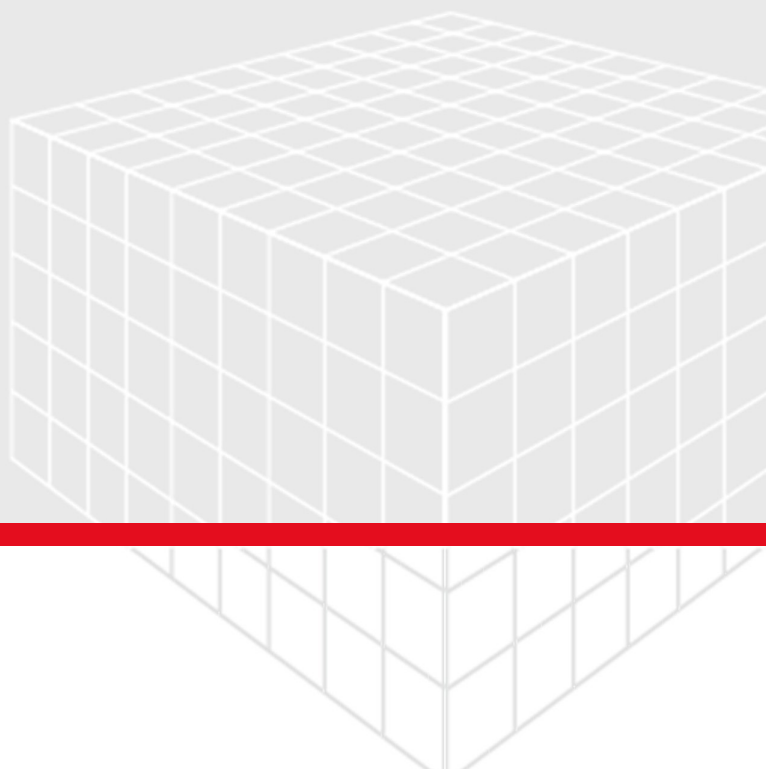


BatteryDict

User Guide

GEODICT Release 2026

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GEODICT

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BatteryDict

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1 BatteryDict

BatteryDict simulates the performance of secondary lithium-ion batteries during charging and discharging on the micro and meso scale. With the Battery Designer, virtual cells can be created, based on 3D structures of electrode materials with a representative elementary volume (REV). The numerical calculation of the electrochemical processes governing ionic transport in the different material phases and across their interfaces are based on local charge and neutrality together with a Butler-Volmer reaction model.

A battery cell in BatteryDict consists of four different components: cathode, anode, separator, and the current collectors. The current collectors are represented as standardized layers, while the separator can be modeled as an effective material. The cathode and anode are individually modeled structures, consisting of multiple active materials, binders and other conductive additives, and electrolyte. Up to four different active materials and up to four conductive additives and binders can be processed for each electrode. It is also possible to perform half cell simulations for single electrode structures, without designing the complete half cell first.

It is possible to run a fully resolved simulation on the created microstructure. This very accurate solution provides results that are fully resolved on the micro scale. Two solvers are provided for fully resolved simulations, the LIR solver and the BESTmicro solver.

BatteryDict additionally allows to run homogenized simulations with the BESTmeso solver that are much faster than the fully resolved simulation. A homogenized model that is created from the given battery structure is used in this case with effective parameters computed in GeoDict.

It is additionally possible to define charging profiles with different stopping criteria. This functionality is especially useful to simulate consecutive charging and discharging processes in the battery.

The relaxation of a battery cell after charging or discharging can be simulated as additional steps in the charging profiles.

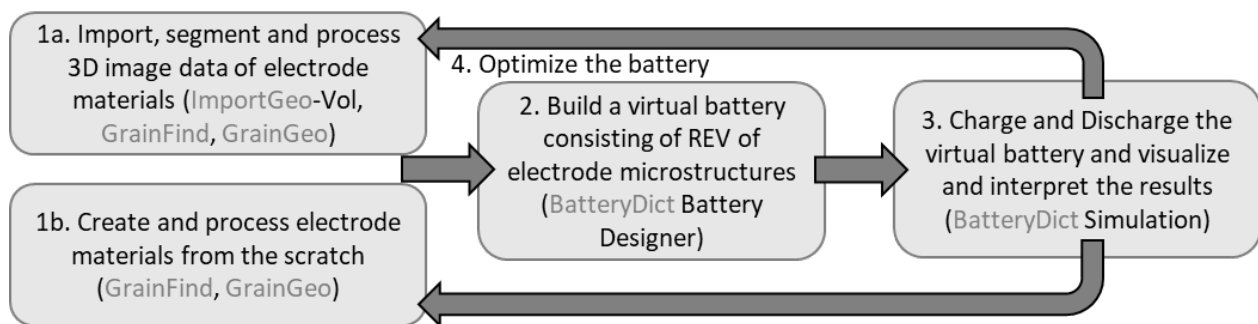
The functionality to compute mechanical deformations of a battery cell due to Lithium intercalation (BatteryDict-Degradation) is also possible. This add-on to BatteryDict allows to study mechanical stresses and strains due to deformations of the active materials in the battery cell from a previously run charging or discharging simulation.

The input data for the electrode models can be either scanned data from μ CT or FIB-SEM images of real cathode and anode materials, or realistic structures created in GeoDict. BatteryDict is capable of handling voxel-based structures, with a volume large enough (REV) to simulate the behavior of a real battery electrode. For each active material, the Open-Circuit Potential (OCV) curve can be specified and the characteristic values for ionic and electronic transport in the active materials, electrolyte and binder or binder and carbon black (represented as one CBD-phase), respectively, can be set. The separator and current collectors are represented as homogeneous materials with a specified thickness.

The models used for simulation and the parameters to be defined are explained in more detail in the section [Theoretical Background](#)^[7]. The different simulation options are outlined in their corresponding topics (see list of topics [below](#)^[5]). The results of the simulations and their interpretation are discussed.

The characteristic application for BatteryDict is to simulate and optimize the charging performance of a battery cell, based on realistic electrode microstructures. To analyze or model electrode microstructures, also the use of other GeoDict modules is emphasized. Many properties of the microstructure are vital for the performance of a battery, like porosity, pore size distribution, surface area, tortuosity, thermal conductivity, thermal flux, electric conductivity, electric flux, thermal expansion, permeability, diffusivity, etc.. The GeoDict modules GrainGeo, GrainFind, PoroDict, FlowDict, DiffuDict, and ConductoDict can be used to analyze these properties and to obtain detailed information about the microstructure of the electrodes.

With ImportGeo-Vol, 3D image data can be imported and segmented and be further processed with the modules mentioned above. GrainFind and GrainGeo are powerful tools to create Statistical Digital Twins based on image data or realistic microstructures from scratch.



New in GeoDict 2026

- **LIR improvements:**

- All result fields can now also be produced by the LIR solver.
- Now, [concentration dependent parameters](#)^[73] for electrolyte can also be considered using the LIR solver.

- **Experiment tab** in [Charge Battery](#)^[79] and [Charge Electrode](#)^[141]:

- The parameters are reorganized for a better overview of boundary conditions and start and end conditions.
- The new boundary condition [Power Density](#)^[80] is available.
- It is now possible to define an [Initial Voltage](#)^[81].

- Two new **simulation types** are available in [Charge Battery](#)^[85] and [Charge Electrode](#)^[143]:

- [Calculate Homogenized Parameters](#)^[85] without running a charging simulation.
- [Calculate Equilibrium Potential Curve](#)^[85] to only estimate the cell potential in equilibrium without running a charging simulation.

- With the [Charge Homogenized Battery](#)^[117] and [Charge Homogenized Electrode](#)^[152] commands you can run homogenized simulations directly without providing a geometry.
- Find the two new [GeoApps](#)^[192] to compute electrochemical properties:
 - Fast charging of batteries reduces the accessible cell capacity. The GeoApp [Battery Capacity Test](#)^[192] allows prediction of accessible cell capacity for different charge rates.
 - Calculate the complex -valued resistance called "impedance" using the GeoApp [Electrochemical Impedance Spectroscopy](#)^[200].
- **Result fields** in [Charge Battery](#)^[92] and [Charge Electrode](#)^[142]:
 - The new result field **Interface Current Density** is now available.
- With the new material parameter [Electrolyte Lithium Concentration of Exchange Current Measurement](#)^[35], you can directly use your exchange current density measurements of your electrolyte materials with any lithium concentration in equilibrium without recalculating the maximum exchange current density.

Learn to use BatteryDict

- [Theoretical Background](#)^[7]
Learn about the equations solved in BatteryDict and parameter definitions. Additionally, learn how to add battery materials to the GeoDict material database.
- [Battery](#)^[46]
In this section a complete battery cell is considered consisting of current collectors, separator, anode and cathode. Design, analyze and charge or discharge a digital battery.
- [Electrode](#)^[135]
In this section, only a half cell is considered consisting of anode or cathode. Lithiate or delithiate an electrode.
- [Degradation](#)^[166]
Compute mechanical deformations of a battery cell due to lithium intercalation.
- [Battery GeoApps](#)^[192]
Determine electrochemical properties with the Battery GeoApps.
- [References](#)^[205]
See the references for more relevant literature.



Join the conversation

Visit the Community on [GeoDict Forum](#) to be inspired and get answers to top questions.

Find illustrative application examples on the [website](#).
Our tutorials and seminar videos give you a first hands-on experience. They are collected in the [Learning Center](#).
Send your [Support Request](#) to our technical Support.

1.1 Theoretical Background

Upon charging a typical secondary Li-ion battery, the Li^+ ions initially stored in the active material of the cathode are transported to the anode side. During this process, the cathode active material is oxidized and Li^+ ions de-intercalate and diffuse through the electrolyte, towards the anode. This electrochemical process is induced by the applied charging potential, that drives the transport of free electrons through the cathode active material and through the binder with carbon black to the current collector. On the anode side, electrons flow from the current collector through the carbon black and active material. The active material of the anode is reduced by the Li^+ intercalation.

During discharging, Li^+ ions are transported in a corresponding process to the cathode side, while the electron flow powers the consumer device. The amount of lithium an electrode material can store per volume determines the volumetric energy density. The resulting cell potential is given by the difference between the electrochemical potential of the cathode and the electrochemical potential of the anode.

Governing equations and explanations

- [State of Charge \(SOC\) and State of Lithiation \(SOL\)](#)^[8]
Depending on context, we distinguish different definitions of state of charge.
- [Fully Resolved Simulation](#)^[12]
Fully resolved simulation of charging and discharging process.
- [Homogenized Simulation](#)^[18]
Homogenized simulation of charging and discharging process.
- [Boundary Conditions](#)^[24]
Boundary conditions at the current collectors.
- [Stopping Criteria](#)^[24]
Stopping Criteria for Charging Simulations.
- [Overpotentials and Heat Production](#)^[26]
Overpotentials and Heat Production in Battery Charging Simulations.
- [Degradation Simulations](#)^[30]
Degradation simulations in BatteryDict.
- [Simulation Parameters](#)^[31]
Simulation parameters for charging simulations.
- [Add Custom Materials](#)^[37]
Adding custom electrochemical materials with the needed experimental data.
- [Overlapping OCV Curves](#)^[44]
Overlapping OCV Curves for several Active Materials.
- [Solver Convergence](#)^[45]
Learn about possible reasons why the solver does not converge.

1.1.1 State of Charge (SOC) and State of Lithiation (SOL)

Depending on context, we distinguish different definitions of state of charge:

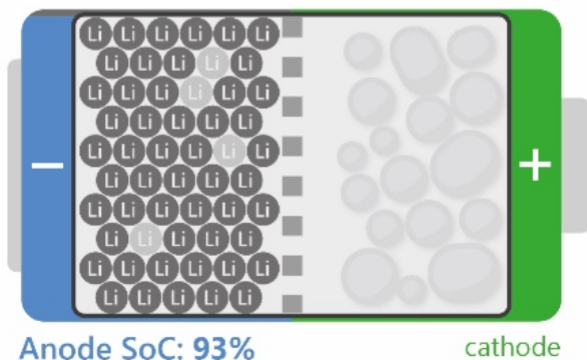
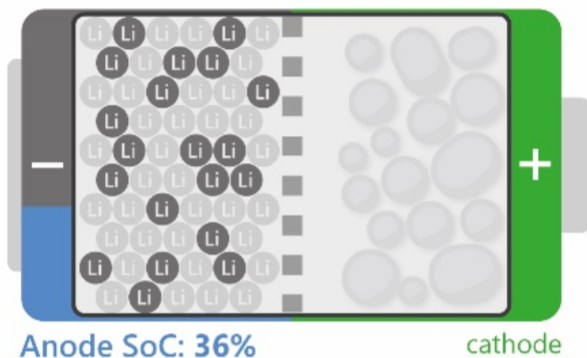
✓ Anode state of charge

The **Anode state of charge** measures the momentary Li-ion content of the anode relative to the maximal Li-ion content of the anode. The Li-ion content is the volume integral of the Li-ion concentration.

This means, for the fully resolved model, for each active material voxel, the SOC is the voxel's Li-ion concentration divided by the voxel's [maximum Li-ion concentration](#)³¹. The anode SOC is the mean value of the voxel SOC's of all active-material voxels within the anode.

For the homogenized model, the anode SOC is the integral of the active material's SOC over all anode voxels.

Anode State of Charge



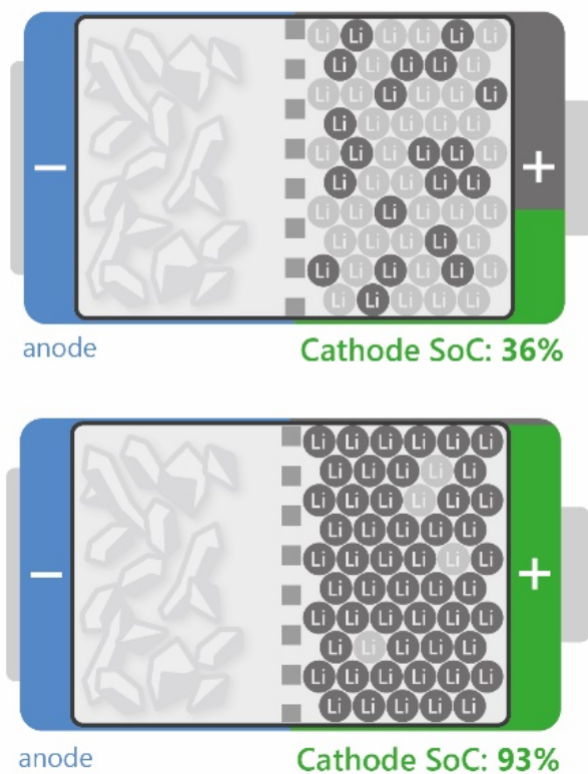
✓ Cathode state of charge

The **Cathode state of charge** measures the Li-ion content of the cathode relative to the maximal Li-ion content of the cathode. The Li-ion content is the volume integral of the Li-ion concentration.

This means, for the fully resolved model, for each active material voxel, the SOC is the voxel's Li-ion concentration divided by the voxel's [maximum Li-ion concentration](#)^[31]. The cathode SOC is the mean value of the voxel SOC's of all active-material voxels in the cathode.

For the homogenized model, the cathode SOC is the integral of the active material's SOC over all cathode voxels.

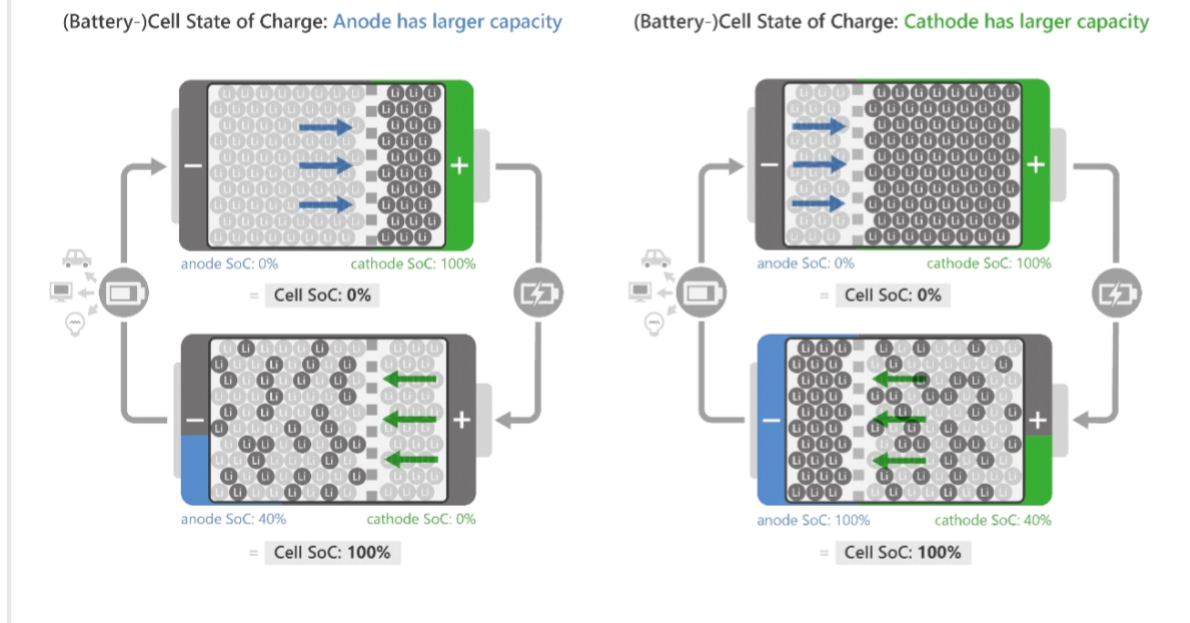
Cathode State of Charge



✓ Cell state of charge

The **Cell state of charge** describes the overall state of charge of the battery cell. In BatteryDict, it is 0% if one of the following conditions is met: the anode is empty, or the cathode is full. It is 100% if one of the following conditions is met: the anode is full or the cathode is empty.

For a half cell simulation the lithium reservoir has always the same capacity as the other electrode. To get a numerically stable solution, the state of charge can be set in GeoDict between 5% and 95%, see also [Fully Resolved](#) ¹⁵.



✓ Material state of lithiation

In BatteryDict's fully resolved model on voxel scale, each voxel has a unique material ID. In simulations with the homogenized model using the BESTmeso solver, a voxel can represent a porous electrode with electrolyte and solid volume fractions. Lithium ions intercalate or deintercalate from active materials during lithiation or delithiation, therefore the lithium composition x of these materials changes during the (dis)charge process. Each material has a maximum lithium composition and a minimum lithium composition.

For anode materials, the minimum lithium composition usually is the status without intercalated lithium ions (e.g., for graphite). Analogously, the maximal lithium composition is the maximum amount of lithium ions that can reversibly be intercalated into the material.

For cathode materials, the maximum lithium composition is usually the stoichiometric lithium composition (e.g., $x=1$ for $\text{Li}_x\text{Ni}_{0.33}\text{Mn}_{0.33}\text{Co}_{0.33}\text{O}_2$). The minimum lithium composition is the lithium composition where the maximal amount of lithium ions is removed reversibly from the structure. Often the minimum lithium composition does not mean that all lithium was taken out of the material because the potential rises to values where the material would get intrinsically unstable while some lithium is still present in the material.

For both anode and cathode materials, BatteryDict works with lithium concentrations instead of lithium compositions on a voxel scale basis. BatteryDict estimates for each

active material voxel (in the fully resolved simulation) or each porous electrolyte voxel (in the homogenized model) a certain “material state of lithiation” by comparing the current lithium concentration c_s in the material to the maximum lithium concentration c_{max} of the material. This material state of lithiation (SOL) is defined as

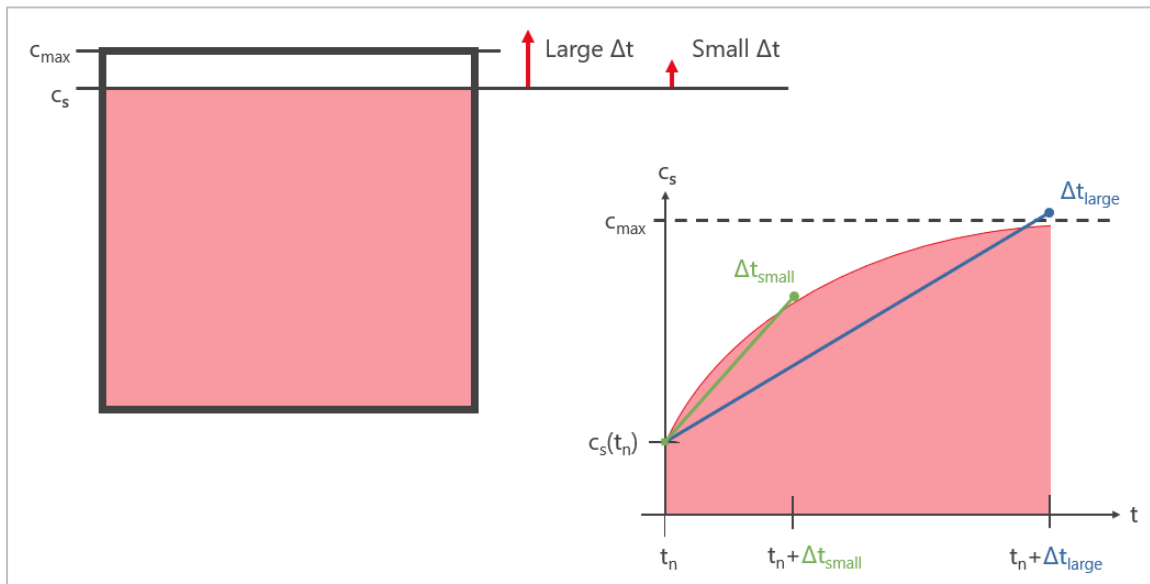
$$SOL = \frac{c_s}{c_{max}} \cdot 100\% \quad (1)$$

where c_s is the (removable) lithium concentration in the active material and c_{max} is the maximum (removable) lithium concentration of the material. Due to this definition, the SOL in an active material’s voxel will always have a value between 0% (minimum lithium composition) and 100% (maximum lithium composition) and the removable lithium concentration assigned to the voxel is in the range between 0 and c_{max} . The active material voxels in fully-resolved model or the porous electrode voxels in homogenized model obtain always material SOL between 0% (i.e., $c_s \geq 0$) and 100% (i.e., $c_s \leq c_{max}$).

When time steps are set too large and a voxel’s lithium concentration is close to the maximum lithium concentration, the lithium concentration might exceed the maximum lithium concentration in this time step and prevent convergence; analogously, voxels that are close to a lithium concentration of 0 might result in negative lithium concentrations with large time steps and prevent convergence.

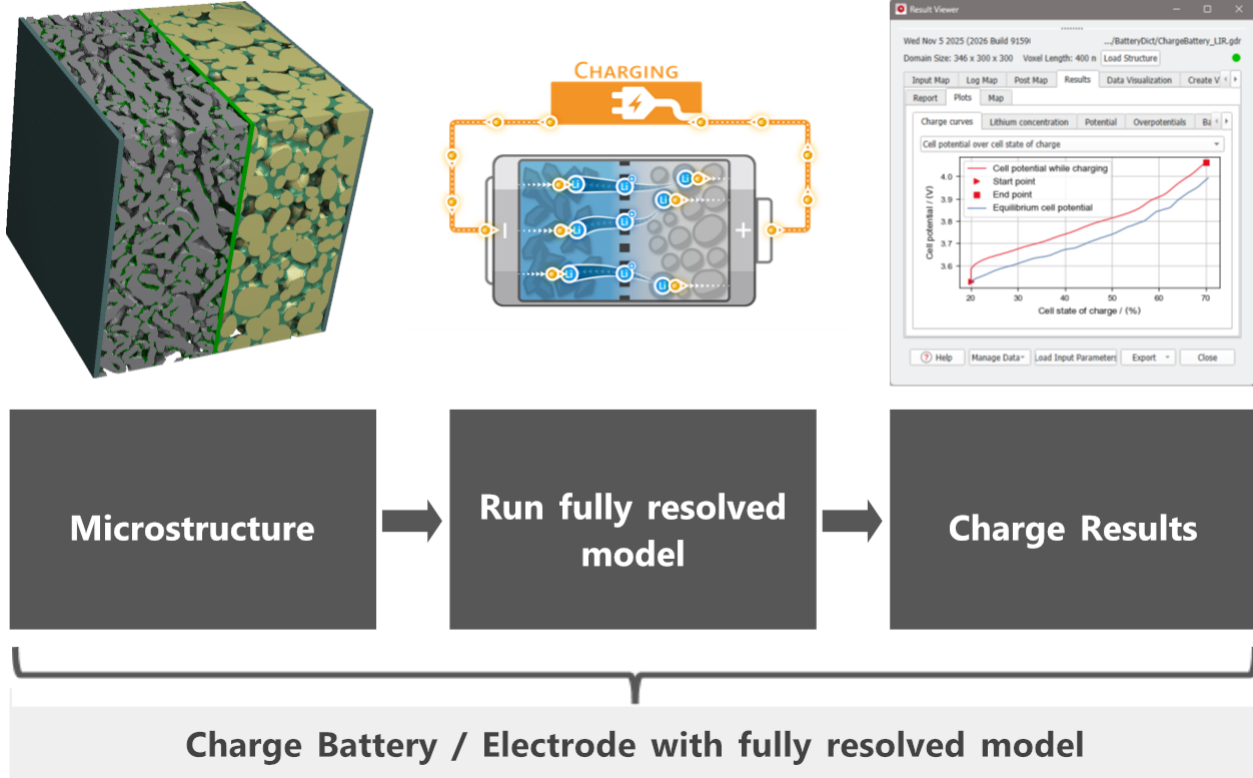
In such circumstances, the solver usually tries smaller time steps to converge to a meaningful result.

Note that the material SOL will usually not coincide with the lithium composition x because the minimum (removable) lithium concentration for cathode materials might be $x > 0$ and the maximum (removable) lithium composition for anode materials might be $x < 1$.



1.1.2 Fully Resolved Simulation

Run a fully resolved charging simulation directly on the microstructure for a very detailed insight into the processes of the battery, e.g., local ion concentration while charging.



The main physical principles, describing the charging or discharging simulation in BatteryDict, are conservation of mass for lithium atoms and conservation of charge.

To describe the cell behavior, a fully resolved model is applied that describes on the micrometer scale the relevant transport process. As the length scale considered in BatteryDict is above the scale where positive and negative charges can be resolved, it is sufficient to consider the distribution of lithium concentrations and potentials. The basis of the battery cell model are the conservation equations for lithium ions and electrical charges, respectively:

$$\frac{\partial c}{\partial t} = -\nabla \cdot \vec{N} \quad (2)$$

$$0 = \nabla \cdot \vec{j} \quad (3)$$

Here, c is the concentration of lithium ions, $\vec{N}$ their flux and $\vec{j}$ the electronic / ionic current density. In the different domains (active material or electrolyte) different constitutive relations apply for the fluxes $\vec{N}$ and $\vec{j}$.

✓ In the active material

In the active material lithium ions recombine with an electron and are therefore electrically neutral. Hence, they are independent of electrical potentials and undergo only diffusive motion driven by gradients in the lithium concentration. The ion flux is given by

$$\vec{N}_s = -D_s \nabla c_s \quad (4)$$

where D_s is the diffusion constant of lithium in the solid material.

The diffusion of ions in the active material is therefore described by the equation

$$\frac{\partial c_s}{\partial t} = \nabla \cdot (D_s \nabla c_s) \quad (5) \text{ Diffusion}$$

In the active material domain, the electrical current is carried by electrons. Therefore, the electronic current density is simply given by Ohm's law

$$\vec{j}_s = -\kappa_s \nabla \varphi \quad (6) \text{ Ohm's law}$$

Where κ_s is the electronic conductivity and φ_s the electrical potential. Thus, it follows

$$0 = \nabla \cdot \vec{j}_s = -\nabla \cdot (\kappa_s \nabla \varphi_s) \quad (7)$$

✓ In the electrolyte

In the electrolyte, the flow of charged species (lithium and counter ions) are responsible for the electrical current. Under the assumption of electroneutrality it is sufficient to consider only the transport of lithium ions. Since they are charged, their motion is influenced by two driving forces, the differences in the ion concentration and in the potentials, such that the ionic current density is given by

$$\vec{j}_e = -\kappa_e \nabla \varphi_e + \kappa_e (1 - t_+) \frac{RT}{F} \nabla \log c_e \quad (8)$$

where κ_e is the ionic conductivity and t_+ the transference number which (in the absence of concentration gradients) describes the fraction of current carried by the positive lithium ions. R is here the universal gas constant, T the temperature and F Faraday's constant.

To simplify the complexity, this equation assumes a constant activity of lithium ions such that the activity does not appear in the model. Additionally, we note, that the

second term sometimes can be found in the literature with an additional factor of 2. This needs to be taken into account consistently in the determination of the transference number.

The charge conservation and electroneutrality equation in the electrolyte is therefore

$$0 = \nabla \cdot \vec{j}_e = -\nabla \cdot (\kappa_e \nabla \varphi_e) + \nabla \cdot \kappa_e \left((1 - t_+) \frac{RT}{F} \nabla \log c_e \right) \quad (9) \text{ Charge conservation and electroneutrality}$$

Similar as the current density, also the ion flux depends on concentration and potential gradients. With the ionic diffusion constant D_e the flux in the electrolyte can be formulated as

$$\vec{N}_e = -D_e \nabla c_e + \frac{t_+ \vec{j}_e}{F} \quad (10)$$

This leads to the diffusion and migration equation in the electrolyte

$$\phi \frac{\partial c_e}{\partial t} = \nabla \cdot (D_e \nabla c_e) - \nabla \cdot \frac{t_+ \vec{j}_e}{F} \quad (11) \text{ Diffusion and migration}$$

where ϕ is the porosity.

Further explanation about the theoretical background for the ion transport in the electrolyte can be found in [Latz et al., 2011](#)^[205].

For solid electrolytes the transference number t_+ is always 1. Therefore, there is no concentration gradient in the solid electrolyte. Thus, for solid electrolytes the equations in the electrolyte simplify to constant lithium concentration

$$\frac{\partial c_e}{\partial t} = 0 \text{ and } \nabla c_e = 0 \quad (12) \text{ Constant lithium concentration}$$

and for the charge conservation and electroneutrality it follows

$$0 = \nabla \cdot \vec{j}_e = -\nabla \cdot (\kappa_e \nabla \varphi_e) \quad (13) \text{ Conservation and electroneutrality}$$

lity for solid electrolytes

✓ In the Carbon Binder Domain (CBD-Phase)

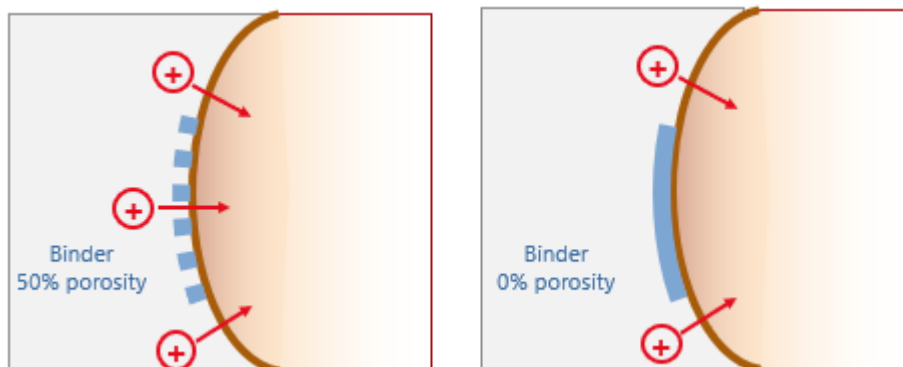
The Carbon Binder Domain (CBD Phase) is represented by respective voxels in the battery structure. The CBD phase can either be simulated as a non-porous material or as a porous material with non-resolved micropores (see [Electrochemistry](#)^[77]). In the GeoDict material database, the material of "PVDF Binder and Carbon Black" is shipped as an effective material representing the CBD properties.

For non-porous binder, the CBD phase is a pure electron conductor. So, only Ohm's law is solved (see equation (7)^[13] for the active material). At interfaces to active materials, electrons can be transferred from CBD phase to active material and vice versa.

For porous binder, there is a solid fraction of the CBD phase and a pore fraction of the CBD phase. The solid fraction of the CBD phase conducts electrons and Ohm's law is solved considering the effective electronic conductivity of the porous binder. The pore phase of the CBD phase is filled with electrolyte and conducts lithium ions. For this fraction, the equations for the electrolyte as stated above (diffusion and migration equation (11) [Diffusion and migration](#)^[14] and charge conservation and electroneutrality equation (9) [Charge conservation and electroneutrality](#)^[14] are solved.

For the interface of non-porous binder and active material, a (de)intercalation of lithium ions is not possible. For the interface of porous binder and active material, a (de)intercalation of lithium ions to/from the pore fraction of the porous binder that is filled with electrolyte is possible. BatteryDict considers that the interfacial area of active material to porous binder is only partly available for lithium intercalation.

See the sketch below. The ion exchange is calculated with the Butler-Volmer equation. See equation (15) [Butler-Volmer interface current density](#)^[16].



✓ Interface between Electrolyte and Active Material

On the interface between electrolyte and active material lithium ions move from the electrolyte into the active material on intercalation or vice versa on deintercalation. This flux of ions is continuous across the interface and its magnitude is given by the Butler-Volmer current density i_{se} such that the interface conditions for the fluxes and current densities are given by

$$\begin{aligned}\hat{n} \cdot \vec{N}_e &= \hat{n} \cdot \vec{N}_s = i_{se}/F \\ \hat{n} \cdot \vec{j}_e &= \hat{n} \cdot \vec{j}_s = i_{se}\end{aligned}\quad (14)$$

here, $\hat{n}$ is the interface normal pointing from solid into electrolyte. Hence, a positive i_{se} corresponds to deintercalation while a negative sign indicates an intercalation reaction. The Butler-Volmer interface current density depends on concentrations and potentials on both sides of the interface and is given by

$$i_{se} = 2 i_{0,max} \sqrt{\left(1 - \frac{c_s}{c_{max}}\right) \frac{c_s}{c_{max}}} \sqrt{\frac{c_e}{c_{e,i_0^{meas}}}} \cdot 2 \sinh\left(\left(\varphi_s - \varphi_e - U_0\right) \frac{F}{2RT}\right) \quad (15) \text{ Butler-Volmer interface current density}$$

Here, $i_{0,max}$ is the **Maximum Exchange Current Density** in equilibrium, $c_{e,equ}$ the lithium concentration of the electrolyte in equilibrium (see below), and U_0 the open-circuit potential of the active material versus lithium.

For Li-ion concentration $c_s = 0$ or $c_s = c_{max}$, the square root $\sqrt{\left(1 - \frac{c_s}{c_{max}}\right) \frac{c_s}{c_{max}}}$ in the Butler-Volmer interface current density gets 0, which can lead to numerical solver problems. As stated in [State of Charge \(SOC\) and State of Lithiation \(SOL\)](#)^[10], the SOC is related to the Li-ion concentration in the active materials. Therefore, the range of the cell and electrode state of charge can only be set between 5% and 95% in the [Charge Battery](#)^[81] and the [Charge Electrode](#)^[141] dialogs. A real battery in experimental conditions usually is set to operate in a certain voltage window (compare also the different [stopping criteria](#)^[24]) to avoid permanent damage of the cell. The relevant voltage window usually is in a SOC range smaller than the range between 5% and 95% SOC and therefore can be fully covered in the simulation.

Furthermore, during the intercalation of Li-ions from the electrolyte into the active material, these Li-ions attain one electron per ion and become neutral in charge. During the de-intercalation of Li from the active material into the electrolyte, every Li atom loses one electron and becomes a positively charged Li-ion.

Hence, in the solid material, the charge transport is performed solely by electrons, whereas in the electrolyte, the charge transport is performed solely by ions.

For solid electrolytes the term $\sqrt{\frac{c_e}{c_{e,i_0}^{meas}}}$ is always 1, because the Li-ion concentration in the electrolyte does not change and thus, c_e is always $c_{e,equ}$.

✓ Interface between Electrolyte and Lithium Reservoir

For the simulation of a single electrode, the other electrode is modeled as a never-ending lithium reservoir, not limiting the battery performance. Therefore, there exist no c_s and c_{max} and the Butler-Volmer interface condition (equation (15) [Butler-Volmer interface current density](#)^[16]) simplifies to

$$i_{se} = 2 i_{0,max} \sqrt{\frac{c_e}{c_{e,equ}}} \cdot 2 \sinh\left((\varphi_s - \varphi_e - U_0) \frac{F}{2RT}\right)$$

(16) Butler-Volmer interface current density (lithium reservoir)

The build-in default value for the **Maximum Exchange Current Density** of a lithium reservoir for the default electrolyte concentration of 1200 mol/m³ is:

$$i_{0,max} = 640 \frac{A}{m^2} \frac{\sqrt{1200 \text{ mol/m}^3}}{\sqrt{1000 \text{ mol/m}^3}} \approx 700 \frac{A}{m^2}$$

This is based on an assumed exchange current density between the lithium reservoir and the electrolyte of 640 A/m² at an electrolyte concentration of 1000 mol/m³, see [Kremer et al., 2020](#)^[206].

