Simulation notes 3

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May 24, 2016

1 Some figures

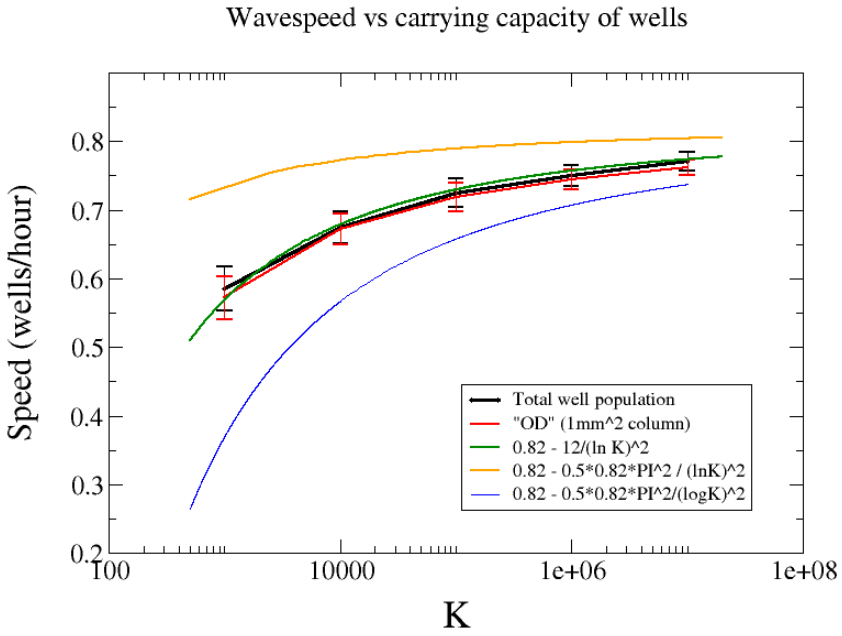


Figure 1: This is the same plot from last set of notes of the wavespeed vs carrying capacity for the full simulation of the experiments. The green line is the arbitrary fit of a $1/(\ln K)^2$ correction I did by eye before, but here the orange and blue curves are of the form in the paper you sent me: $v \sim \sqrt{Dr}\left[2 - \frac{\pi^2}{(\log N)^2}\right]$. It's a much stronger effect if I use the $\log_{10}$. I haven't read the references in that paper yet, so I'm not 100% sure if we should be expecting an actual fit, or just a qualitative agreement with our simulation? The approximation is valid for "large K" and if I chose a higher maximum value than I guessed in this plot, the fit could be good for large K.

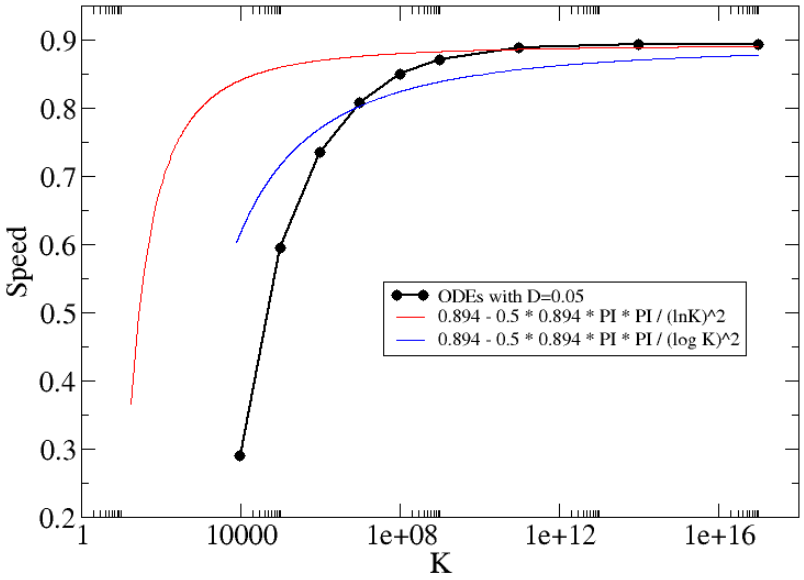


Figure 2: I also simulated the equations we discussed using the simples ODEs: $\frac{dn_i}{dt} = D\left(n_{i+1} + n_{i-1} - 2n_i\right) - n_i g(n_i/k)$ using the LB growth rate and D=0.05. Plotted here is the wavespeed vs carrying capacity and the expected K-dependence from the paper you sent. The dependence of speed on carrying capacity is much stronger here. NOTE: I'm not sure how reliable this plot is anymore – I just noticed that the wavespeed depends on the timestep I've chosen. I need to check if this is a bug, or if it's that the simple Euler method I used to solve the equations isn't good enough – I think it should match the plot produced from the tau-leaping algorithm in the next figure.

