

The above two plots use the fits that are provided in the science reports paper as follows:

Occupation Fit:

$$\rho(x, t) = \rho_0 \operatorname{erfc}\left(\frac{x}{\sqrt{4Dt}}\right) \quad (1)$$

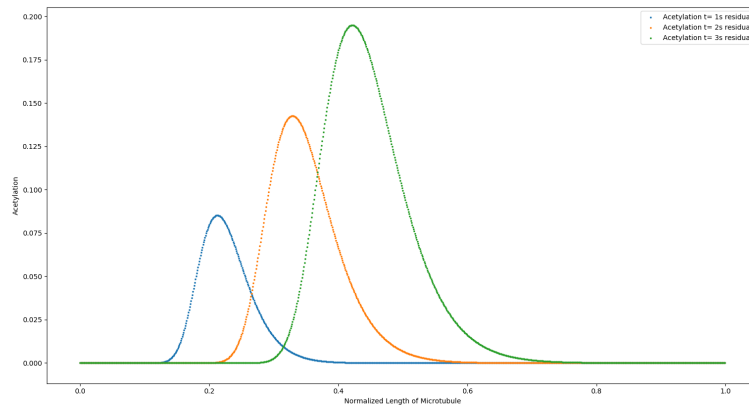
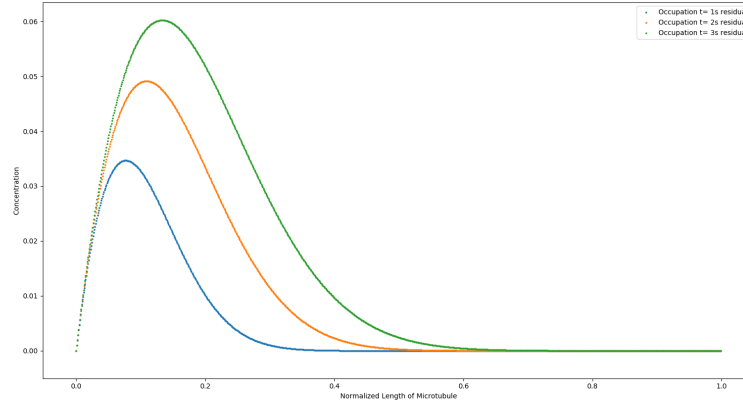
Acetylation Fit:

$$a(x, t) = 1 - \exp(-\rho_0 \Gamma t ((1 + 2z^2) \operatorname{erfc}(z) - 2z \exp(-z^2)/\sqrt{\pi})) \quad (2)$$

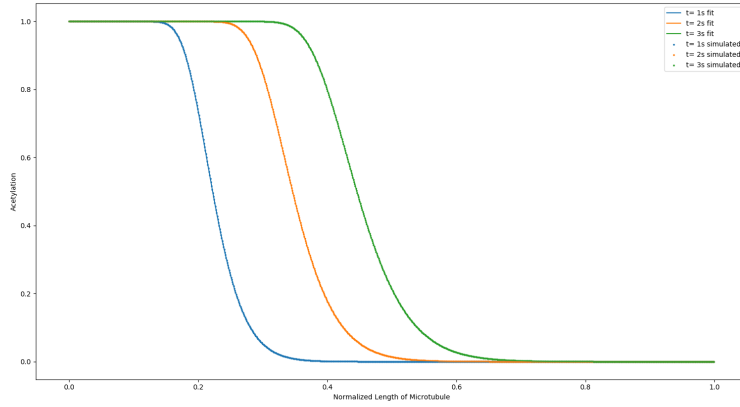
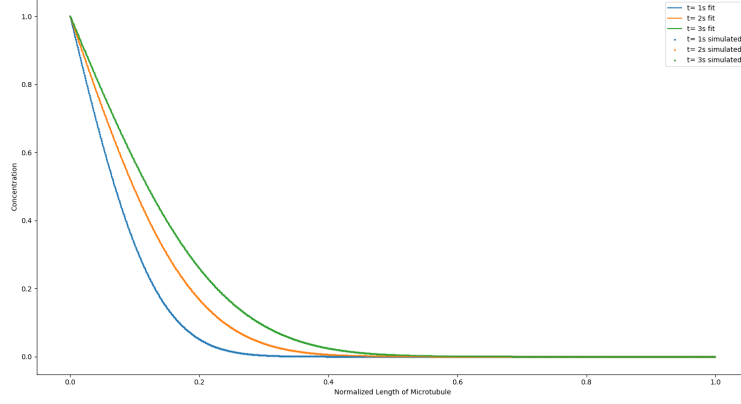
where

$$z = \frac{x}{\sqrt{4Dt}}$$

Below are the residuals for each of these fits



Next I looked at what happened if I just didn't have the ρ_0 terms within the fits.



