Report – Changing the charge of impermeant anions

22 March 2021

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| Experiment: | Change charge of impermeant anions in both compartments from -0.85 to -1.1 and observe effect |
| Hypothesis: | Driving force of chloride in that compartment will decrease |
| Starting values: | 2 compartments at default values: |

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| Simulation settings: | 20 min sim  1ms time step  Dynamic atpase  Dropping z in both compartments from -0.85 to -1.1  Start of z drop @ 4 mins, end z drop @14 mins |
| Final values: |  |
| Relevant graphs |  |
| Boundary graph: |  |
| Conclusions: | * Membrane potential changes to a new set point * Definite change in chloride driving force * My volume change was significantly higher than Kira’s * Similar change in driving force as seen in Kira’s * Compartments not quite at steady state |

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| Experiment: | Dropping the impermeant charge in 1 compartment only. |
| Hypothesis: |  |
| Starting values: |  |
| Simulation setup: | Runtime = 20 mins  Timestep = 1ms  Dynamic atpase  Changing the impermeant anion concentration in compartment 1 only at 4 mins for -0.85 to -1.1. stopping the change @14 mins |
| Final values: |  |

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| Relevant graphs |  |
| Boundary dynamic |  |
| Conclusions | * The compartment that did not change its impermeant concentrations had a lower final steady state voltage * If you drop the impermeant charge the driving force in that compartment changes * Rate of volume change in the compartment with the change mimic the rate at which the impermeant concentrations in that compartment are changing. * Still major fluxes at the end of the simulation… will need to increase the time. * Not sure why so much chloride is moving into the more negative compartment at the end. * Need to repeat the simulation but for longer (30 mins instead of 20) |

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| Experiment | Same as above (changing impermeant average charge in only one compartment) but for longer simulation time |
| Hypothesis: | As above |
| Starting values: | As above |
| Simulation setup | 35 min duration  1ms time step  Dynamic atpase  Change average charge in compartment 1 from -0.85 to -1.1, starting @4 mins, ending @14 mins |
| Final values |  |
| Relevant graphs: |  |
| Boundary graphs: |  |
| Conclusions | * Reducing the charge actually drops the Vm in the neighbouring compartment * Reducing the charge increases the driving force for chloride * Seeing the perfect loop scenario come up again * My final values are not quite matching kira’s analytical… go back to the drawing board |