Project Description:

There is currently work being done to model the performance of lithium air batteries in the CORES Research group. There is an existing working model that predicts analyzes the possible reactions that can take place in a carbon-based cathode for the battery. Various particle geometries are also being examined for the cell. This particular project will remove existing parts of the model that cover the topics of conservation of mass and energy, conservation of species, mass transport, chemical reactions, and thermodynamics. Efforts will be made to rebuild the removed parts to learn more about electrochemical modeling and overall lithium air battery model. I want to understand the effect of the geometry of the oxide particles affect lithium air battery performance. Similar batteries, such as Na-Air batteries, focus on creating particles with shapes that would create large active sites and help with adhesion to the carbon films [1], enhancing battery performance.

The removed parts can be determined by the professor or by another student. All in all, this project will cover rebuilding an existing model.

[1] https://www.nature.com/articles/am2016104/

Derivations:

1.1 Relating thermodynamics and Kinetics

$$\Delta G_{rxn} = \Delta G^o_{rxn} + RTln(\prod_k a_k^{vk}) = 0$$

$$\Delta G_{rxn} = \Delta G^o_{rxn} + RTln(\prod_k (\frac{\gamma_k C_k}{C_k^o})^{v_k} = 0$$

$$0 = k_{fwd} \prod_k (\gamma_k C_k)^{v_k^1} - k_{rev} \prod_k (\gamma_k C_k)^{v_k''}$$

$$k_{fwd} \prod_k (\gamma_k C_k)^{v_k^1} = k_{rev} \prod_k (\gamma_k C_k)^{v_k''}$$

$$\frac{k_{fwd}}{k_{rev}} = \frac{\prod_k (\gamma_k C_k)^{v_k^1}}{\prod_k (\gamma_k C_k)^{v_k''}}$$

$$\frac{k_{fwd}}{k_{rev}} = \frac{\prod_k (exp(\frac{-\Delta G_{rxn}}{RT})^{1/v_k} C_k^o)^{v_k''}}{\prod_k (exp(\frac{-\Delta G_{rxn}}{RT})^{1/v_k} C_k^o)^{v_k'}}$$

$$\frac{k_{fwd}}{k_{rev}} = exp(\frac{-\Delta G_{rxn}}{RT}) \prod_k \frac{C_k^o v_k''}{C_k^o v_k'}$$

$$\frac{k_{fwd}}{k_{rev}} = exp(\frac{-\Delta G_{rxn}}{RT}) \prod_k C_m^{o\,\sum_{k,m} v_k}$$

1.2 Relating mass action kinetics and the Butler-Volmer Form

$$i_{M-A} = n_{elec}F[k_{fwd} \prod C_{ac,k}^{v_k'} - k_{rev} \prod C_{ac,k}^{v_k''}]$$

$$i_{M-A} = n_{elec}F[k_{fwd}^{*} exp(\frac{-\beta n_{elec}F\eta}{RT}) \prod C_{ac,k}^{v_k'} - k_{rev}^{*} exp(\frac{(1-\beta) n_{elec}F\eta}{RT}) \prod C_{ac,k}^{v_k''}]$$

$$\eta = \Delta\Phi - \Delta\Phi_{eq}$$

$$\Delta\Phi_{eq} = \frac{-\Delta G_{rxn}^{o}}{n_{elec}F} = 0$$

$$k_{fwd} = k_{rev} exp(\frac{-\Delta G_{rxn}^{o}}{RT}) \prod_k C_m^{o\,\sum_{k,m} v_k}$$

$$i_{M-A} = n_{elec}F[k_{fwd}^{*} exp(\frac{-\beta n_{elec}F\eta}{RT}) \prod C_{ac,k}^{v_k'} \prod C_{ac,k}^{\beta v_k'} - k_{rev}^{*} exp(\frac{(1-\beta) n_{elec}F\eta}{RT}) \prod C_{ac,k}^{v_k''}]$$

$$i_{M-A} = n_{elec}F k_{rev}^{*}[exp(\frac{-\beta n_{elec}F\eta}{RT}) \prod C_{ac,k}^{\beta v_k'} - exp(\frac{(1-\beta) n_{elec}F\eta}{RT}) \prod C_{ac,k}^{v_k''}]$$

$$i_{M-A} = n_{elec}F k_{fwd}^{*}[exp(\frac{-\beta n_{elec}F\eta}{RT}) \prod C_{ac,k}^{\beta v_k^{2\prime}} - exp(\frac{(1-\beta) n_{elec}F\eta}{RT}) \prod C_{ac,k}^{\beta v_k''}]$$

$$C_{ac,k}^{\beta v_k} = \frac{k_{fwd}}{k_{rev}}$$

$$i_{M-A} = n_{elec}F k_{fwd}^{*} \frac{k_{fwd}}{k_{rev}^{*}}[exp(\frac{-\beta n_{elec}F\eta}{RT}) \prod C_{ac,k}^{\beta v_k'} - exp(\frac{(1-\beta) n_{elec}F\eta}{RT}) \prod C_{ac,k}^{(1-\beta) v_k''}]$$

$$i_o = n_{elec} F k_{fwd}^{*(1-\beta)} k_{rev}^{\beta} \prod C_{ac,k}^{\beta v_k'} - \prod C_{ac,k}^{\beta v_k''}]$$

$$i_{M-A} = i_o [exp(\frac{-\beta n_{elec} F \eta}{RT}) - exp(\frac{(1-\beta) n_{elec} F \eta}{RT}) \prod]$$