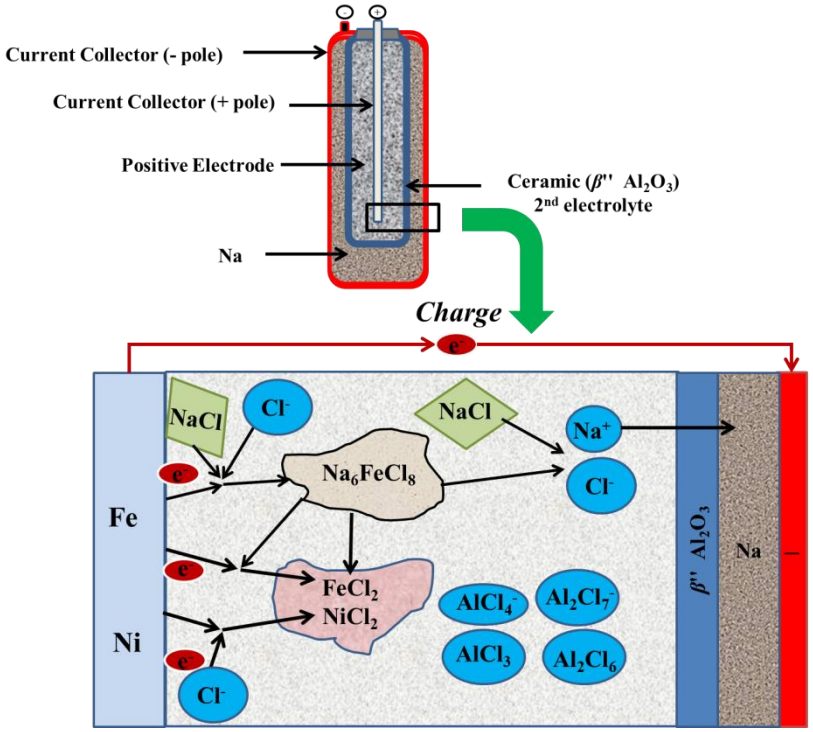
Mathematical Modeling of a sodium-metal chloride battery

Objective: Investigating reaction mechanisms in the positive electrode of sodium-metal chloride in order to predict the experimental data during charge, charge, and open circuit condition



Description of Research: Develop a simplified 0D model which includes only the kinetic source term for exploring several reaction mechanisms by using MATLAB DAEs solver and Global Optimization Toolbox.

Using the best mechanism with optimal kinetic parameters in 1D model in COMSOL Multi-physics environment for higher charge-discharge rates

Main Questions:

How does the $NiCl_2$ reduction occur on the iron plateau during discharge?

How the XRD observation about $NiCl_2$-$FeCl_2$ phase can be described in terms of the model expressions?

How the voltage relaxation time can be explained when we turn off the current (open circuit experiment) during charge and discharge?

Overall Cell Reaction

$$M + 2NaCl \underset{\text{Discharge}}{\overset{\text{Charge}}{\rightleftharpoons}} MCl_2 + 2Na$$

M = Fe, Ni

Major Challenges:

Finding a reaction mechanism which is able to predict the charge-discharge and OCV data at different Fe-Ni compositions and rates

Finding a reaction mechanism which is able to describe the XRD observations

Solving the model stiff DAE system in reasonable computation time for optimization purposes

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