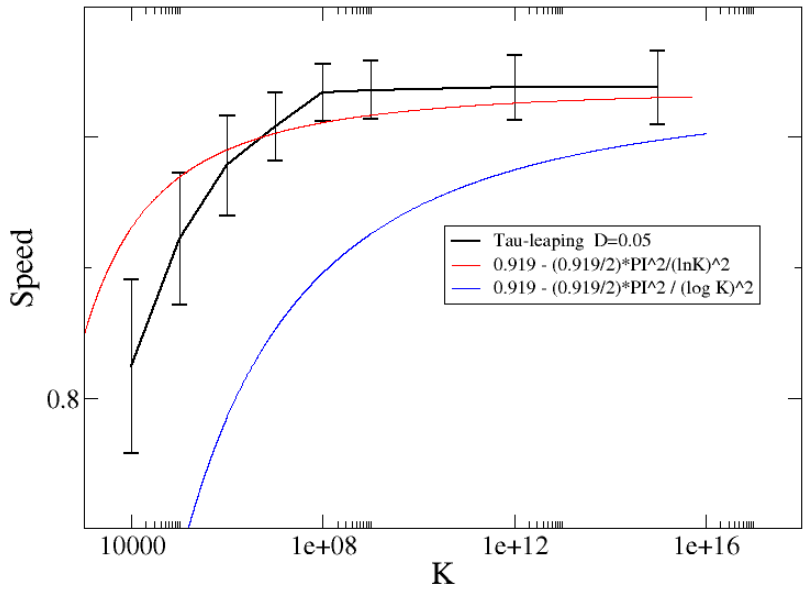


Figure 3: I also made the same plot but using a stochastic tau-leaping algorithm where bugs jump between wells with rate D and replicate with the LB growth rate. We see similar qualitative behaviour but obviously quantitatively it's different from the full well simulations since the diffusion constants D represent totally different processes. In the simulations, Figure 1, increasing K from 10^4 to 10^7 increased the speed from 0.572 wells/h to 0.762. Increasing K similarly when using the Tau-leaping algorithm in this figure sees the speed increase from 0.812 wells/h to 0.904, a smaller difference (although admittedly this is for this one arbitrary choice of $D = 0.05$.)

