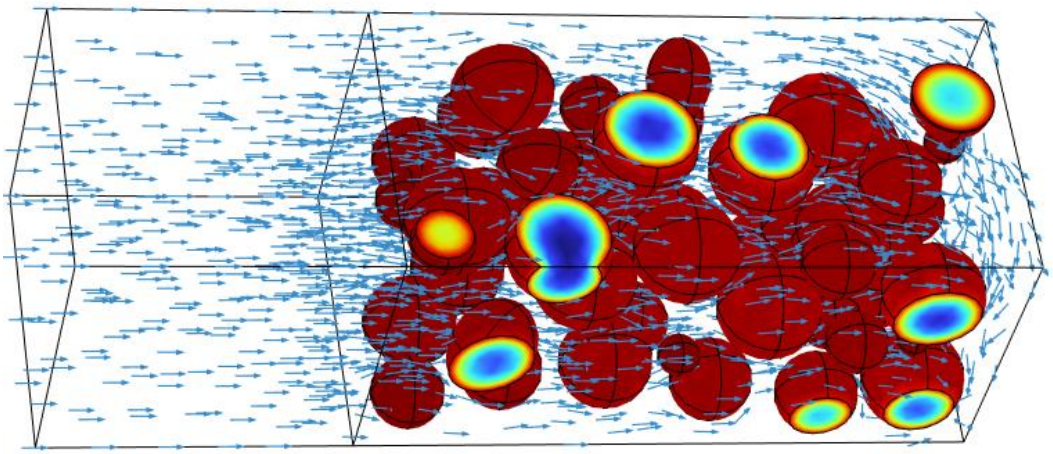
Li-ion half-cell battery model

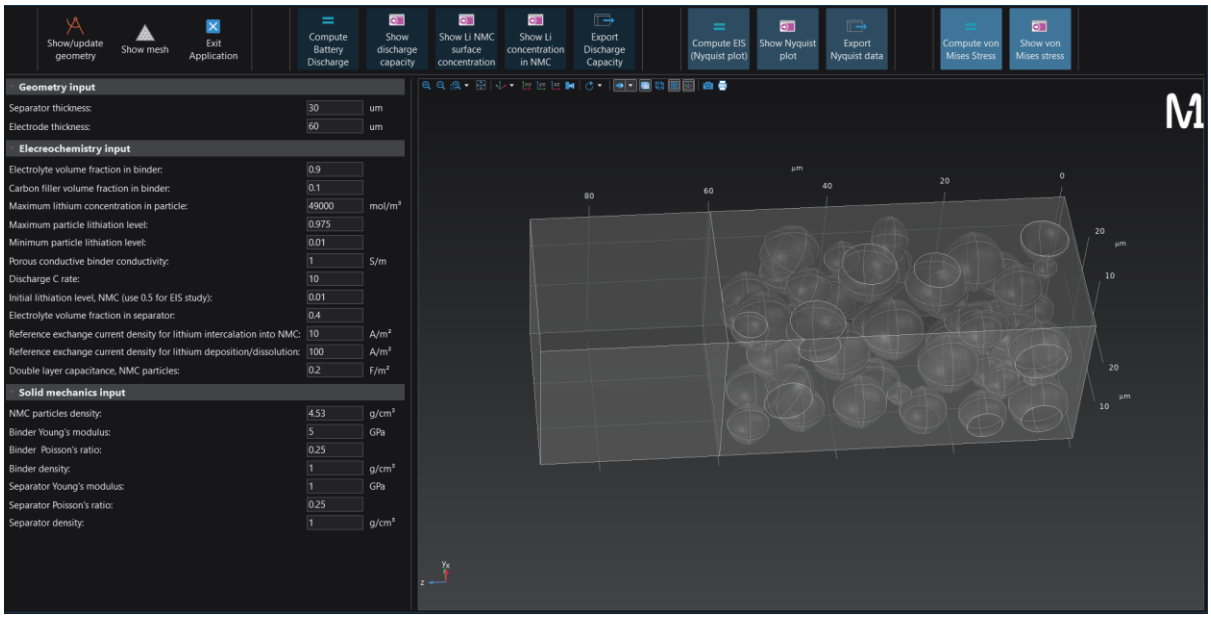
Application description



Contents

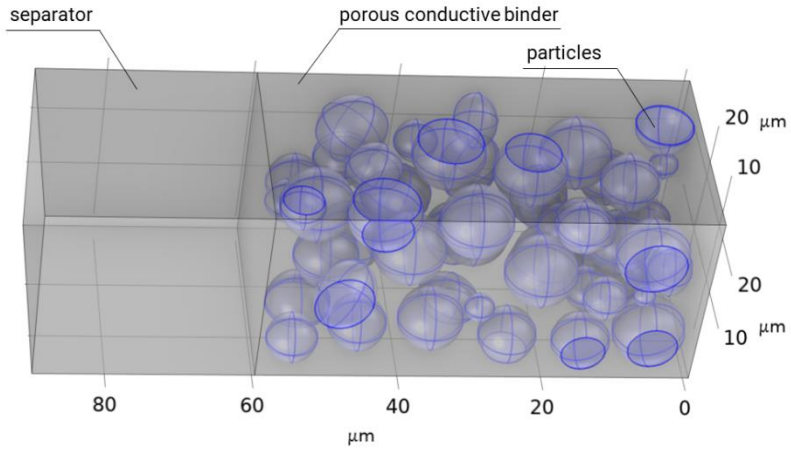
I. Introduction: what does the app do?

