Report – Experiment B:

Formally demonstrating non-isopotential compartments in a multi-compartment model

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| **Experiment-B1** | * 9 Comp + Soma model, fluxing impermeants in comp 3 and 7 * Poor experiment, too many changes to know what was going on. * Useful in that I found several errors which were corrected. |
| **Experiment-B2** | * 10 Comp model, fluxing impermeants in comp 2 * Unexpected changes occurring in final compartment * Possibly due to an error in the electrodiffusion calculations as I was using concentrations rather than moles to transfer ion |
| **Experiment-B3** | * Made changes to the electrodiffusion order and made use of moles as opposed to concentrations. * Success in replicating figure 8C, but with only 4 compartments |
| **Experiment-B4** | * Confirming the results of experiment B3 just with 8 compartments instead of 4 * Successfully extrapolated to 8 compartments. * Not quite at steady state, but clearly show the non-isopotential multicompartmental model with constant Cl driving force |

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| Title | Experiment-B1 |
| Setup: | 9 compartments with a soma. Fluxes into compartment 2 and 7. |
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| Outcome: | “Failed experiment”. Observed that there were errors in the electrodiffusion calculations, and difficult to pinpoint because there were 2 anion fluxes going on. |

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| Title | Experiment-B2 |
| Aim | Sanity check on the multicompartmental model. **Fluxing impermeants in compartment 2 only**. Direct replica of figure 8C. |
| Starting conditions | * Compartment 10 appears higher up on the table as it is listed alphabetically, but the compartment is actually adjacent to compartment 9. |
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| End of simulation |  |
| Mid anion flux |  |
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| Conclusions | * Strange to see the major fluxes that occur in compartment 10 * It seems like compartment 10 is doing the heavy lifting during the anion flux but returns to close to baseline, whereas compartment 2 has permanent changes. * In Kira’s 8C, compartment 10 does not bear the changes **during** the anion flux. In the mid simulation heatmaps of fig8C compartment 10 behaves as the other compartments * The way in which the values change in compartment 10 almost seem as if there is a dynamic x influx, but it appears to be related to the fact the volume is changing. * This is possibly because compartment 10 is not buffered by 2 adjacent compartments in terms of electrodiffusion. * The heatmap of the simulation end is what we would expect, apart from the smaller changes in compartment 10 * Better compartment names in future to avoid the compartment 10 listing issue. |
| Plan | * Electrodiffusion order of operation must be making compartment 10 bear the brunt of the experiment. * Relook at the electrodiffusion code and correct error. |

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| Title | Experiment-B3 |
| File name: | Experiment-B3-4 |
| Aim | 4 compartments, flux in compartment 2   * Ensure all the compartments have a drop in voltage when impermeant anions are added and that the final compartment does not act any differently to the others |
| Setup | Realized I can run the simulation for 1 minute with a very short flux and get the same outcome. |
| Results |  |
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| Heatmap during impermeant anion addition |  |
| Heatmap at the end of the simulation |  |
| Outcome: | Success in replicating Kira’s 8C, just with 4 compartments.   * Membrane potentials drop in all the compartments. * Compartment 4 is not acting differently to other compartments. * Similar driving forces at the end of the simulation * Simulation could be run for a bit longer to get to a steady state |
| Plan: | Run the same experiment but with 8 compartments to confirm these findings  Find a way to better represent the boundary graph |

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| Title | Experiment-B4 |
| File name | “ Experiment-B4” |
| Aim | Replicating B3, just with 8 compartments to see if the effect continues with a larger model. |
| Starting values | Dt =10^-6  ATPase – variable  Area Scale - on |
| Result |  |
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| Heat map mid anion flux |  |
| Heatmap @ end of simulation |  |
| Conclusion | * Success in replicating results from Experiment B3 with 8 compartments. * Model behaving as anticipated * Unfortunately, did not reach steady state yet at the end |
| Plan | * Think of ways to make boundary graph more informative * Proceed with testing of GABAergic inputs |