✓ Interface between two Active Materials

At interfaces between active material grains, exchange of Li ions is possible only if both grains are modeled with the same material ID in GeoDict. In case of different material IDs, no exchange of Li ions is possible between the grains. Especially, if different grains of the same active material are assigned to separate Material IDs in the GeoDict structure, no ion exchange happens between the IDs.

✓ Interface between Active Materials and Separator

In case the separator is modeled as [non-porous material](#)^[74], it is considered as filled with electrolyte throughout the simulation and the interface is modeled in the same way as the [interface between electrolyte and active materials](#)^[15] or the [interface between electrolyte and lithium reservoir](#)^[17].

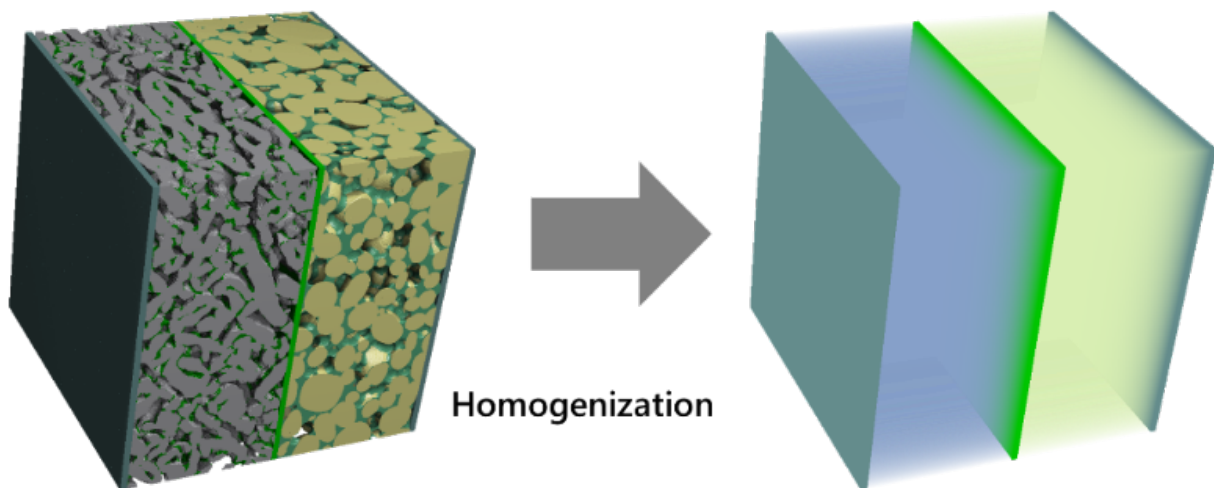
Also, in the case of a porous separator with [effective properties](#)^[74], it is always assumed that the direct interface between separator and active material is completely filled with some electrolyte. The whole interface is therefore described by the equations for [interaction between electrolyte and active material](#)^[15]. The same is valid for the interface between separator and a lithium reservoir.

1.1.3 Homogenized Simulation

Fully resolved charging and discharging simulations are based on the voxel geometry and thus fully resolve the micro-structure of the battery. But basically, the charge transport in a battery is one-dimensional. Therefore, BatteryDict also provides a pseudo-2D Newman model (also called DFN-model) simulation with the BESTmeso solver. Although it does not fully resolve the structures within the battery cell, it can provide an approximation for the charging-curve and takes much shorter computation time.

Fully resolved Model

Homogenized Newman Model



In this model, BatteryDict first calculates input parameters for the homogenized simulation, such as ionic diffusivity and electrical conductivities, see [below](#)^[22]. These effective parameters depend both on the geometry of the structure and on the material properties of the fully resolved model. With these parameters, the homogenized simulation is able to consider the different characteristics of anode and cathode.

In the next step, the battery structure is then recomposed of representative effective voxels. These voxels are arranged in 1D in the x-direction. Each voxel in the 1D model is now not completely filled with active material, electrolyte or binder, but consists of a mixture of the different materials. The voxel therefore has both active material and electrolyte properties. Ionic and electronic current are computed in this 1D model in charging direction (currently x-direction) and are linked by a Butler-Volmer exchange current.

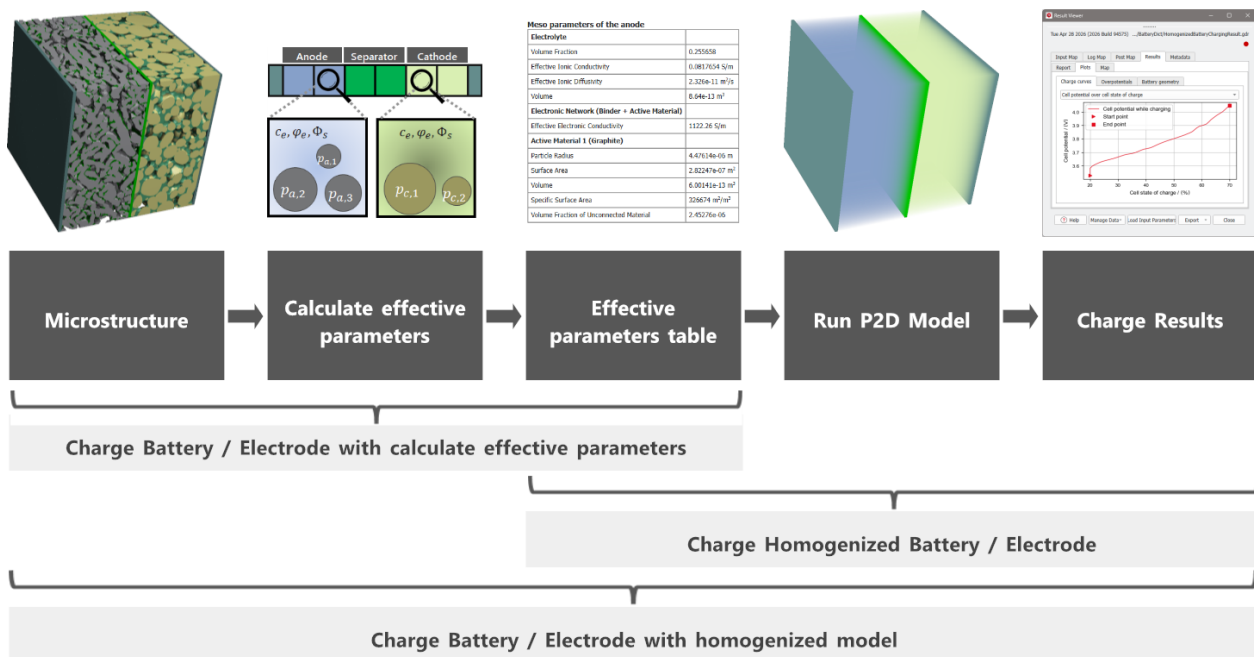
Each of the 1D voxels contains a sphere-shaped representative active particle for every active material. The effective radius of these spheres is calculated analyzing the fully resolved

microstructure and gives a second degree of freedom. This has no spatial dimension and is thus called "pseudo-dimension". Therefore, the method is called pseudo-2D. With the representative active material particles, it is possible to simulate diffusion of Lithium inside the active material, even if only 1D representative effective voxels are used for the simulation. This is necessary to be able to compute the overpotentials during the charging or discharging simulation. These overpotentials depend on the Lithium concentration at the active materials surface.

The effective parameters are calculated separately for anode and cathode and assigned to the anode and cathode voxels respectively. The concentrations and potentials computed during the charging or discharging simulation however can be different for each voxel.

BatteryDict offers three options for the homogenized model:

1. You can start from the microstructure and [calculate only the effective parameters](#)^[85] of the structure.
2. Alternatively, if you already know the effective parameters, you can only run a [homogenized charging simulation](#)^[117].
3. Or, you can do [both at once](#)^[85]. Calculate the effective parameters and run a charging simulation on the homogenized battery.



✓ Homogenized Model Equations

In the homogenized model, each voxel consists of a mixture of active material and electrolyte. Therefore, the system of partial differential equations solved by the BESTmeso solver does not consist of separate equations for active material, the electrolyte and the interface between them as in the fully resolved model.

The homogenized model uses a volume averaged 1D version of the microscopic model outlined in [Latz et al., 2013](#)^[205]. This is basically identical to the DFN-model.

The equations of the fully resolved model for diffusion and migration as well as for charge conservation and electroneutrality of the electrolyte (equations (11) Diffusion and migration^[14] and (9) Charge conservation and electroneutrality^[14]) and Ohm's law for the active materials (equation (7)^[13]) are therefore supplemented by additional source terms. These source terms account for the Butler-Volmer current from electrolyte to active material and vice versa through the (no longer resolved) interface between these materials. The 1D movement of Lithium ions and electrons is described by the following three equations:

$$\frac{\partial(\varepsilon_e c_e)}{\partial t} = \nabla \cdot (D_{eff,e} \nabla c_e) - \nabla \cdot \frac{t_+ j_e}{F} + \nabla \cdot \frac{j_e}{F} \quad (17)$$

$$\nabla \cdot \vec{j}_e = -\nabla \cdot (\kappa_{eff,e} \nabla \varphi_e) + \nabla \cdot \left[\kappa_{eff,e} (1 - t_+) \frac{RT}{F} \nabla \log c_e \right] = \sum_{p \in P} a_p i_{BV,p} \quad (18)$$

$$\nabla \cdot \vec{j}_s = -\nabla \cdot \kappa_{eff,s} \nabla \varphi_s = -\sum_{p \in P} a_p i_{BV,p} \quad (19)$$

The equation of diffusion in the active materials transforms to a radial diffusion on the representative active particle scale:

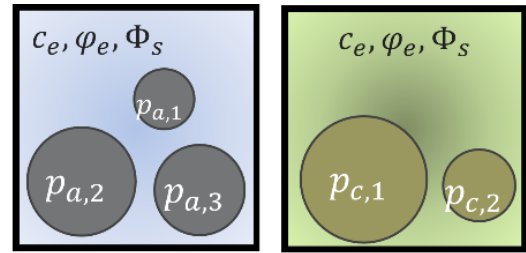
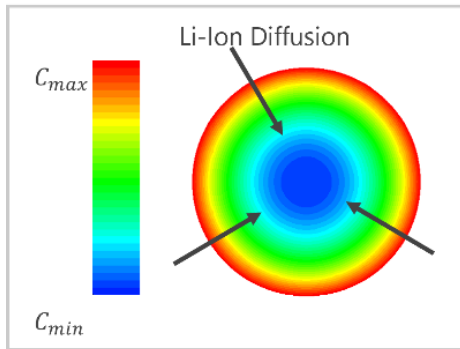
$$\forall p \in P : \frac{\partial c_{s,p}}{\partial t} = -\nabla \cdot \vec{N}_{s,p} = 0 \quad (20)$$

and

$$\vec{N}_{s,p} \cdot \vec{n}|_{r=R_p} = F^{-1} i_{BV,p} \quad (21)$$

with the flux

$$\vec{N}_{s,p} = -D_{s,p} \nabla c_{s,p} \quad (22)$$




Radial Diffusion
 for each representative particle

Finally, the Butler-Volmer interface condition depends now on the overpotential at the boundary of the spherical particles.

$$i_{se} = 2 i_{0,max} \sqrt{\left(1 - \frac{c_s}{c_{max}}\right) \frac{c_s}{c_{max}}} \sqrt{\frac{c_e}{c_{e,i_0^{meas}}}} \cdot 2 \sinh\left(\left(\varphi_s - \varphi_e - U_0\right) \frac{F}{2RT}\right) \quad (23)$$

In the fully resolved model, the interface is located between active material and electrolyte voxels. In contrast to this, the interface in the homogenized model is within the 1D voxels and not resolved in the structure.

Parameters, appearing in the equations above are:

Electrolyte	
ε_e	Volume fraction of electrolyte in the electrode
$D_{eff,e}$	Effective ionic diffusivity of electrolyte
t_+	Transference number
$\kappa_{eff,e}$	Effective ionic conductivity
Active Materials and Binder	
$\kappa_{eff,s}$	Effective electric conductivity of active materials and binder

Active Materials

P	Number of active materials
$D_{s,p}$	Ionic diffusivity of active material p
R_p	Effective radius of spherical particle of active material p
a_p	Specific surface area between electrolyte and active material p

Representative active material particle

c_e	Lithium concentration in electrolyte
$c_{s,p}$	Lithium concentration in active material p
$c_{s,p,max}$	Maximum Lithium concentration in active material p
φ_e	Electrochemical potential in electrolyte
$\varphi_{s,p}$	Electrochemical potential in active material p

Constants

F	Faraday number
R	Gas constant
T	Absolute temperature

✓ Computation of effective properties from the micro model

The computation of effective properties in the homogenized model precedes charging or discharging simulations, which are run with BESTmeso solver. For a full battery simulation, effective parameters for each electrode are calculated separately.

The computed effective properties can be found in the Result Map of charging or discharging simulation under **FoundMesoParameters** and are displayed in the [Results](#)

[Report](#)^[96]. In the case of an electrode simulation, calculated effective parameters are always listed under **Cathode**.

The following effective properties are computed:

For electrolyte:

- $D_{eff,e}$ - effective ionic diffusivity
- $\kappa_{eff,e}$ - effective ionic conductivity

Both properties are computed for the x-direction of the electrode, using algorithms of ConductoDict with EJ solver, assuming symmetric boundary conditions of the structure and taking into account the (non-zero) electrolyte diffusivity and conductivity respectively. The diffusivity or conductivity constants for all active materials are set to zero. In case of porous binder, effective ionic diffusivity and conductivity are used, for non-porous binder both constants are also set to zero.

For active materials and binder:

- $\kappa_{eff,s}$ - effective electronic conductivity

The parameter is computed using the same setting as for electrolyte (ConductoDict algorithms with EJ solver, computation in X-direction of the electrode, symmetric boundary conditions). In this case, the conductivity of electrolyte is set to zero, while for all active materials and binder their electronic conductivity is considered.

For active materials:

- R_p - effective radius of representative spherical particle of active material p
- a_p - specific surface area between electrolyte and active material p

The computation of effective radius is similar to the algorithm Estimate Grain Diameters in the GrainFind module. The effective radius for each active material is found as the average radius of all particles of this active material. All particles are considered as spheres in this estimation.

The specific surface area is calculated as voxelized area between electrolyte and connected voxels for each active material. The voxel connectivity is checked according to the algorithm, which is explained in [Analyze Battery](#)^[56] for the structure with symmetric tangential boundary conditions.

The volume fraction of unconnected material is also considered when computing the transferred charges and the SOC in order that it matches to the fully resolved model. The electrochemical cell behavior, i.e., the shape of the charging curve, is not affected.

For separator:

In case of porous separator, the effective values for ionic conductivity and ionic diffusivity and the porosity are used in the same way as for [fully resolved simulations](#)^[74].

1.1.4 Boundary Conditions

A battery can be operated in two modes, either by prescribing the current or the voltage. Define the boundary conditions in the [Experiment](#)^[80] tab of the option's dialog.

In the first case, the cell potential is a simulation result and in the second case, it is a time-dependent current that is computed. In a current-controlled simulation, the current can be specified in three different ways: Prescribing the electronic current directly (in A), the current density (in A/m²), or the C-rate. Using the C-rate is useful since it allows an intuitive understanding of the load that is applied on the cell without the need to know the cell capacity. Note that the same C-rate might correspond to different currents for different geometries with different capacity! Similarly, the same current density might correspond to a different current if the cross section of the cell changes. So be aware of this relation when comparing different simulation cases.

Battery charging and discharging with constant potential can be simulated. In case of constant potential, the time-dependent current, charge rate, etc. are not constant anymore and can be analyzed for the charging simulation in the GeoDict Result Viewer.

Additionally, it is possible to define a [charging profile](#)^[83]. This allows to simulate the charging or discharging with different boundary conditions at the current collectors one after the other. Relaxation of the battery or electrode after charging and discharging can be simulated as separate step in the charging profile.

1.1.5 Stopping Criteria

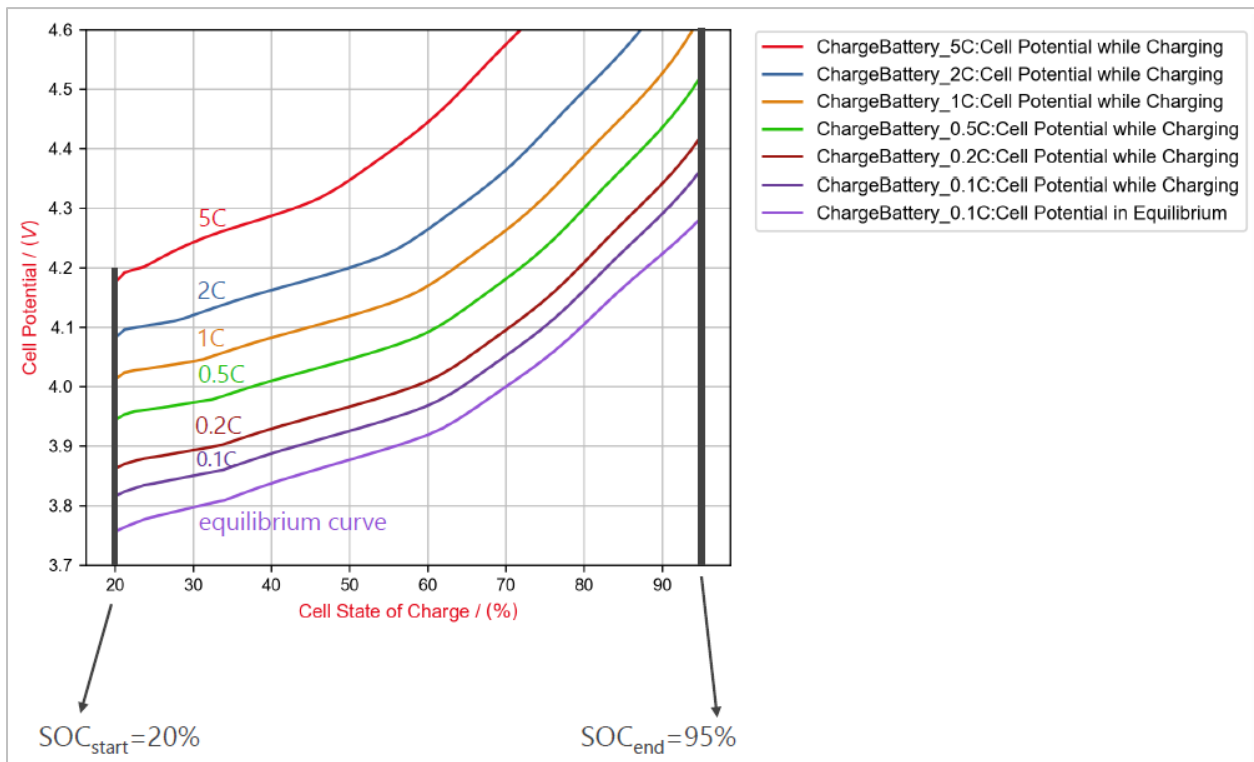
Different stopping criteria for a charging simulation can be defined. Define initial and final state-of-charge for the whole battery or for both electrodes or define initial and final voltage.

If a charging profile is defined, additionally a reached cell potential, charge rate, current density, or current can be defined as stopping criterion. Setting the stopping criterion in the GeoDict GUI is explained for simple charging profiles [here](#)^[80] and for more complex profiles [here](#)^[83].

In the following, as an example, the difference between the stopping criteria final state-of-charge and final cell potential is shown for simulations with constant charge rate.

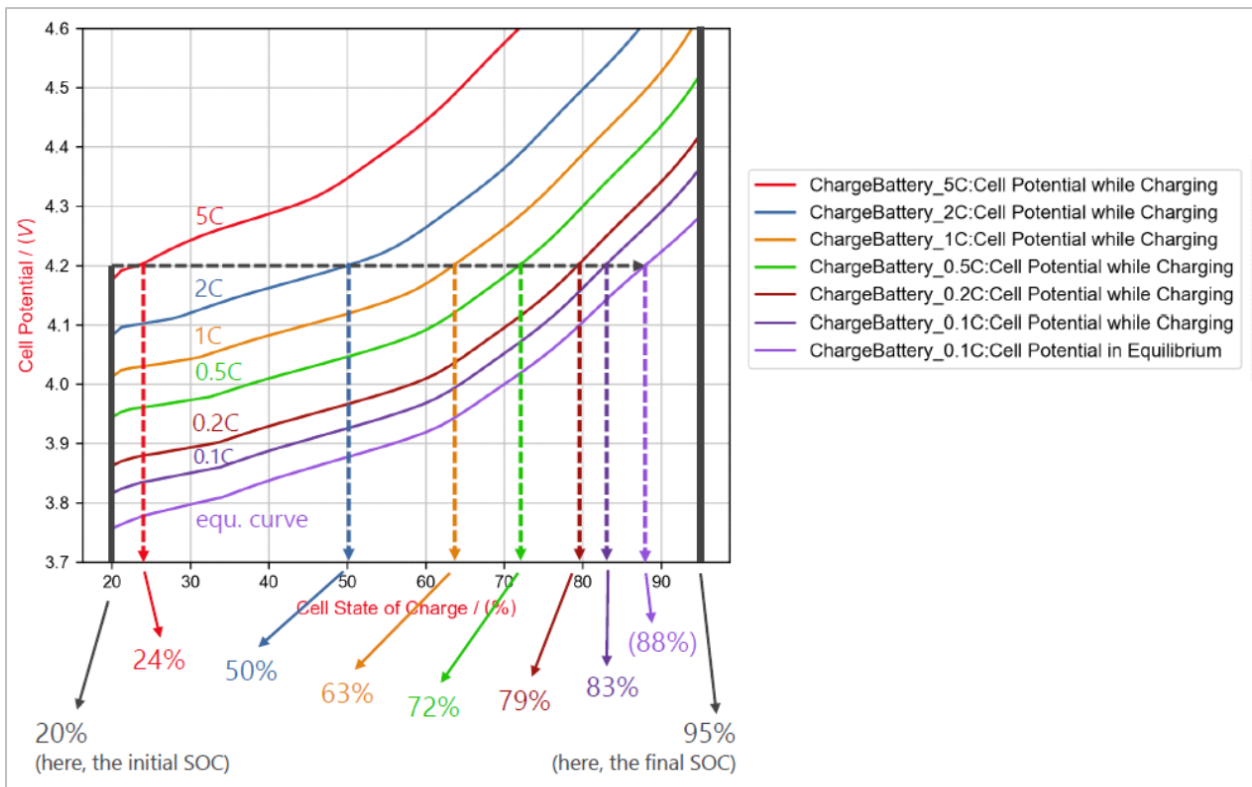
For simulations with constant charge rate, the time evolution of the cell potential depends on the charge rate selected. The higher the charge rate, the larger the deviation of the cell potential curve from the equilibrium charge curve, since the overpotentials get larger for higher charge rates (see also [Overpotentials and Heat Production](#)^[26]).

In the following figure, a charging simulation from state-of-charge 20% till 95% is shown for different charge rates using an example structure.



For the stopping criterion final state-of-charge, the computation always runs until the final state-of-charge is reached, here 95%. Depending on the charge rate, the cell potential reached for this final state-of-charge, is very different. Especially for high charge rates, it might not be possible to reach this stopping criterion at all, or the voltages reached may be unphysically high.

On the other hand, if a final potential – here 4.2 V - is defined as stopping criterion, the state-of-charge reached at the end of the simulation will vary depending on the charge rate, while the cell potential remains the same. In the following figure, the reached state-of-charge at the end of the simulation is indicated for simulations with different charge rates. As a result of the varying state-of-charge at the end of the simulation, the capacitance of the battery differs depending on the charge rates.



1.1.6 Overpotentials and Heat Production

Overpotentials of the (dis-)charging process, can be visualized for a finished simulation in the [Result Viewer](#) ¹⁰⁵.

Overpotentials are the reason why the real charging curve deviates from the equilibrium potential curve in the charging process. The equilibrium potential curve is the cell potential in equilibrium for each state-of-charge.

To charge the battery with an increased charge rate, an additional potential, i.e., additional energy, is necessary due to the inner resistivities of the battery cell. In the same way, while discharging, these resistivities are responsible for the potential difference compared to the equilibrium potential. Less energy can be taken out of the battery which produces heat instead, compared to the equilibrium situation. These differences are characterized by the overpotentials. The larger the charge rate, the higher the overpotentials get.

The overpotentials are usually computed over the whole structure while the heat production is also computed per voxel.

The overpotentials for the battery / electrode are calculated by summing up the weighted local overpotentials, which are calculated per voxel / voxel face.



Note! While in the GUI always a positive current is entered, internally the algorithm considers the current as positive or negative depending on the following four cases:

- Battery charging: negative current
- Battery discharging: positive current

- Electrode delithiation: negative current
- Electrode lithiation: positive current

In GeoDict, three sources of overpotential and heat production are considered:

✓ Kinetic

Kinetic overpotentials define the additional potential necessary for bringing the lithium ions from the electrolyte into the active materials of cathode or anode. They are computed from the Butler-Volmer expression.

Separately for anode and cathode interface the kinetic overpotentials are given by

$$\eta_{Kin} = -\frac{1}{I} \sum_{\text{all interface voxel faces}} [i_{se} A (\varphi_s - \varphi_e - U_0)] \quad (24) \text{ Kinetic overpotential}$$

where i_{se} is the local Butler-Volmer current density, φ_s the solid potentials, φ_e the electrolyte potential, U_0 the open-circuit potential, A the voxel face area (voxel length)², and I the total current.

The local kinetic heat production is given by

$$P_{Kin} = i_{se} A (\varphi_s - \varphi_e - U_0) \quad (25) \text{ Local kinetic heat production}$$

✓ Diffusive

Diffusive overpotentials result from the distribution of lithium ions in the active materials of an electrode that is not uniform during charging or discharging. E.g., during charging, lithium ions enter the anode active materials at the surface of the grains and diffuse into the grains. The slower this diffusion in the active materials, the higher the difference in the distribution of lithium and the higher the additional potential necessary for keeping a desired charge rate. If the simulation is started from an equilibrium situation, these concentration differences in the active materials increase during the simulation. The diffusive overpotentials can be time-dependent and might get higher the longer the charging process is running.

The diffusion overpotentials are given separately for anode and cathode active material by

$$\eta_{D-AM} = -\frac{1}{I} \sum_{\text{all interface voxel faces}} [i_{se} A (U_0(c_s) - \bar{U}_0(soc))] \quad (26) \text{ Diffusive overpotential}$$

in active
material

where i_{se} is the Butler-Volmer current density, $U_0(c_s)$ the open-circuit potential as function of local surface concentration c_s , $\bar{U}_0(soc)$ the open-circuit potential as function of global electrode SOC in equilibrium, A the voxel face area (voxel length)², and I the total current.

For one active material, the global electrode SOC is calculated as follows:

$$soc = \frac{\sum c_s}{\sum c_{max}} \quad (27)$$

where the values for all active material voxels are summed up. This means that the c_s and therefore also the $U_0(c_s)$ varies in the sum. $\bar{U}_0(soc)$, on the other hand, always has the same value. For electrode blends, the calculation of the equilibrium state at a given electrode SOC becomes more involved. The lithium contents of the electrode must be distributed between the materials such that all the material specific open-circuit voltages take the same value. Since U_0 and c_{max} generally differ between materials, the average calculation [\(27\)](#) is no longer applicable, and more advanced computations must be performed.

The local diffusive heat production for the active material is then given by

$$P_{D-AM} = -F \frac{\partial U_0}{\partial c_s} \frac{\vec{N}^2}{D} V \quad (28) \text{ Local diffusive heat production in active material}$$

where F is the Faraday constant (96485.33289 C/mol), N is the local ion flux density in a cell, V is the volume of a single voxel (voxel length)³, and D is the local diffusivity.

A diffusive overpotential can also build up in the electrolyte due to concentration gradients that can form during charging in the electrolyte. Please note that overpotential due to concentration gradients in the separator is accounted to the diffusive overpotential of the electrolyte.

The diffusion overpotential for the electrolyte are given by

$$\eta_{D-El} = \frac{1}{I} \sum_{\text{all electrolyte voxels}} \left[\vec{i} \frac{RT}{F c_e} (1 - t_+) \nabla c_e V \right] \quad (29) \text{ Diffusive overpotential in electrolyte}$$

where $\vec{i}$ is the local current density, R the universal gas constant, T is the temperature, F is the Faraday constant, c_e lithium concentration in electrolyte, t_+ is the transference number, V is the volume of a single voxel (voxel length)³, and I the total current.

The local diffusive heat production for the electrolyte is given by

$$P_{D-El} = \frac{R T}{D_e c_e} \left(\vec{N} - \frac{t_+}{F} \vec{i} \right)^2 V$$

(30) Local diffusive heat production in electrolyte

✓ Resistive

Resistive overpotentials define the additional potential necessary to overcome bulk electrical resistivities in the charging process. These resistivities depend on the electrical bulk conductivities of the different battery materials. For electrodes, it relates from the electronic conductivities of the binder and active materials in this electrode, as well as the corresponding current collector. For the electrolyte, it relates to the ionic conductivity of the electrolyte and separator.

The resistive overpotentials are given separately for anode, cathode, and electrolyte by

$$\eta_{\Omega} = -\frac{1}{I} \sum_{\text{all voxels}} \left[\frac{\vec{i}^2}{\kappa} V \right]$$

(31) Resistive overpotential

where i is the current density in the respective material, for anode and cathode resistive overpotential κ is the electrical conductivity in the respective material (ionic conductivity for the electrolyte's resistive overpotential and electronic conductivity for the electrodes' resistive overpotential), V is the voxel volume (voxel length)³, and I the total current.

The local resistive heat production is given by

$$P_{\Omega} = \frac{\vec{i}^2}{\kappa} V$$

(32) Local resistive heat production



Note! In the Result Viewer of the *.gdr result file, these three kinds of [overpotentials](#)^[105] are shown separately. In this way, it is possible to analyze which process in the battery causes the largest amount of additional potential during charging and is responsible for the largest potential loss during discharging.

The different overpotentials sum up to the total overpotential.



Note! A charging simulation provides produced heat results in three different ways:

The first one is the produced heat as power in the [report](#)^[95]. This is the integral over all heat production parts over all time steps.

The second one is the produced areal heat power as a power density found under the [Plots](#)^[97] tab in the Result Viewer. For the anode and cathode, the resistive heat production in the current collectors and binder is added to the resistive, kinetic, and diffusive heat production in the active materials. For the electrolyte, the resistive and the diffusive heat production in the electrolyte are added. For both, the resulting value is transformed to the areal power over time.

The third result is a 3D visualization of the [thermal power density](#)^[110]. For each voxel all three heat production components are summed up.

1.1.7 Degradation Simulations

Use [BatteryDict-Degradation](#)^[166] for the simulation of battery volumetric changes due to lithium intercalation of active materials.

After a finished charging or discharging simulation of a battery or a half cell, the mechanical expansion or contraction of the cell as well as the stresses and strains resulting from this deformation can be computed. To this purpose, ElastoDict's FeelMath solver is called internally from BatteryDict-Degradation.

The expansion, Δl , of an active material in each coordinate direction depends on the changes in lithium concentration during charging simulation,

$$\Delta l = (c_{s,end} - c_{s,start}) \cdot \alpha \cdot l \quad (33) \text{ Expansion}$$

with α the concentration expansion coefficient, $c_{s,start}$ and $c_{s,end}$ the lithium concentration at the start and end of the (charging) simulation and l the length of the material in the coordinate direction under consideration. It is computed analogously to the thermal expansion of a material due to [temperature change](#).

Note that the concentration expansion coefficient used in BatteryDict-Degradation is a coefficient for the linear expansion in each coordinate direction. In literature, one can often find the maximal volumetric expansion due to intercalation. To get the coefficient required here, use

$$\alpha = \frac{\sqrt[3]{\frac{V_0 + \Delta V_{max}}{V_0}} - 1}{c_{max}} = \frac{\sqrt[3]{1 + \frac{\Delta V_{max,\%}}{100}} - 1}{c_{max}} \quad (34) \text{ Concentration expansion coefficient}$$

where V_0 is the initial volume, ΔV_{max} is the maximum absolute volume change due to lithium intercalation, $\Delta V_{max,\%}$ is the maximum relative volume change in percent, and c_{max} is the maximum (removable) lithium concentration. Also refer to [Wenzler et al., 2023](#)^[205].

1.1.8 Simulation Parameters

The parameters occurring in the equations of charging simulations are explained in the following:

✓ Maximum Lithium Concentration

The **Maximum Lithium Concentration** c_{max} that can be stored to or taken out of the active material. This is not the maximum lithium concentration of the active material itself, but the difference between the minimum and maximum reachable lithium concentration. Usually, the minimum reachable lithium concentration of common active materials used in cathodes is not zero. The reason is that often the last lithium ions cannot be removed or could only be removed with a cell potential that is so high that it could damage the battery. c_{max} can be calculated from the maximum experimentally accessible specific capacity of a material $Q_{spec,max}$ when determining the open circuit voltage potential (see below), the material density ρ , and Faraday's constant F :

$$c_{max} = \frac{Q_{spec,max} \cdot \rho}{F}$$

(35)
Maximum
lithium
concentration

Its unit is mol/m³, i.e., the concentration is provided as amount of accessible lithium ions per volume.

✓ Electronic Conductivity

Measures a material's ability to conduct electrons. Active materials and non-porous binders / conductive additives are pure electron conductors. Porous binders / conductive additives also conduct ions in the electrolyte-filled pore space.

✓ Ionic Conductivity

Measures the electrolyte's ability to conduct ions (such as Li ions). GeoDict can consider the concentration dependence of ionic conductivity constants for [electrolyte](#)^[73].

Electrolyte and separator are pure ion conductors. Porous binders / conductive additives also conduct electrons in the solid part.

✓ Ionic Diffusion Constant

Measures a material's ability to equilibrate differences in concentration. The ionic diffusion constant in active materials is often measured via Galvanostatic Intermittent Titration Technique (GITT), where the reaction of a half cell to a current pulse and the subsequent relaxation is recorded, see [Weppner et al., 1977](#)^[205]. It can also be measured by Electrochemical Impedance Measurements (EIS), see [Ecker et al., 2015](#)^[205]. The ionic diffusion constant of an active material can depend on the [material SOC](#)^[10]. GeoDict can consider the concentration dependence of ionic diffusion constants for [electrolyte](#)^[73].

✓ Maximum Exchange Current Density

Since GeoDict 2025 this replaces the **Butler-Volmer Rate Constant** known from earlier GeoDict releases.

This new parameter has many advantages:

- It has a physical interpretation which is easier to understand,
- It can be determined by experiments much more easily,
- It has the unit of the current density, which is the same unit for all cases.

If you are used to the **Butler Volmer Rate Constant** from previous GeoDict releases, you may find it useful to find the **Butler Volmer Rate Constant** in the BatteryDict GUI directly below the **Maximum Exchange Current Density** as shown [here](#)^[71]. It is computed automatically from the entered value for **Maximum Exchange Current Density**.

The **Maximum Exchange Current Density** is not a material parameter of one material alone but depends on the active material as well as on the electrolyte. It is necessary to define the interface condition between voxels of active material and those of electrolyte. It characterizes "how easy" ions can be exchanged between active material and electrolyte.

First, the derivation of **Butler-Volmer Interface Current Density** i_{se} , as calculated in BatteryDict is shown. The Butler-Volmer equation found in literature is (see [Ecker et al., 2015](#)^[205])

$$i_{se} = \frac{I_D}{S} = j_0 \left(\exp \left[\frac{\alpha z F}{RT} \eta_D \right] - \exp \left[- \frac{(1 - \alpha) z F}{RT} \eta_D \right] \right) \quad (36) \text{ Butler-Volmer equation}$$

with the current I_D , the contact area S between electrode's active material(s) and electrolyte, the exchange current density j_0 , the charge transfer coefficient α , the charge number z (which is $z = 1$ for a lithium-ion battery), and the overpotential η_D . Considering $\alpha = 0.5$, the Butler-Volmer equation simplifies to

$$i_{se} = 2j_0 \sinh\left[\frac{F}{2RT}\eta_D\right] \quad (37)$$

For insertion electrodes, literature provides a relation of the exchange current density to the lithium concentration in the electrolyte and the lithium concentration in the solid with considering the charge transfer coefficient $\alpha = 0.5$ ([Ecker et al., 2015](#)^[205])

$$j_0 = k_0 F \sqrt{c_s c_e (c_{max} - c_s)} = k_{BV} \sqrt{c_s c_e (c_{max} - c_s)} \quad (38)$$

where the **Butler-Volmer Rate Constant** is defined as $k_{BV} = k_0 \cdot F$ with a particle transfer rate k_0 and Faraday's constant F .

