Report

30 March 2021

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| Aim: | Replicate Kira’s 4c – adding impermeant anions (1mM) mid simulation |
| Hypothesis: |  |
| Starting values: | Default 2 compartments |
| Simulation setup: | 20 min sim, 1ms time step  Variable ATPase  Adding 1mM impermeants between 6 and 12 minutes |
| Final values |  |
| Relevant graphs | Graphs not rendering well. |
| Boundary graph |  |
| Conclusion | * Success * Compartment not at equilibria * Same voltage dynamics as Kira’s 4c * Volume change is not identical… mine only increases by 0.1 pL while Kira’s increases by a bit more, but dynamic is identical |

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| Aim: | Add extracellular impermeant anions (Kira 4D) |
| Hypothesis: |  |
| Starting values: | Default. |
| Simulation setup: | 2 compartments  Add 60mM extracellular impermeants between 400 and 800s  20 min sim total duration |
| Final values: |  |
| Relevant graphs |  |
| Boundary graph |  |
| Conclusion | * Success in replicating the dynamics of extracellular impermeant anion addition |

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| Aim: | Replicating Kira’s 5A – By dropping the impermeant anion charge mid experiment, we should be able to change the driving force slightly |
| Hypothesis |  |
| Starting values | Defaults (z =-0.85) |
| Setup | 2 compartments, changing the charge of impermeants in both to -1 between 300s and 800s  Total simulation run time = 20mins |
| Final values |  |
| Relevant graphs |  |
| Boundary graph |  |
| Conclusions | * Not quite at equilibrium * Dynamics generally are in line with Kira’s * My volumes change more than Kira’s – this needs to be investigated further * Similar slight change to driving force |

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| Aim | Replicate Kira’s 5B – Part 1 – start simulation with -1.2 impermeant anion charge and see if I get the same values as the analytical |
| Hypothesis |  |
| Starting values | Default compartment starting values just with 2 compartments that have impermeant charges of -1.2 |
| Setup: | 15 minute simulation. No change to anions mid simulation. Dynamic atpase. |
| Final values |  |
| Relevant graphs |  |
| Boundary graph |  |
| Conclusion: | Reache |

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|  | asd asdasd – Matches Kira’s analytical solution   * Reaches steady state * Success   R- asd |

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| Aim: | Replicate Kira’s 5b by starting the sim with impermeant anion charge of -0.5 |
| Hypothesis |  |
| Starting values: | 2 default compartments with -0.5 average intracellular impermeant charge |
| Setup: | 15 Min simulation. Charges all set from the beginning of the sim. Dynamic Atpase. No changes mid simulation |
| Final values |  |
| Relevant graphs |  |
| Boundary graph |  |
| Conclusion | * Success * Replicates Kira’s 5B successfully at higher impermeant anion charge * Model reaches steady state |

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| Aim | Replicating Kira’s 5C – dropping the charge of impermeant anions mid simulation |
| Hypothesis |  |
| Starting values | Default 2 compartments with z= -0.85 |
| Setup | Drop z in both compartments from -0.85 to -1.1 .. starting the drop at 400s, end the drop at 1200s. Total time 30 mins  Dynamic Atpase. |
| Final values |  |
| Relevant graphs |  |
| Boundary graph |  |
| Conclusion | * Did not reach equilibrium * Values are slightly different to Kira’s in terms of Vm and volumes * Dynamics look good * Redo experiment with a longer time frame |