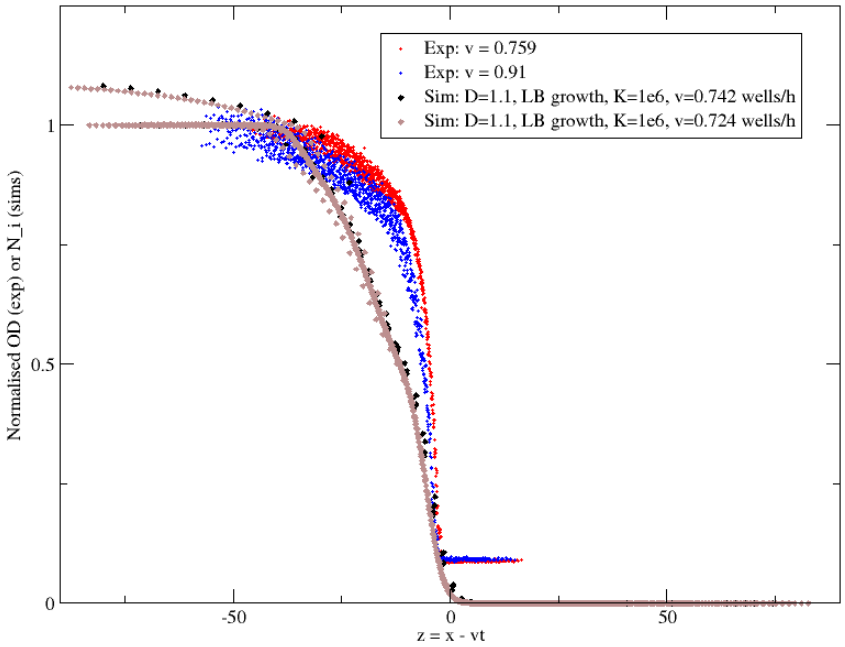


Figure 4: Plotted here are some wave profiles from the simulations (brown diamonds) and 2 of Bartek's experiments (blue and red). The simulations use the experimentally determined LB growth rate. On the y-axis is the "normalised" OD for the experiments (max value was about 2.25 in all experimental data sets), or well population for simulations ($K = 10^6$). On the x-axis I plot $z = x - vt$ where I have converted all distances to mm instead of wells, which is what Bartek's data consists of. I had never made this sort of plot before – the shape of the simulation wavefront is actually quite strange and doesn't match the shape observed in experiments so well. Question for Bartek: the range of z in your data sets isn't always the same but I don't understand why not? The length of the experiment in the simulations is (wellwidth $*$ number of wells + 1 mm $*$ number of channels) $= 3.25 * 24 + 1 * 23 = 101$ mm; the data sets you gave me have a z-range of either 64 or 72 mm. I'm not sure if I should be scaling them by some number?

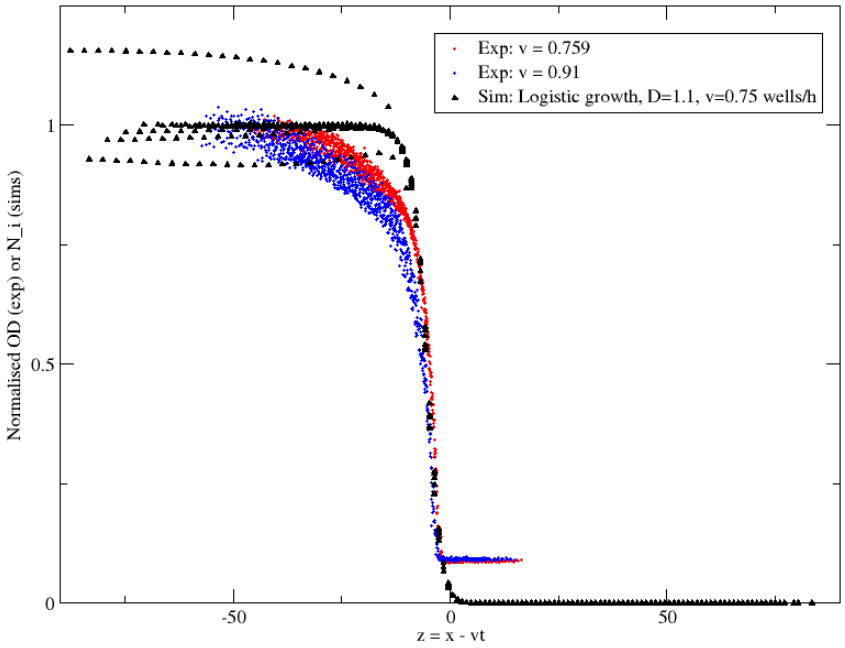


Figure 5: Using our original logistic growth the waveform found from the simulation (black triangles) is much steeper than the experimentally observed profile. Something I noticed a while ago but forgot about is that the population is always higher in the end wells. This is the reason that some of the simulation data sits above the value of 1. I don't know if this is obviously expected or not (easier to get trapped in an end-well) or it's more just that there is more bacteria in the initial well (since it has the initial population too) and I've not left the simulation long enough to correct this?

