|  |  |
| --- | --- |
| Aim: | Replicate Kira’s 4c – adding impermeant anions (1mM) mid simulation |
| Hypothesis: |  |
| Starting values: | Default 2 compartments |
| Simulation setup: | 30 min sim, 1ms time step  Variable ATPase  Adding 1mM impermeants between 6 and 12 minutes |
| Final values |  |
| Relevant graphs |  |
| Boundary graph |  |
| Conclusion | * Success * Replicates Kira’s essentially identically |

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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 |  |
| Setup | 2 compartments, changing the charge of impermeants in both to -1 between 400s and 1000s  Total simulation run time = 20mins |
| Final values |  |
| Relevant graphs |  |
| Boundary graph |  |
| Conclusions | * Reach same equilibria as Kira * Change in chloride driving force with drop in average charge of impermeants |

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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 |

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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: | See if I can replicate Kira’s figure 8 |
| Sim Setup: |  |
| Final values: |  |
|  |  |
| Boundary graph | Not rendering |
| Conclusion | Matches Kira’s figure 8 |

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| Aim | Observe the effect of changing the charge of impermeants in one compartment on the boundary dynamic |
| Hypothesis | Equilibrium will be reached where there is a non-zero flux of ions |
| Setup |  |
| Final values |  |
| Relevant graphs |  |
| Boundary graph |  |
| Conclusion | * Non-isopotential steady state * Transmembrane and transcompartmental flux at steady state |