When this relation is inserted into equation (37)^[33] above and the overpotential is equal to $\eta_D = (\varphi_s - \varphi_e - U_0)$, the equation describing the **Butler-Volmer Interface Current Density** i_{se} in BatteryDict is obtained,

$$i_{se} = 2k_{BV} \sqrt{c_s c_e (c_{max} - c_s)} \sinh\left[(\varphi_s - \varphi_e - U_0) \frac{F}{2RT}\right] \quad (39) \text{ Butler-Volmer interface current density}$$

The k_{BV} can be computed from the **Maximum Exchange Current Density** as follows:

$$k_{BV} = 2 \frac{i_{0,max}}{c_{max} \sqrt{c_{e,i_0}^{meas}}} \quad (40)$$

$i_{0,max}$ is the **Maximum Exchange Current Density** in equilibrium electrolyte concentration at 50% lithiation (material SOC = 50%). It replaces the k_{BV} used until GeoDict 2025.

$$i_{0,max} = \frac{1}{2} c_{max} \sqrt{c_{e,i_0}^{meas}} k_{BV} \quad (41) \text{ Maximum Exchange Current Density}$$

From version 2026, GeoDict takes care of calculating k_{BV} from your measurements. Simply provide the maximum exchange current density $i_{0,max}$ and the electrolyte

lithium concentration of exchange current density measurement c_{e,i_0}^{meas} . This works as follows:

To obtain a value of $i_{0,max}$ from the measured exchange current densities at different [material SOLs](#) ^[10] of the electrode material, the experimental data for i_{se} are fit to a modified equation [\(38\)](#) ^[33] using $c_s = c_{max} \cdot \frac{SOL}{100\%}$:

$$i_{se} = 2 \cdot i_{0,max} \sqrt{\left(1 - \frac{c_s}{c_{max}}\right) \frac{c_s}{c_{max}}} \sqrt{\frac{c_e}{c_{e,i_0}^{meas}}} \cdot 2 \sinh\left((\varphi_s - \varphi_e - U_0) \frac{F}{2RT}\right) \quad (42) \text{ User-defined exchange current density}$$

Note that it might be necessary to convert literature data for j_0 from a function of lithium composition to a function of SOL as described in [\(47\) Material SOL](#) ^[36]. The next figure shows the experimental data j_0 as a function of SOL for NMC333 and a reference electrolyte (EC/DMC/EMC 1:1:1, salt LiPF₆, concentration 1 mol/L) as reported in [Schmalstieg et al., 2018, Part 1](#) ^[205] and [Schmalstieg et al., 2018, Part 2](#) ^[205]. The **Maximum Exchange Current Density** is now easy to determine as the maximum of this half circle, which is about 1.34 A/m² at the electrolyte lithium concentration 1000 mol/m³. Both values are then to be entered in the material database.

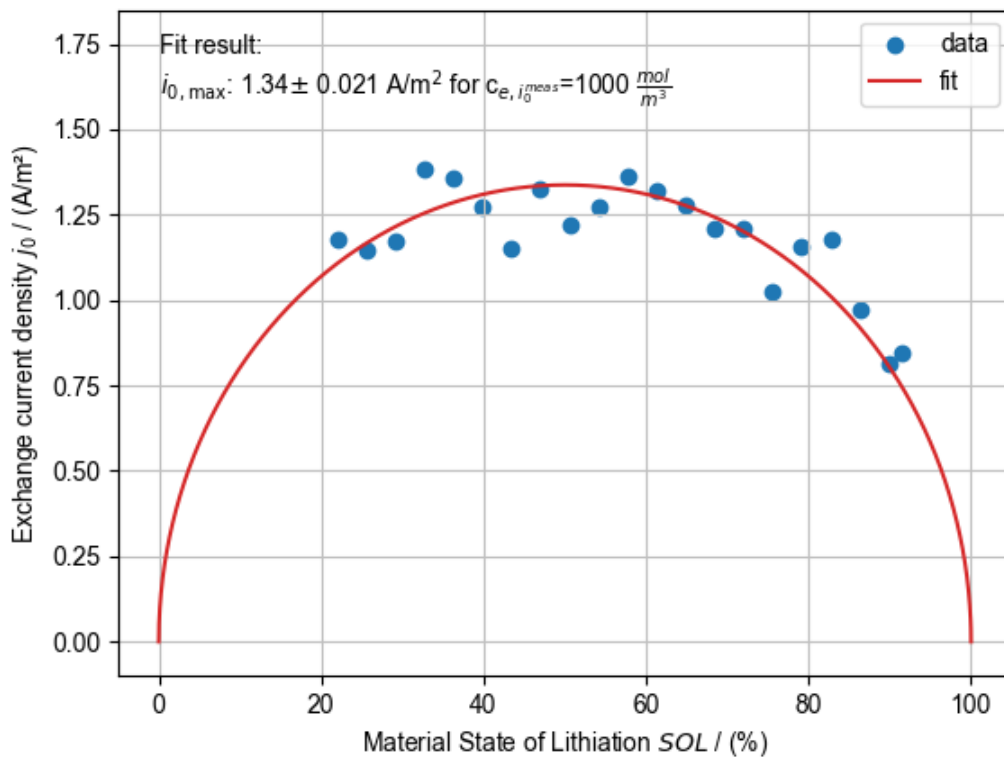


Figure 1: Measured data for j_0 of NMC333 at 15°C from the Supplementary Information of [Schmalstieg et al., 2018, Part 2](#)^[205] as a function of electrode SOC and fit to the data using the above equation. The fit results in $i_{0,max} = 1.34 \text{ A/m}^2$ for $c_{e,i_0}^{meas} = 1000 \text{ mol/m}^3$

✓ Electrolyte Lithium Concentration of Exchange Current Measurement

This parameter is needed as a reference for the [Maximum Exchange Current Density](#)^[32]. It defines the lithium concentration in equilibrium when measuring the exchange current density.

✓ Open-Circuit Potential (OCV) Function

This is also known as Open-Circuit Voltage, hence the abbreviation OCV. The open-circuit potential is directly related to the chemical potential of lithium within the active material. Experimentally, it is determined by measuring the potential difference between the respective electrode and a lithium counter electrode in equilibrium, i.e., without load applied to the electrode. To this end, either relaxation steps are introduced before measurement at a distinct SOL or a "quasi-OCV" function is measured at very low charging rates, e.g., of C/100 [Schmalstieg et al., 2018, Part 1](#)^[205]. The open circuit potential is generally path-dependent, i.e., it can vary between the charging or discharging process. This phenomenon is known as OCV hysteresis and is observed when the chemical potential of the electrode varies between lithium intercalation and lithium deintercalation ([Barai et al., 2015](#)^[205]). Additionally, it depends on the electrode state of lithiation and is therefore a function of the material state of lithiation (see also [State of Charge \(SOC\) and State of Lithiation \(SOL\)](#)^[10]).

$$SOL = \frac{c_s}{c_{max}} \cdot 100\% \quad (43)$$

In literature, the OCV function is often provided as a function of the specific capacity Q_{spec} , e.g., in mAh g⁻¹ against the potential vs Li/Li+ ([Nitta et al., 2015](#)^[205]). The maximum experimentally accessible specific capacity of a material is denoted as $Q_{spec,max}$ and the OCV curve ends at this specific capacity. Figure 4(e) from [Nitta et al., 2015](#)^[205] shows an example from literature for various cathode materials. In this case, the x-axis of the OCV function must be transformed from the specific capacity Q_{spec} to the material SOL by the equation:

$$SOL(Q_{spec}) = \frac{Q_{spec}}{Q_{spec,max}} \cdot 100\% \quad (44)$$

GeoDict interpolates the OCV curve between the points provided for the OCV function of the material. For the interpolation it is necessary that the OCV function is monotonous, i.e., the OCV must increase with decreasing material SOC.

Sometimes, data in literature are also provided as a function of lithium composition. For instance, for cathode materials the lithium composition x ranges from the maximal lithium composition ($x_{max} = 1$ for stoichiometric NMC333 ($\text{Li}_x\text{Ni}_{0.33}\text{Mn}_{0.33}\text{Co}_{0.33}\text{O}_2$)) to the minimally reachable lithium composition x_{min} . This minimally reachable lithium composition can be calculated via the maximum experimentally accessible specific capacity $Q_{spec,max}$ and the theoretical capacity $Q_{spec,theo}$, which is calculated with the equation:

$$Q_{spec,theo} = \frac{n_{Li}}{M} F \quad (45)$$

where n_{Li} is the number of lithium atoms per unit cell in the maximally lithiated material, M is the molar mass, and F Faraday's constant. For cathode materials, the minimum lithium composition is found by comparing $Q_{spec,max}$ to $Q_{spec,theo}$, for instance for NMC333:

$$x_{min} = 1 - \frac{Q_{spec,max}}{Q_{spec,theo}} \approx 0.27 \quad (46)$$

The material SOL as a function of lithium composition x is then given via linear transformation. E.g., for a cathode material such as NMC333:

$$SOL(x) = \frac{100}{1 - x_{min}} (x - x_{min}) \quad (47) \text{ Material SOL}$$

✓ Equilibrium Lithium Concentration

Concentration of lithium ions in the electrolyte solution. This is the lithium concentration of the electrolyte if it is in thermodynamic equilibrium. As soon as the battery starts charging or discharging, local concentration gradients will build up in the electrolyte.

✓ Transference Number

In the absence of concentration gradients, the transference number measures the fraction of ionic current carried by lithium ions. GeoDict can consider the concentration dependence of [transference number](#)^[73] for the electrolyte.

✓ Concentration Expansion Coefficient

The concentration expansion coefficient is needed to calculate the material expansion upon lithium intercalation using [BatteryDict-Degradation](#)^[166]. The expansion coefficient is calculated with the equation [\(34\) Concentration expansion coefficient](#)^[30].

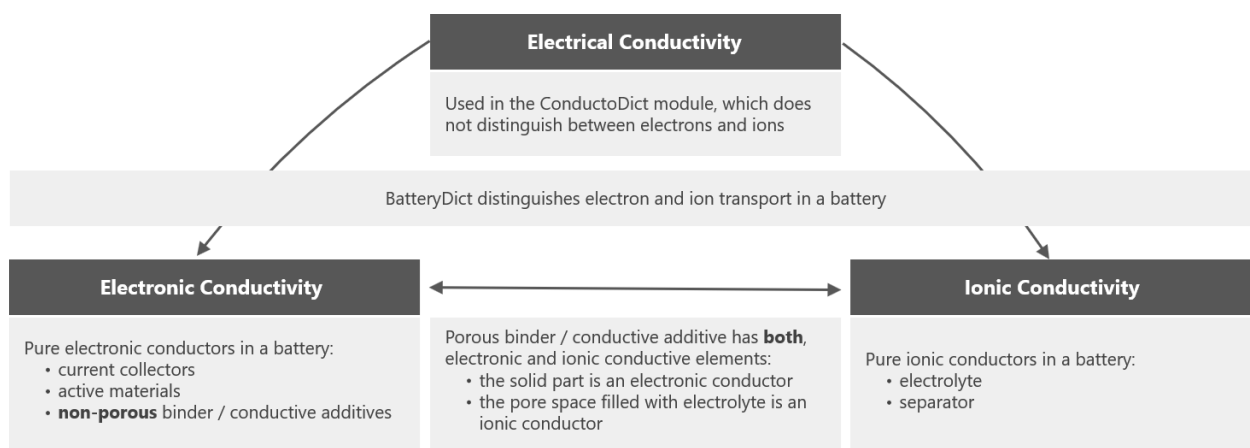
1.1.9 Add Custom Materials

GeoDict provides standard materials in the GeoDict material database for electrolyte, active materials, and binder and carbon black or other conductive additives.

The following material parameters are required to add new materials for electrochemical simulations to the GeoDict material database:

For all materials, save the changes in the material database by clicking **Save Database**. The new material can now be used like any of the standard materials delivered with GeoDict.

Note, that the material database does not differentiate between ionic and electronic conductivity. Instead you define the electrical conductivity and the material's role in the battery defines if it is an ionic or electronic conductor.



Materials for Charge Battery / Electrode

Electrolyte

✓ Mandatory Parameters

- Role in battery cell must be set to electrolyte (Electrochemistry tab)
- Equilibrium lithium concentration (Electrochemistry tab)
- Ionic diffusivity (Electrochemistry tab)
- Transference number (Electrochemistry tab)

- Electrical Conductivity (Electrical Conductivity tab, enter the ionic conductivity of your electrolyte)

The screenshot shows the 'Material Database' window. On the left, a tree view under 'Fluid' has 'Electrolyte' selected. The main panel has the 'Electrical Conductivity' tab active. The 'Role in Battery Cell' is set to 'Electrolyte'. The following parameters are entered:

Parameter	Value
Equilibrium Lithium Concentration / (mol/m ³)	1200
Ionic Diffusivity / (m ² /s)	3e-10
Transference Number t_+ / (1)	0.399

Buttons at the bottom include 'Add Material', 'Copy Material', 'Delete Material', 'Help', 'Save Database', and 'Close'.

For solid electrolytes no parameters need to be entered in the **Electrochemistry** tab, GeoDict automatically considers the transference number $t_+ = 1$ for solid electrolytes.

The screenshot shows the 'Material Database' window. On the left, a tree view under 'Solid' has 'LPSCI' selected. The main panel has the 'Solid' tab active. The 'Role in Battery Cell' is set to 'Electrolyte'. No other parameters are entered in this tab.

The corresponding [Maximum Exchange Current Density](#)³⁹ must be defined for all active materials, that will be used with the new electrolyte.

✓ Optional Parameters

Concentration dependent values for ionic conductivity, ionic diffusion constant, and transference number in electrolyte.

Concentration dependent values can be added under the **Metadata** tab, by clicking **Edit Parameters** and entering the values.

The screenshot shows the BatteryDict GUI with the 'Metadata' tab selected. The 'Edit Parameter-Map' dialog is open, displaying a table of parameters and their values. The table has three columns: Key, Unit, and Value. The parameters listed are:

Key	Unit	Value
Valoen2005ElyteIonicDiffuConcentration	mol/m ³	0, 50, 100, 150, 200, 250, 300, ...
Valoen2005ElyteIonicDiffuValues	m ² /s	5.32E-10, 5.15E-10, 4.98E-10, ...
Valoen2005ElyteIonicConduConcentration	mol/m ³	0, 50, 100, 150, 200, 250, 300, ...
Valoen2005ElyteIonicConduValues	S/m	0, 0.130066025, 0.249489343, ...
Landesfeind2019ElyteTransfeNumConcentration	mol/m ³	0, 50, 100, 150, 200, 250, 300, ...
Landesfeind2019ElyteTransfeNumValues	1	0.5121971, 0.498124258, 0.48428967, ...
Park2017ElyteIonicDiffuConcentration	mol/m ³	250, 300, 350, 400, 450, 500, ...
Park2017ElyteIonicDiffuValues	m ² /s	1.65536E-09, 1.57486E-09, 1.4..., ...
Park2017ElyteIonicConduConcentration	mol/m ³	250, 300, 350, 400, 450, 500, ...
Park2017ElyteIonicConduValues	S/m	0.201843342, 0.2825387, 0.35..., ...
Park2017ElyteTransfeNumConcentration	1	0.44, 0.45, 0.45, 0.45, 0.45, 0..., ...

The 'Edit Parameter-Map' dialog also shows a 'Number of Rows' field set to 11. The 'OK' button is highlighted.

However, this is only useful to have a reference. To use them in the BatteryDict GUI, store them in *.txt file as shown [here](#)^[73].

Click **OK** to return to the **Metadata** tab of the material database.

Copy the values from the **Metadata** tab for the charging simulations to the [Charge Battery](#)^[73] or [Charge Electrode](#)^[141] dialog.

Active material

✓ Mandatory parameters

- Role in battery cell must be set to active material (Electrochemistry tab)
- Density (Solid tab)
- Maximum Lithium Concentration (Electrochemistry tab)
- Ionic Diffusivity (Electrochemistry tab)
- Open-circuit potential (OCV) function curve (Electrochemistry tab)
- Maximum Exchange Current Density (Electrochemistry tab): This value depends not only on the active material, but also on the electrolyte. It can be therefore defined for different electrolyte materials.
- Electrolyte Lithium Concentration of Exchange Current Measurement (Electrochemistry tab): This parameter is needed as a reference value for the Maximum Exchange Current Density
- Electrical Conductivity (Electrical Conductivity tab)

GeneralSolidMechanical PropertiesElectrochemistryThermal ConductivityElectrical ConductivityMetadata

Role in Battery Cell:

Active Material

Preferred Electrode Type

Anode

Maximum Lithium Concentration / (mol/m³)

31090

Ionic Diffusivity / (m²/s)

2e-14

Electrolyte Selection

Edit Electrolyte

Default

Delete

Rename

Add Electrolyte

Add

Maximum Exchange Current Density / (A/m²)

4

Electrolyte Lithium Concentration of Exchange Current Measurement / (mol/m³)

1000

Butler-Volmer Rate Constant / (A m⁻²/mol⁻¹s)

8.13709e-06

Open-Circuit Potential (OCV) Function U₀

☒ Open-Circuit Potential Has Hysteresis

	Material State of Lithiation / (%)	Potential for Lithiation / (V)
1	0	0.43667
2	5.92	0.22889
3	7.427	0.21133
4	8.934	0.20978
5	10.441	0.20711

Number: 55

Insert Row

Delete Row

Import...

	Material State of Lithiation / (%)	Potential for Delithiation / (V)
1	0	0.43667
2	6.674	0.22778
3	8.288	0.22133
4	9.903	0.21933
5	11.625	0.218

Number: 53

Insert Row

Delete Row

Import...

Potential for Lithiation and Delithiation / (V)

Optional parameters

- Mechanical Properties for computation of mechanical deformations with [BatteryDict-Degradation](#)
- Concentration dependent diffusivity and electrical conductivity (possible via **Expert Settings** only, please contact support@math2market.de for details).

Binder / Conductive Additive

Mandatory parameters

- Role in battery cell must be set to Binder / Conductive Additive (Electrochemistry tab)
- Effective electrical conductivity

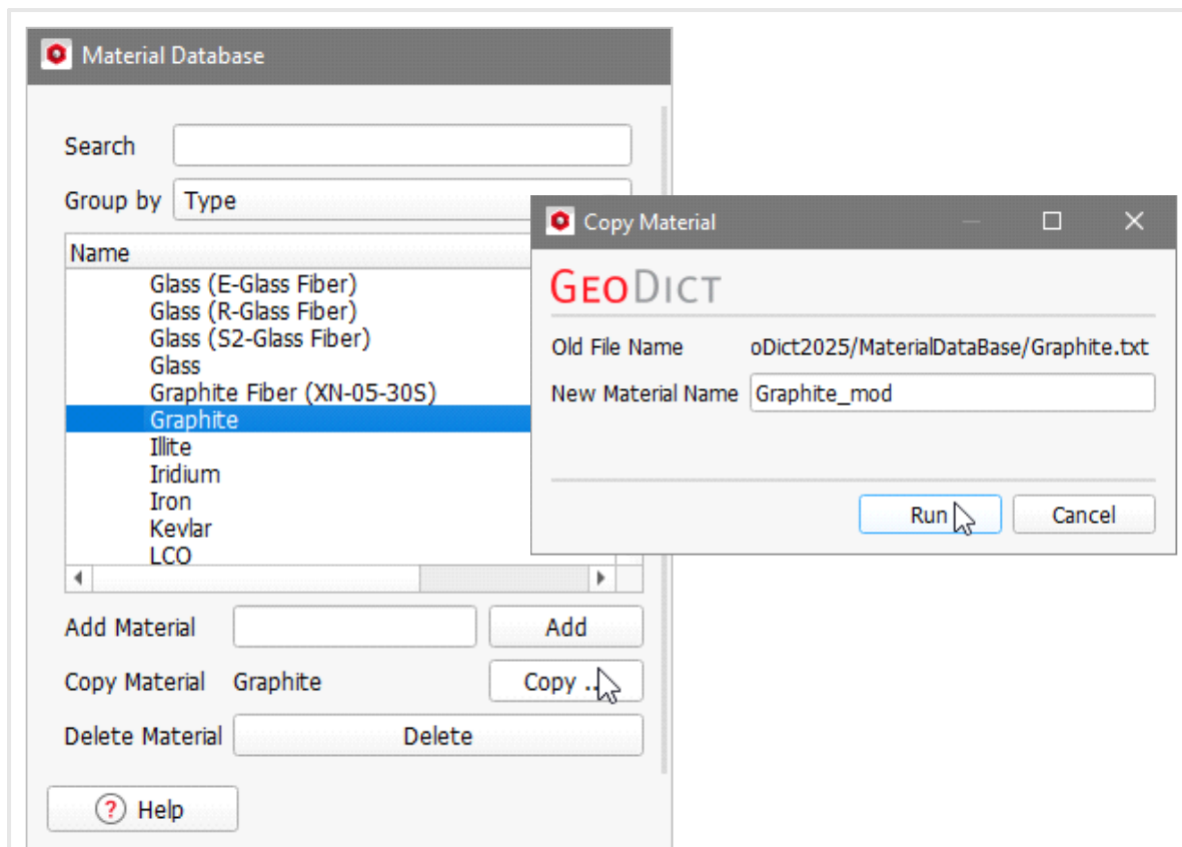
Materials for Degradation

To be able to use an active material in a degradation simulation with BatteryDict-Degradation, apart from the mandatory material parameters for a charging simulation (see [above](#)³⁷), the concentration expansion coefficient and the mechanical parameters need to be defined.

The GeoDict material database currently provides the materials Graphite, NMC333, NMC532, NMC622, NMC811, LNO, LCO, LFP, LMO, LTO, NCA, and Silicone with these parameters.

✓ Define a new material

To define the parameters for another material, select the material in the material database. For example, select Graphite as shown here. To avoid changing the material parameters delivered with GeoDict, first create a **Copy** of the material. Save it with a new name in the material database.

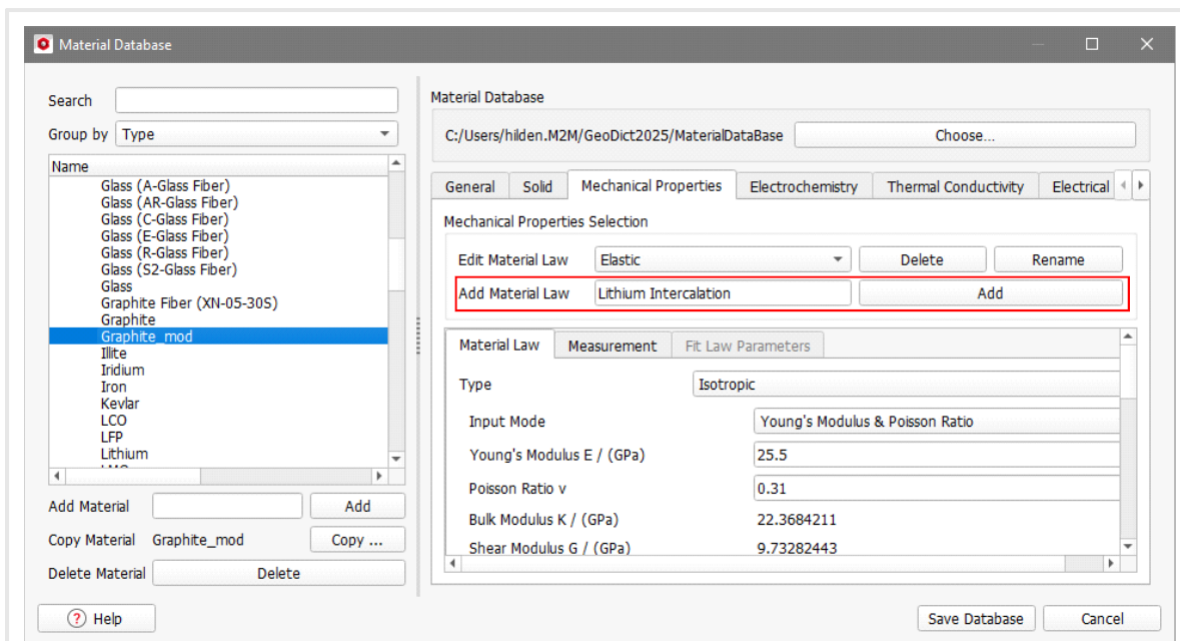


If all parameters are set as described [below](#)⁴², save the database.

For other materials of the battery cell (electrolyte, in case of solid electrolyte, binder and carbon black, current collectors and separator), mechanical parameters need to be defined as well to be able to use them in a [degradation simulation](#)¹⁶⁷.

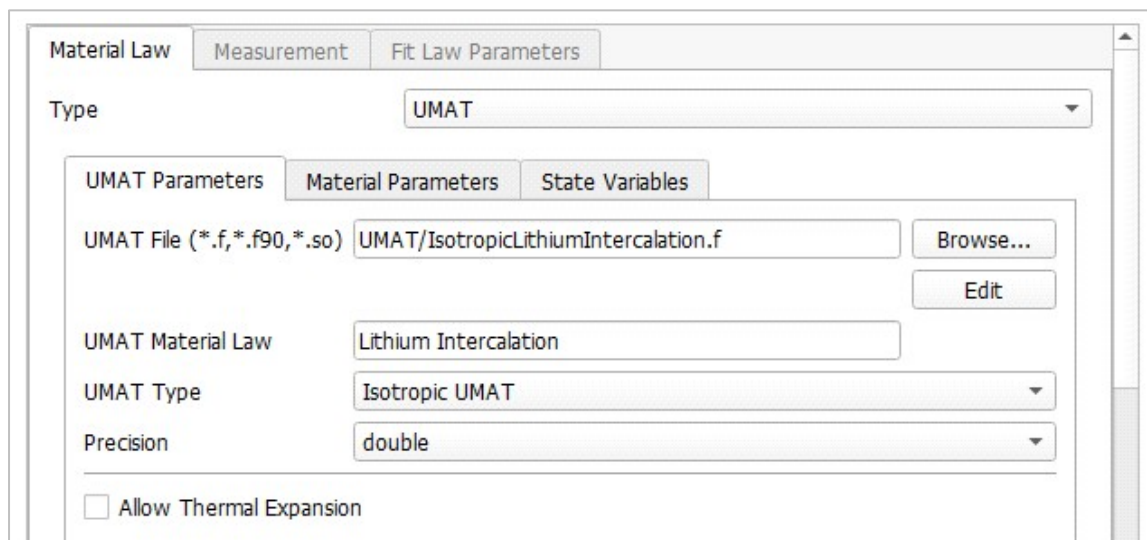
✓ Define a Material Law

On the **Mechanical Properties** tab, add the name of a new Material Law and call it, e.g., **Lithium Intercalation** and click **Add**.



On the **Material Law** tab below, choose the Type **UMAT**. Two UMAT files for concentration dependent expansion are provided in the UMAT folder of your GeoDict installation. For isotropic expansion, select the file **IsotropicLithiumIntercalation.f**, for transversal isotropic expansion the file **LithiumIntercalation.f**.

On the subtab **UMAT Parameters**, browse to the file you want to use. Set the appropriate **UMAT Type** and choose the **Precision** desired for the computation. We recommend using double precision.



On the subtab **Material Parameters**, define now **Young's Modulus**, **Poisson Ratio** and **Concentration Dependent Expansion Coefficient** for the isotropic case. The lithium concentration expansion coefficient is used for volume expansion during lithiation with BatteryDict-Degradation, measured, e.g., by electrochemical dilatometry.

Material Law: Measurement, Fit Law Parameters

Type: UMAT

UMAT Parameters, Material Parameters, State Variables

	Material Parameter	Value	Description
1	E	25.5	Young's Modulus / GPa
2	nu	0.31	Poisson Ratio
3	alpha	1.19e-06	Concentration Expansion Coefficient / (m³/mol)

For the transverse isotropic case, with the **UMAT LithiumIntercalation.f**, define the **Young's modulus** and the **Concentration Expansion Coefficient** in longitudinal and transversal direction, the transversal plane and parallel plane **Poisson Ratio** and the **Shear modulus**.

Material Law: Measurement, Fit Law Parameters

Type: UMAT

UMAT Parameters, Material Parameters, State Variables

UMAT File (*.f, *.f90, *.so): UMAT/LithiumIntercalation.f

UMAT Material Law: Lithium Intercalation

UMAT Type: Isotropic UMAT

Precision: double

☐ Allow Thermal Expansion

Material Law: Measurement, Fit Law Parameters

Type: UMAT

UMAT Parameters, Material Parameters, State Variables

	Material Parameter	Value	Description
1	E1	32	Longitudinal Young's Modulus / GPa
2	E2	32	Transversal Young's Modulus / GPa
3	nu12	0.32	Transversal Plane Poisson Ratio
4	nu23	0.32	Parallel Plane Poisson Ratio
5	G12	12.12	Shear modulus in parallel direction
6	alpha1	1.4e-06	Longitudinal Concentration Expansion Coefficient
7	alpha2	1.4e-06	Transversal Concentration Expansion Coefficient

Number of Rows: 7

Load... Save...

1.1.10 Overlapping OCV Curves

If several active materials are used in an electrode, an additional check controls that the value ranges of the open-circuit potential (OCV) curves of all materials overlap. Otherwise, there is no well-defined equilibrium state of the battery cell, which is the starting point for the simulation.

OCVs are the driving force in a battery that make lithium ions flow from materials with low OCV to materials with high OCV. If a battery is used in an electrical device and the two electrodes are conductively connected, ions flow from the negative electrode (low OCV) to the positive electrode (high OCV). The charging process requires an additional external driving force (the charging device) to cause ions to flow in the opposite direction.

If one of the electrodes is composed of several active materials, the OCV-curves of the active materials differ (at least a bit). Since the active materials in an electrode are conductively connected, there will be a driving force that will move ions from particles with low OCV to particles with high OCV. This process continues until all active materials within the electrode have the same OCV value and the electrode is in equilibrium.

In BatteryDict, the Cell-SOC or the electrode-SOC determine the initial amount of charge (i.e., lithium ions) stored in the electrode. Before starting the simulation, the solver will try to distribute this initial amount of charge between the different active materials of an electrode. This is done in such a way that the electrode is in equilibrium, i.e., that the OCVs are equal. This can only be achieved if the OCV curves of the active materials share common values.

1.1.11 Solver Convergence

The solver in BatteryDict strives to perform a physically accurate simulation for any given set of material parameters (like conductivities), material structure parameters (morphological), and simulation parameters (like the applied current). This is done by calculating the time evolution of the battery simulation step-by-step.

First, the solver works to establish the initial state or equilibrium state for every simulation in BatteryDict. Then, the solver undertakes performing time steps. In every time step, the solver first attempts a time step with the “maximum time step” given by the user. If this time step does not result in a physically meaningful state of the battery cell, the solver reduces the time step and tries again. This time-step reduction is repeated until the solver finds a physically meaningful state. If it cannot find one, the solver produces a warning message indicating that “Time step has not converged”.

In some cases, the cell-potential might rise well above any reasonable end-of-charging voltage, like for example if a large charge rate is applied. The solver might reach 10 V or even 100 V, but at some point, it will stop. In these kinds of situations, the cell-potential diverges, but the solver produces a meaningful and helpful result.

However, there are other situations in which the cell-potential does not diverge, but the solver stops regardless of that and as mentioned above, the solver has not converged.

In BatteryDict, the possible reasons why the solver does not converge are revealed in warnings, shown before the solver starts and written into the [report](#)⁹⁴. The warnings help figuring out why the solver stopped and include:

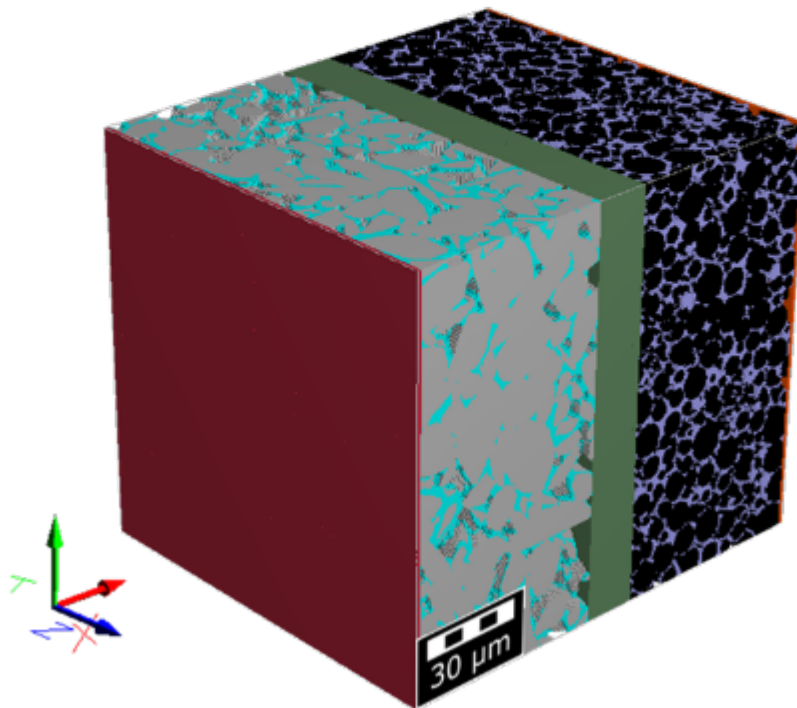
1. **Having very large particles with very low ionic diffusion at a very fast charge rate:** If grains of the active material are large or the diffusion is slow, the lithium takes a long time to get from the active surface to the core of the active material grain or from the core of the grain to the surface. In this case it can happen that the lithium concentration at the surface of the active material gets larger than the maximum lithium concentration defined for the material or even smaller than zero. This can also happen, if the active surface is small, the charge rate is high, or if there are at least two active materials and one of them is nearly filled or nearly empty.
2. **Having chosen untested material parameters:** different tests have been carried out during the development of BatteryDict to identify material parameters that should lead to converging simulations.
3. **Sometimes an error message “error -9” appears.** This happens, if the operating system ended the process, for example if not enough RAM is available. To prevent this, use [Estimate Memory](#)⁶⁴ before running a simulation.

1.2 Battery

In this section a complete battery cell is considered consisting of current collectors, separator, anode and cathode.

Design and analyze the battery geometry and simulate charging or discharging, either [fully-resolved](#)^[12] or [homogenized](#)^[18].

Material Information:	
	ID 00: Electrolyte [Electrolyte] [invis.]
	ID 01: Anode Current Collector (Solid)
	ID 02: Graphite [Anode Active Material 1]
	ID 06: PVDF Binder + Carbon Black [Anode Binder 1]
	ID 10: Separator (Fluid)
	ID 11: NMC333 [Cathode Active Material 1]
	ID 15: PVDF Binder + Carbon Black [Cathode Binder 1]
	ID 19: Cathode Current Collector (Solid)



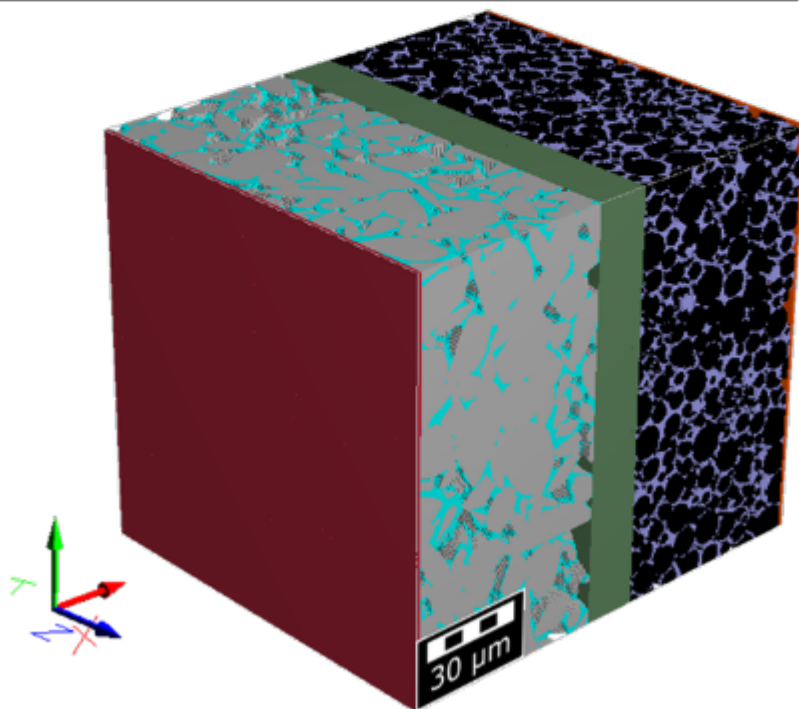
Commands available for battery structures:

- [Design Battery](#)^[47]
Use the Design Battery command to design a battery cell from two electrodes.
- [Analyze Battery](#)^[56]
Analyze the connection and volume of different materials for the designed battery structure.
- [Charge Battery](#)^[62]
Start a charging or discharging simulation.
- [Charge Homogenized Battery](#)^[117]
Run homogenized charging simulations directly without providing a battery geometry.

