Report

14 April 2021

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| Aim | Sanity check 1.  3 compartments, changing z in all. Jp variable. (Will repeat below with Jp Constant)  Expect it to behave as the single compartment (i.e. Kira 6A) |
| Setup | \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*  Compartment settings:  \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*  Comp1 Comp2 Comp3  Radius 5.000000e-05 5.000000e-05 5.000000e-05  Length 2.500000e-04 2.500000e-04 2.500000e-04  Volume 1.963495e-12 1.963495e-12 1.963495e-12  Na\_i 1.400000e-02 1.400000e-02 1.400000e-02  K\_i 1.226650e-01 1.226650e-01 1.226650e-01  Cl\_i 5.000000e-03 5.000000e-03 5.000000e-03  X\_i 1.549000e-01 1.549000e-01 1.549000e-01  z\_i -8.500000e-01 -8.500000e-01 -8.500000e-01  ATPase pump rate 1.036427e-06 1.036427e-06 1.036427e-06  KCC2 pump rate 2.072854e-08 2.072854e-08 2.072854e-08  Vm 0.000000e+00 0.000000e+00 0.000000e+00  Ek 0.000000e+00 0.000000e+00 0.000000e+00  ECl 0.000000e+00 0.000000e+00 0.000000e+00  \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*  Extracellular anion concentrations:  \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*  Na: 145.0 mM  K: 3.5 mM  Cl: 119.0 mM  X: 29.5 mM  \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*  Simulation settings:  \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*  Total time (mins): 30.0  Timestep (ms): 1.0  ATPase Model type: J\_ATP = p \* (Na\_in/Na\_out)^3  Pump rate: 0.1  Area scale type: Constant  \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*  Impermeant anion changes:  \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*  No change of intracellular impermeant anion concentration mid simulation  All compartments : change in intracellular impermeant anion charge - valence: -1.0, between: 400.0s and 1000.0s  No change of extracellular impermeant anion concentration mid simulation |
| Final values: | Cl driving force: 11.42mV |
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| Boundary: |  |
| Conclusion: | * Voltage in all compartments drop, as it does in Kira’s * Minimal, but certain change in driving force * Slight increase in sodium concentration * Change to concentration of impermeants follows the change of charge * All compartments at steady state * **Model behaving as expected. Next step to do the same but with constant ATPase** |

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| Aim | Sanity check as above.  3 compartments  Drop z in all compartment. ATPase **constant.**  Expect to see a higher increase in sodium than above, and constant driving force. |
| Setup | \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*  Compartment settings:  \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*  Comp1 Comp2 Comp3  Radius 5.000000e-05 5.000000e-05 5.000000e-05  Length 2.500000e-04 2.500000e-04 2.500000e-04  Volume 1.963495e-12 1.963495e-12 1.963495e-12  Na\_i 1.400000e-02 1.400000e-02 1.400000e-02  K\_i 1.226650e-01 1.226650e-01 1.226650e-01  Cl\_i 5.000000e-03 5.000000e-03 5.000000e-03  X\_i 1.549000e-01 1.549000e-01 1.549000e-01  z\_i -8.500000e-01 -8.500000e-01 -8.500000e-01  ATPase pump rate 1.036427e-06 1.036427e-06 1.036427e-06  KCC2 pump rate 2.072854e-08 2.072854e-08 2.072854e-08  Vm 0.000000e+00 0.000000e+00 0.000000e+00  Ek 0.000000e+00 0.000000e+00 0.000000e+00  ECl 0.000000e+00 0.000000e+00 0.000000e+00  \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*  Extracellular anion concentrations:  \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*  Na: 145.0 mM  K: 3.5 mM  Cl: 119.0 mM  X: 29.5 mM  \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*  Simulation settings:  \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*  Total time (mins): 30.0  Timestep (ms): 1.0  ATPase Model type: Constant  Pump rate: 0.1  Area scale type: Constant  \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*  Impermeant anion changes:  \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*  No change of intracellular impermeant anion concentration mid simulation  All compartments : change in intracellular impermeant anion charge - valence: -1.0, between: 600.0s and 1200.0s  No change of extracellular impermeant anion concentration mid simulation |
|  | Cl driving force =14.23mV |
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|  | Sodium should be accumulating according to Kira’s! In mine sodium keeps on dropping likely due to the ATPase rate |
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| Conclusion | The ATPase set at constant is at such a high rate the leak channel can’t account for it….  The ATPase rate here is super important.  Seems like it needs to be less than the leak rate for sodium to accumulate |

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| Aim | Repeat the experiment above.  I found that my constant ATPase rate was possibly too fast and now I have changed it to be the ATPase rate at the beginning of the Sim (like Kira’s)  I expect to see the leak channel letting more sodium in than in the previous experiment and hope to see Na increase by +- 3mM when ATPase is constant.  3 comps.  Drop in z from -0.85 to -1.0 in all comps.  Constant ATPase. Constant Area scale. |
| Setup: | \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*  Compartment settings:  \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*  Comp1 Comp2 Comp3  Radius 5.000000e-05 5.000000e-05 5.000000e-05  Length 2.500000e-04 2.500000e-04 2.500000e-04  Volume 1.963495e-12 1.963495e-12 1.963495e-12  Na\_i 1.400000e-02 1.400000e-02 1.400000e-02  K\_i 1.226650e-01 1.226650e-01 1.226650e-01  Cl\_i 5.000000e-03 5.000000e-03 5.000000e-03  X\_i 1.549000e-01 1.549000e-01 1.549000e-01  z\_i -8.500000e-01 -8.500000e-01 -8.500000e-01  ATPase pump rate 1.036427e-06 1.036427e-06 1.036427e-06  KCC2 pump rate 2.072854e-08 2.072854e-08 2.072854e-08  Vm 0.000000e+00 0.000000e+00 0.000000e+00  Ek 0.000000e+00 0.000000e+00 0.000000e+00  ECl 0.000000e+00 0.000000e+00 0.000000e+00  \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*  Extracellular anion concentrations:  \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*  Na: 145.0 mM  K: 3.5 mM  Cl: 119.0 mM  X: 29.5 mM  \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*  Simulation settings:  \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*  Total time (mins): 30.0  Timestep (ms): 1.0  ATPase Model type: Constant  Pump rate: 0.1  Area scale type: Constant  \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*  Impermeant anion changes:  \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*  No change of intracellular impermeant anion concentration mid simulation  All compartments : change in intracellular impermeant anion charge - valence: -1.0, between: 600.0s and 1200.0s  No change of extracellular impermeant anion concentration mid simulation |
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|  | driving force = 11.14mV |
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| Na channel activation |  |
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| Boundary |  |
| Conclusion: | * Sodium is increasing and therefore the Vm drops as expected when z is dropped. * This matches what is shown by Kira * Driving force changes are also observed * Very close to an equilibrium being reached |