Report 19 May

|  |  |
| --- | --- |
| **Experiment-A1** | 3 compartments – fluxing impermeants **(z=-1)** at a rate of **0.2mM/min**   * Observed slight non-isopotential effect, final z =-0.8506 |
| **Experiment-A2** | 3 compartments – fluxing impermeants **(z=-1)** at a rate of **0.5 mM/min**   * Increased effect, final z = -0.8515 |
| **Experiment-A3** | 3 compartments – fluxing impermeants **(z=-1)** at a rate of **4 mM/min**   * Increased effect, final z= -0.866 |
| **Experiment-A4** | 3 compartments – fluxing impermeants **(z=-2)** at a rate of **10 mM/min**   * Dramatically increased effect, final z =-1.2 |
| **Experiment-A5** | 3 compartments – fluxing impermeants **(z=-2)** at a rate of **10 mM/min** with **ATPase constant**   * Similar effect with constant ATPase, perhaps just getting to a steady state quicker. |
| **Experiment-A4-2** | Same as A4 just with longer time frame to try get an equilbrium |

\*HDF5 Data files for all experiments are saved on the GITHUB repository so can be recalled for future graphing or additional investigation.

Contents

[Experiment-A1 2](#_Toc72923661)

[Experiment-A2 9](#_Toc72923662)

[Experiment-A3 14](#_Toc72923663)

[Experiment-A4 19](#_Toc72923664)

[Experiment-A5 24](#_Toc72923665)

[Experiment A4-2 28](#_Toc72923666)

|  |  |
| --- | --- |
| Title | Experiment-A1 |
| Aim |  |
| Setup | Change z and x in comp 2  \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*  Compartment settings:  \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*  Empty DataFrame  Columns: []  Index: []  \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*  Extracellular anion concentrations:  \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*  Na: 145.0 mM  K: 3.5 mM  Cl: 119.0 mM  X: 29.5 mM  \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*  Simulation settings:  \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*  Total time (mins): 10.0  Timestep (ms): 0.001  ATPase Model type: J\_ATP = p \* (Na\_in/Na\_out)^3  Pump rate: 0.1  Area scale type: Am = Surface Area / volume  \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*  Impermeant anion changes:  \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*  Comp2 : increase intracellular impermeant anion concentration - 2.0 mM, valence: -1.0, between: 120.0s and 300.0s  No change of intracellular impermeant anion charge mid simulation  No change of extracellular impermeant anion concentration mid simulation |
|  |  |
|  |  |
|  |  |
|  |  |
|  |  |
|  |  |
|  |  |
|  |  |
|  |  |
|  |  |
|  |  |
|  |  |

|  |  |
| --- | --- |
| Title | Experiment-A2 |
| Aim | Same experiment as above, just increased the flux rate from 0.2mM/min to 0.5mM/min to see if I could exaggerate the effect |
|  | \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*  Compartment settings:  \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*  Empty DataFrame  Columns: []  Index: []  \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*  Extracellular anion concentrations:  \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*  Na: 145.0 mM  K: 3.5 mM  Cl: 119.0 mM  X: 29.5 mM  \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*  Simulation settings:  \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*  Total time (mins): 10.0  Timestep (ms): 0.001  ATPase Model type: J\_ATP = p \* (Na\_in/Na\_out)^3  Pump rate: 0.1  Area scale type: Am = Surface Area / volume  \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*  Impermeant anion changes:  \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*  Comp2 : increase intracellular impermeant anion concentration - 2.0 mM, valence: -1.0, between: 120.0s and 300.0s  No change of intracellular impermeant anion charge mid simulation  No change of extracellular impermeant anion concentration mid simulation |
|  |  |
|  |  |
|  |  |
|  |  |
|  |  |
|  |  |
|  |  |
|  |  |
| Conclusion | Successful experiment. Changing the flux rate did amplify the phenomenon. Next step is to increase the flux rate further |

|  |  |
| --- | --- |
| Title | Experiment-A3 |
| Aim | Same as above, just increasing the flux rate from 0.5 mM/min to 4mM/min |
|  | \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*  Compartment settings:  \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*  Empty DataFrame  Columns: []  Index: []  \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*  Extracellular anion concentrations:  \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*  Na: 145.0 mM  K: 3.5 mM  Cl: 119.0 mM  X: 29.5 mM  \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*  Simulation settings:  \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*  Total time (mins): 10.0  Timestep (ms): 0.001  ATPase Model type: J\_ATP = p \* (Na\_in/Na\_out)^3  Pump rate: 0.1  Area scale type: Am = Surface Area / volume  \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*  Impermeant anion changes:  \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*  Comp2 : increase intracellular impermeant anion concentration - 2.0 mM, valence: -1.0, between: 120.0s and 400.0s  No change of intracellular impermeant anion charge mid simulation  No change of extracellular impermeant anion concentration mid simulation |
|  |  |
|  |  |
|  |  |
|  |  |
|  |  |
|  |  |
|  |  |
|  |  |
|  | Successful experiment. Changing the flux rate did amplify the phenomenon. Next step is to increase the flux rate further.  The final valence is -0.865. In Kira’s her final valence wass -0.93 so th next step is to increase the rate and decrease the z of the incoming impermeants. |