1.2.1 Design Battery

Use the **Design Battery** command to design a cuboid battery cell from two electrodes. **Design Battery** will add a separator and current collectors.

Material Information:	
	ID 00: Electrolyte [Electrolyte] [invis.]
	ID 01: Anode Current Collector (Solid)
	ID 02: Graphite [Anode Active Material 1]
	ID 06: PVDF Binder + Carbon Black [Anode Binder 1]
	ID 10: Separator (Fluid)
	ID 11: NMC333 [Cathode Active Material 1]
	ID 15: PVDF Binder + Carbon Black [Cathode Binder 1]
	ID 19: Cathode Current Collector (Solid)



Designing Batteries:

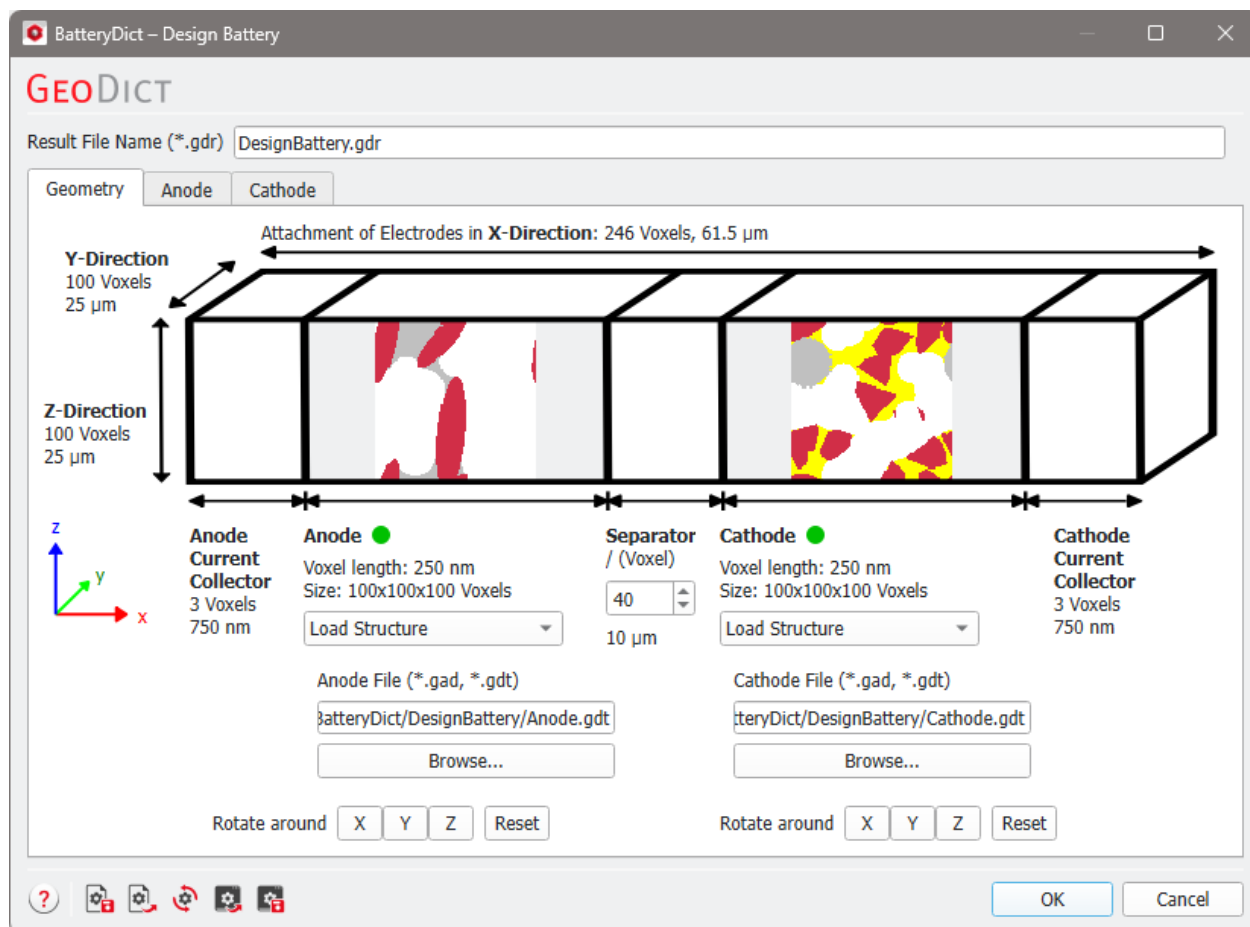
- [Options](#)⁴⁸
Define the parameters for your battery generation.
- [Results](#)⁵¹
View the results of Design Battery.
- [More Flexible Geometries](#)⁵⁵
Instead of generating a cuboid battery geometry with Design Battery, also arbitrary battery geometries can be used for charging simulations. Learn about the requirements for such structures.
- [All Solid State Batteries](#)⁵⁵
Create batteries with solid electrolytes.

Options

To design a battery using BatteryDict, choose **Battery** and **Design Battery** from the pull-down menus and click **Edit** to choose the options.

The **Design Battery** dialog opens, containing three tabs where to define the morphology of the battery ([Geometry](#)^[49] tab) and the constituent materials for [Anode](#)^[51] and [Cathode](#)^[51].

After all parameters are set, click **OK** in the **Design Battery** dialog, to keep the parameters selected in memory, or **Cancel** to discard the parameters.



Click **Design** in the BatteryDict section of the GUI to create the battery.

If the battery is created successfully, a result file with the name chosen for **Result File Name (*.gdr)** is created in the selected project folder, as well as a structure file (*.gdt) in the subfolder with the same name.

Tabs of Design Battery:

- [Geometry](#)^[49]
Define the electrodes and the separator thickness for the battery geometry.
- [Anode and Cathode](#)^[51]
Define anode and cathode materials.

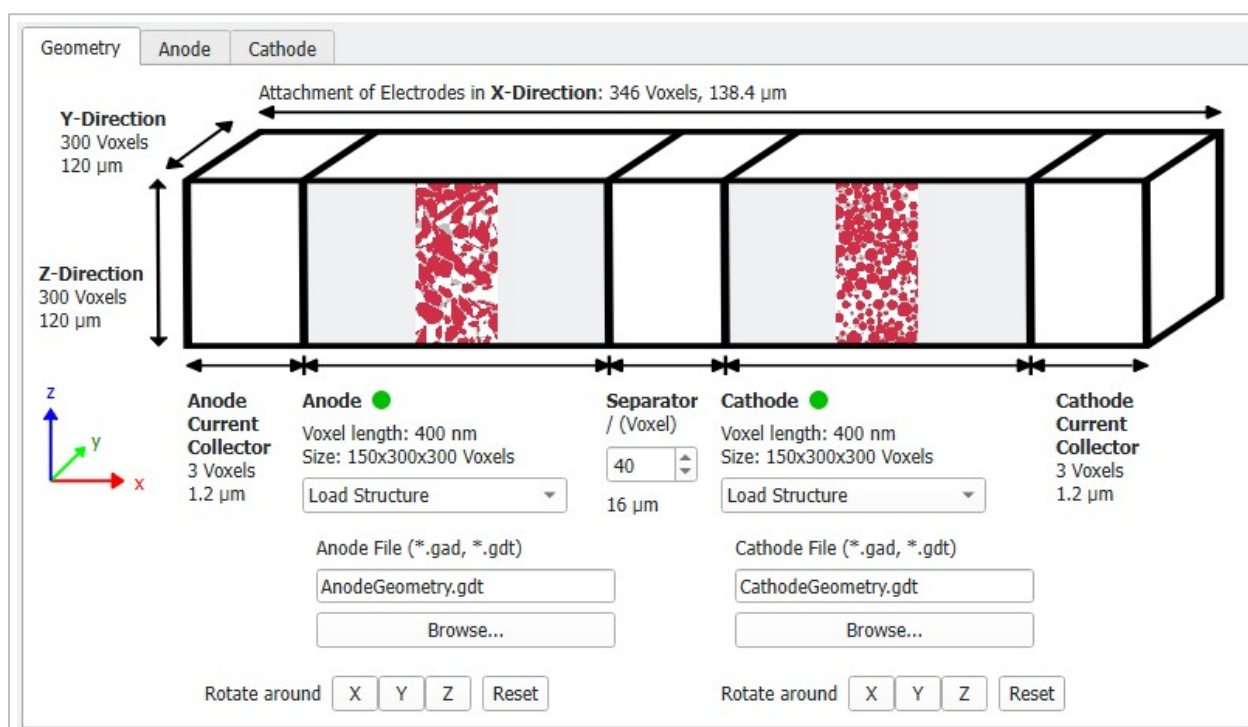
Geometry

Define the geometry for the battery.

For both electrodes, either the current structure loaded in the GeoDict visualization area can be used, a previously saved structure can be loaded, or the electrode can be modeled as a lithium reservoir.



Know how! In the topic [Charge Electrode](#)¹³⁵, we show how to simulate the charging of a half cell starting from the microstructure of a single electrode with the **Electrode – Charge Electrode** command. Note, that it is not necessary to create the geometry of the whole half cell first.



For the example battery shown here, anode and cathode structure are created with the Bimodal Electrode GeoApp.

Choose **Load Structure** and use the **Browse** buttons to select an input file for anode and cathode, in *.gad or *.gdt GeoDict structure file formats. If the built-in default settings are used for the dialog, a default structure for anode and cathode from the GeoDict installation folder (BatteryDict/DesignBattery sub folder) is loaded.



After selecting electrode files, a 2D representation of the anode and of the cathode appears in the dialog.

A red dot is visible for the anode and cathode, if no files are loaded at all.

Anode ● The chosen file is invalid.	Separator / (Voxel) 40	Cathode ● Voxel length: 400 nm Size: 150x300x300 Voxels
---	--	--

A yellow dot appears if a file is loaded but the dimensions or voxel length of the anode and the cathode do not match.

Anode ● Voxel length: 250 nm Size: 100x100x100 Voxels	Separator / (Voxel) 40	Cathode ● Voxel length: 400 nm Size: 150x300x300 Voxels
--	--	--

A green dot appears if the anode and cathode files are loaded successfully, the dimensions of the two match each other, and the voxel length is the same for both microstructures.

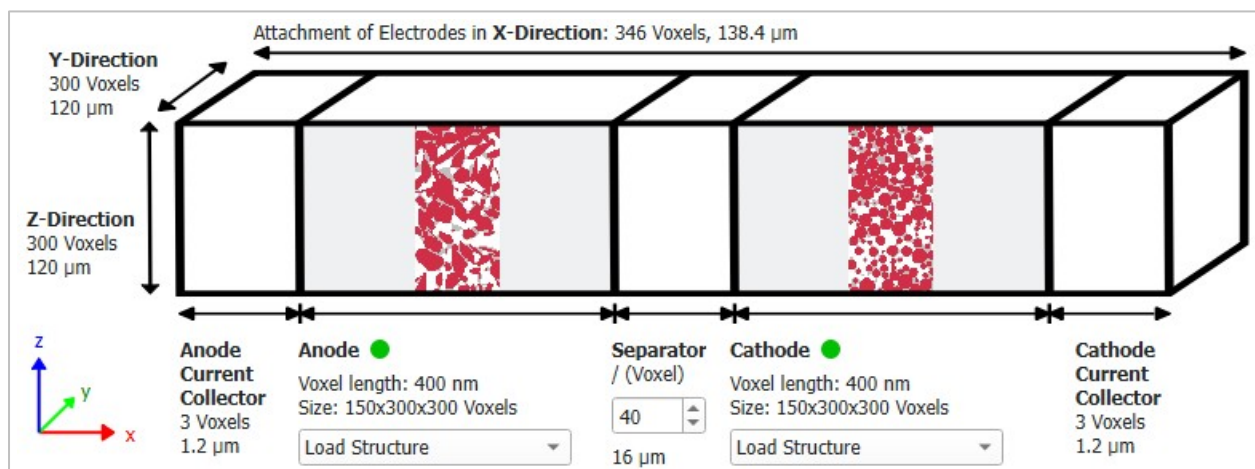
Anode ● Voxel length: 400 nm Size: 150x300x300 Voxels	Separator / (Voxel) 40	Cathode ● Voxel length: 400 nm Size: 150x300x300 Voxels
--	--	--

The **Rotate around X, Y and Z** buttons are used to rotate the structure 90° around the X, Y, or Z-axis. Click **Reset** to go back to the original orientation of anode and cathode in the battery structure.

Rotate around	X	Y	Z	Reset	Rotate around	X	Y	Z	Reset
---------------	----------------------------------	----------------------------------	----------------------------------	--------------------------------------	---------------	----------------------------------	----------------------------------	----------------------------------	--------------------------------------

The **Size** of anode and cathode are shown as the number of voxels in each direction below the diagram of the battery, and the **Voxel Length** is also displayed. After choosing anode and cathode, the total number of voxels and total length of the complete battery structure are displayed for each direction above and to the left of the diagram.

The number of voxels of the **Separator** can be defined in the dialog. The default is 40 voxels ($\approx 10 \mu\text{m}$ for 250 nm voxel length). The length of anode and cathode current collector is fixed to be three voxels and cannot be changed.



Anode and Cathode

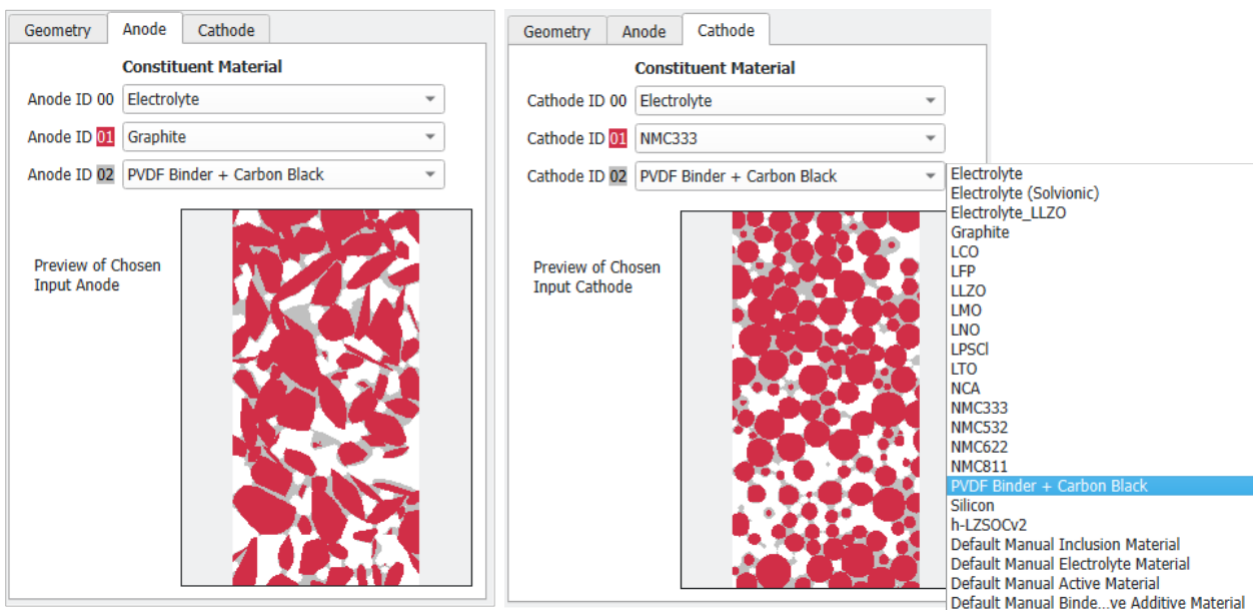
The next step is to assign electrolyte and active materials, as well as binder and carbon black to the materials available in the structures of anode and cathode.

Under the **Anode** and **Cathode** tabs all material IDs of the anode and cathode structure are assigned to a material

- electrolyte,
- up to four different binder materials or other conductive additive phases per electrode,
- up to four different active materials per electrode,
- or inclusion.

In the example shown here, both the anode and cathode consist of only one active material.

Built-in default materials from the GeoDict material database can be selected from the pull-down menu. Materials and corresponding parameters can be changed when performing a charging simulation later on.

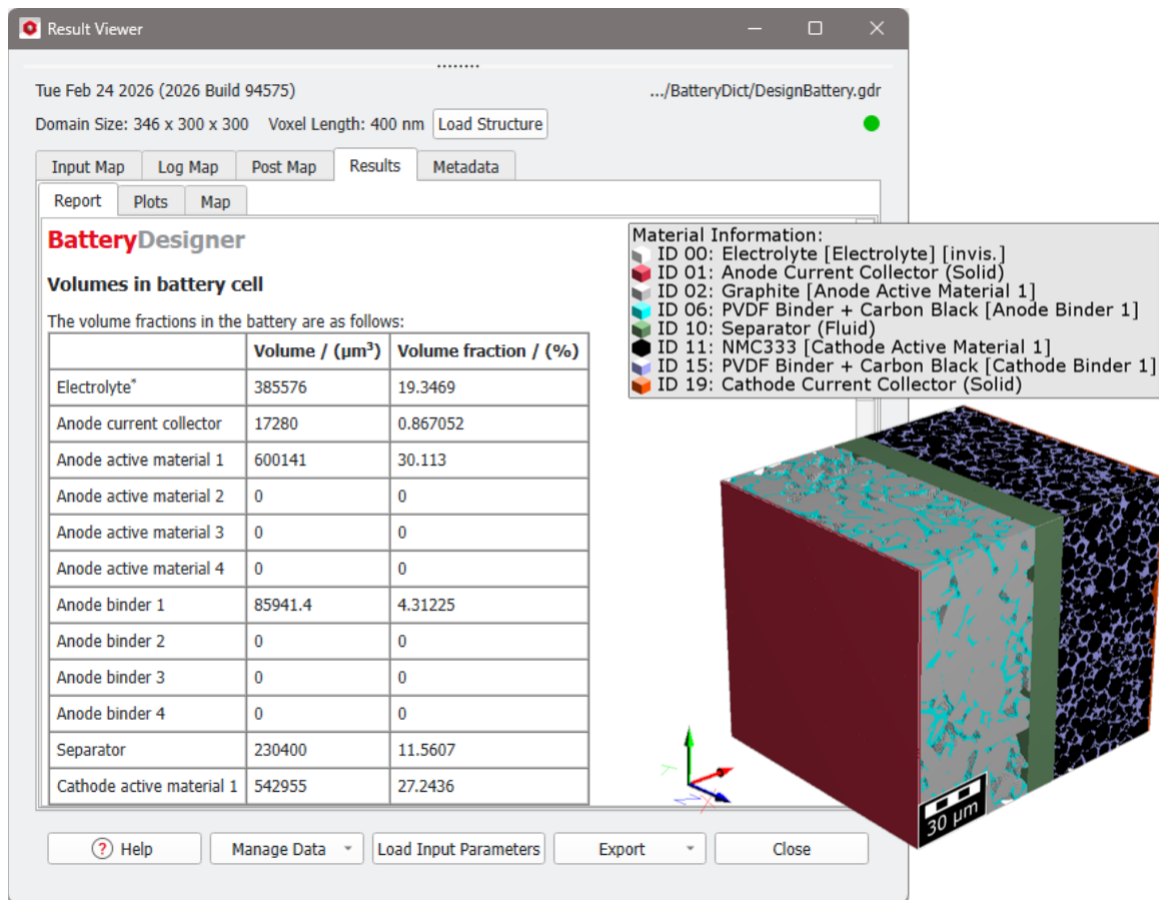


If one of the materials should have no active role in the battery charging process, assign it to the **Default Manual Inclusion Material**. In that case, no conduction is possible in this material. It has no potential and does not contain lithium.

It is possible to define up to four conductive additives in one electrode. Choose **Default Manual Binder & Carbon Black Material** and later, in the [Charge Battery](#) ⁶⁸ dialog, assign them the role “**Binder / Conductive Additive**” and set them to **Manual**.

Results

After running **Design Battery** successfully, a GeoDict result file (.gdr) is written and the **Result Viewer** for this result file opens automatically. The created battery structure is available in memory and shown in the visualization area of the GeoDict GUI.

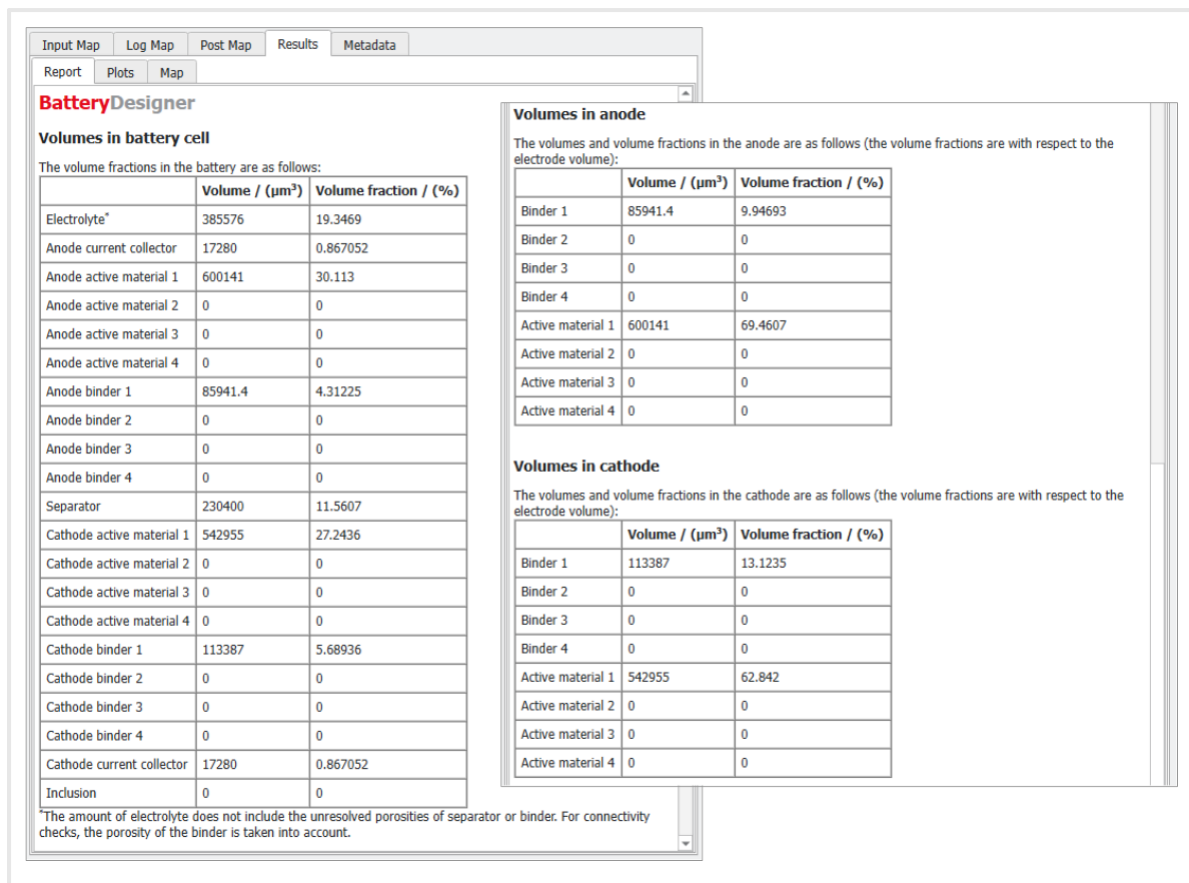


The .gdr file can be reopened at any time by choosing **File - Open Results (*.gdr)** in the menu bar. The **Result Viewer** opens at the Results tab.

More details about the general options can be found in the Result Viewer chapter.

✓ Report

The **Results - Report** subtab lists the information on the volume fractions of the different materials for the whole battery, as well as for anode and cathode separately.



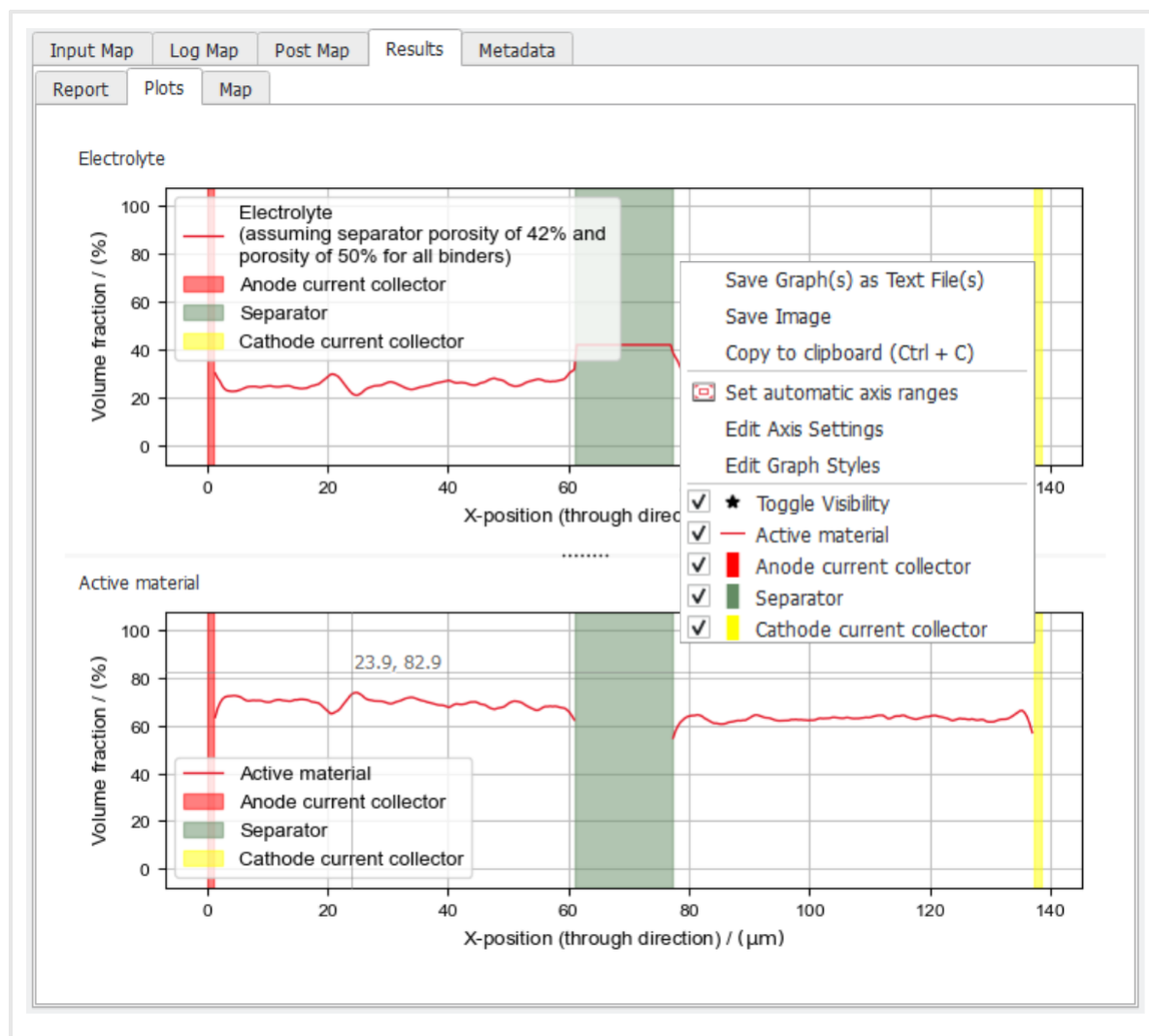
✓ Plots

Under the **Results - Plots** subtab, the volume fraction distributions over the whole battery as averaged values over each slice in y- and z-direction are shown for the electrolyte and the active material.

In the electrolyte-volume-fraction plot the binder is represented as a solid material while the separator is represented as porous, leading to the constant area in the separator area of the plot. Later, in the analysis of the battery or a charging simulation, binder can be considered as porous material.

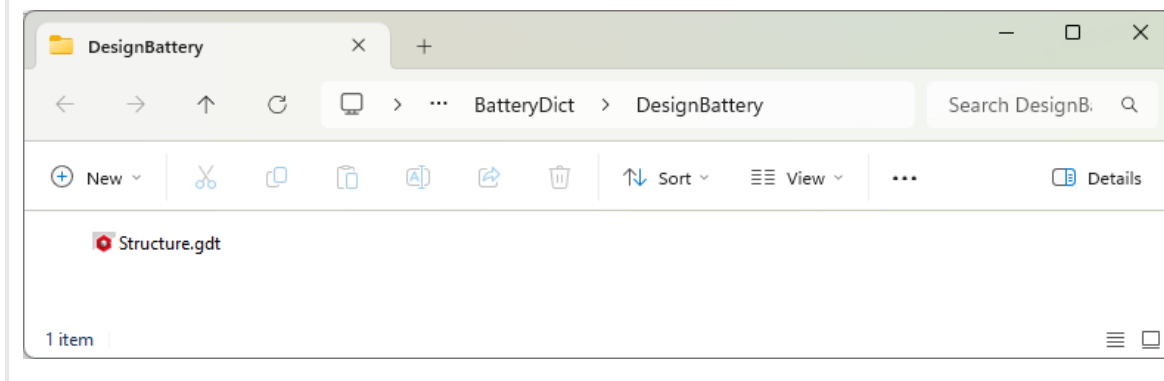
No values are shown for the active material volume fraction at the separator and both current collectors, since these areas do not contain active material.

By right-clicking with the mouse in one of the plots, axis and graph settings can be changed, the components can be set to visible or invisible, and the graph can be saved as image, *.txt file, or be copied to the clipboard.



✓ Result Folder

After the generation of a battery structure, a GeoDict result file (.gdr) is created in the selected project folder. A subfolder with the same name as the result file contains the generated battery structure.



More Flexible Geometries

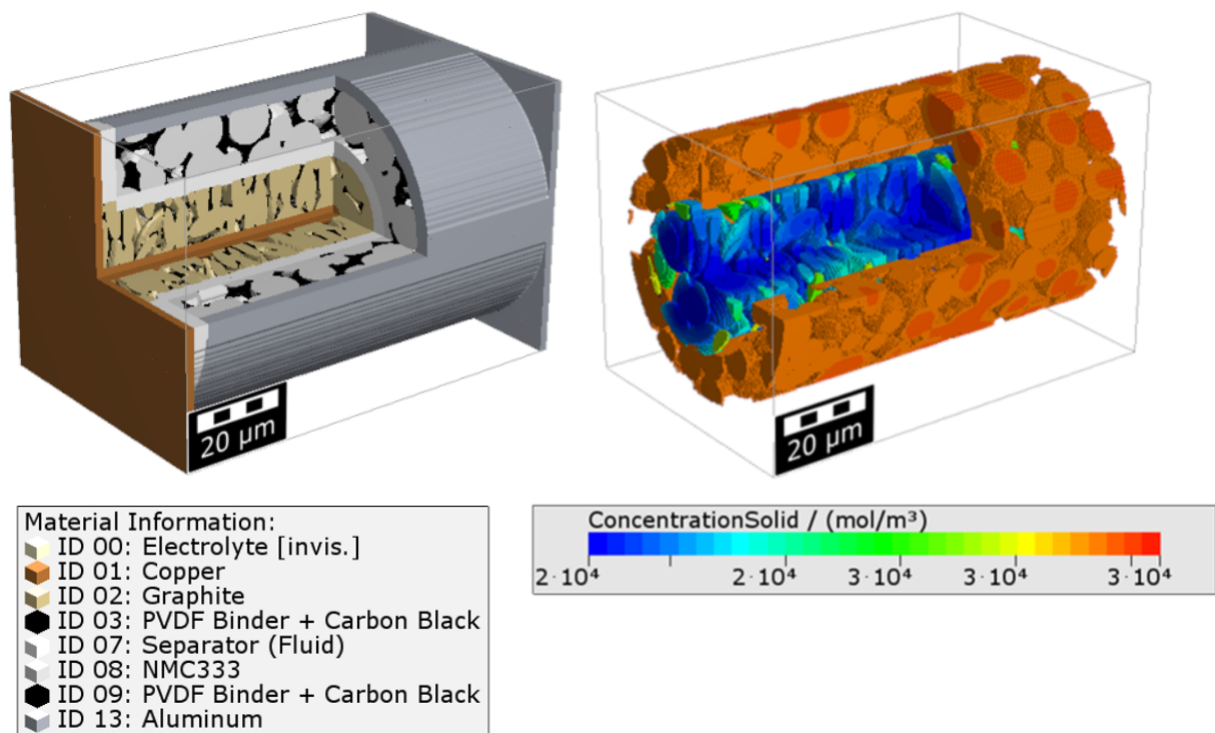
While **Design Battery** only generates cuboid battery geometries^[49], it is possible to use arbitrary battery geometries for charging simulations. They can be generated with the GeoDict structure generators or can stem from 3D scans.

Regarding the current collectors of non-cuboid geometries, it is necessary that they cover the whole surface of the structure in x-direction.

That means that the anode current collector needs to cover the whole structure in negative x-direction. The cathode current collector needs to cover the whole structure in positive x-direction.

For geometries with circular cross sections, current collectors can be positioned as shown in the figure below. The volume field visualization on the right shows the ion concentration in the solids for this geometry.

Additionally, the geometry needs to be chosen in such a way that no short-circuit of both current collectors exists. This means that the cathode and anode current collectors must not touch each other and must also not be connected directly via active material.



All Solid State Batteries

It is also possible to simulate the charging of all solid state batteries. The geometry is designed in the same way as for batteries with fluid electrolyte, using **Design Battery**^[47], however we recommend some adjustments afterwards.

The GeoDict material database provides one solid electrolyte material: LPSCI. But you can add your own electrolytes to the database as described [here](#)^[37].

For the active material in the battery, the [Maximum Exchange Current Density](#)^[39] with the electrolyte should be defined. For LPSCI, the material NMC811 already provides a **Maximum Exchange Current Density**.

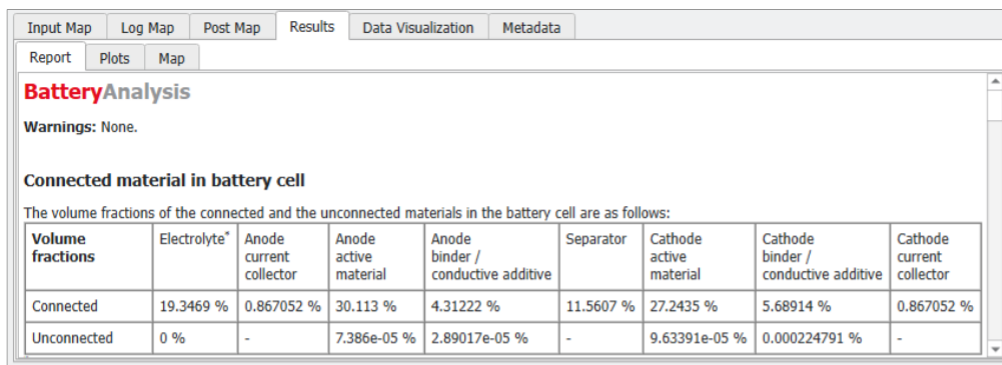
When you use LPSCI with a lithium reservoir, we recommend to change the **Maximum Exchange Current Density** $i_{0,max}$ to 320 A/m², which is cited by [Singh et al., 2023](#)^[205] for the exchange current density between lithium and the solid electrolyte LPSCI. Find more information on charging simulations with solid electrolytes refer to the topic [All Solid State Batteries](#)^[116].

To avoid issues in the charging simulation, make sure to reassign the material ID of the separator so that it matches the material ID of the solid electrolyte. This is also illustrated in the [All Solid State Batteries](#)^[116] topic. The BatteryDict GUI automatically detects this when you set the electrolyte to solid.