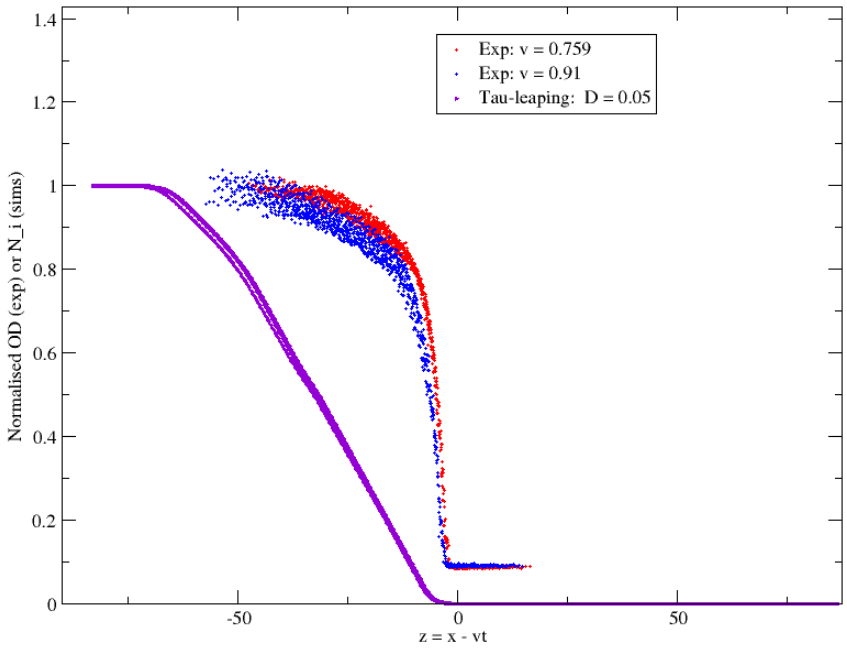
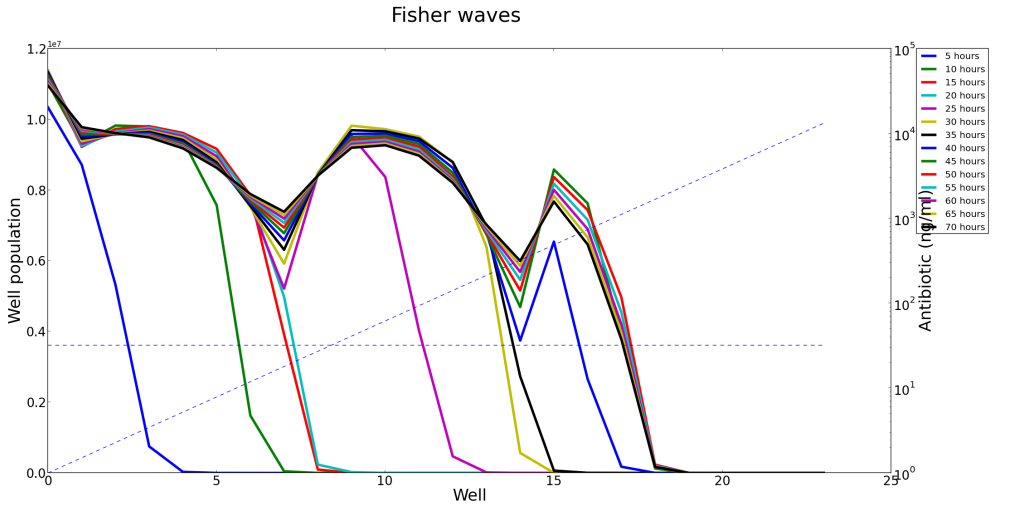
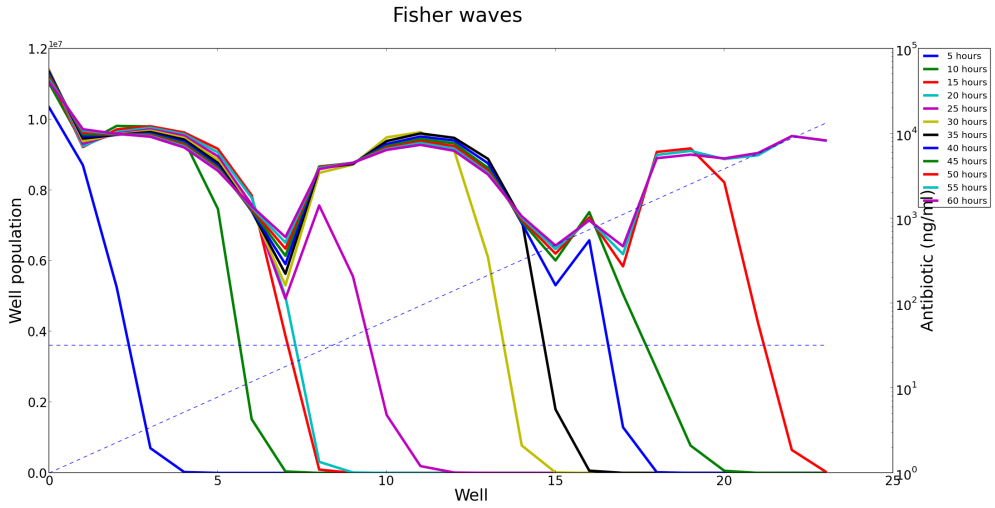


