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Module 3 Concept Repository

- The charge/energy capacity of a given battery is calculated using reduction potential of the anode and cathode. In the reaction, $2Li + S \leftrightarrow Li_2S$, the anode half (oxidation) reaction is $2Li \leftrightarrow 2Li^+ + e^-$ and the cathode half (reduction) reaction is $2e^- + s \leftrightarrow S^{2-}$. $E_{cell} = E_{cathode} - E_{anode} = -0.407 - 3.05 = 2.633$ V as a reference potential. This is not a good estimate due to error as reduction potential is not a constant and changes with concentration and therefore state of charge. This estimate is more of a maximum. The difference between the concentration is the concentration polarization calculated by the Nerst equation. Through conversion g/mol and g/cm^3, this gives 13.882 g Li + 32.06 g S = 45.95 g Total, and 26 cm^3 Li + 15.5 cm^3 S = 41.5 cm^3 Total. E=QV where charge Q is moles of electrons e^- in this case 2 times Faradays constant F=96,485 C/mol. Charge Capacity is Q=(2)(96,485)=192,970 C. E=QV=(192,970 C)(2.633V) = 508,100 J. Energy Capacity is E= E(1 Wh/3600 J) = 141 Wh and Specific Energy is E/m= (141 Wh)/(45.95 g)=3070 Wh/kg and Energy Density is E/V= (141Wh)/(41.4 cm^3)=3400 Wh/L. These calculations have error because you are assuming all reactant are fully used, you are only using active materials in computations since batteries contain more than active materials and electrolyte, and during battery operation, theoretical potential will not be maintained.
- The relationship between state of battery charge and open-circuit voltage is nonlinear and has a curve accessed with it. Therefore, the equation is $_{Qmin}\int^{Qmax} E_{ref}(Q)dQ/(m_{active}+ m_{passive})$ and a SOC-OVC curve is needed where $E_{ref}(x) = E_{cathode}(1-x)- E_{anode}(x)$ and E= $Q_{xmin}\int^{xmax} E_{ref}(x)dx/(m_{active}+ m_{passive})$
- Batteries can be modeled using static or dynamic models. These models follow the form where u(t) are an input signal and y(t) are an output signal which can be a Voltage or Current. A static model is in the form is y(t) = g(u(t)). A dynamic model is in the from x'(t) = f(x(t), u(t)), y(t)=g(x(t), u(t)). x(t) is a state variable that can be a charge stored, etc.
- Batteries have capacitive, resistive, and inductive behavior. A resistor is any subsystem that can be modeled as a static relationship between voltage and current. This can be derived be the slope of a nonlinear function of voltage and current or polarization curve. A capacitor is any component or subsystem whose output voltage is a static function of accumulated charge. A model of this is where u(t) is current, x(t) is stored charge and y(t) is voltage. x'(t)= u(t) and y(t)=g(x). Here the Slope is dV/dQ=1/C where C is capacitance in farads. The typical bulk capacitance of a battery is in thousands of farads. An inductor is any device or effect where current is a static function of integral of voltage with respect to time. A model of this is y(t) is current, x(t) and current, and u(t) is voltage where x'(t) = f(u(t)) and y(t)=x(t) where dI/dt= V/L where L is in henrys
- To analyze the impedance of a battery, an oscillatory current input is given to the battery and voltage response is measured. All spinning vectors/oscillatory inputs and outputs can be written as $Ae^{j(wt+\varphi)}$. For example, in a simple circuit, $I=I_0 e^{jwt}$ and $V= I_0R e^{jwt}$. Here impedance Z=V/I=R. For impedance of a capacitor, $Z=V/I= V_0 e^{jwt}/ C V_0jw e^{jwt}=1/jwC=-j/wC$. For impedance of an inductor, Z=jWL. Impedance of capacitor and inductor changes with frequency $w=2\pi f$ and does not with impedance of a resistor. The impedance is the magnitude of impedance vector changing

with frequncy. Impedance of a parallel RC circuit is Z=-j/wRC. This can be visualized graphically using imaginary vs real phasor of oscillatory input and output.

- The Nyquist plot follows the input I_0 e^{jwt} to the battery and battery output V= V_0 $e^{(wt+\varphi)}$ where Z= V_0 $e^{(wt+\varphi)}$/ I_0 e^{jwt} = (V_0 / I_0)$e^{(j\varphi)}$ as a function of omega in the imaginary vs real domain.
- In the EIS plot the negative imaginary is plotted vs the real. The nature of a battery is predominantly resistance and capacitive with inductive effects on taking place at higher frequencies, with this plot being more appropriate to represent the plane.
- For a series RC circuit, Zeq=R-j/wC, as w=infinity Z=R=0, for w=0, Z= infinity.
- For a parallel RC circuit, Zeq= 1/(1/R+jwC)=R(1-jwRC)/(1+$(wRC)^2$). This would graph a semicircle on Nyquist/EIS plot. With radius R/2, where as w=0, Z=R, w=infinity, Z=0.
- To combine multiple EIS you use Kirchhoff Laws to find Zeq. A typical battery EIS has a large imaginary impedance at w=0, and inductive effects at w=infinity. As a function frequency is Z(w1)= Re(z(w1))+Im(z(w)). At intermediate value of w it is oscillatory.
- To report battery testing, you must record safe ranges of voltage, current, and temperature as minimum and maximum. Record charge and discharge capacity and protocol such as a CCV cycle or a truncated CCV cycle. Also record the OCV/SOC curves and terminal voltage vs charge/discharge capacity. Record cycle life for the battery and EIS plot.
- To test and report battery cell voltage you report based on safety consideration which are maximum voltage and minimum voltage. To test for capacity you must apply a slow constant voltage constant current charge and discharge test. To record cycling performing. You report the terminal voltage as a function of charge capacity with Vmax and Vmin and this is reported for different C-rate for discharge and charge.
- Factors that affect cycling performance for a battery are C-rate, temperature, and sometimes pressure. To record calendar life and cycle life this is tabulated with state of charge, calendar, and different temperatures. Battery life calendar lives are accelerated with high temperatures and then fitted to avg operating temperatures. Cycle life is reported with charge or discharge capacity as a function of a number of cycles. This can be reported for different variations affected by depth of discharge, temperature, and C-rate. Higher temperature and high c-rate decreases cycle life. Factors affecting calendar life are state of charge and temperature.
- To test battery impedance, the battery cell is taken a state of charge and you let it rest until equilibrium, then a small sinusoidal input current and the resulting sinusoidal input voltage with a DC offset is measured, the gain (V/I) and phase difference is measured between the two phases of the current and voltage. The gain and phase are set equal to the magnitude and angle of the z vector of the complex plane. Except tis is flipped din the EIS plot. This is performed at multiple frequencies. This can be done with EIS machines or a current function generator and oscilloscope to generate a solution.