1.2.2 Analyze Battery

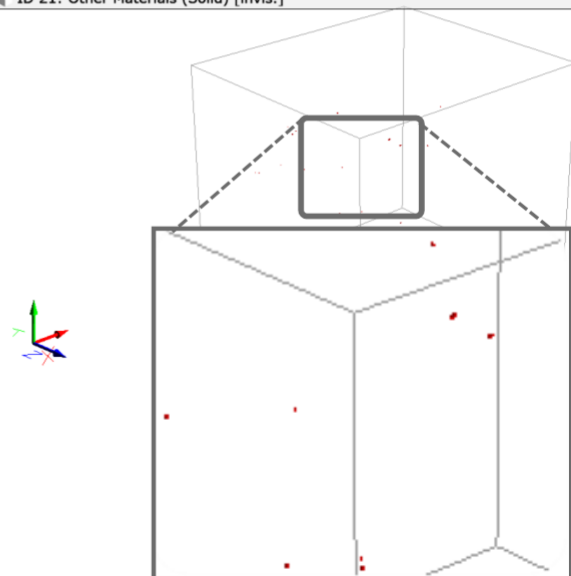
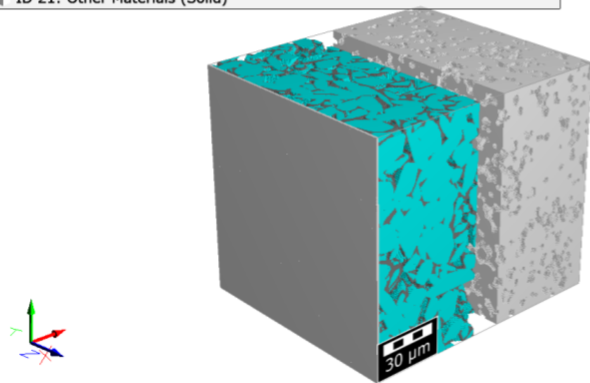
Analyze a battery structure to:

- Identify connected and unconnected materials
- Display volume fractions in anode and cathode
- Verify correct cathode / anode balancing
- Reduce unconnected material for improved energy density.



Material Information:
 ID 00: Electrolyte And Separator (Fluid) [invis.]
 ID 01: Graphite [Anode Active Material 1 With Ionic Connection]
 ID 02: Graphite [Anode Active Material 1 Without Ionic Connection]
 ID 09: PVDF Binder + Carbon Black [Anode Binder 1 With Ionic Connection]
 ID 21: Other Materials (Solid)

Material Information:
 ID 00: Electrolyte And Separator (Fluid) [invis.]
 ID 01: Graphite [Anode Active Material 1 With Ionic Connection] [invis.]
 ID 02: Graphite [Anode Active Material 1 Without Ionic Connection]
 ID 09: PVDF Binder + Carbon Black [Anode Binder 1 With Ionic Connection] [invis.]
 ID 21: Other Materials (Solid) [invis.]

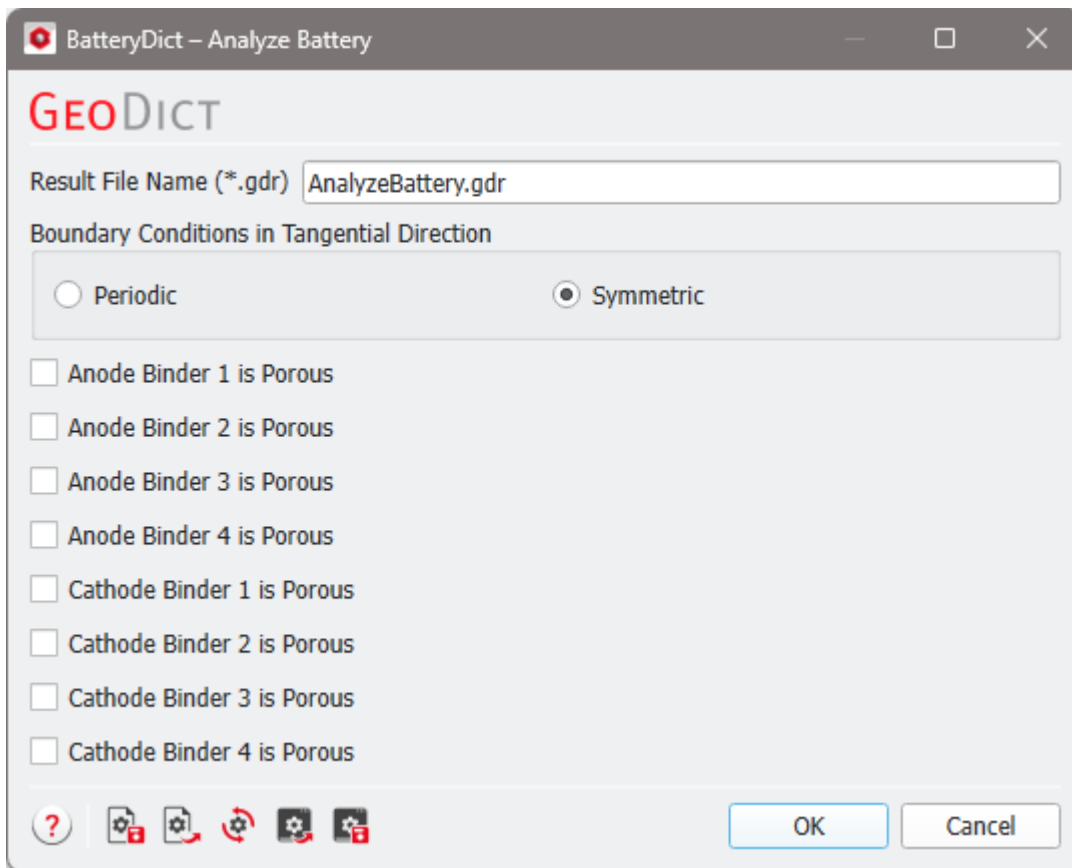


The Analyze Battery command:

- [Options](#)⁵⁷
Define the parameters to analyze your battery structure.
- [Results](#)⁵⁸
View the Analyze Battery results.

Options

Click **Edit** to open the options dialog.



First, define the **Result File Name (*.gdr)** and the **Tangential Boundary Conditions**.

Periodic or **Symmetric** boundary conditions can be selected. For periodic boundary conditions, the structure is assumed to repeat periodically in y- and z-direction and for symmetric boundary conditions, the structure is mirrored in y- and z-direction.

Boundary conditions are applied while identifying connected and unconnected material, since this depends on the continuation of the material in y- and z-direction. For a charging simulation, it can be chosen independent of the value selected here. Connected and unconnected material is identified again during charging simulation dependent on the boundary conditions selected then.

Make sure the **Anode Binder# is Porous** and/or **Cathode Binder# is Porous** checkboxes are selected if the binder (or other conductive additive) is a porous material whose micropores (not resolved on the voxel scale) contain electrolyte.

Click **Analyze** in the BatteryDict section to start the analysis. When it is finished, the **Result Viewer** opens. The results are explained in the [Results](#) topic.

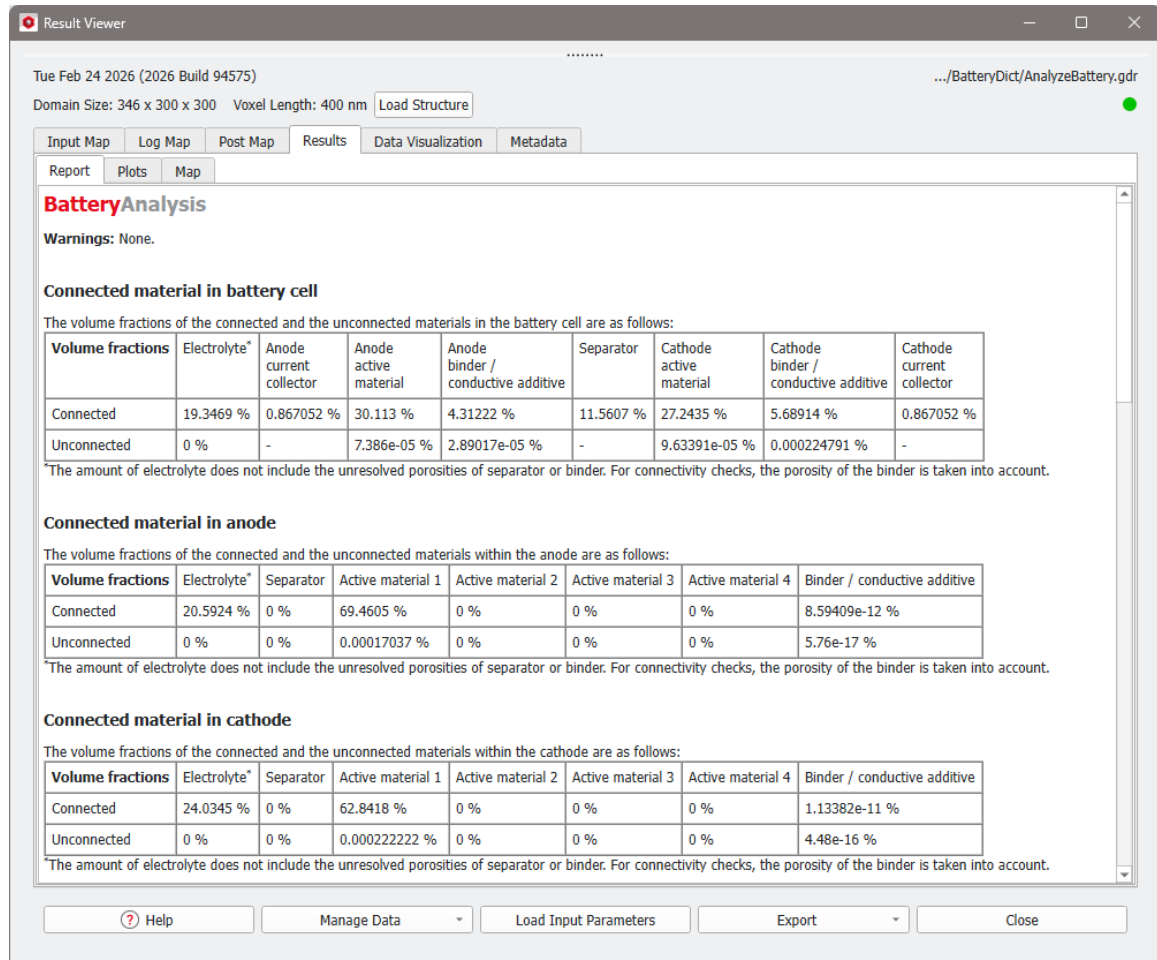
Results

After successful completion of a battery analysis, the GeoDict Result Viewer opens for the results.

✓ Report

The **Results – Report** subtab shows the information on electronic connectivity. The volume fractions of the connected and unconnected parts for the different battery components are listed. First, these volume fractions are shown for the whole battery cell, then for anode and cathode separately. The volume fractions are given in respect to the complete volume of the battery structure.

Because unconnected parts do not contribute to the battery's performance, the goal is to keep their fraction as small as possible.



The screenshot shows the 'Result Viewer' window with the 'Results' subtab selected. The 'BatteryAnalysis' report is displayed, showing volume fractions for connected and unconnected materials in the battery cell, anode, and cathode.

BatteryAnalysis
Warnings: None.

Connected material in battery cell
The volume fractions of the connected and the unconnected materials in the battery cell are as follows:

Volume fractions	Electrolyte*	Anode current collector	Anode active material	Anode binder / conductive additive	Separator	Cathode active material	Cathode binder / conductive additive	Cathode current collector
Connected	19.3469 %	0.867052 %	30.113 %	4.31222 %	11.5607 %	27.2435 %	5.68914 %	0.867052 %
Unconnected	0 %	-	7.386e-05 %	2.89017e-05 %	-	9.63391e-05 %	0.000224791 %	-

*The amount of electrolyte does not include the unresolved porosities of separator or binder. For connectivity checks, the porosity of the binder is taken into account.

Connected material in anode
The volume fractions of the connected and the unconnected materials within the anode are as follows:

Volume fractions	Electrolyte*	Separator	Active material 1	Active material 2	Active material 3	Active material 4	Binder / conductive additive
Connected	20.5924 %	0 %	69.4605 %	0 %	0 %	0 %	8.59409e-12 %
Unconnected	0 %	0 %	0.00017037 %	0 %	0 %	0 %	5.76e-17 %

*The amount of electrolyte does not include the unresolved porosities of separator or binder. For connectivity checks, the porosity of the binder is taken into account.

Connected material in cathode
The volume fractions of the connected and the unconnected materials within the cathode are as follows:

Volume fractions	Electrolyte*	Separator	Active material 1	Active material 2	Active material 3	Active material 4	Binder / conductive additive
Connected	24.0345 %	0 %	62.8418 %	0 %	0 %	0 %	1.13382e-11 %
Unconnected	0 %	0 %	0.000222222 %	0 %	0 %	0 %	4.48e-16 %

*The amount of electrolyte does not include the unresolved porosities of separator or binder. For connectivity checks, the porosity of the binder is taken into account.

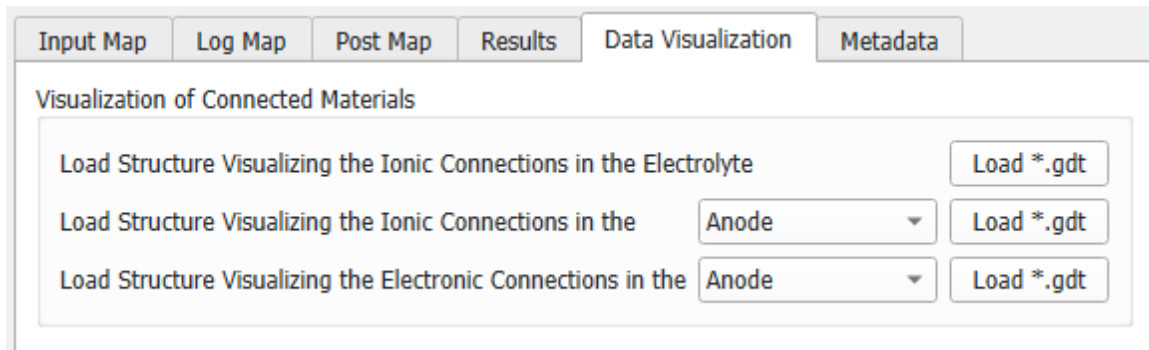
After the section that explains which parts of the battery are connected or unconnected, the **Results – Report** tab shows a table listing each component's volume and its volume fraction for the whole cell, as well as for the anode and cathode separately. The same information is also included in the [Battery Designer](#)⁵¹ result file.

✓ Plots

Under the **Results - Plots** subtab, the porosity, and the distribution of active material over the whole battery are shown as averaged values over each slice in Y- and Z-direction. This is the same plot as shown for a result file of the [Battery Designer](#)⁵¹.

✓ Data Visualization

To visualize the location of connected and unconnected parts of the battery components, load structure files located in the **Analyze Battery** result folder from the **Data Visualization** tab.



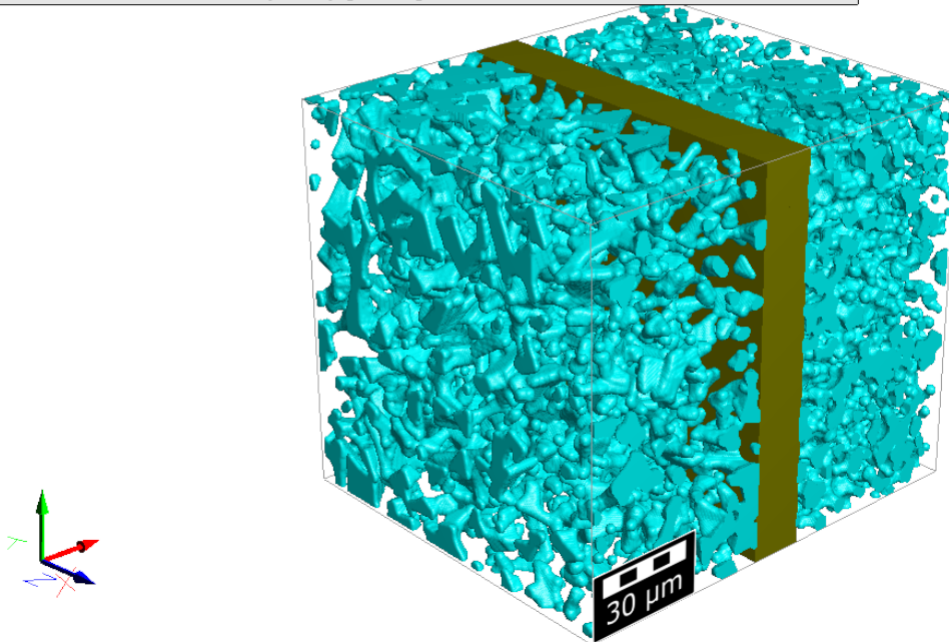
Structure files that show both electronic and ionic connections are available for the anode, cathode, and electrolyte. They are stored in the [result folder](#).

As an example, the image below shows the structure visualizing the ionic connection within the electrode; in this example battery there is no unconnected electrolyte.

In the **Color & Visibility** tab of the GUI side bar, the binders and solid materials are hidden while the electrolyte is set to visible. For more details on visualization options, refer to the GeoDict Visualization chapter.

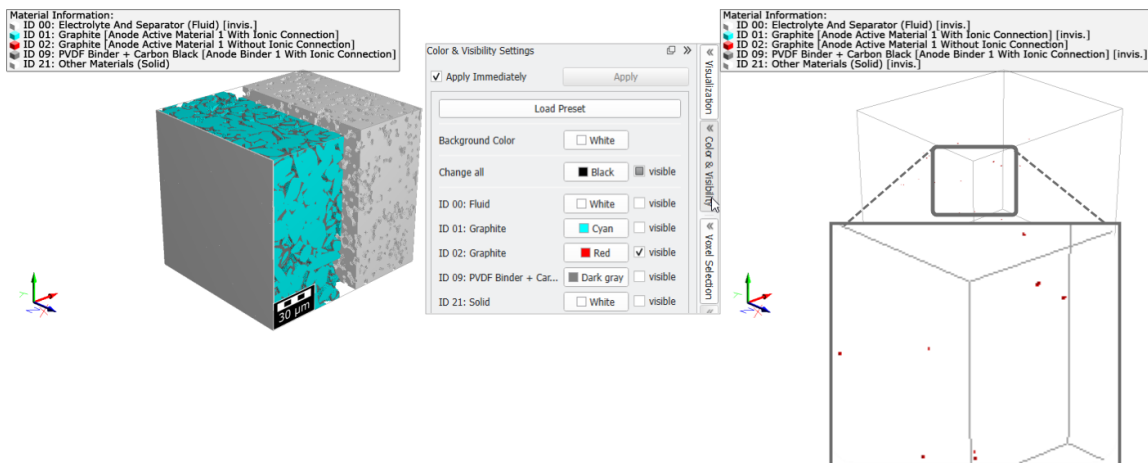
Material Information:

- ID 00: Electrolyte [Electrolyte With Ionic Connection]
- ID 02: PVDF Binder + Carbon Black [Non-porous Anode Binder 1] [invis.]
- ID 06: Separator With Ionic Connection (Fluid)
- ID 08: PVDF Binder + Carbon Black [Non-porous Cathode Binder 1] [invis.]
- ID 21: Solid Materials (Solid) [invis.]

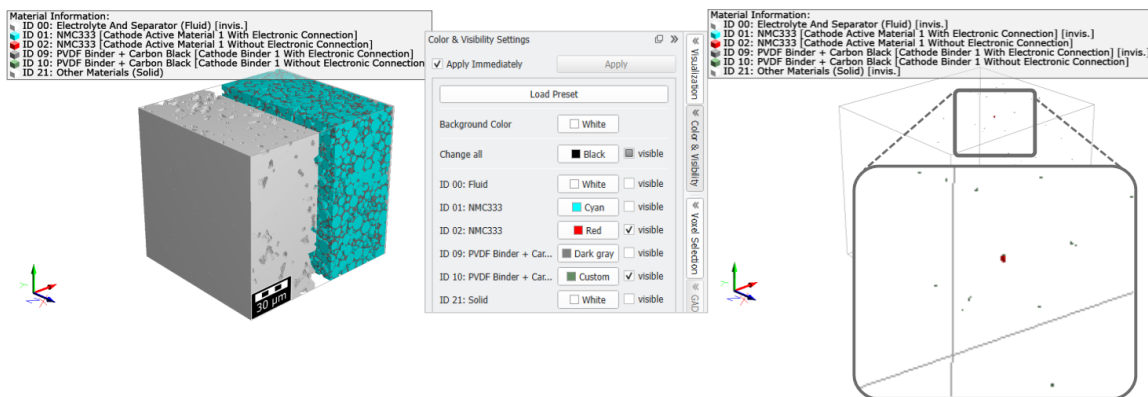


The result gives further insights to the electrode's connectivities. Details of the ionic connections in the anode become visible when you hide every material ID except for

the unconnected anode active material. Then zoom in to see the small spots where that active material has no ionic connection.

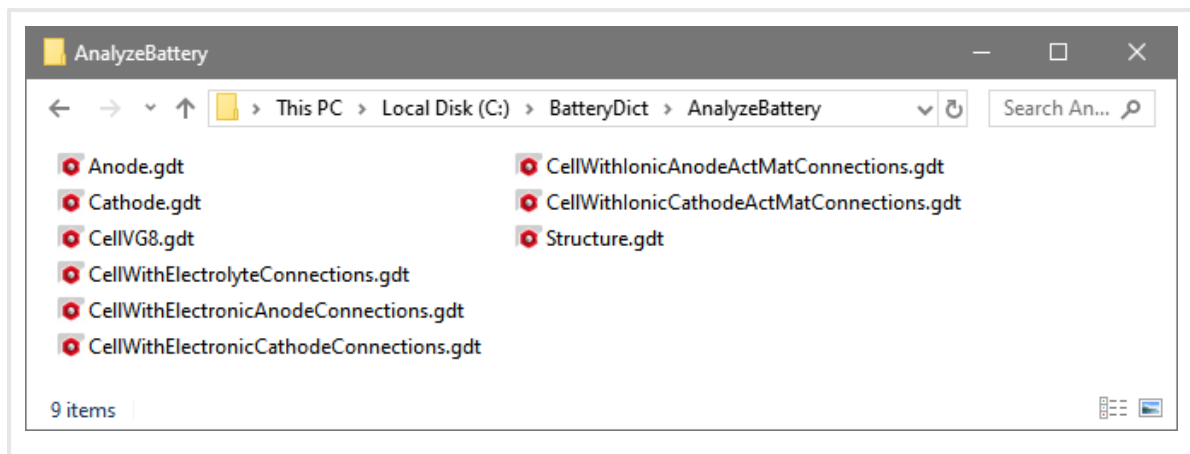


Below find also an example for the electronic connectivity result in the cathode. Here, also parts of the binder have no electronic connectivity.



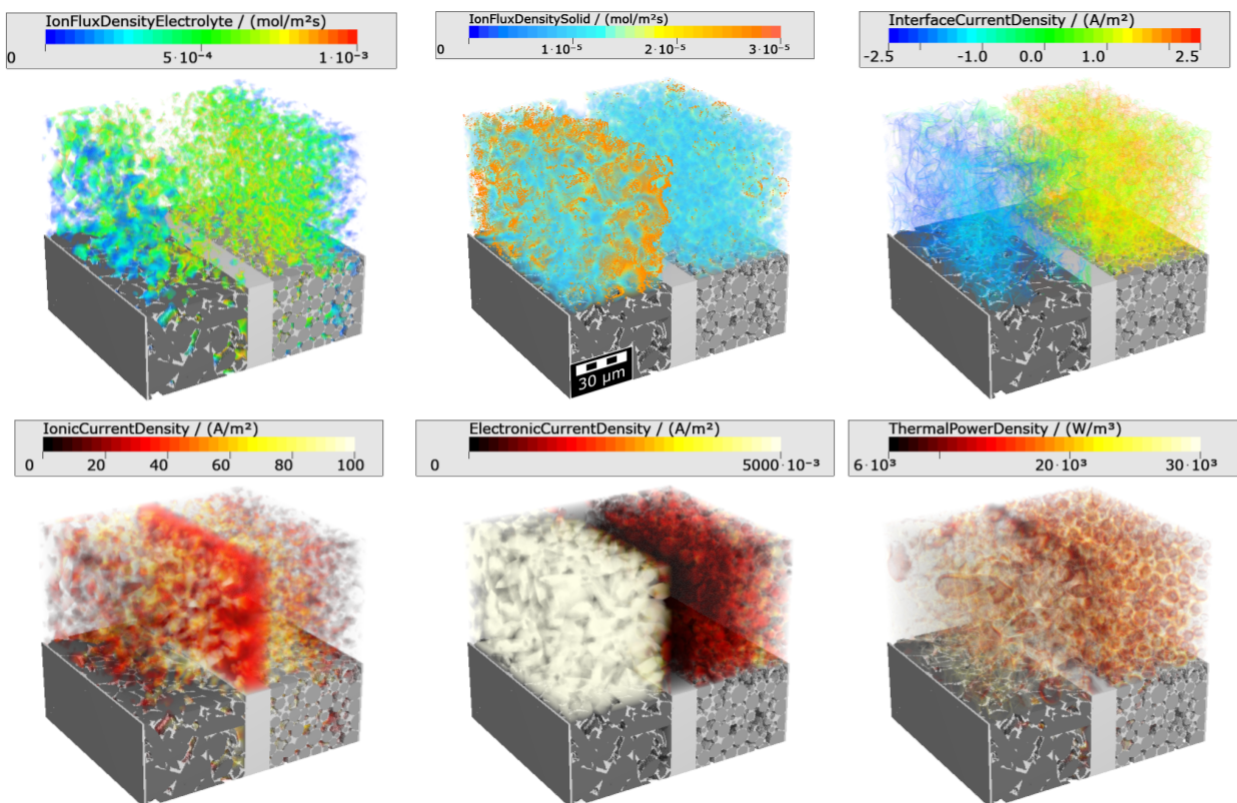
✓ Result Folder

After the analysis of a battery structure, a GeoDict result file (.gdr) is created in the selected project folder. A subfolder with the same name as the result file contains the used battery structure (**Structure.gdt**) and several files generated for, or by, the analysis: The input structures used for both electrodes (**Anode.gdt** and **Cathode.gdt**), as well as the GeoDict structure files showing electronic and ionic connections in the active materials, the electrolyte, and the binder and carbon black are available (**CellWith...Connections.gdt**).



1.2.3 Charge Battery

Simulate battery charging and discharging with multiple solver options. All solvers support concentration-dependent parameters in the electrolyte and active materials. Run fully-resolved or homogenized simulations or only compute the effective parameters of the microstructure that are needed for a homogenized simulation. The [Theoretical Background](#)⁷ section provides details about the underlying models.



The Charge Battery command:

- [Options](#)⁶³
Define the parameters for your charging simulation.
- [Results](#)⁹³

The Charge Battery command:

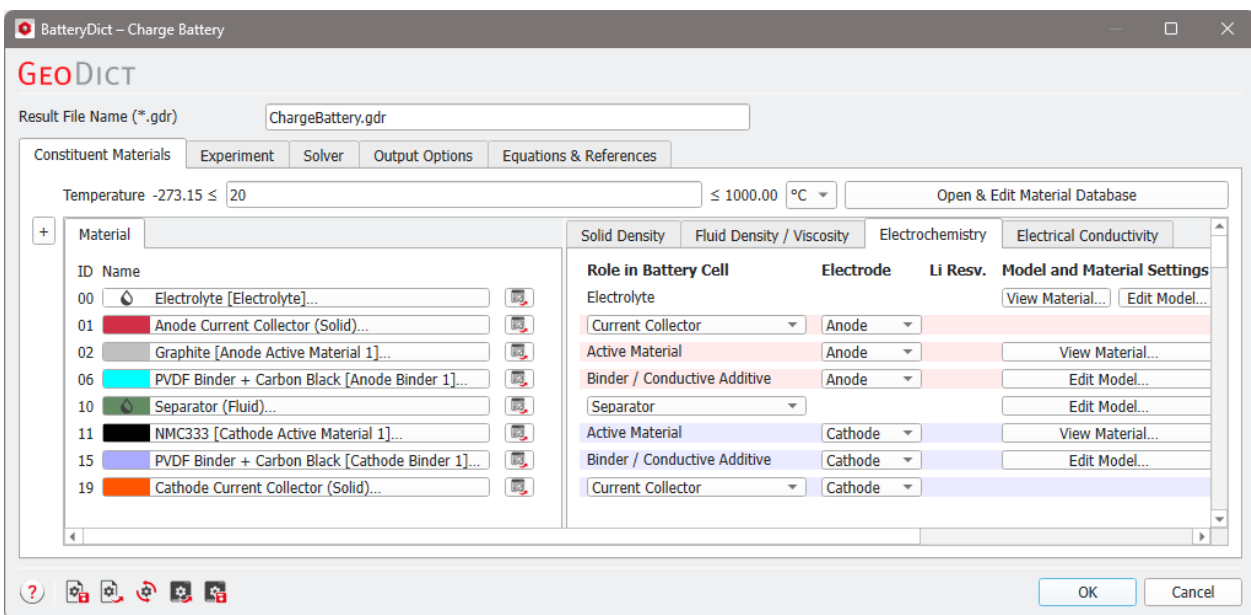
View the results of the charging or discharging simulation.

- [All Solid State Batteries](#)¹¹⁶

How to set up a charging simulation with solid electrolytes.

Options

Choose **Battery** and **Charge Battery** from the pull-down menus in the BatteryDict section and click **Edit** to adjust the charging parameters.



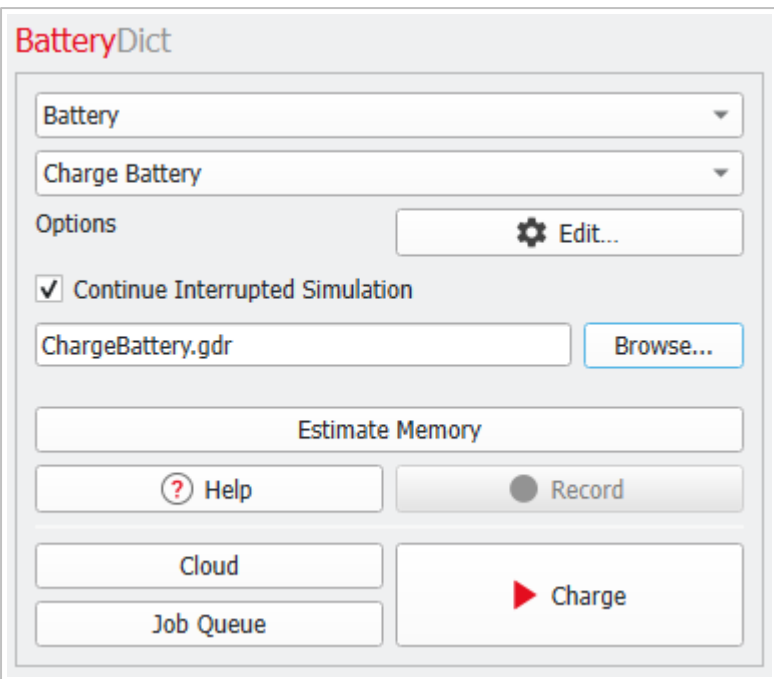
Additionally, the options **Estimate Memory** and **Continue Interrupted Simulation** become available in the BatteryDict section.

✓ Continue Interrupted simulation

It is possible to continue a previously interrupted charging simulation.

Check **Continue Interrupted Simulation**.

Browse for a GeoDict result file, created earlier with the command **Battery – Charge Battery**, and continue an unfinished simulation by selecting **Charge**.



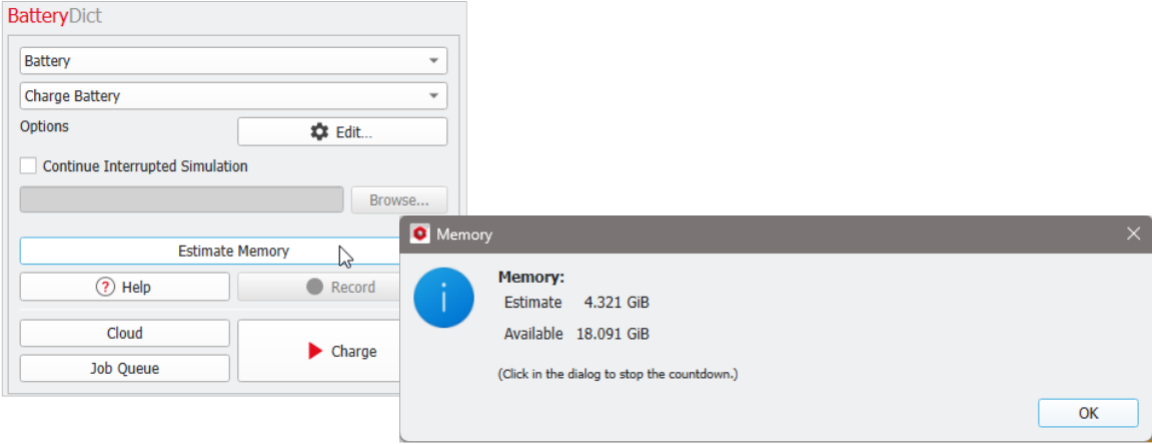
Continuing an interrupted simulation is possible, if a previously run charging simulation was stopped from the progress dialog and GeoDict could create a result file.

Cancel Stop Continue

If the simulation was canceled instead of being interrupted, it is not possible to continue the simulation later

✓ Estimate Memory

If you are unsure whether the simulation can be executed on your hardware, use the **Estimate Memory** button before starting the simulation.



Memory:

Estimate	4.321 GiB
Available	18.091 GiB

(Click in the dialog to stop the countdown.)

OK

Tabs of Charge Battery:

- [Constituent Materials](#) ⁶⁵

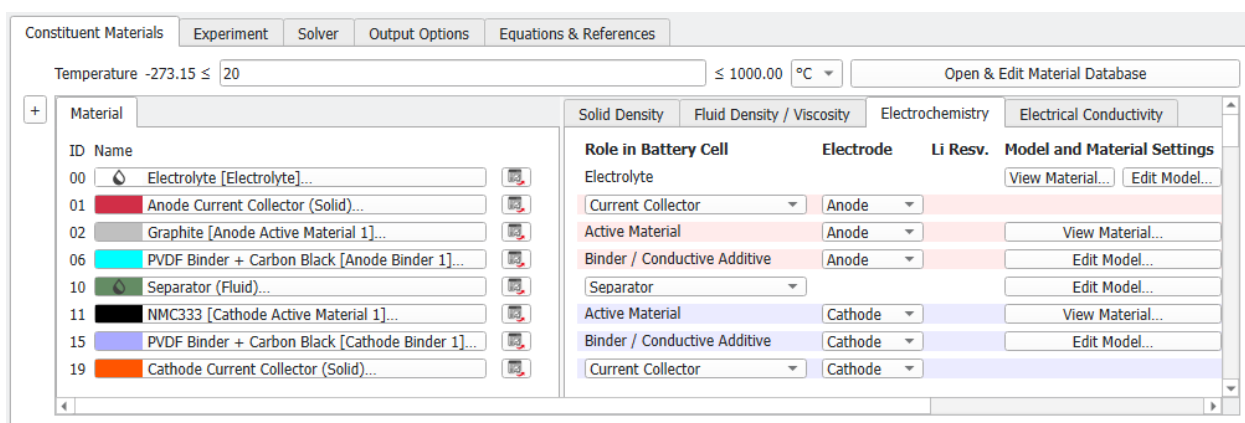
Tabs of Charge Battery:

Define the properties for all materials in the battery cell.

- [Experiment](#)⁷⁹
Edit the experiment parameters for charging, discharging, or a charging profile.
- [Solver](#)⁸⁵
Define the solver and parallelization for the simulation.
- [Output Options](#)⁹²
Decide which 3D result fields should be saved.

Constituent Materials

The properties of all materials of the battery structure are defined on the **Constituent Materials** tab.



The **Temperature** defines the temperature during simulation in Kelvin (K), Celsius (°C), or Fahrenheit (°F). The material properties of active materials and electrolyte can strongly depend on the temperature.

This temperature-dependence of the material properties can currently be derived from the entries in the material database only for the electrical conductivity and density.

However, the temperature-dependent ionic diffusivity and the exchange current density are not yet available in the material database. Consequently, while the electrical conductivity values can be adjusted based on the selected temperature — provided that the temperature dependence is included in the database entry — the other material parameters must be manually modified to ensure consistency with the chosen temperature. To facilitate comparisons of simulations at different temperatures, we recommend duplicating the relevant materials in the database for each new temperature and updating the material properties accordingly.

Material IDs of the structure and the assigned materials are listed on the left under **Material**.