Figure 6: Shown here is the waveform from the stochastic simulation using the tau-leaping algorithm (purple triangles) with the LB growth data. It has a very different shape from the experimental waves, looking almost linear, but this is maybe expected since we are simulating a very different process.


Fisher waves
Well population
Antibiotic (ng/ml)
Well
1e7
5 hours
10 hours
15 hours
20 hours
25 hours
30 hours
35 hours
40 hours
45 hours
50 hours
55 hours
60 hours
65 hours
70 hours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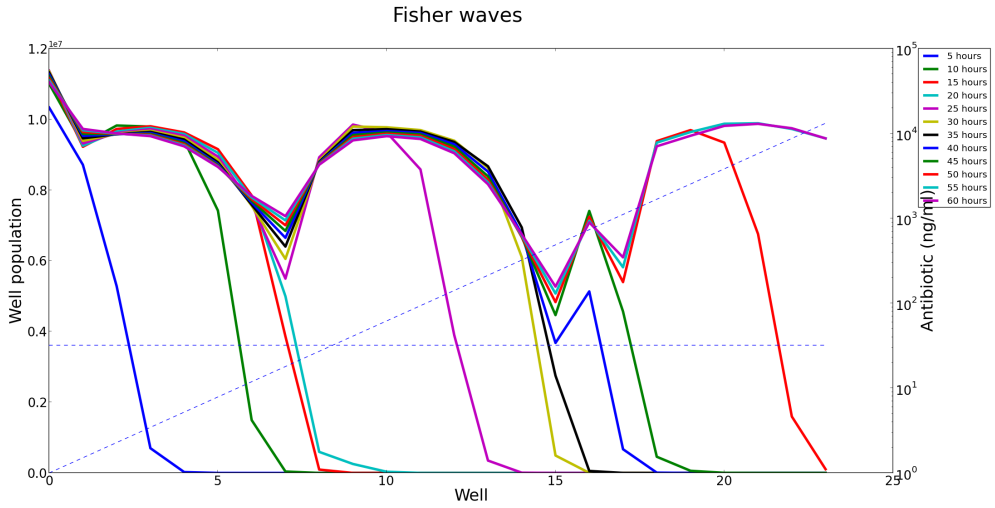