|  |  |
| --- | --- |
| Title | Experiment-A4 |
| Aim | Same experiment as above but trying to amplify the phenomenon even further by changing the flux rate from 4mM/min to 10mM/min. And from z=-1 to z=-2  …. 10 mM/min does sound biologically implausible, but this high rate will hopefully allow me to run shorter simulations and get the same response.  In Kira’s last multicompartment figure she had a final average charge of -0.93mv. |
|  | \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*  Compartment settings:  \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*  Empty DataFrame  Columns: []  Index: []  \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*  Extracellular anion concentrations:  \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*  Na: 145.0 mM  K: 3.5 mM  Cl: 119.0 mM  X: 29.5 mM  \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*  Simulation settings:  \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*  Total time (mins): 10.0  Timestep (ms): 0.001  ATPase Model type: J\_ATP = p \* (Na\_in/Na\_out)^3  Pump rate: 0.1  Area scale type: Am = Surface Area / volume  \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*  Impermeant anion changes:  \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*  Comp2 : increase intracellular impermeant anion concentration - 2.0 mM, valence: -2.0, between: 60.0s and 420.0s  No change of intracellular impermeant anion charge mid simulation  No change of extracellular impermeant anion concentration mid simulation |
|  |  |
|  |  |
|  |  |
|  |  |
|  |  |
|  |  |
|  |  |
|  | * Success in amplifying the effect – Non-isopotential compartments with equal chloride driving forces. * Experiment is not quite at equilibrium, perhaps run for a bit longer. * My final charge is approximately -1.2, which is lower than Kira’s (-0.93) |

|  |  |
| --- | --- |
| Title | Experiment-A5 |
|  | Exact same as above but with constant atpase |
|  | \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*  Compartment settings:  \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*  Empty DataFrame  Columns: []  Index: []  \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*  Extracellular anion concentrations:  \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*  Na: 145.0 mM  K: 3.5 mM  Cl: 119.0 mM  X: 29.5 mM  \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*  Simulation settings:  \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*  Total time (mins): 10.0  Timestep (ms): 0.001  ATPase Model type: Constant  Pump rate: 0.1  Area scale type: Constant  \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*  Impermeant anion changes:  \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*  Comp2 : increase intracellular impermeant anion concentration - 2.0 mM, valence: -2.0, between: 60.0s and 420.0s  No change of intracellular impermeant anion charge mid simulation  No change of extracellular impermeant anion concentration mid simulation |
|  |  |
|  |  |
|  |  |
|  |  |
|  |  |
|  |  |
|  | * Similar dynamic to the above, constant ATPase perhaps gets to the equilbirium slightly quicker |

|  |  |
| --- | --- |
| Title | Experiment A4-2 |
| Aim | Replicating A4 but trying to get it to reach equilibrium.   * 12 min run instead of 10 minute * 5 mins of anion flux instead of 6 mins (60s – 360s)   Flux rate of 10mm/min. z=-2. Dt=10^-6. Variable ATPase |
|  | \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*  Compartment settings:  \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*  Empty DataFrame  Columns: []  Index: []  \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*  Extracellular anion concentrations:  \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*  Na: 145.0 mM  K: 3.5 mM  Cl: 119.0 mM  X: 29.5 mM  \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*  Simulation settings:  \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*  Total time (mins): 12.0  Timestep (ms): 0.001  ATPase Model type: J\_ATP = p \* (Na\_in/Na\_out)^3  Pump rate: 0.1  Area scale type: Am = Surface Area / volume  \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*  Impermeant anion changes:  \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*  Comp2 : increase intracellular impermeant anion concentration - 2.0 mM, valence: -2.0, between: 60.0s and 360.0s  No change of intracellular impermeant anion charge mid simulation  No change of extracellular impermeant anion concentration mid simulation |
|  |  |
|  |  |
|  |  |
|  |  |
|  | No major differences between experiment 4A – if graphs are needed here just get from the HDF5 file |