Investigation of capacity limitations with AutoLion-1D™

Introduction

One common question from clients is what limits cell capacity under different operating conditions? With graphite-based cells with common cathode materials such as NMC or LFP, the diffusion process in the graphite active material typically limits the cell’s discharge capacity, particularly at low temperatures and high C-rates. In this case study, we highlight this point through an illustrative example.

Technology Used

AutoLion-1D™

Setup

- A 5Ah LFP/graphite power cell was designed in AutoLion-1D™. Materials database values were used.
- Three cells with different anode particle radii are used: 10 µm, 5 µm, and 1 µm; in all three cells every other geometric (electrode thickness, electrode capacity, porosity, etc.) remain the same.
- In these plots, we define depth of charge (DOD) as the discharged capacity divided by the cell material design capacity.
- Stoichiometry (“stoich”) is defined by the ratio of the solid-phase Li concentration to the material maximum solid-phase Li concentration ($c_s/c_{s,max}$) locally within the active material.
- Isothermal simulations were performed for all cases; all cells were initially at 100% SOC.

Results

Figure 1: Voltage vs. DOD discharge at -10°C for anode particle radii of 10 µm (green dash-dot), 5 µm (red dash), and 1 µm (blue solid); 1C rate discharge.

Figure 2: Voltage vs. DOD discharge at 25°C for anode particle radii of 10 µm (green dash-dot), 5 µm (red dash), and 1 µm (blue solid) 1C rate discharge.
Figure 3: Voltage vs. DOD discharge at 40°C for anode particle radii of 10 µm (green dash-dot), 5 µm (red dash), and 1 µm (blue solid) 1C rate discharge.

Figure 4: Voltage vs. DOD discharge at 25°C for anode particle radii of 10 µm (green dash-dot), 5 µm (red dash), and 1 µm (blue solid) 5C rate discharge.

Figure 5: Active material particle Li stoichiometry ($c_s/c_{s,max}$) vs. normalized particle radius ($r/R$) at end of discharge at -10°C, for anode particle radii of 10 µm, 5 µm, and 1 µm. Solid blue line is at anode/current collector interface; red dashed line is at anode/separator interface. 1C rate discharge.

Figure 6: Active material particle Li stoichiometry ($c_s/c_{s,max}$) vs. normalized particle radius ($r/R$) at end of discharge at 25°C, for anode particle radii of 10 µm, 5 µm, and 1 µm. Solid blue line is at anode/current collector interface; red dashed line is at anode/separator interface. 1C rate discharge.