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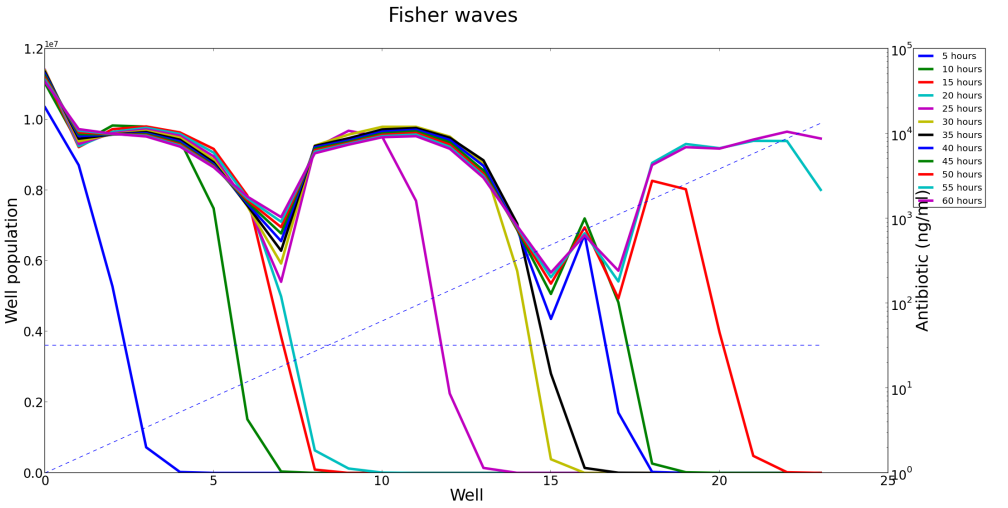
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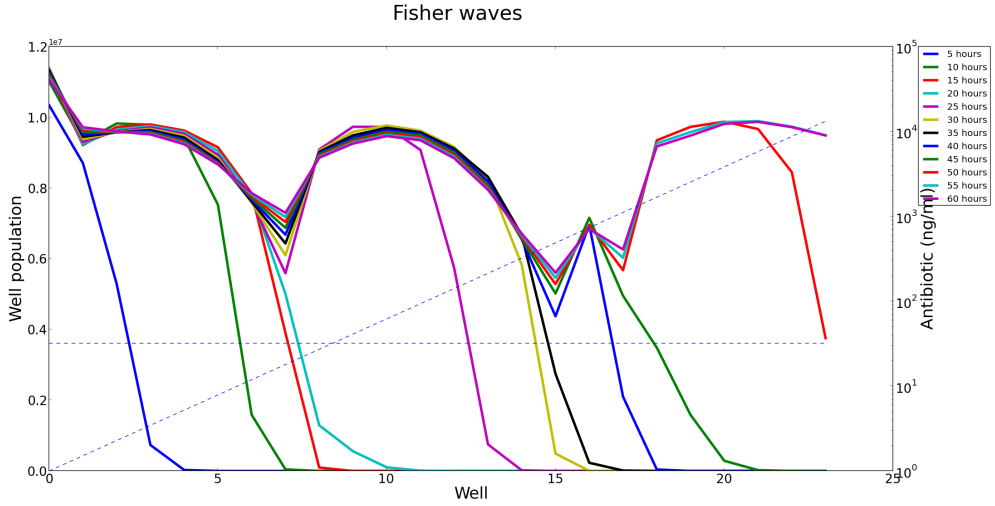
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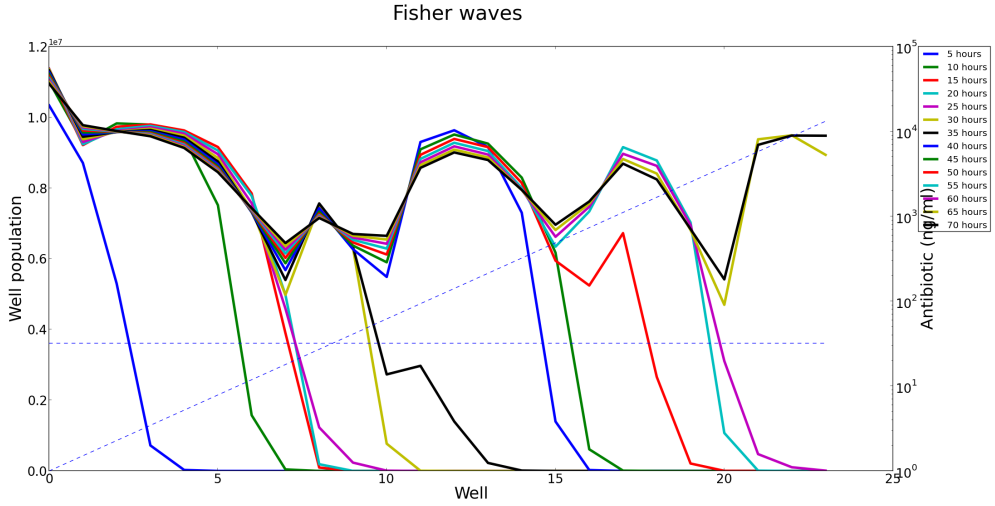
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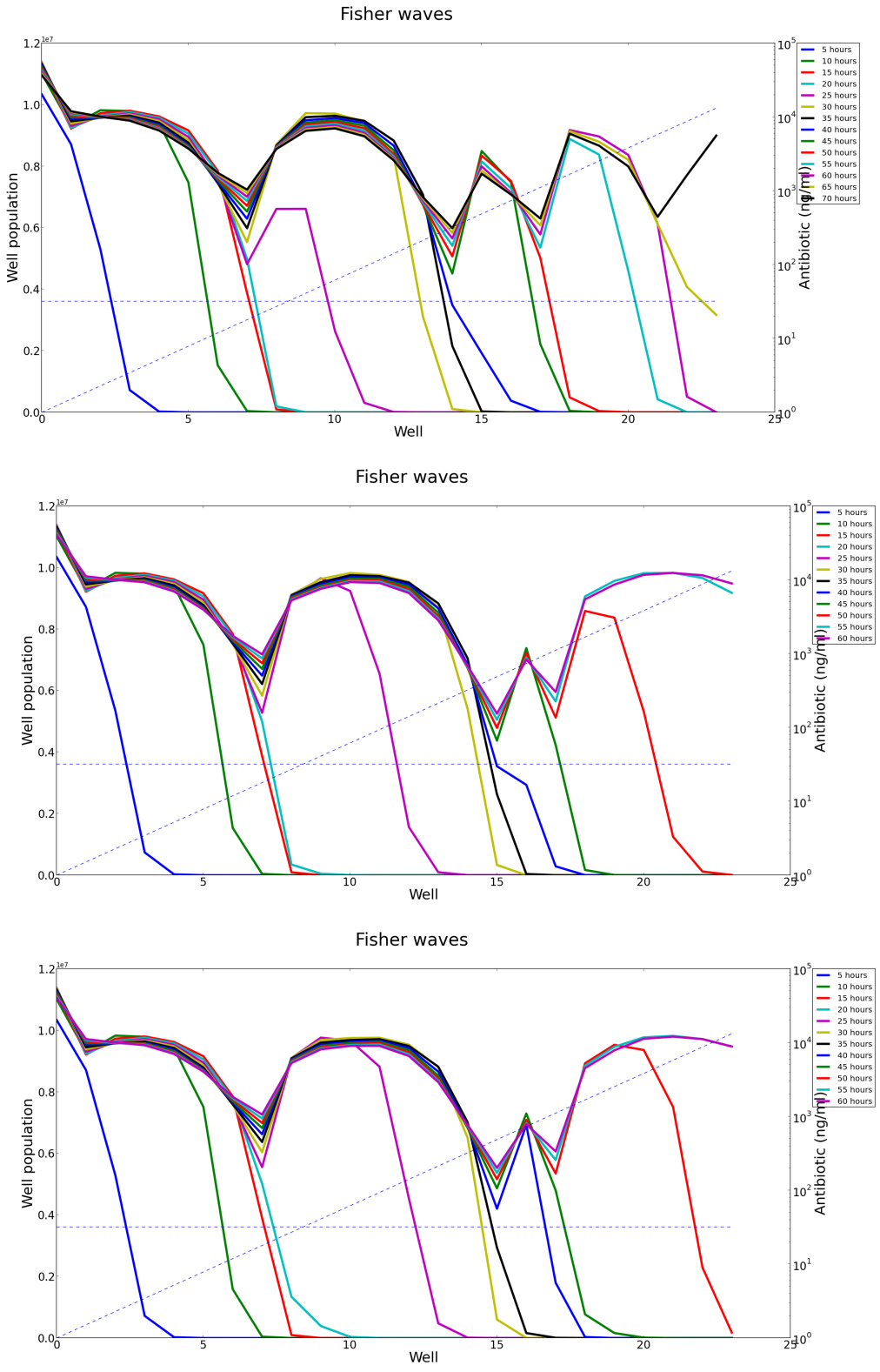

Figure 9: I meant to include this figure in the last set of notes. It shows the progression of the population for a carrying capacity per well of $K = 10^7$ and maximum ciprofloxacin concentration of 20 000 ng/ml. 8 out of 9 runs reached the final well and this figure shows that this process can occur in different ways but that some may be more likely than others: out of the 8 runs that reached the final well, 6 appear to follow the same mutational pathway while the other 2 do something different. I think it would be relatively easy to make some plots showing the probability of different mutational pathways for different concetration profiles and will do it this week unless you think it's not of interest.