Report

23 March 2021

* Trying to replicate impermeant related analytical findings
* I saw yesterday that some of my anion fluxes results were not matching with the analytical so I am trying to go back and see at which logical step the results weren’t correct
* Starting with replicating Kira’s 4A and 4B
* I suspect at Kira’s 4C and 4D something is going wrong with my model

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| Experiment | Replicating Kira 4A – start with 30mM impermeant anions and see if it converges at steady state: |
| Hypothesis: | * Achieves steady state * Achieves above values based on analytical * Expect final volume roughly equal to 0.6pL |
| Starting values: | * Default 2 compartments * Impermeants in both set to 30 |
| Simulation settings | No anion fluxes |
| Final values |  |
| Relevant graphs |  |
| Boundary graph |  |
| Conclusion | * Success wrt to final concentrations and voltages * Slight differences in final volumes… need to relook at Kira’s volume equations * Rate of change of impermeants and volumes much quicker in mine than in Kiras |

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| Experiment | Replicating Kira’s 4B, starting with very high impermeant concentration and see if I converge on the same values and at a similar rate |
| Hypothesis | Convergence but not same rate (as shown in 4A above) |
| Starting values |  |
| Simulation settings |  |
| Final values |  |
| Relevant graphs |  |
| Boundary |  |
| Conclusions | * Same voltages as kira * Not exactly at steady state * Model is behaving as predicted and reaches near identical values to the analytical. |

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| Experiment | Replicating Kira’s 4c – adding impermeant anions during the simulation |
| Hypothesis | If I change the impermeants from 155 to 156 (adding 1mM), I’ll increase the volume by 0.2 pL (2.2pL) and the Vm and ECl will drop temporarily while the impermeants are being fluxed in. Volume will show a permanent change (why) but the impermeant concentration will decrease |
| Starting values |  |
| Simulation setup |  |
| Final values |  |
| Relevant graphs |  |
| Boundary graph |  |
| Conclusion | * Kira’s voltage drops initially much more than mine * Kira’s volume increases much more than mine * My default (starting) impermeant concentration is 150 vs. Kira’s of 155 so that changes the dynamic slightly … need to rerun the same simulation but with 155 as my default x * My peak impermeant didn’t go up as much as expected… that basically affects the volume and voltage so something is wrong there… |