This app simulates a 3D heterogeneous NMC (Nickel-Manganese-Cobalt) electrode structure, which is based on an experimental microstructure of the NMC cathode. The app is based on the Doyle-Fuller-Newman lithium-ion battery model. The discharge capacitance, electrochemical impedance spectroscopy (EIS), and solid mechanics calculations can be performed with this app. The application interface looks as follows:



II. Geometry and system description

The half-cell battery model is comprised of three main parts – active particles (e.g., NMC 111, $LiNi_{0.33}Mn_{0.33}Co_{0.33}O_2$), separator and porous conductive binder. The particles size distribution is based on experimental data, and it is predefined for this particular application. However, users can also input their own particle data based on x-ray tomography from a csv file. The geometry of the model is depicted in figure below where the dimensions of the cathode are 30×30×60 μm^3 and of the separator – 30×30×30 μm^3. The particles are surrounded by homogenized (the polymeric binder, carbon conductor and electrolyte are represented by the same domain) porous conductive binder and electrolyte phase. The anode is not explicitly included in the model but only implicitly through a boundary condition on the left side of the separator. The boundary condition on the right side of the cathode represents the current collector where inward electrode current is applied.



III. Simulated properties

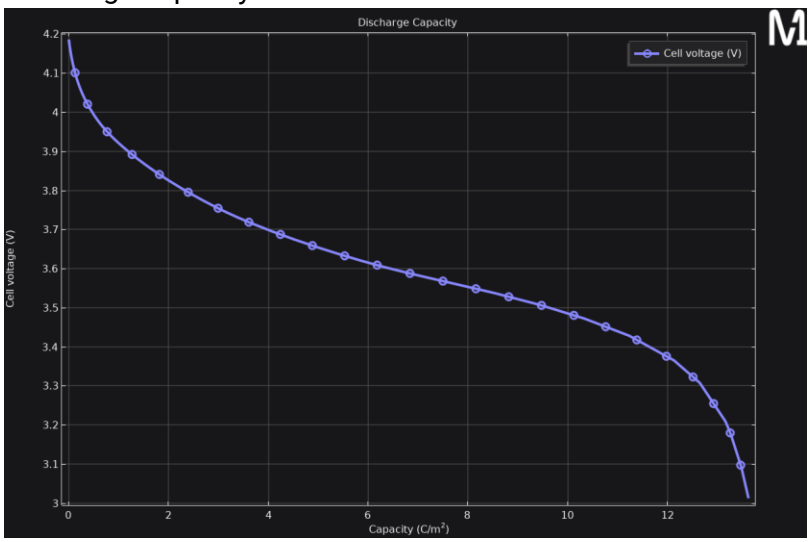
Three predefined properties are simulated with the “compute” buttons in the main menu.

- Electrochemical and morphological properties (discharge capacity, Li^+/NMC surface concentration, Li^+ concentration in NMC)
- Electrochemical impedance spectroscopy (Nyquist plot)
- Mechanical properties (von Mises stress)

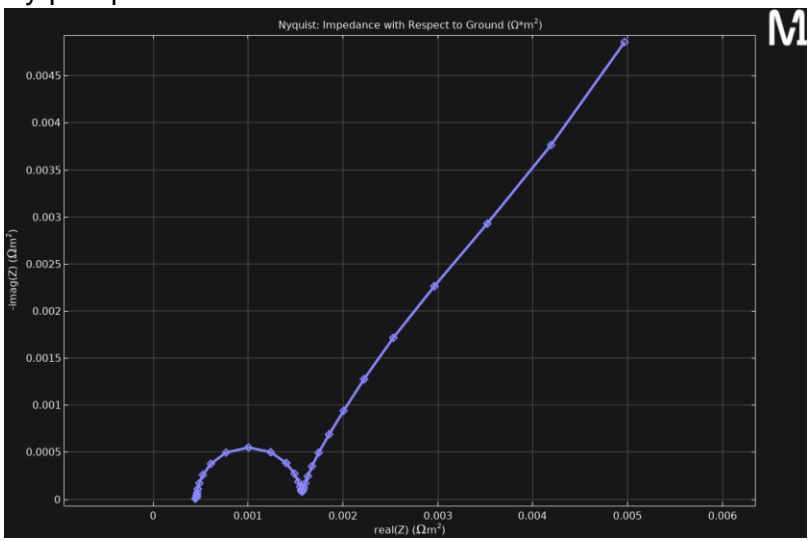
After the specific calculation is done, the results can be displayed with the “show” buttons next to the specific compute study. The three predetermined computations are grouped together with their respective results for easier navigation. Furthermore, the discharge capacity and Nyquist plot data can be exported to text files, CSV or Excel files for further external analysis and use. All results (plots and images) can also be exported as an image file with the snapshot button ( ).