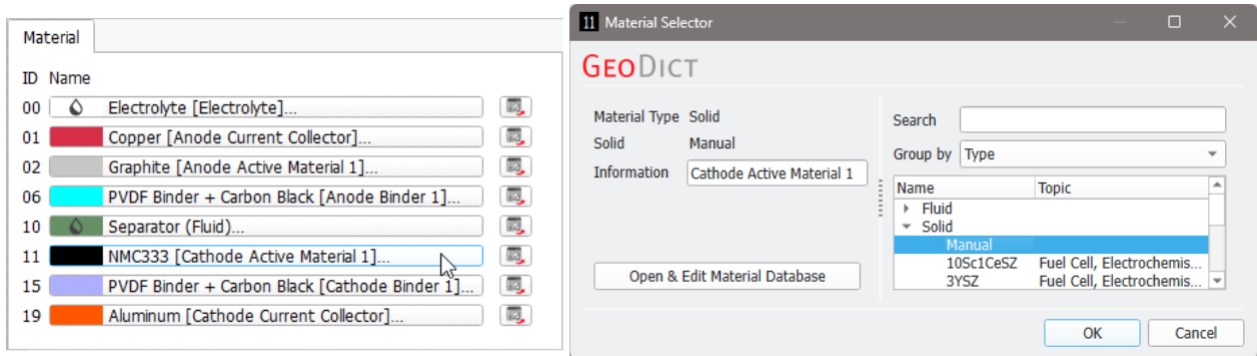
Material properties are organized into four different subtabs on the right, **Solid Density**, **Fluid Density / Viscosity**, **Electrochemistry**, and **Electrical Conductivity**.

The Constituent Materials subtabs:

- [Material](#)⁶⁶
Define the material IDs of the structure and the assigned materials.
- [Solid Density and Fluid Density / Viscosity](#)⁶⁷
Define the density and the viscosity for the constituent materials.
- [Electrochemistry](#)⁶⁸
Set the electrochemical roles of the materials and define the material parameters.
- [Electrical Conductivity](#)⁷⁸
Define the electronic or ionic conductivity for the constituent materials.

Material

The assigned materials can be changed by clicking the material of an ID to open the **Material Selector** dialog. Choose another material from the database, or select **Manual**, to edit the material's properties.



Click the **Material Report** button, available on the right of each material, to access all parameters of the material, relevant to the charging simulation.

ID	Name	
00	Electrolyte [Electrolyte]...	
01	Copper [Anode Current Collector]...	
02	Graphite [Anode Active Material 1]...	
06	PVDF Binder + Carbon Black [Anode Binder 1]...	
10	Separator (Fluid)...	
11	Cathode Active Material 1 (Solid)...	
15	PVDF Binder + Carbon Black [Cathode Binder 1]...	
19	Aluminum [Cathode Current Collector]...	

Report for Material with ID 02		
Key	Unit	Value
Type		Solid
Name		Graphite
Information		Anode Active Material 1
▼ SolidProperties		
CurrentLaw		1
NumberOfLaws		1
▼ MaterialLaw1		
Name		Material Law 1
Density	kg/m ³	2260
▼ ElectricalConductivity		
CurrentLaw		1
NumberOfLaws		2
▼ MaterialLaw1		
Type		Isotropic
Name		Powder - Isotropic
Beta	S/m	2120
▶ MaterialLaw2		
▼ Electrochemistry		
▼ LiIonBattery		
BatteryMaterialType		ActiveMaterial
▼ ActiveMaterial		
ElectrodeType		Anode
IsLithiumReservoir		false
MaxLiConcentration	mol/m ³	31090
LiDiffusivity	m ² /s	2e-14
NumberOfElectrolytes		1
▶ Electrolyte1		
▶ OpenCircuitPotential		

Solid Density and Fluid Density / Viscosity

On these two subtabs, the **Solid Density** and the **Fluid Density / Viscosity** are shown (for materials from the GeoDict material database) or can be selected (for **Manual** materials). While the fluid properties are only available for fluids, the solid properties are only available for solids.

Material	Solid Density	Fluid Density / Viscosity	Electrochemistry	Electrical Conductivity
ID Name	Density / (kg/m ³) Temp. Range / (°C)			
00 Electrolyte [Electrolyte]...	-	-	-	-
01 Copper [Anode Current Collector]...	Material Law 1 8939.8	-269.15 , 999.85	-	-
02 Graphite [Anode Active Material 1]...	Bulk 2260	-	-	-
06 PVDF Binder + Carbon Black [Anode Binder 1]...	Material Law 1 1914	-	-	-
10 Separator (Fluid)...	-	-	-	-
11 Cathode Active Material 1 (Solid)...	Manual Law 1 4700	-	+	-
15 PVDF Binder + Carbon Black [Cathode Binder 1]...	Material Law 1 1914	-	-	-
19 Aluminum [Cathode Current Collector]...	Material Law 1 2700.09	-253.15 , 659.85	-	-

Material	Solid Density	Fluid Density / Viscosity	Electrochemistry	Electrical Conductivity
ID Name	Density / (kg/m ³) Dyn. Viscosity / (kg/(m s)) Temp. Range / (°C)			
00 Electrolyte [Electrolyte]...	Material Law 1 1300	0.01	-	-
01 Copper [Anode Current Collector]...	-	-	-	-
02 Graphite [Anode Active Material 1]...	-	-	-	-
06 PVDF Binder + Carbon Black [Anode Binder 1]...	-	-	-	-
10 Separator (Fluid)...	-	-	-	-
11 Cathode Active Material 1 (Solid)...	Manual Law 1 0	0	-	+
15 PVDF Binder + Carbon Black [Cathode Binder 1]...	-	-	-	-
19 Aluminum [Cathode Current Collector]...	-	-	-	-

Electrochemistry

In the **Electrochemistry** subtab, materials are highlighted according to the electrode they belong to. All anode materials (active materials, binder and carbon black, and the current collector) are highlighted in pink, all cathode materials in purple.

Material	Solid Density	Fluid Density / Viscosity	Electrochemistry	Electrical Conductivity
ID Name				
00 Electrolyte [Electrolyte]...			Electrolyte	
01 Copper [Anode Current Collector]...			Current Collector	
02 Graphite [Anode Active Material 1]...			Active Material	
06 PVDF Binder + Carbon Black [Anode Binder 1]...			Binder / Conductive Additive	
10 Separator (Fluid)...			Separator	
11 NMC333 [Cathode Active Material 1]...			Active Material	
15 PVDF Binder + Carbon Black [Cathode Binder 1]...			Binder / Conductive Additive	
19 Aluminum [Cathode Current Collector]...			Current Collector	

✓ Electrochemical Role

If a material from the GeoDict material database is selected for a Material ID (e.g., for ID 02 in the example shown), all parameters are set according to the database values. The electrochemical role of the material (here: Anode Active Material) is shown and the electrochemical parameters can be displayed by clicking the **View Material** button for electrolyte and active materials. For all electrochemical roles of the materials, the database values for **Solid Density**, **Fluid Density / Viscosity**, and **Electrical Conductivity** are shown on the correspondent subtabs. For more details on the parameters displayed and selectable see [Parameter Options Dialogs](#) ⁷⁰.

02 Graphite [Anode Active Material 1]... Active Material Anode View Material...

GeoDict

Maximum Lithium Concentration / (mol/m³) 31090

Ionic Diffusivity / (m²/s) 2e-14

Electrolyte Selection

Currently Selected Electrolyte: Default

Used Electrolyte Profile: Default

Maximum Exchange Current Density / (A/m²) 4

Electrolyte Lithium Concentration of Exchange Current Measurement / (mol/m³) 1000

Butler-Volmer Rate Constant / (A m^{-2.5}/mol^{1.5}) 8.13709e-06

Open-Circuit Potential (OCV) Function U₀

☒ Open-Circuit Potential Has Hysteresis

Material State of Lithiation / (%)	Potential for Lithiation / (V)
1 0	0.43667
2 5.92	0.22889
3 7.427	0.21133
4 8.934	0.20978
5 10.441	0.20711

Material State of Lithiation / (%)	Potential for Delithiation / (V)
1 0	0.43667
2 6.674	0.22778
3 8.288	0.22133
4 9.903	0.21933
5 11.625	0.218

Number of 55 Insert Row Delete Row Import...

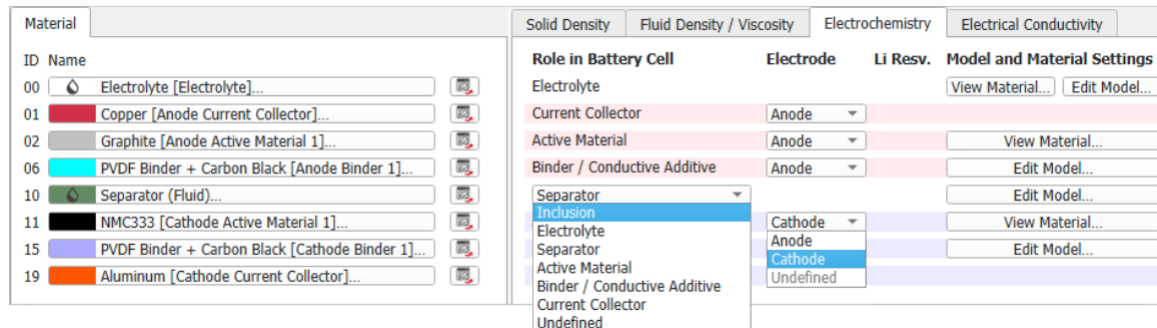
Number of 53 Insert Row Delete Row Import...

Potential for Lithiation and Delithiation / (V)

Material State of Lithiation / (%)

OK Cancel

If a material is set to manual, the electrochemical role of the material and the electrode it belongs to can be selected or changed, and the electrochemical parameters can be modified.

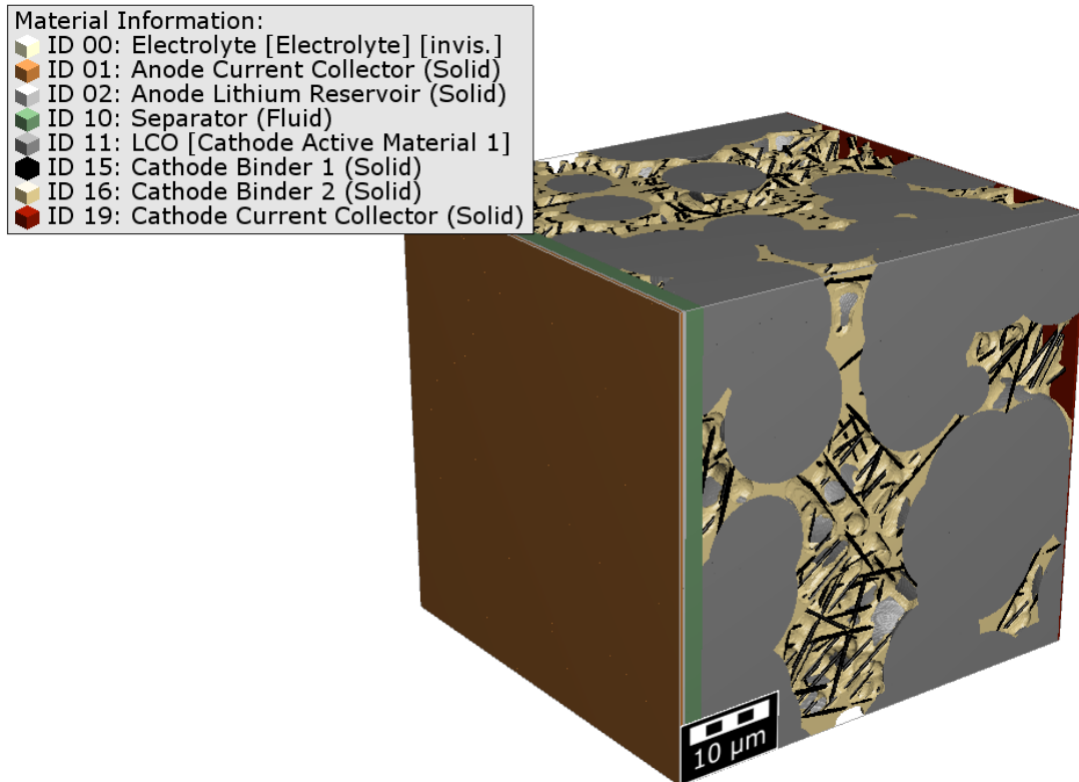


The electrochemical roles **Separator**, **Anode Current Collector**, and **Cathode Current Collector** can each be selected only for one material in the structure.

For each electrode, up to four **Active Materials** and four **Binder / Conductive Additives** can be defined.

In the following example, a half cell charging simulation of a LCO cathode versus a lithium reservoir is considered. Thus, instead of an anode a lithium reservoir is considered. The cathode contains LCO, PDVF binder and carbon black, and carbon fibers. The LCO is assigned the **Active Material** role, while the binder has the role **Binder / Conductive Additive** and can be marked as porous.

Carbon fibers are entered as a manual material with the same **Binder / Conductive Additive** role. In the [model parameter dialog](#)^[77] they must be set to non-porous so that they conduct only electrons. Consequently, the carbon fibers function as conductive additives within the electrode.



The simulation cannot be started if one of the materials has the role **Undefined** or if the electrode type is **Undefined** for an active material, binder & carbon black, or a current collector. If a material does not participate in the charging process, set its electrochemical role to **Inclusion**. No conduction is possible for a material defined as **Inclusion**. It has no potential and does not contain lithium.

If the box **Lithium reservoir** is checked for a **Cathode Active Material** or an **Anode Active Material**, the **Edit Material** button changes to an **Edit Model** button and allows to change the [Maximum Exchange Current Density](#)^[32]. The active material is in this case modeled as a lithium reservoir (necessary for half cell simulations). The solver will treat this material as a never-ending reservoir, not limiting the battery performance. Only one material can be modeled as lithium reservoir. Note that the lithium reservoir is modeled as a **Manual** material. Assigning **Lithium** from the material database will not work to model a lithium reservoir in BatteryDict.

Parameter Options Dialogs

Clicking **Edit Material** opens the property dialog for active materials or electrolyte for editing the values, **Edit Model** allows to change the electrolyte, binder / conductive additive or separator model. See below for more details.

Parameter dialogs for active materials, binder / conductive additive, separator, and electrolyte are explained in the following. For an explanation of the meaning of the parameters, see [Simulation Parameters](#)^[31].

✓ **Active Material Parameter Dialog**

The active material parameter dialogs are available for active materials from the **Electrochemistry** subtab.

For database materials, view the parameters by clicking **View Material**.

For manual materials, edit the parameters by clicking **Edit Material**.

For all active materials, the simulation parameters [Maximum Lithium Concentration](#)^[31], [Ionic Diffusivity](#)^[31], [Maximum Exchange Current Density](#)^[32], [Electrolyte Lithium Concentration of Exchange Current Measurement](#)^[35], and [Open-Circuit Potential \(OCV\) Function \$U_0\$](#) ^[35] need to be defined.

For your convenience, GeoDict computes the **Butler-Volmer Rate Constant** from the entered values as shown in equation (40)^[33] to compare the material parametrization to BatteryDict simulation parameters used until GeoDict 2024. This lets you confirm that you are employing identical effective settings for the simulation as in previous GeoDict versions. The conversion between these two parameters **Maximum Exchange Current Density** and **Butler-Volmer Rate Constant** is explained [here](#)^[32].

If a material from the GeoDict material database is used for an active material, values are shown in the **Active Material** dialog. They are shown in gray and cannot be changed.

In case **Manual (Solid)** is selected as active material, the simulation parameters can be set in the **Active Material** dialog.

Active Material

GEO DICT

Maximum Lithium Concentration / (mol/m³) 31090

Ionic Diffusivity / (m²/s) 2e-14

Maximum Exchange Current Density / (A/m²) 4

Electrolyte Lithium Concentration of Exchange Current Measurement / (mol/m³) 1000

Butler-Volmer Rate Constant / (A m⁻²/mol⁻⁵) 8.13709e-06

Open-Circuit Potential (OCV) Function U_0

☒ Open-Circuit Potential Has Hysteresis

Material State of Lithiation / (%)	Potential for Lithiation / (V)
1 0	0.43667
2 5.92	0.22889
3 7.427	0.21133
4 8.934	0.20978
5 10.441	0.20711
6 11.948	0.20178

Material State of Lithiation / (%)	Potential for Delithiation / (V)
1 0	0.43667
2 6.674	0.22778
3 8.288	0.22133
4 9.903	0.21933
5 11.625	0.218
6 13.348	0.21022

Number of f: 55 [Insert Row] [Delete Row] [Import...]

Number of f: 53 [Insert Row] [Delete Row] [Import...]

Potential for Lithiation and Delithiation / (V)

Material State of Lithiation / (%)

OK Cancel

The parameters of the material most recently chosen for this ID, taken from the GeoDict material database, are displayed and can be edited.

Values defining the **Open-Circuit Potential Function** can be modified directly in the table. Additionally, the number of value points can be changed by deleting or inserting new rows. Another possibility is to import the **Open-Circuit Potential Function** from a text file with two columns. The first column contains the material state of lithiation in percent, and the second column shows the related potential.

The chosen function is displayed as **Potential for Lithiation and Delithiation** over **Material State of Lithiation** in the plot on the right of the table.

If the **Open-Circuit Potential Function** is different for lithiation and delithiation, check the box **Open-Circuit Potential Has Hysteresis** and define one OCV function for lithiation and a different one for delithiation.

In case the active material of an electrode is defined as Lithium reservoir, with **Edit Model**, the **Maximum Exchange Current Density** can be defined in respect to the **Electrolyte Lithium Concentration of Exchange Current Measurement**.

No other parameters need to be set for a lithium reservoir, since it will be considered as a never-ending reservoir of lithium, not limiting the battery performance.

✓ Electrolyte Material Parameter Dialog

The electrolyte parameter dialog sets the parameters for simulations that do not use concentration-dependent properties for the electrolyte.

For structures containing resolved liquid-electrolyte voxels, the dialog can be accessed from the **Electrochemistry** subtab.

In the special case where no electrolyte is defined in the structure other than through porous materials, the dialog is available at the top of the **Constituent Materials** tab instead.

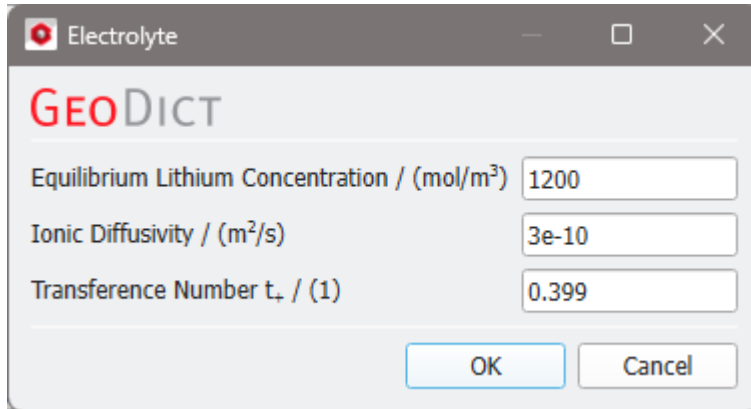
For database materials, view the parameters by clicking **View Material**.

For manual materials, edit the parameters by clicking **Edit Material**.

For the electrolyte, the [Equilibrium Lithium Concentration](#)^[36], [Ionic Diffusivity](#)^[31], and [Transference Number](#)^[36] need to be defined by clicking **Edit Material** for manual

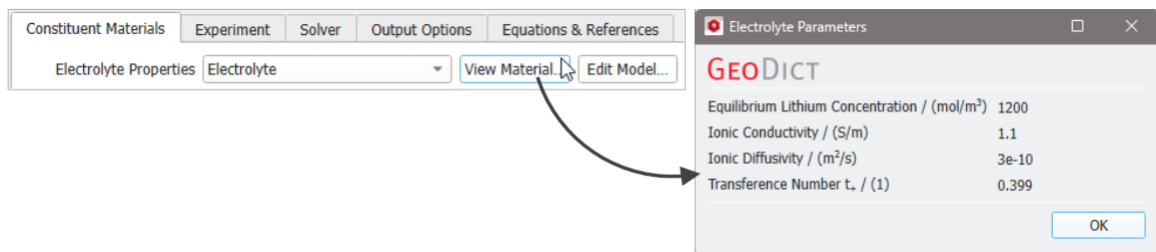
materials. If a material from the GeoDict material database is selected for the electrolyte, values are shown when clicking **View Material**, but cannot be changed.

Set the electrolyte to **Manual (Fluid)** or **Manual (Solid)** and click **Edit Material** to modify the parameters.

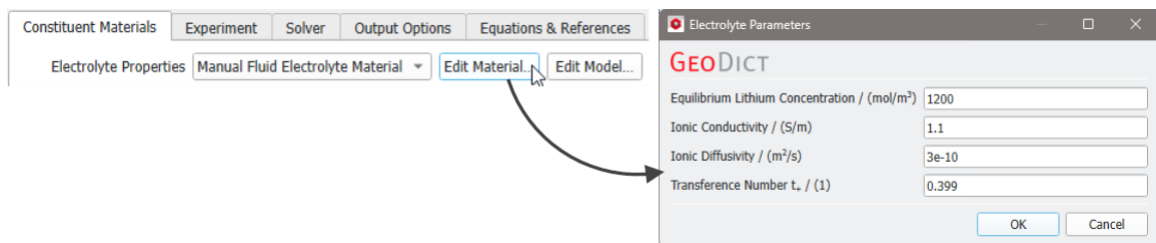


The ionic conductivity of the electrolyte is the value for the electrical conductivity defined on the **Electrical Conductivity** tab. In the case of electrolyte materials, the electrical conductivity corresponds to the ionic conductivity, since they have no electronic conductivity.

If no material ID with material defined as electrolyte exists, the electrolyte can be defined in the upper part of the **Constituent Materials** tab. The electrolyte's properties defined here are used when the separator or a binder material is modeled with [non-resolved pores](#).



When a manual Electrolyte material is selected, its properties appear in the **Electrolyte Parameters** dialog and can be adjusted there.



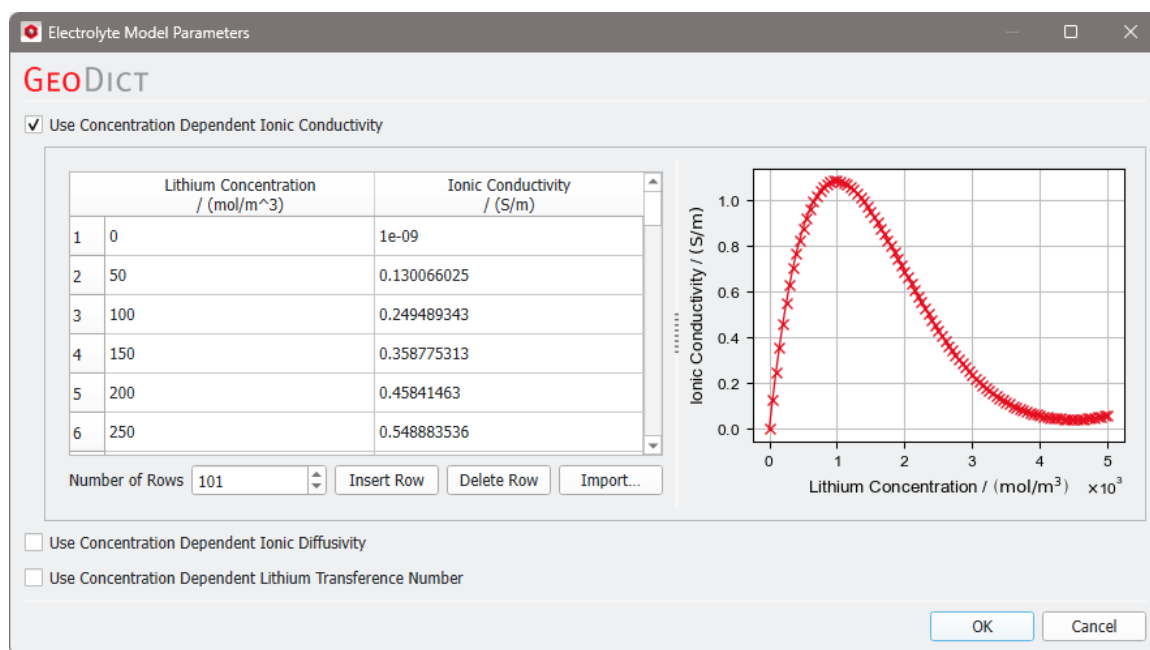
✓ Electrolyte Model Parameter Dialog

The electrolyte model parameter dialog allows you to set electrolyte properties that depend on the lithium concentration.

For structures containing resolved liquid-electrolyte voxels, the dialog can be accessed from the **Electrochemistry** subtab.

In the special case where no electrolyte is defined in the structure other than through porous materials, the dialog is available at the top of the **Constituent Materials** tab instead.

Click the **Edit Model** button for the electrolyte to open the **Electrolyte Model Parameters** dialog. Check the parameter(s) that should be modeled concentration dependent.



Insert the concentration dependent parameters either manually or import them from a *.txt file. The *.txt file must consist of two columns with the lithium concentration values on the left and the concentration dependent values on the right, separated by an empty space. For the default values such a *.txt file would look as follows:

```

1 0 1e-09
2 50 0.130066025
3 100 0.249489343
4 150 0.358775313
5 200 0.45841463
6 250 0.548883536
7 300 0.630644021
8 350 0.704144032
9 400 0.769817676
10 450 0.828085432
11 500 0.879354349
12 550 0.92401826
13 600 0.962457981
14 650 0.995041523

```

✓ Separator Model Parameter Dialog

The separator model parameter dialog is available for the separator material from the **Electrochemistry** subtab. The separator is treated as a homogeneous material, i.e., by default its porosity is not resolved in the microstructure. Edit the parameters by clicking **Edit Model**. Here you can decide whether the separator should be treated as bulk electrolyte material or modeled as a porous solid material.

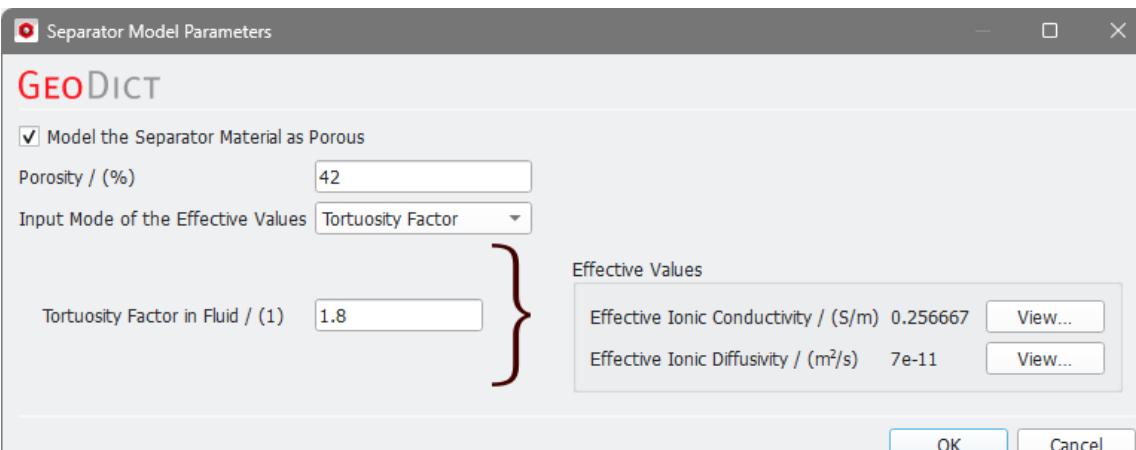
If the **Model the Separator Material as Porous** checkbox is unchecked, the separator inherits the same properties as bulk electrolyte. This is reasonable when the separator's microstructure does not significantly influence ion transport compared with bulk electrolyte.

If separator properties are influenced by the separator microstructure, check **Model the Separator Material as Porous** and define the porosity of the separator. An **Effective Ionic Conductivity** and an **Effective Ionic Diffusivity** to account for the influence of the separator microstructure are necessary in this case.

Set the **Input Mode of the Effective Values** to **Tortuosity Factor** to define the tortuosity factor in the fluid. The effective values are computed from the tortuosity factor, the porosity, and the electrolyte properties. The effective diffusivity D_{eff} (and analogous the ionic conductivity) is calculated by the equation

$$D_{eff} = \frac{\varepsilon}{\kappa_{fluid}} \cdot D_0 \quad (48)$$

where ε is the porosity, κ_{fluid} the tortuosity factor in the fluid, and D_0 the diffusivity of the electrolyte (see also the Compute Tortuosity GeoApp). In case the electrolyte properties are [not concentration dependent](#)⁷³, effective values are displayed directly in the dialog.



Separator Model Parameters

GEODICT

☒ Model the Separator Material as Porous

Porosity / (%)

Input Mode of the Effective Values

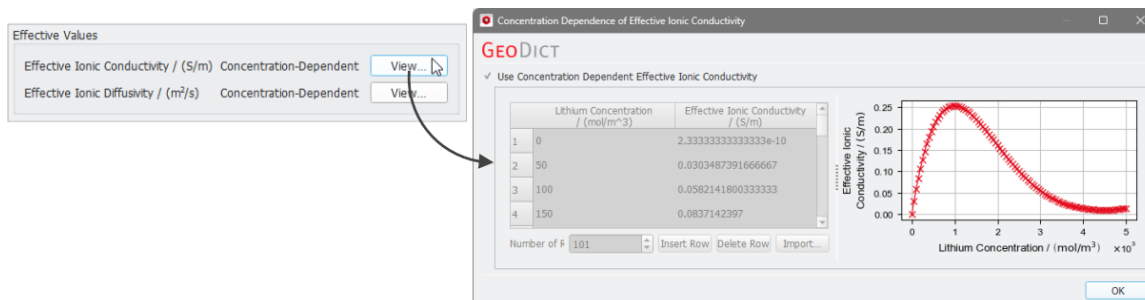
Tortuosity Factor in Fluid / (1)

Effective Values

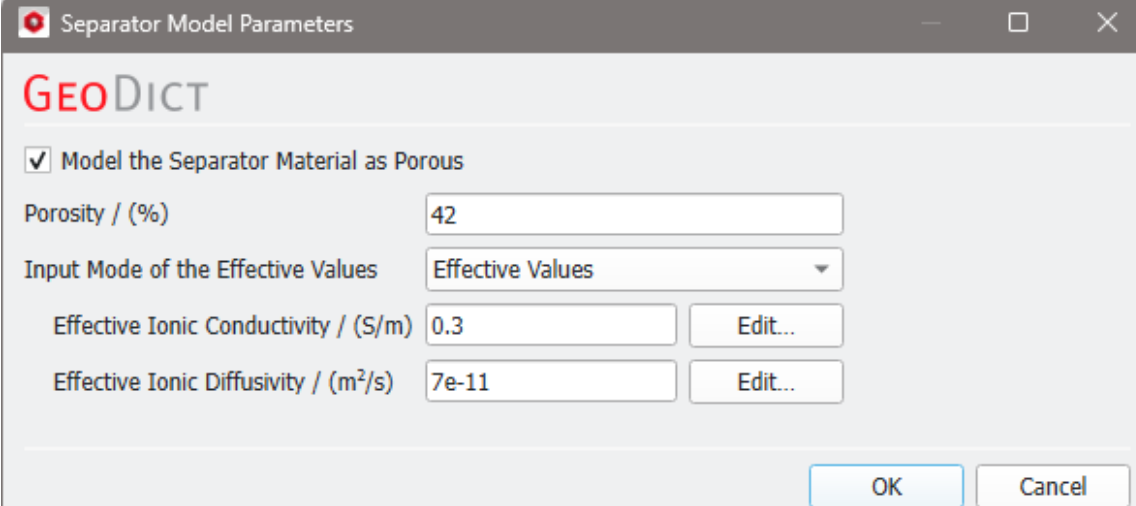
Effective Ionic Conductivity / (S/m)

Effective Ionic Diffusivity / (m²/s)

When the electrolyte uses concentration-dependent properties (e.g., ionic conductivity), the separator's effective parameters also vary with lithium concentration. Click **View** to show the concentration dependence of the effective values.



To define the effective values directly, choose **Effective Values** as **Input Mode of the Effective Values**.



Separator Model Parameters

GEODICT

☒ Model the Separator Material as Porous

Porosity / (%)

Input Mode of the Effective Values

Effective Ionic Conductivity / (S/m)

Effective Ionic Diffusivity / (m²/s)



Know how!

If your structure model contains solid voxels of the separator and resolved pores that are filled with electrolyte, you have two options to model this in BatteryDict:

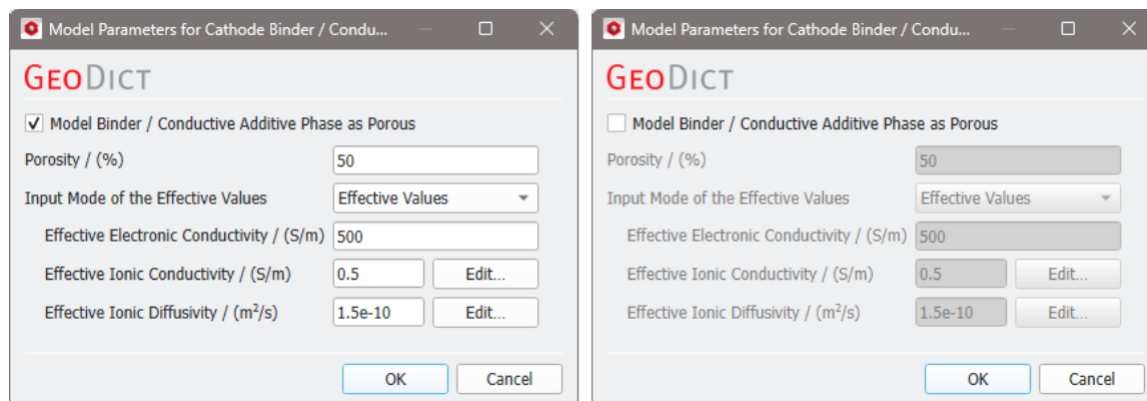
1. **Inclusion approach:** In the **Electrochemistry** tab, label the solid voxels of the separator as Inclusion instead of treating them as a separator.
2. **Homogenized separator material approach:**
 - a. Use DiffuDict to compute the tortuosity of the resolved separator structure.
 - b. In the charging simulation, replace that resolved separator geometry with a homogenized separator geometry.
 - c. Set the separator material to Porous and enter the porosity and tortuosity values you obtained from the DiffuDict simulation.

✓ Binder / Conductive Additive Model Parameter Dialog

The binder / conductive additive parameter dialogs are available for binders and conductive additives defined as **Binder / Conductive Additive** phase from the [Electrochemistry](#)^[68] subtab. Edit the parameters by clicking **Edit Model**.

For a conductive additive or non-porous binder, leave the box **Model Binder / Conductive Additive as Porous** unchecked. In this case, only the electronic conductivity of the material is used for the simulation. This value is defined by the electrical conductivity on the [Electrical Conductivity](#)^[78] tab. For materials with no ionic conductivity, [electrical and electronic conductivity are equivalent](#)^[37]; this is the case for conductive additives such as carbon fibers.

To model binder and carbon black with unresolved pores filled with electrolyte, check **Model Binder / Conductive Additive Phase as Porous**. In this case, define the **Porosity** of the binder or other conductive additive material.



The **Effective Electronic Conductivity**, the **Effective Ionic Conductivity**, and the **Effective Ionic Diffusivity** can be defined in two different ways by choosing the **Input Mode of the Effective Values**:

1. Select **Effective Values** to define the properties directly.
2. Choose **Tortuosity Factors** to set tortuosity factor values for both solid and fluid.

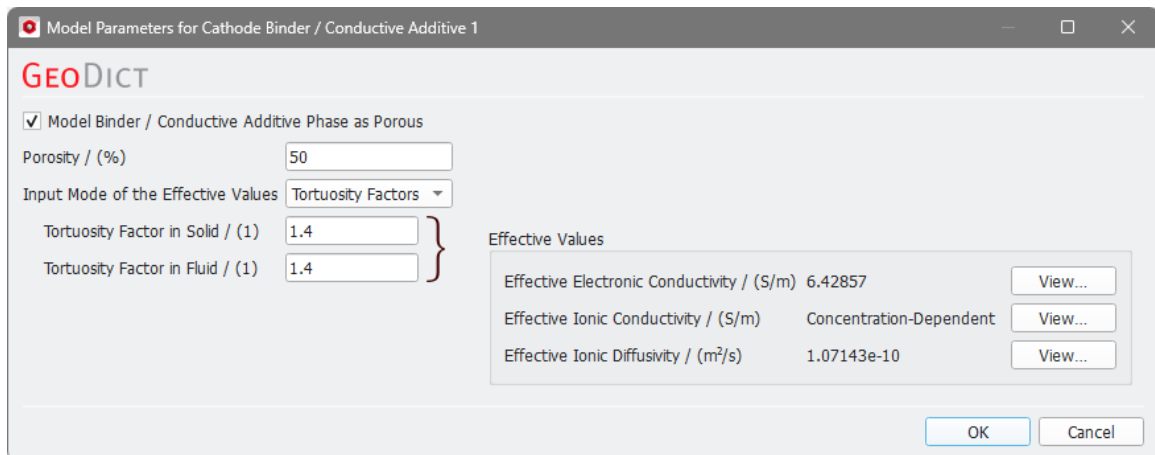
Effective values are computed and shown on the right of the dialog in case electrolyte values are not concentration dependent. They cannot be changed there.

