Report

11 April 2021

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| Aim: | Understand boundary dynamics when impermeant charge is changed mid-simulation |
| 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  \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*  Timing:  \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*  Total time (mins): 30.0  Timestep (ms): 1.0  \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*  Extracellular anion concentrations:  \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*  Na: 145.0 mM  K: 3.5 mM  Cl: 119.0 mM  X: 29.5 mM  \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*  ATPase settings:  \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*  Model type: J\_ATP = p \* (Na\_in/Na\_out)^3  Pump rate:  \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*  Impermeant anion changes:  \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*  No change of intracellular impermeant anion concentration mid simulation  Comp2 : change in intracellular impermeant anion charge - valence: -1.2, between: 400.0s and 900.0s  No change of extracellular impermeant anion concentration mid simulation |
| Final Values |  |

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| Graphs |  |
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| Boundary |  |
| Conclusion | * ATPase seems crucial for the balance… * When dropping the impermeant anions, appears that ATPase in adjacent compartments need to increase their rate * Next step is to do the same experiment with ATPase off |

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| Aim: | Assess the role of the adjacent ATPase when the impermeant anion charge drops in a compartment |
| 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  \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*  Timing:  \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*  Total time (mins): 30.0  Timestep (ms): 1.0  \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*  Extracellular anion concentrations:  \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*  Na: 145.0 mM  K: 3.5 mM  Cl: 119.0 mM  X: 29.5 mM  \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*  ATPase settings:  \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*  Model type: Constant  Pump rate:  \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*  Impermeant anion changes:  \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*  No change of intracellular impermeant anion concentration mid simulation  Comp2 : change in intracellular impermeant anion charge - valence: -1.2, between: 400.0s and 900.0s  No change of extracellular impermeant anion concentration mid simulation |
| Final vals |  |
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| Conclusion | * Similar dynamics with the variable ATPase just at different values. * System is still able to maintain the chloride driving force difference irrespective of the constant pump rate. * Contradicts the single compartment findings where there is no driving force change. |