The calculated results include the following characteristics:

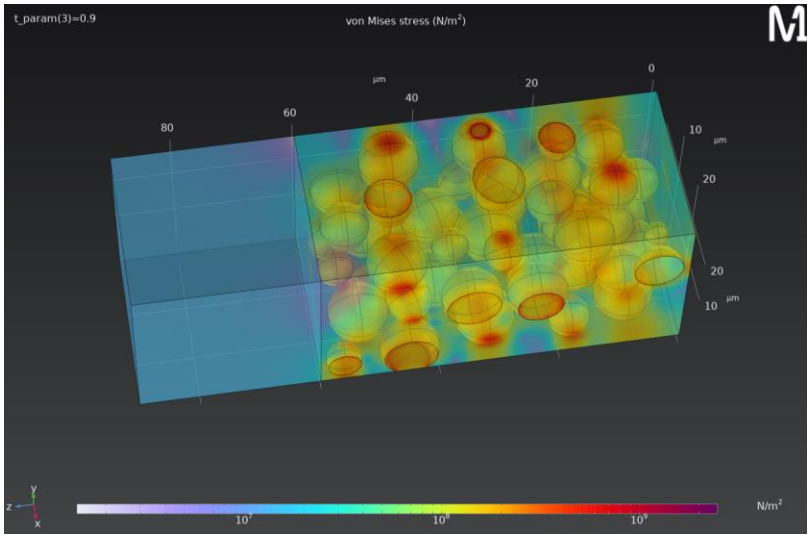
1. Discharge capacity



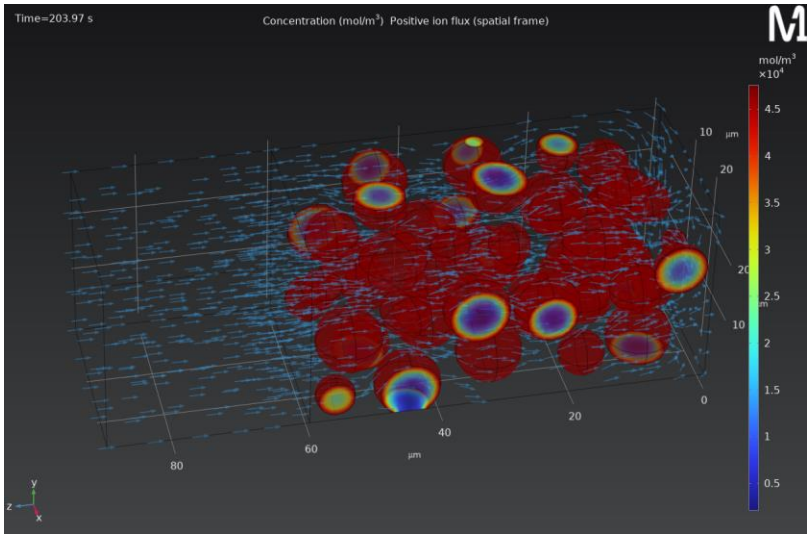
2. Nyquist plot



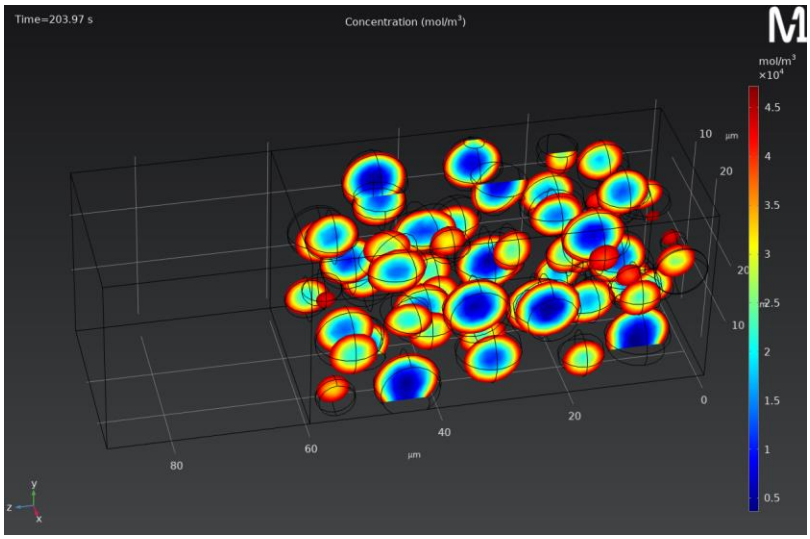
3. von Mises stress



4. Li/NMC surface concentration



5. Li concentration in NMC



IV. Model parameters

Most of the physical parameters of the model can be varied with the parameter's toolbar shown below. The parameters are divided into three main groups – geometry, electrode (electrochemical) and solid mechanics properties. The geometry in the model is predefined, thus only the electrode and separator thicknesses can be varied. The general (electrochemical) materials properties determine the electrochemical performance of the cell; thus, they affect mostly the discharge and the EIS calculations. The mechanical properties are used in the von Mises stress calculation. The default parameters of the model are listed when the application is started.

Parameter's toolbar