The effective electronic conductivity σ_{eff} is calculated by the equation

$$\sigma_{eff} = \frac{1 - \varepsilon}{\kappa_{solid}} \cdot \sigma_0 \quad (49)$$

where ε is the porosity, κ_{solid} the tortuosity factor in the solid, and σ_0 the electronic conductivity of the (non-porous) binder / conductive additive material. The ionic conductivity and ionic diffusivity are calculated using the provided tortuosity factor in the fluid and the parameters from the electrolyte with the same equation as given above for the separator.

For details, see also the Compute Tortuosity GeoApp.



For concentration dependent electrolyte properties click **View** to show the concentration dependence of the effective values as shown for the [separator parameters](#)⁷⁴.

Electrical Conductivity

For numerical reasons, the [electrical conductivity](#)³⁷ of the current collectors and the lithium reservoir used in the simulations should be limited to 1000 S/m instead of using the physical conductivities of the metals, to avoid large contrasts in electrical conductivities in the battery structure. 1000 S/m is a sufficiently high value for the electrical conductivity to not be a limiting factor during the charging simulations. Reducing the electrical conductivities to this

value will not influence the overall battery performance but allowing a faster convergence of the solver. In some cases, when the electron conductivity of the electrode (active material and binder network) is very low, the conductivity contrast to the current collectors is very high and the simulation might diverge. In this case, it may help to decrease the conductivity values for the current collectors even further.

Therefore, the lithium reservoir and **Manual** materials for the current collectors have 1000 S/m as electrical conductivity by default. If the material for the current collector is not set to **Manual**, but to a material from the GeoDict material database (e.g., copper or aluminum), make sure that the **Material Law Current Collector** is selected for the electrical conductivity to limit the electrical conductivity to 1000 S/m.

ID

Name

00

Electrolyte [Electrolyte]...

01

Copper [Anode Current Collector]...

02

Graphite [Anode Active Material 1]...

06

PVDF Binder + Carbon Black [Anode Binder 1]...

10

Polypropylene [Separator]...

11

Cathode Active Material 1 (Solid)...

15

PVDF Binder + Carbon Black [Cathode Binder 1]...

19

Aluminum [Cathode Current Collector]...

Solid Density	Fluid Density / Viscosity	Electrochemistry	Electrical Conductivity				
Material Law		Long. / (S/m)	Trans. 1 / (S/m)	Trans. 2 / (S/m)	Temp. Range / (°C)	Mixing Rule	Fluid Con. / (S/m)
Iso. Law	Isotropic	1.1	1.1	1.1	-	Single Phase	-
Current Collector	Isotropic	1000	1000	1000	-	Single Phase	-
Powder - Isotropic	Isotropic	2120	2120	2120	-	Single Phase	-
Isotropic	Isotropic	18	18	18	-	Single Phase	-
Isolator	Isotropic	0	0	0	-	Single Phase	-
Manual Law 1	Isotropic	0.814	0.814	0.814	-	Single Phase	-
Isotropic	Isotropic	18	18	18	-	Single Phase	-
Current Collector	Isotropic	1000	1000	1000	-	Single Phase	-
Iso. Law							
Current Collector							

On this tab, the separator's conductivity is shown as 0 S/m by default. However, the value shown here does not have any influence on the simulation.

In case the porosity of the separator is not modeled, it gets the same ionic conductivity as the electrolyte. In case the separator is modeled as porous material, you define its ionic conductivity using the settings in the dialog [Separator Model Parameters](#).

Experiment

All parameters defining the charging simulation of the battery are defined on this tab.

Constituent Materials	Experiment	Solver	Output Options	Equations & References
Experiment Type		Charge Battery Cell		
Boundary Conditions in Through Direction		Charge Rate		
Charge Rate / (1)		1		
Start and End Condition		Minimum and Maximum Cell SOC >>> Charge >>>		
Range of the Cell State of Charge / (%)		20.00 70.00		
☐ Use Upper Cut-Off Voltage / (V)		4.3		
☐ Max. Simulated Time / (s)		3600		
Boundary Conditions in Tangential Direction		Symmetric		

✓ Experiment Type

From the pull-down menu **Experiment Type**, select the appropriate entry to simulate the charging or discharging of the battery cell or set a charging profile. Here, a charging simulation is chosen. For the experiment types **Charge Battery Cell** and **Discharge Battery Cell** select the [Boundary Conditions in Through Direction](#)^[80] and the [Start and End Condition](#)^[81]. How to Set a **Charging Profile** is explained [here](#)^[83].

✓ Boundary Conditions in Through Direction

The **Boundary Conditions in Through Direction** can be specified by a **Charge Rate**, a **Current Density**, by defining the **Current**, by defining the **Cell Potential**, or the **Power Density**.

- With a **Charge Rate** defined, the applied current is related to the cell's maximum capacity from 0% state of charge to 100% state of charge and is a measure of the duration of the battery charging. For example, a charge rate of 1 for a battery with capacity of 1 Ah means that the battery is charged completely in 1 hour with a constant current of 1 Ampere (A). This time is unrelated to the simulation time, but instead to the time that the charging process itself requires. A charge rate of 2 means that charging the same battery with a current of 2 Ampere takes 1/2 hour.

Boundary Conditions in Through Direction	Charge Rate
Charge Rate / (1)	1

- Defining the **Current Density** instead means that the applied the applied current density (in A/m²) is defined directly.

Boundary Conditions in Through Direction	Current Density
Current Density / (A/m ²)	10

- Defining the **Current** instead means that the applied current (in A) is defined directly.

Boundary Conditions in Through Direction	Current
Current / (A)	1e-11

- If **Cell Potential** is selected, the voltage is kept at a constant value during the simulation, and the current is a time-dependent value. Define a [Cut-Off Current](#)^[81] as end condition.

Boundary Conditions in Through Direction	Cell Potential
Cell Potential / (V)	3.5

- Defining the **Power Density** in W/m² means that the applied current density is dynamically adjusted so that the product of cell potential and current density - i.e., the power density - remains constant throughout the simulation.

Boundary Conditions in Through Direction	Power Density
Power Density / (W/m ²)	20

✓ Start and End Condition

The **Start and End Condition** for the charging simulation can be defined in several ways:

Start and End Condition	Minimum and Maximum Cell SOC	>>> Charge >>>
Range of the Cell State of Charge / (%)	20.00	70.00
☐ Use Upper Cut-Off Voltage / (V)	4.3	
☐ Max. Simulated Time / (s)	3600	

- as minimum and maximum percentage of the [state of charge](#)^[8] of the whole cell (**Minimum and Maximum Cell SOC**)

Start and End Condition	Minimum and Maximum Cell SOC	>>> Charge >>>
Range of the Cell State of Charge / (%)	20.00	70.00

- for the anode SOC and cathode SOC individually (**Anode and Cathode SOC**s),

Start and End Condition	Anode and Cathode SOC	>>> Lithiate >>>
Range of the Anode State of Charge /	20.00	70.00
		<<< Delithiate <<<
Range of the Cathode State of Charge	20.00	70.00

- by selecting an initial .cap file from a previous BatteryDict simulation and defining a final SOC (**Initial *.cap File and Final Cell SOC**). This option is especially useful for simulating a charging or discharging process, starting from a non-equilibrium condition after a previous discharging or charging simulation.

Start and End Condition	Initial *.cap File and Final Cell SOC ▾	
Initial *.cap File (*.cap)		Browse...
Final Cell SOC / (%)	70	

- or, by defining an initial voltage value and a final SOC (**Initial Voltage and Final Cell SOC**). This option can be used together with **Use Upper (Lower) Cut-Off Voltage** to define a voltage window for your charging (discharging) simulation.

Start and End Condition	Initial Voltage and Final Cell SOC ▾	
Initial Equilibrium Voltage for Charging / (V)	2.8	
Final Cell SOC / (%)	70	



Important! To get a numerically stable solution, the state of charge for the whole cell as well as for anode and cathode separately can be set only between 5% and 95%, see also [Theoretical Background - Fully Resolved](#)^[15].

Depending on the selected [boundary conditions](#)^[80], it is possible to set additional an end conditions to the simulation.

- Limit the voltage in a simulation by checking **Use Upper / Lower Cut-Off Voltage**. The voltage will not exceed this limit. I.e., if the cut-off voltage is reached, the charging will end. This option is not available for the boundary condition Cell Potential.

☒ Use Upper Cut-Off Voltage / (V)	4.3
---	----------------------------------

- If Cell Potential is set as boundary condition in through direction, select the **Cut-Off Current** as an end condition to the simulation to be **Charge Rate**, **Current Density** or **Current**. For example, consider charging a battery at constant **Cell Potential**, and selecting a **Cut-Off Charge Rate**. The simulation starts with the entered SOC value and charges the battery at the provided constant cell potential, for example at 3.5 V. During the charging, the charge rate decreases with the increasing SOC. As soon as the charge rate is lower than the entered **Cut-Off Charge Rate**, the simulation stops.

Cut-Off Current	Current ▾	
Current / (A)	1e-13	Charge Rate Current Density Current

- When checking **Max. Simulated Time**, the simulation ends if the charging process exceeds the entered **Max. Simulated Time**. Note that **Max. Simulated Time** does not denote the duration given to the solver. Instead it specifies how long the simulated battery is charged or discharged. For an example, let us consider a battery that is charged from 20% state-of-charge to 70% state-of-charge at a charge rate of 1C. The battery takes 30 min to charge. If the **Max. Simulated Time** is set to 600

seconds (10 min), in this example the battery will only be charged from 20% to 36.67% state-of-charge.

☒ Max. Simulated Time / (s)

600



Note! The simulation is stopped as soon as the first of the provided end conditions is met, i.e., either the set final SOC is reached, the cut-off voltage / current is reached, or the max. simulated time is exceeded.



Know how! If a simulation diverges, it is often helpful to reduce the voltage window covered in a charging simulation.

✓ Charging Profile

Charging Profiles are a series of charging, discharging, and relaxation simulations that are performed sequentially for the same structure.

Experiment Type
Set a Charging Profile
Initial Cell Condition
Equilibrium Cell SOC
Initial Cell SOC / (%)
20

	(Dis-)Charge or Relaxation?	Type of Boundary Condition	Applied BC Value	Stopping Criterion at Boundary	Stopping BC Value	Stopping Cell SOC / (%)	Stopping Time / (s)
1	Charge Battery Cell	Charge Rate / (1)	1	Cell Potential / (V)	3.8	50	☐ 1800
2	Charge Battery Cell	Cell Potential / (V)	3.8	Charge Rate / (1)	0.01	50	☒ 3600
3	Discharge Battery Cell	Charge Rate / (1)	1	Cell Potential / (V)	3.55	20	☐ 1800
4	Discharge Battery Cell	Cell Potential / (V)	3.55	Charge Rate / (1)	0.01	20	☒ 3600

Number of Rows
4
Insert Row
Delete Row

Overall Stopping Conditions:
☐ Max. Simulated Time / (s)
3600

If **Set a Charging Profile** is selected as [Experiment Type](#), the starting point for the first simulation can be defined

- as an **Equilibrium Cell SOC** (Select an initial Cell SOC between 5% and 95%, that defines the initial equilibrium state),

Experiment Type
Set a Charging Profile
Initial Cell Condition
Equilibrium Cell SOC
Initial Cell SOC / (%)
20

- as an **Equilibrium Voltage** (enter the voltage for the initial equilibrium state of the battery),

Experiment Type	Set a Charging Profile ▼
Initial Cell Condition	Equilibrium Voltage ▼
Initial Equilibrium Voltage / (V)	3.6

- or, by selecting a **.CAP File** of a previous simulation.

Experiment Type	Set a Charging Profile ▼
Initial Cell Condition	CAP File ▼
Initial *.cap File (*.cap)	InitialCAP.cap
	Browse...

The starting point for the following simulations, defined in the charging profile table, is always the final state of the previous one.

To define a charging profile, choose as many rows for the table as simulation steps desired by entering the **Number of Rows**. Select for each step, if the battery is charged, discharged, or if relaxation is simulated.

For **charging** or **discharging**, define the **Type of Boundary Condition** (BC) and the corresponding **Applied BC Value**, in the same way as for [simple charging simulations](#)^[80]. The same options for the boundary condition (**Charge Rate**, **Current Density**, **Current**, **Cell Potential**, and **Power Density**) are available.

For charging or discharging, next, the first stopping criterion for the selected boundary condition (**Stopping Criterion at Boundary**) is chosen for each simulation step. The available options depend on the **Type of Boundary Condition**.

- If **Charge Rate**, **Current Density**, **Current**, or **Power Density** is selected as BC, only a cut-off **Cell Potential** is possible as stopping criterion at boundary.
- For **Cell Potential** as BC, the stopping criterion at boundary can be chosen between a cut-off **Charge Rate**, **Current Density**, and **Current**.

Enter the **Stopping BC Value** for the first stopping criterion, for the second stopping criterion a stopping state-of-charge for the whole cell (**Stopping Cell SOC / %**) and for the (optional) third stopping criterion a **Stopping Time**. The computation ends for each simulation step, if the first one of the stopping criteria is reached. The next simulation step will continue from this state.

For **relaxation**, no boundary conditions need to be defined, only the stopping time as the only possible stopping criterion of the relaxation step. In a relaxation step, the return of the battery cell to an equilibrium state after charging or discharging is simulated. The solver settings, including the time step, are set by BatteryDict to optimize the simulation time required for the relaxation step.

(Dis-)Charge or Relaxation?	Type of Boundary Condition	Applied BC Value	Stopping Criterion at Boundary	Stopping BC Value	Stopping Cell SOC / (%)	Stopping Time / (s)
1 Charge Battery Cell ▾	Charge Rate / (1) ▾	1	Cell Potential / (V) ▾	3.8	50	☐ 1800
2 Charge Battery Cell ▾	Cell Potential / (V) ▾	3.8	Charge Rate / (1) ▾	0.01	50	☒ 3600
3 Discharge Battery Cell ▾	Charge Rate / (1) ▾	1	Cell Potential / (V) ▾	3.55	20	☐ 1800
4 Relaxation ▾						☒ 3600

✓ Boundary Conditions in Tangential Directions

Periodic or **Symmetric** boundary conditions can be selected for the **Boundary Conditions in Tangential Directions**.

Boundary Conditions in Tangential Direction Symmetric ▾

Periodic

Symmetric

For **periodic** boundary conditions, the structure is assumed to repeat periodically in Y- and Z-direction and for **symmetric** boundary conditions, the structure is mirrored in Y- and Z-direction and the Li⁺ ions and electrons are reflected at the boundary in Y- and Z-direction. The connected and unconnected parts of the active materials and electrolyte depend on the boundary conditions, so they are determined when the simulation begins.

Solver

Under the **Solver** tab, select the type of simulation to run and the solver to use when solving the system of partial differential equations, as well as the solver options.

Constituent Materials Experiment **Solver** Output Options Equations & References

Simulation Type Fully Resolved Simulation ▾

Solver Type LIR ▾

Parallelization 16 Threads Edit...

Time Step

Time Step Input Mode Automatic ▾

LIR **BESTmicro** BESTmeso

☒ Error Bound Error Bound ▾ 0.01

☐ Maximum Iterations 100000

☐ Maximum Run Time / (h) 240

▶ Advanced Options

✓ Simulation Type

Select the **Simulation Type** to one of the following:

- The **Fully Resolved Simulation**¹² runs directly on the voxels of the battery structure. It is therefore very accurate, and, in addition to charge curves, also provides solution files with results resolved on the voxel scale and slice mean plots.
- The **Homogenized Simulation**¹⁸ is much faster than the fully resolved simulation. It uses an advanced pseudo 2D-Newman-model (DFN-model) which is a simplified model, that is created from the given structure. The effective parameters for this simulation are computed in GeoDict. It returns a charge curve as well, but no solution

fields resolved on the voxel scale.

- The **Calculate Homogenized Parameters** option does not run a charging simulation. Instead it only computes the effective parameters from the structure that are needed for a pseudo-2D Newman model (DFN-model) simulation. The [Experiment](#)^[79] and [Output Options](#)^[92] tabs are grayed out. The calculated parameters can be loaded into the [Charge Homogenized Battery](#)^[120] dialog for fast simulations on an already homogenized battery.
- The last option is to **Calculate Equilibrium Potential Curve**. The [Experiment](#)^[79] and [Output Options](#)^[92] tabs are grayed out, because the full simulation is not performed. The cell potential in equilibrium is determined considering only geometry and material information.

✓ Solver Type

For a **Fully Resolved Simulation**, select **LIR** or **BESTmicro** for **Solver Type**.

For the **Homogenized Simulation**, only the **BESTmeso** solver is available.

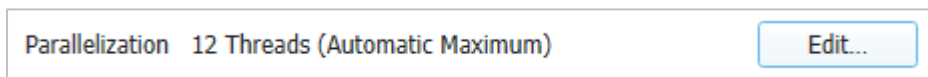
If using any of the other two simulation types none of the solvers are used.

For the **LIR** solver, [additional parameters](#)^[90] for the computation can be defined.

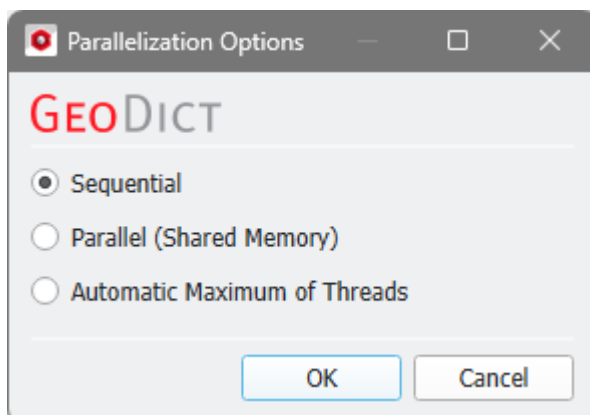
✓ Parallelization

Control how many threads are used for the computation. Parallelization is possible if your license and hardware allow it.

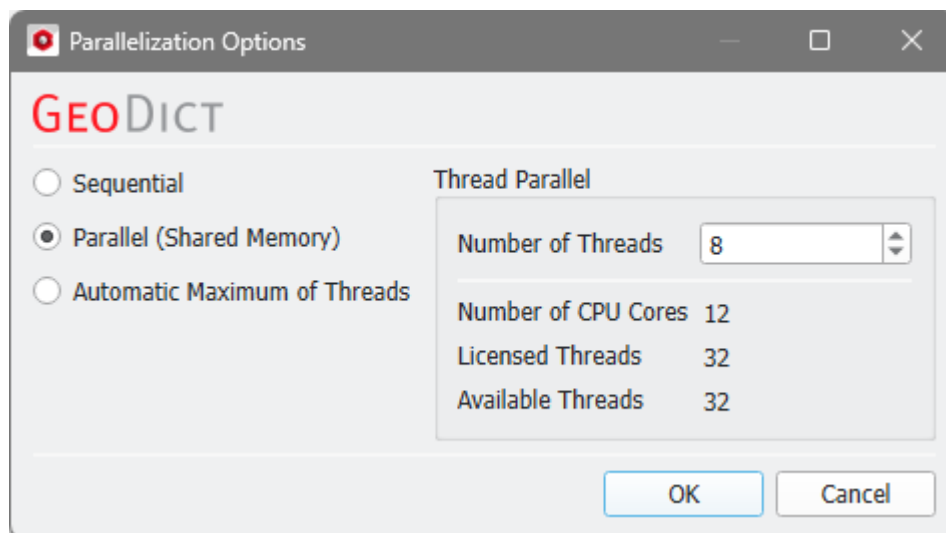
The **Parallelization Options** dialog opens when clicking the **Edit** button and you can choose between **Sequential**, **Parallel (Shared Memory)**, or **Automatic Maximum of Threads**.



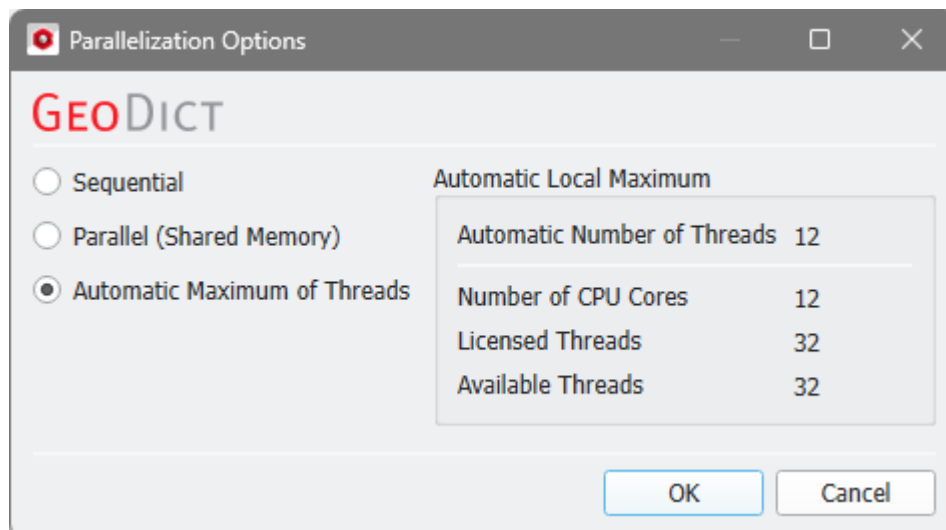
Selecting **Sequential** will not apply parallelization and only one thread is used for the computation.



When **Parallel (Shared Memory)** is selected, the **Number of Threads** can be entered. Below, the **Number of CPU Cores** that the current machine has, the maximum number of **Licensed Threads** and the number of those licensed threads that are available (**Available Threads**) are shown in the dialog. Of course, the maximal number of parallel processes you can use, is the smallest of those three numbers.



If **Automatic Maximum of Threads** is selected, the number of parallel processes is automatically selected for optimal speed, based on the CPU cores and licensed parallel processes.



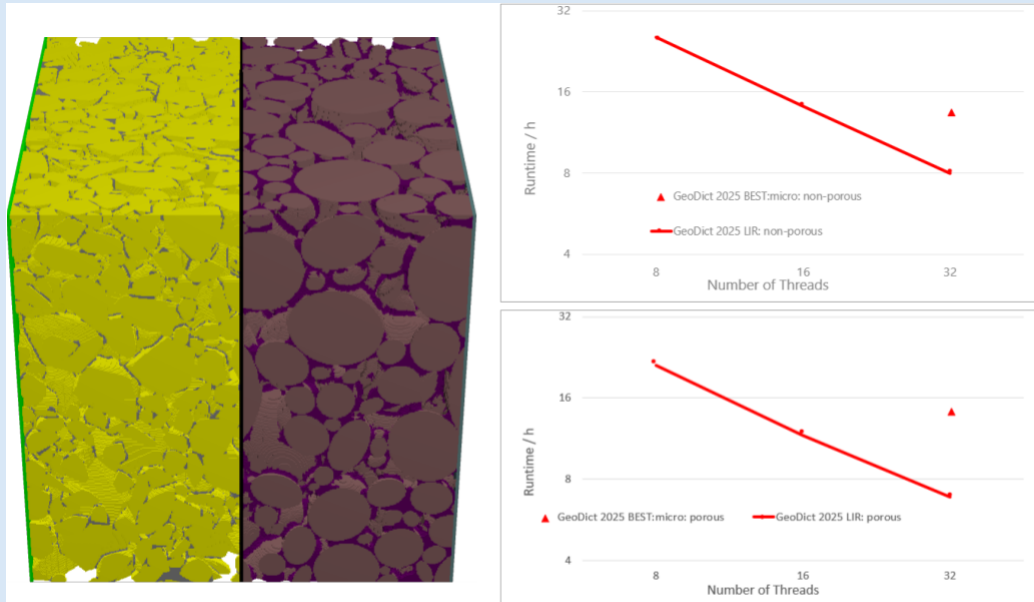
The **Automatic Local Maximum** of processes is automatically selected, which is the minimum of **Number of CPU Cores**, **Licensed Threads**, and **Available Threads**.



Note! As an example for the parallelization, a full battery structure of size 409 x 400 x 400 voxels with 200 nm voxel length is used to simulate the charging from the cell state of charge 20% till 70%. The computation is run on a server

with 2 x Intel E5-2697A v4 processors with 16 cores each, running with a maximum of 3.60 GHz, and 1 TB RAM.

The simulations are computed with GeoDict 2025.



When the binder is considered as solid (first plot), the LIR solver needs only 2/3 of the runtime compared to BESTmicro.

The LIR solver needs only 8.3 GB of RAM which is 4% of the memory required by BESTmicro. The speedup for LIR solver is nearly optimal.

When the binder is considered as porous (second plot). The LIR solver needs 9.4 GB of RAM, only 4% of the memory required by BESTmicro. The runtimes of LIR and BESTmicro with 32 threads are 6.9 h and 14 h.

✓ Time Step

In the **Time Step** panel an option for the **Time-Step Input Mode** may be selected.



Any of the battery solvers calculates the time evolution of the given Li-ion battery. It starts at the initial state, which has time = 0 in the [result plots](#)⁹⁷. It takes the time step defined as maximum time step size and tries to find the battery state at time = last time + time step by searching an equilibrium solution fulfilling the given system of differential equations. If no solution can be found for this time step size, it reduces the time step size, and the solver starts again. This procedure is repeated until an appropriate time step size is found. This time step size is used for the next steps in the

simulation as well. After several successful steps with a certain time step size, the solver tries to increase this time step size again, to reduce overall computation time. With the **Time-Step Input Mode**, the maximum time-step size can be influenced. For more information on time steps see [State of Charge \(SOC\) and State of Lithiation \(SOL\)](#)^[107].

- Choosing **Automatic**, the solver selects the time-step size without restrictions.
- If a **Minimum Number of Time Steps** is defined, at least this number of points are computed for the solution and the maximum time-step size is selected accordingly. If your simulation does not produce enough points in the plots of the result file, then you might want to increase the **Minimum Number of Time Steps**.
- **Maximum Time Step Size** defines the maximum time step in seconds used in the simulation. If the size of the time step is oscillating a lot, the recommendation is to reduce this maximum value.

The time steps that were finally realized in the simulation are saved in the [Result Map](#)^[107] of the GeoDict result file (*.gdr file), created for the charging simulation, under the key **TimeDependentValues:TimeStep**.

If a new battery state is found in a simulation with a charge rate boundary condition, the solver computes the Cell-SOC step of the just found new battery state i via:

$$\Delta(SOC)_i = \Delta t_i \cdot C / (1h) \quad (50)$$

with Δt_i the time step and C the charge rate. So, it is not clear from the start which is the next computed Cell-SOC in a simulation, this depends on the time step.

Example:

- Charge Rate $C = 5$
- Time Step Size $\Delta t_i = 2.5 \text{ s}$
- Cell-SOC step $\Delta(SOC)_i = 2.5 \cdot \frac{5}{1h} = 2.5 \text{ s} \cdot \frac{5}{3600 \text{ s}} = 0.00347 = 0.347\%$

If you choose to set the current density instead of the charge rate, then the calculation of the Cell-SOC step size depends on the given current density and the cell capacity. Thereby, the cell capacity depends on the battery-geometry and the maximum lithium concentration of the active materials.

In the GeoDict result file (*.gdr file) created for the charging simulation, you can find the time-evolution of the Cell-SOCs in percent as well as the corresponding times in seconds in the [Result Map](#)^[107] under the keys

TimeDependentValues:CellStateOfCharge and **TimeDependentValues:Time**, respectively.

For simple simulations (charge rate ≤ 1 , physical domain size $\leq 5 \text{ }\mu\text{m}$, only one active material per electrode, diffusivities $\geq 1\text{e-}12 \text{ m}^2/\text{s}$, conductivities $\geq 1 \text{ S/m}$ and no warnings during the simulation), the time step size is usually the maximum time step

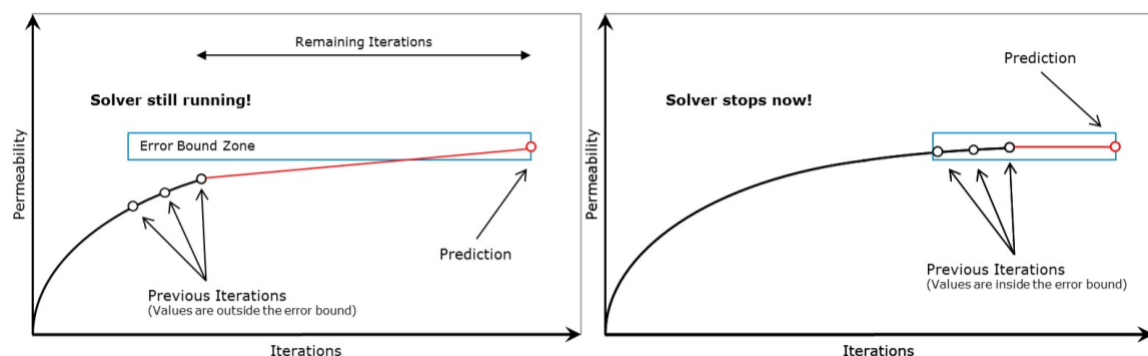
size set. Then, also the Cell-SOC step is a constant value.

However, for more complex simulations (charge rate ≥ 10 , physical domain size $\geq 50 \mu\text{m}$, two active materials in an electrode with different parameters, low diffusivities in the active materials and small conductivities), it might happen that the time step size may be smaller than the maximum time step size defined and not constant over the whole simulation.

✓ LIR Solver Options

With the LIR solver, the partial differential equations of each time step are solved iteratively with an adaptive tree structure. Several solver options can be chosen in the panel on the right.

The stopping criterion **Error Bound** uses the result of previous iterations, and predicts the final solution based on linear and quadratic extrapolation. The solver stops if the relative difference between computed and predicted solution is smaller than the specified error bound. The stopping criterion recognizes oscillations in the convergence behavior and prevents premature stopping at local minima or maxima. A damped convergence curve is fit through the oscillating curve and the solver stops then regarding the damped convergence curve.



If the Krylov method (under LIR - Advanced Options) is activated, which is always the case in BatteryDict, the definition of **Error Bound** is somewhat different. Here, no prediction is made, instead the continuity between neighboring cells and the conservation of mass is checked. The maximal value is normalized by the mean flow and if this value is smaller than the **Error Bound** the simulation stops.

Use the **Maximum Iterations** value or the **Maximum Run Time (h)** stopping criteria causes the solver to stop if the maximal number of iterations and/or the maximal runtime (in hours) is exceeded.

When the solver stops because one of these criteria has been reached, no guarantee on the quality of solution can be given. In this case, a warning is printed into the report. The following possibilities might help:

- Check the corresponding .log file to see how large the residual values and the computed values are. If the computed values are in reasonable range and they do not have changed during the last iterations, you may decide to use the current result.
- Double-check the structure and parameter values. Unphysical parameters or too rough resolution of the structure (leading, e.g., to artificial unconnected components) can cause an iterative solver to fail.



Important! Note that all stopping criteria selected are applied for each time step separately. Thus, the maximal run time defined is not the maximal run time for the whole charging simulation, but for each time step.

Unfold **Advanced Options** to gain access to several advanced solver options.

The **Grid Type** decides what kind of tree structure is used for the simulation.

The default option is **LIR-Tree** and should always be used. The solver uses an adaptive grid structure called LIR-tree and needs up to 10 times less runtime and memory compared to the **Regular Grid** option.

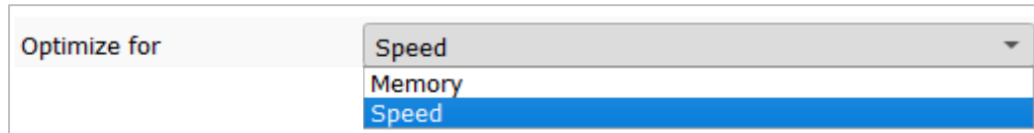
The solver can analyze the result field during the computation and improves the adaptive grid in places where more accuracy is needed. The LIR solver splits cells where a high gradient occurs.

Depending on the material parameters and geometry of the structure, the underlying mathematical problem can vary in complexity, thus influencing the behavior of the solver. The more complex the problem is, the more stable the solver settings should be.

With the **Relaxation** number, the solver is adjusted from **Stable** (which results in higher

number of iterations, slower time stepping, and longer solver run times), to **Fast**, which makes the solver run less iterations but implies the risk that the solver does not converge. The **Relaxation** is a parameter of the [SOR method](#) and must be between 0 and 2 to ensure convergence. For relaxation values smaller than one (<1.0), the simulation is more stable. For relaxation values larger than one (>1.0), the simulation converges faster.

The **LIR** solver can **Optimize for Speed** or **Memory**.

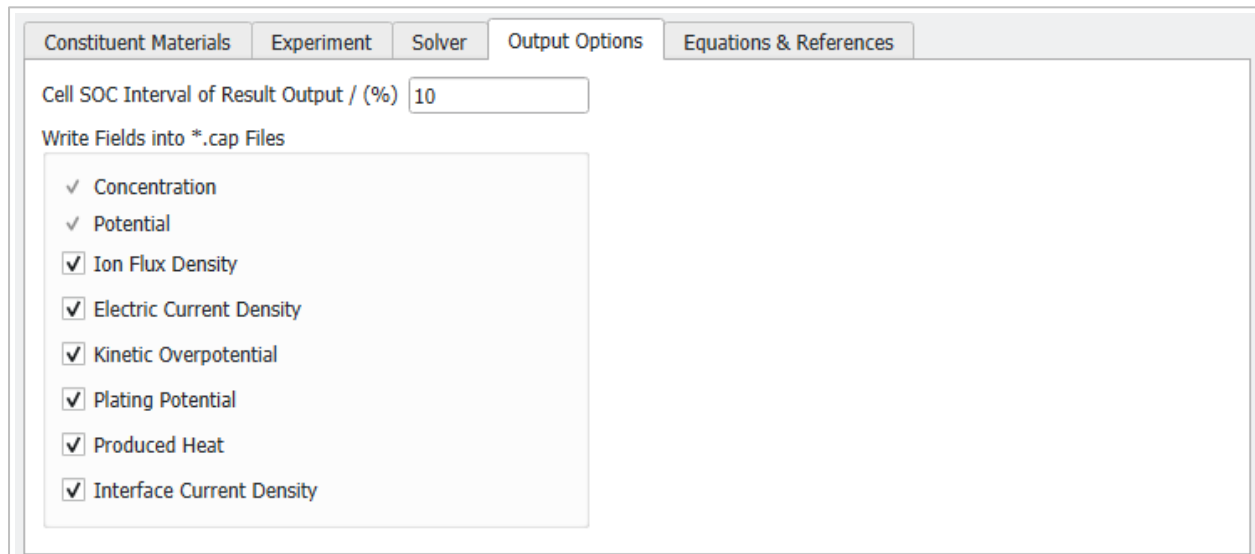


The image shows a software interface with a label 'Optimize for' and a dropdown menu. The dropdown menu is open, showing three options: 'Speed', 'Memory', and 'Speed'. The first 'Speed' option is highlighted in blue, indicating it is the selected option.

- If **Speed** is chosen, the solver constructs additional optimization structures. The runtime is decreased by up to 30% but requires up to 50% more memory compared to the other option.
- If **Memory** is chosen, the runtime is increased by up to 40% but the solver requires up to 50% less memory.

Output Options

Several options can be defined under the output options tab.



The image shows a software interface with several tabs: 'Constituent Materials', 'Experiment', 'Solver', 'Output Options', and 'Equations & References'. The 'Output Options' tab is active. It contains a text input field for 'Cell SOC Interval of Result Output / (%)' with the value '10'. Below this is a section titled 'Write Fields into *.cap Files' which contains a list of checkboxes, all of which are checked: 'Concentration', 'Potential', 'Ion Flux Density', 'Electric Current Density', 'Kinetic Overpotential', 'Plating Potential', 'Produced Heat', and 'Interface Current Density'.

✓ Cell SOC Interval of Result Output

The **Cell SOC interval of result output** defines the interval for the export of intermediate result files in percent of the cell state of charge.

✓ Write Fields into *.cap Files

Select which fields to write into the 3D result files (*.cap).

The lithium ion **Concentration** and the **Potential** are always written.

