glycolysis that it is well-mixed, we can also model cytoplasmic hot spots of metabolic activity and relatively "cold" spots by introducing the spatial dependence. S and P are now functions of t and x, y, and z, and we can add diffusion terms to the ordinary differential equations and turn them into partial differential equations:

$$\frac{\partial S}{\partial t} = D_S\, \Delta S + V_0 - cSP^2$$
$$\frac{\partial P}{\partial t} = D_P \Delta P + cSP^2 - kP$$

Where the Laplacian $\Delta = \nabla^2$, which generalizes the second derivative with respect to the spatial dimensions.