The above two plots use the fits that are provided in the science reports paper without the ρ_0 multiplication in the fits, where ρ_0 is the expected steady state of the system.

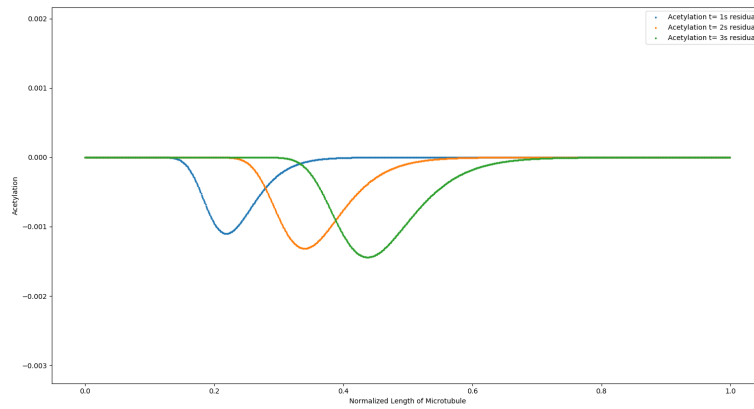
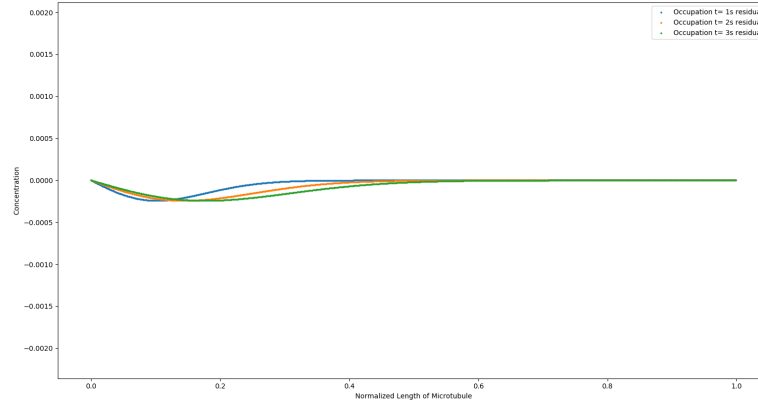
Occupation Fit:

$$\rho(x, t) = \text{erfc}\left(\frac{x}{\sqrt{4Dt}}\right) \quad (3)$$

Acetylation Fit:

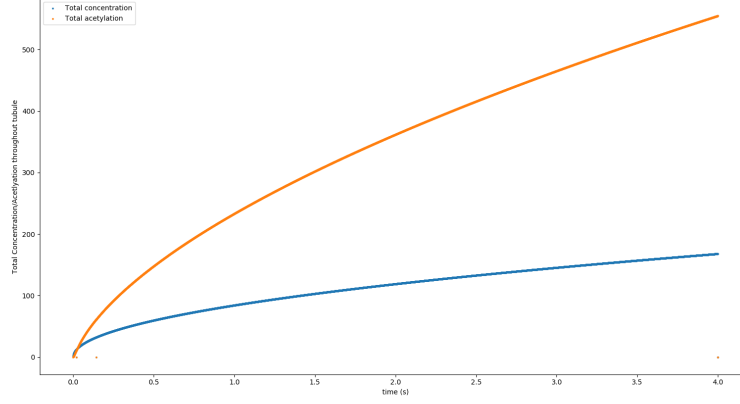
$$a(x, t) = 1 - \exp(-\Gamma t((1 + 2z^2)\text{erfc}(z) - 2z\exp(-z^2)/\sqrt{\pi})) \quad (4)$$

Below are the residuals for each of the above two plots



The shapes in the residuals are similar albeit flipped in sign, however also much smaller.

The final plot I have to show you is the Total Concentration and Acetylation as a function of time.



The tube is discretized into 1024 sites in this case, so if every site was fully acetylated we'd expect the total acetylation to go to 1024. The simulation ran for 4 seconds but I only plotted at 1, 2 and 3 seconds.

One last thing to mention is that Single File Effects are implemented and I am running this with a large ρ_{scale} so that we recover the $D = D_0$ effect.

If $\frac{dt}{d\bar{x}^2} > 0.5$