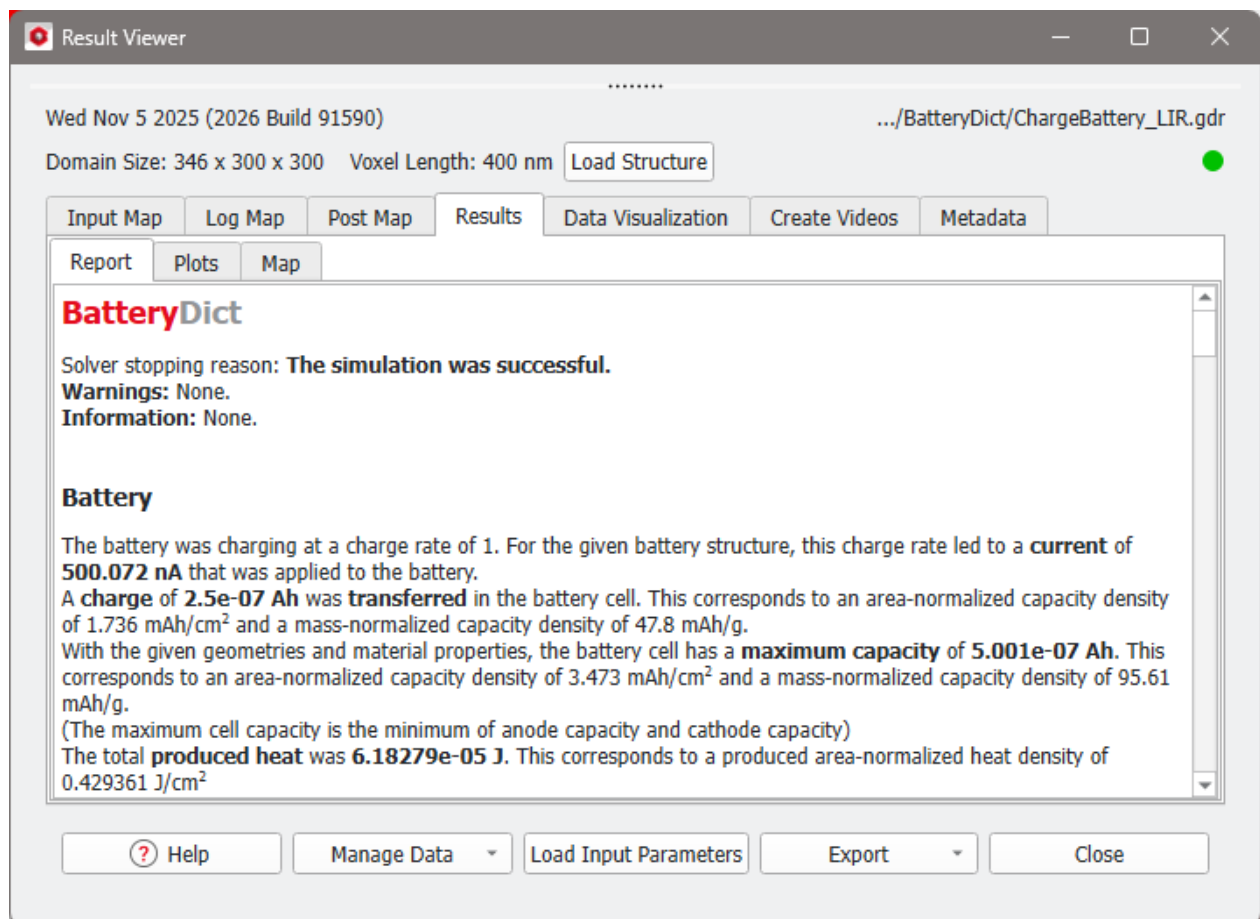
For the other fields, decide which ones you need. Deselecting fields saves disc space.

For a visualization of all result fields see [here](#)^[110].

Results

After a charging simulation has finished, a GeoDict result file (.gdr) is written and the **Result Viewer** of this result file automatically opens. The information of simulation result is shown, can be visualized, or further processed.

These results are accessible at any time by loading the .gdr file from the menu bar (**File - Open Results (*.gdr)**). The **Load Structure** button and the buttons available at the bottom of the **Result Viewer** are the same as for other result files and are explained in the Result Viewer chapter.



Charge simulation results:

- [Results Tab](#)^[94]
Find the computational results as report and as plots.
- [Data Visualization](#)^[107]
View your result fields in 3D.

Charge simulation results:

- [Create Video](#)^[111]
Animate your simulation results.
- [Result Folder](#)^[114]
Find out which files are saved in the result folder.

Results Tab

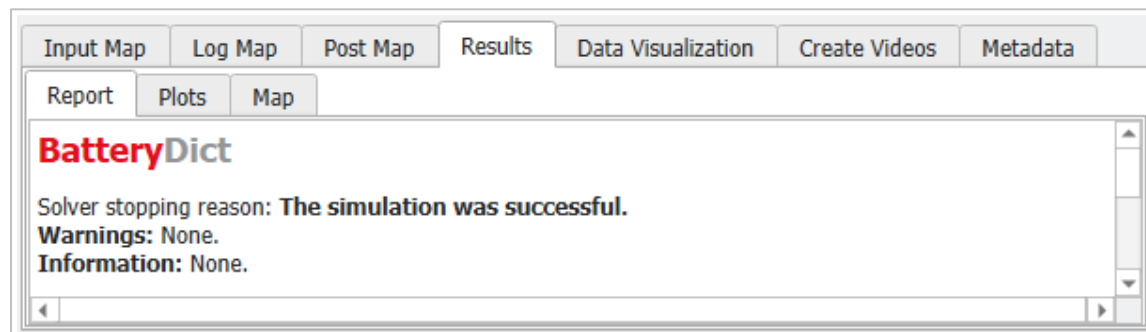
The **Results** tab shows the computational results in several ways, through the subtabs **Report**, **Plots**, and **Maps**.

Report

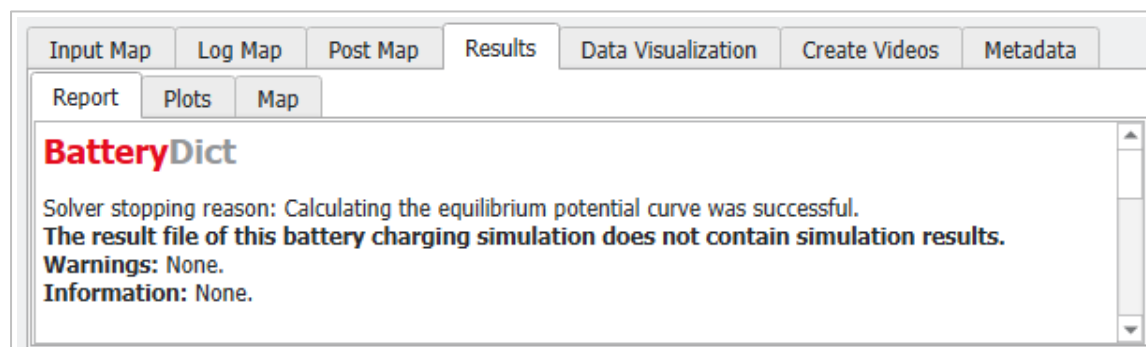
✓ Solver stopping reason

If the solver stopped unexpectedly before one of the stopping criteria defined was reached, the reason for this is shown on top of the report.

In the same way, warnings shown before starting the simulation (e.g., due to the parameters selected) and information about the simulation steps for a charging profile are shown there.



For example, if only the [potential curve in equilibrium](#)^[85] was computed, the first lines look as follows:



This report section is available for all [simulation types](#)^[85].

✓ Battery results

Under the results for **Battery**, the charge rate applied, the applied current, the charge transferred, the maximum capacity of the battery cell and the produced heat are listed.

This report section is available for the [simulation types](#)⁸⁵ **Fully Resolved**, **Homogenized**, and **Equilibrium Potential Curve**.

Battery

The battery was charging at a charge rate of 1. For the given battery structure, this charge rate led to a **current** of **500.072 nA** that was applied to the battery.
A **charge** of **2.5e-07 Ah** was **transferred** in the battery cell. This corresponds to an area-normalized capacity density of 1.736 mAh/cm² and a mass-normalized capacity density of 47.8 mAh/g.
With the given geometries and material properties, the battery cell has a **maximum capacity** of **5.001e-07 Ah**. This corresponds to an area-normalized capacity density of 3.473 mAh/cm² and a mass-normalized capacity density of 95.61 mAh/g.
(The maximum cell capacity is the minimum of anode capacity and cathode capacity)
The total **produced heat** was **6.18279e-05 J**. This corresponds to a produced area-normalized heat density of 0.429361 J/cm²

The maximum capacity of the battery cell, $Q_{B,max}$, is the minimum of the maximum anode capacity, $Q_{A,max}$, and the cathode capacity, $Q_{C,max}$:

$$Q_{B,max} = \min(Q_{A,max}, Q_{C,max}) \quad (51)$$

with

$$Q_{A,max} = l_V^3 \cdot F \cdot \sum_{V \in \{\text{Anode Active Material Voxels}\}} c_{max}(V) \quad (52)$$

and

$$Q_{C,max} = l_V^3 \cdot F \cdot \sum_{V \in \{\text{Cathode Active Material Voxels}\}} c_{max}(V) \quad (53)$$

l_V denotes hereby the voxel length of the structure, F the Faraday constant, and $c_{max}(V)$ the maximum removable lithium concentration of each active material voxel.

✓ Time dependent charge curve table

The table **Time dependent charge curve** below shows part of the time dependent values in a clearly arranged way.

This report section is available for the [simulation types](#)⁸⁵ **Fully Resolved** and **Homogenized**.

Time dependent charge curve:

In the following, we show the **time dependence** of the battery's cell potential, state of charge, and transferred charge. The potential estimation is not given at the same time steps as the values from the full simulation. Therefore, in this table, it is represented by interpolated values. More details are shown in the plot. Moreover, the full data can be found in the result map.

Time / (h:mm:ss)	Cell state of charge / (%)	Anode state of charge / (%)	Cathode state of charge / (%)	Cell potential / (V)	Equilibrium cell potential at cell SOC / (V)	Charge rate	Transferred charge / (Ah)	Transferred area-normalized charge capacity density / (mAh/cm ²)	Transferred mass-normalized charge capacity density / (mAh/g)
0:00:00	20	20	80.65	3.528	3.528	0	0	0	0
0:00:00	20	20	80.65	3.584	3.528	1	0	0	0
0:00:30	20.83	20.83	79.85	3.604	3.539	1	4.167e-09	0.02894	0.7967
0:01:00	21.67	21.67	79.04	3.615	3.546	1	8.335e-09	0.05788	1.593
0:01:30	22.5	22.5	78.24	3.624	3.553	1	1.25e-08	0.08682	2.39
0:02:00	23.33	23.33	77.43	3.631	3.56	1	1.667e-08	0.1158	3.187
0:02:30	24.17	24.17	76.62	3.637	3.568	1	2.084e-08	0.1447	3.984

✓ Meso parameters

The **Meso parameters** are computed for both, the cathode and the anode, as well as the separator. The meso parameters can then be loaded into the [Charge Homogenized Battery](#) ¹²⁰ dialog to run fast homogenized simulations eliminating the need to compute the effective parameters each time.

This report section is available for the [simulation types](#) ⁸⁵ **Homogenized** and **Calculate Homogenized Parameters**.

Meso parameters of the anode		Meso parameters of the cathode		Meso parameters of the separator	
Electrolyte		Electrolyte		Electrolyte	
Volume Fraction	0.255658	Volume Fraction	0.305963	Volume Fraction	0.42
Effective Ionic Conductivity	0.0817654 S/m	Effective Ionic Conductivity	0.15596 S/m	Effective Ionic Conductivity	0.256667 S/m
Effective Ionic Diffusivity	2.326e-11 m ² /s	Effective Ionic Diffusivity	4.44362e-11 m ² /s	Effective Ionic Diffusivity	7e-11 m ² /s
Volume	8.64e-13 m ³	Volume	8.64e-13 m ³		
Electronic Network (Binder + Active Material)		Electronic Network (Binder + Active Material)			
Effective Electronic Conductivity	1122.26 S/m	Effective Electronic Conductivity	12.0798 S/m		
Active Material 1 (Graphite)		Active Material 1 (NMC333)			
Particle Radius	4.47614e-06 m	Particle Radius	3.91099e-06 m		
Surface Area	2.82247e-07 m ²	Surface Area	3.92143e-07 m ²		
Volume	6.00141e-13 m ³	Volume	5.42955e-13 m ³		
Specific Surface Area	326674 m ² /m ³	Specific Surface Area	453869 m ² /m ³		
Volume Fraction of Unconnected Material	2.45276e-06	Volume Fraction of Unconnected Material	3.53621e-06		

✓ Results for electrodes

The connectivity and maximal capacity is shown for both electrodes, respectively.

This report section is available for all [simulation types](#) ⁸⁵.

Anode

Taking only the **connected active material** into account, the **capacity** of the anode is **5.00071e-07 Ah**.
The **unconnected active material** leads to a **capacity** loss of **1.22656e-12 Ah** in the anode.
The **maximal capacity** of the anode material is **5.001e-07 Ah** (the sum of the capacities contributed by connected as well as unconnected active material).

Cathode

Taking only the **connected active material** into account, the **capacity** of the cathode is **5.16958e-07 Ah**.
The **unconnected active material** leads to a **capacity** loss of **1.82808e-12 Ah** in the cathode.
The **maximal capacity** of the cathode material is **5.17e-07 Ah** (the sum of the capacities contributed by connected as well as unconnected active material).

✓ Analyze Battery results

At the end of the **Results-Report** subtab for all **Charge Battery** simulations information about the volumes as already seen in [Design Battery](#)^[51] or [Analyze Battery](#)^[58] are found.

This report section is available for all [simulation types](#)^[85].

Plots

Under the **Results - Plots** subtab, several standard plots for the visualization of the BatteryDict simulation results are available.

The tabs [Charge curves](#)^[97] and [Battery geometry](#)^[106] are available for all [simulation types](#)^[85].

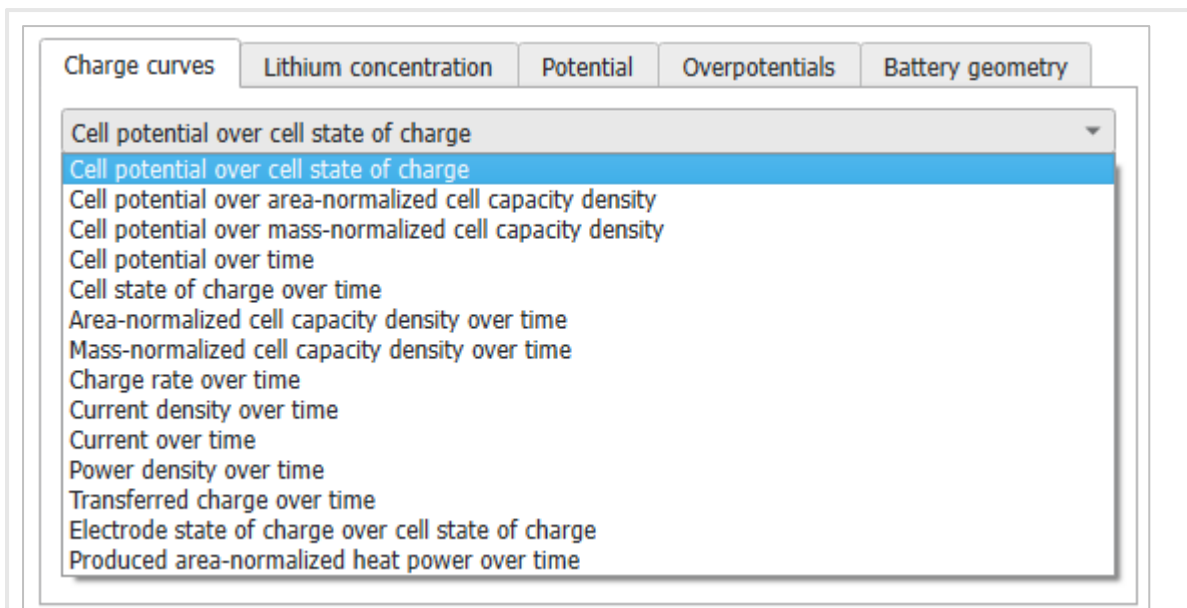
The [Overpotential](#)^[105] plots are available for **Homogenized** and **Fully Resolved** simulations.

For the simulation type **Fully Resolved** additionally the plots for [Lithium concentration](#)^[103] and [Potential](#)^[104] are available. For the homogenized simulation, the voxel and slice-based information shown on these two tabs is not available.

Find out more details about editing plots in the Result Viewer chapter.

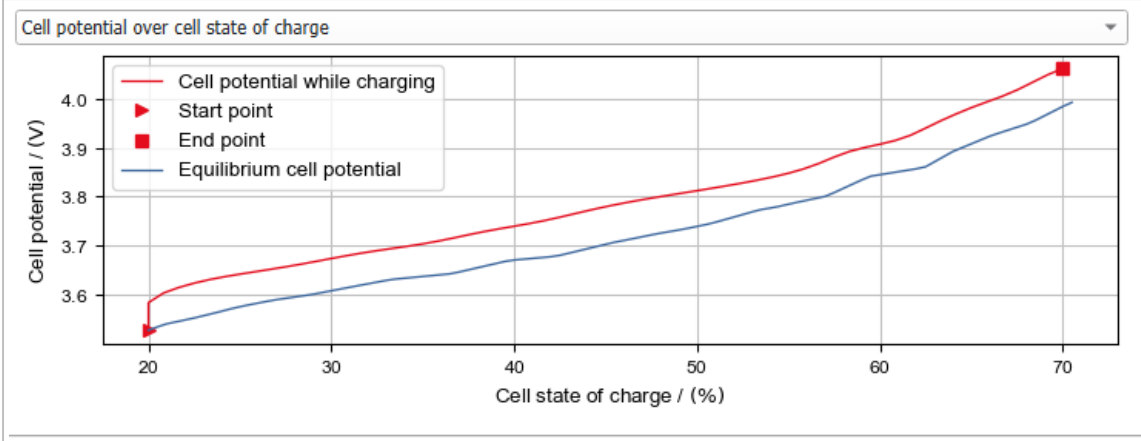
✓ Charge curves

On the tab **Charge curves** you can select different charge curves from the pull-down menu:



- Cell potential over
 - [cell state of charge](#)^[98]
 - [area-normalized cell capacity density](#)^[99]
 - [mass-normalized cell capacity density](#)^[99]
 - [time](#)^[101]
- [Cell state of charge over time](#)^[101]
- Area-normalized cell capacity density over time
- Mass-normalized cell capacity density over time
- [Charge rate over time](#)^[102]
- [Current density over time](#)^[102]
- [Current over time](#)^[102]
- Power density over time
- Transferred charge over time
- Electrode state of charge over cell state of charge
- [Produced area-normalized heat power over time](#)^[102]

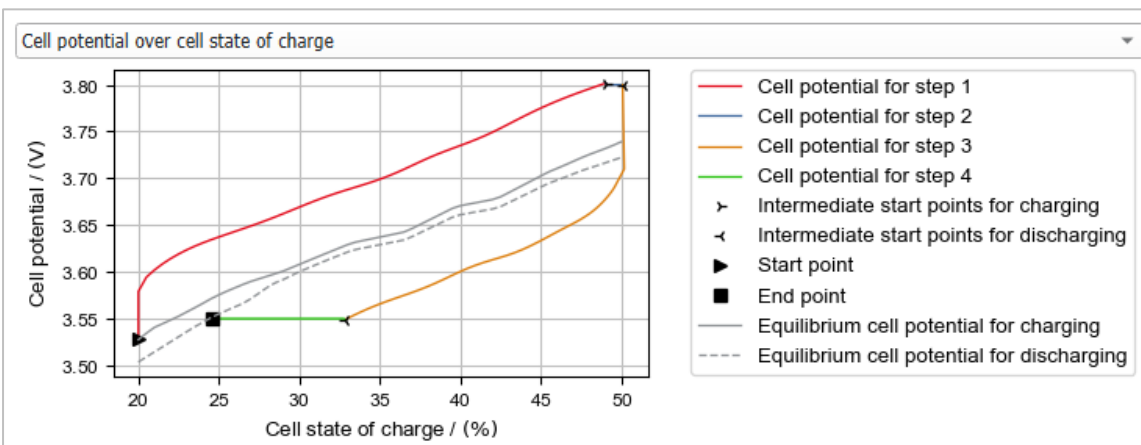
In the **Cell potential over cell state of charge** plot the cell potential while charging or discharging is compared to the cell potential in equilibrium, i.e., while loading in infinite time. When the battery is charged or discharged slowly over an infinite amount of time, it remains in a state of equilibrium. However, when the process is done in a finite amount of time, the battery deviates from this equilibrium state.



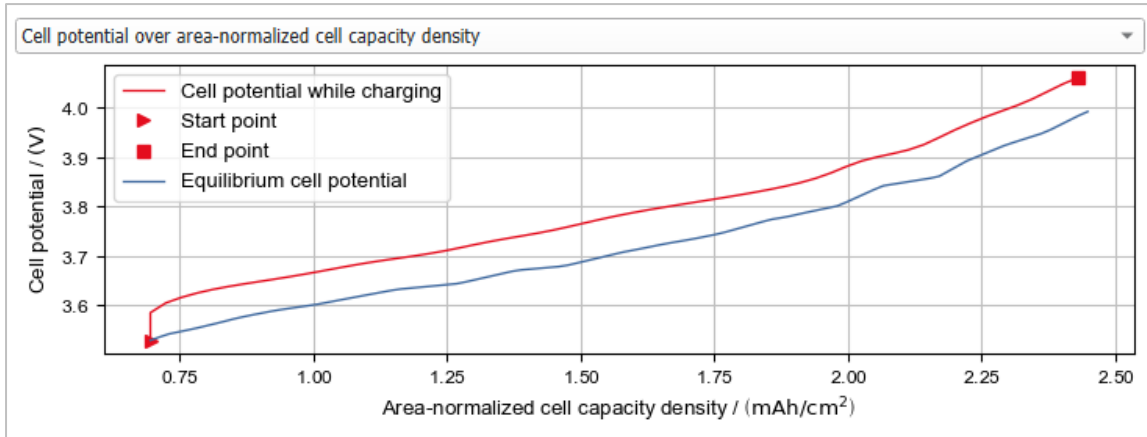
During charging, the curves always show higher values than the equilibrium curve, indicating that charging the battery requires a higher potential than what is observed in equilibrium. On the other hand, during discharging, the curves are always below the equilibrium curve. If **Equilibrium Potential Curve** or **Calculate Homogenized Parameters** was chosen as [simulation type](#)^[85], only the equilibrium curve is shown.

In case a [charging profile](#)^[83] was selected for the simulation, the cell potential is shown for each simulation step in the profile in a different color. If the charging profile consists of charging and discharging steps, the equilibrium cell potential is shown both for charging and discharging.

Start and end point of the whole simulation as well as intermediate start points for the steps are shown in the graph.



The **Cell potential over mass-normalized cell capacity density** and **Cell potential over areal-normalized cell capacity density** plots show the potential depending on the cell capacity density.



The initial cell capacity Q_{start} can be computed from the initial cell SOC and the total cell capacity Q_C . The final cell capacity Q_{fin} is computed analogously.

$$Q_{start} = SOC_{start} \cdot Q_C \text{ and } Q_{fin} = SOC_{fin} \cdot Q_C \quad (54)$$

The transferred charge is the difference between the initial and the final cell capacity.

$$Q_{trans} = Q_{fin} - Q_{start} \quad (55)$$

The initial mass cell capacity density $Q_{start,mass}$ can then be computed from the initial cell capacity and the mass M of the cell. The final mass cell capacity $Q_{fin,mass}$ is again computed analogously.

$$Q_{start,mass} = \frac{Q_{start}}{M} \text{ and } Q_{fin,mass} = \frac{Q_{fin}}{M} \quad (56)$$

The **cell potential over area-normalized cell capacity density** takes the SOC value into account. If for example the starting cell SOC is 20%, the starting cell capacity is $20\% \cdot \text{Total Cell Capacity}$ (also see equation (54) above). This way, the plot cannot have negative values for charging profiles.

For the initial areal cell capacity density $Q_{start,areal}$ follows analogously:

$$Q_{start,areal} = \frac{Q_{start}}{\text{Electrode Area}} = \frac{SOC_{start} \cdot Q_C}{(NY \cdot NZ \cdot VL)^2} \quad (57)$$

For the final areal cell capacity density $Q_{fin,areal}$ follows:

$$Q_{fin,areal} = \frac{Q_{fin}}{Electrode\ Area} = \frac{SOC_{fin} \cdot Q_c}{(NY \cdot NZ \cdot VL)^2} \quad (58)$$

where NY and NZ are the number of voxels in Y- and Z-direction and VL is the voxel length.

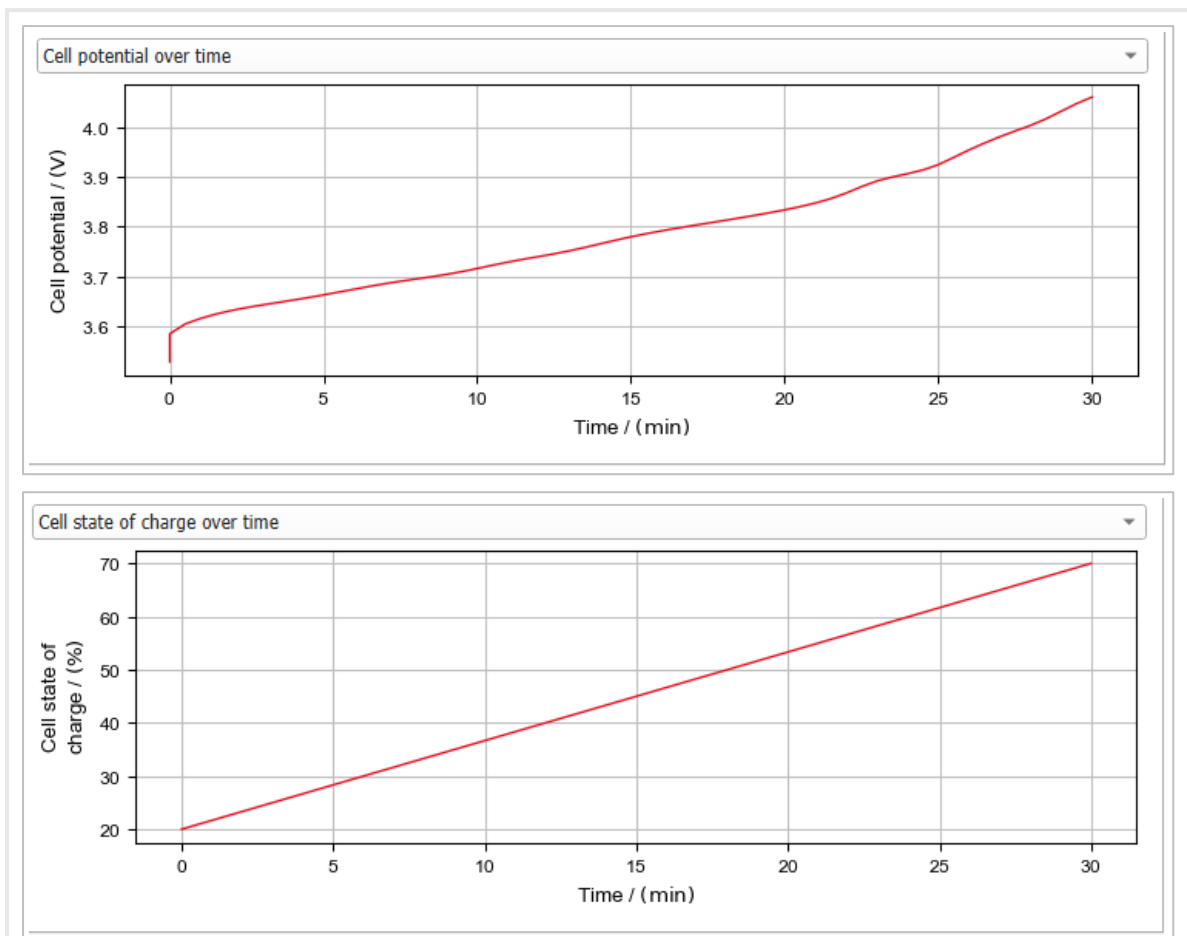
The total cell capacity Q_c (TotalCapacity) and the transferred charge can be found under the **Maps** tab in the **Battery** section. The **Mass** is given under **InputStructure**. The domain size and voxel length are given at the top.

Domain Size: 346 x 300 x 300 Voxel Length: 400 nm			Load Structure
Input Map	Log Map	Post Map	Results
Data Visualization	Create Videos	Metadata	
Report	Plots	Map	
Key	Unit	Value	
ErrorMessage		The simulation was successful.	
CellType		BatteryCell	
FoundGeoParameters			
Battery			
VolumeFractions			
Volumes			
TotalCapacity	Ah	5.000719427e-07	
ConnectedCapacity	Ah	5.000707161e-07	
UnconnectedCapacity	Ah	1.82807544e-12	
TransferredCharge	Ah	2.500359713e-07	
SignedTransferredCharge	Ah	2.500359713e-07	
Anode			
Cathode			
EquilibriumPotential			
TimeDependentValues			
TimeDependentFields			
InputStructure			
Mass	kg	5.230432783e-09	

For our example, the SOC_{fin} is 70%, the total cell capacity Q_c is about 5e-07 Ah, the domain size is 346x300x300 voxel with a voxel length of 400 nm. Thus, for the final areal cell capacity follows:

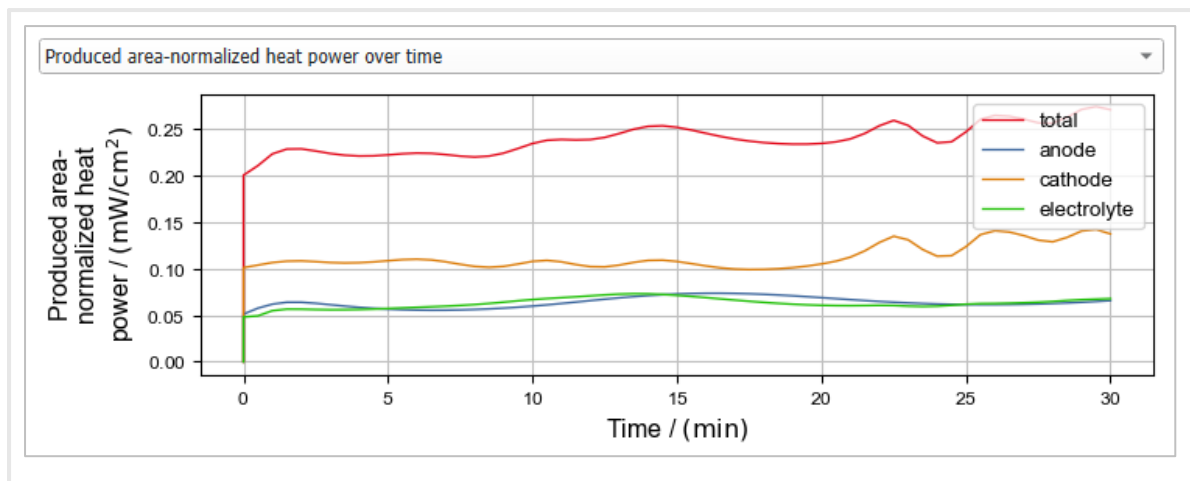
$$Q_{fin,areal} = \frac{0.7 \cdot 5e-07\ Ah}{(300 \cdot 300 \cdot 400\ nm)^2} = \frac{3500e-07\ mAh}{0,000144\ cm^2} = 2.43 \frac{mAh}{cm^2} \quad (59) \text{ Example}$$

Due to simulation with a constant charge rate in the example shown, the state of charge increases linearly with the simulated time. The trend of the **Cell potential over time** is therefore the same as for the **Cell potential over Cell state of charge** and the **Cell state of charge over Time** is a straight line.



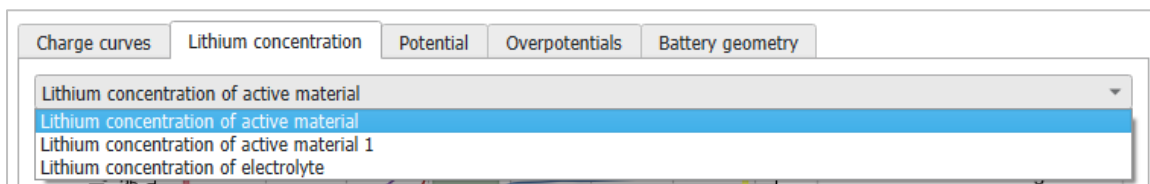
The **Current over time**, as well as the **Current density over time**, and the **Charge rate over time** are constant for the example shown.

The **Produced area-normalized heat power over time** can also be visualized. During charging and discharging, heat is produced. This causes loss of energy and reduces the charging and discharging efficiency of the battery. Additionally, strong heat production at a single spot can cause a security problem, for example if a polymer separator is melting and a short circuit can occur. This plot displays the areal heat power produced over time. In contrast, a [3D visualization](#)^[110] can reveal the specific locations of heat production, helping you determine whether the produced heat is evenly distributed or concentrated in small areas.

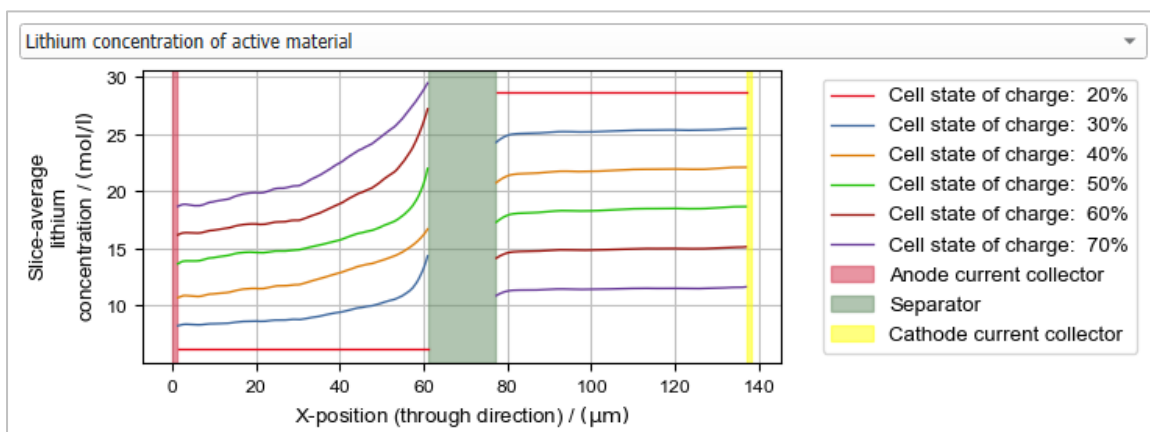


✓ Lithium concentration

The **Lithium concentration** tab shows the mean concentration of lithium ions for each slice in y-z-direction for a constant x value. It can be displayed as **Lithium concentration of electrolyte**, **Lithium concentration of active material** (for all active materials together), or of each active material separately (Lithium concentration of active material 1, Lithium concentration of active material 2, etc.).



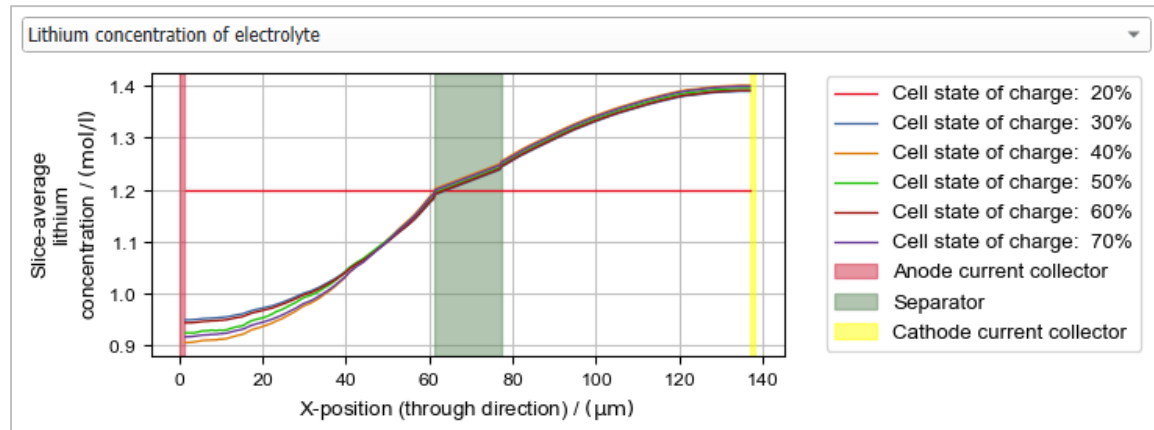
A separate curve is shown in these plots for each state of charge with an intermediate result available. As can be seen in the following plot, the concentration of lithium ions in the cathode (right-part of the plot) is decreasing during charging of the battery, while the concentration in the anode is increasing.



At the beginning of the simulation, the Li-ion concentration of the electrochemically connected part of the electrolyte is constant throughout the battery. Its value is the equilibrium Lithium concentration specified in the settings.

While charging, the cathode releases Li-ions into the electrolyte, causing the Li-ion concentration to increase on the cathode side. Simultaneously, the Li-ions intercalate into the anode.

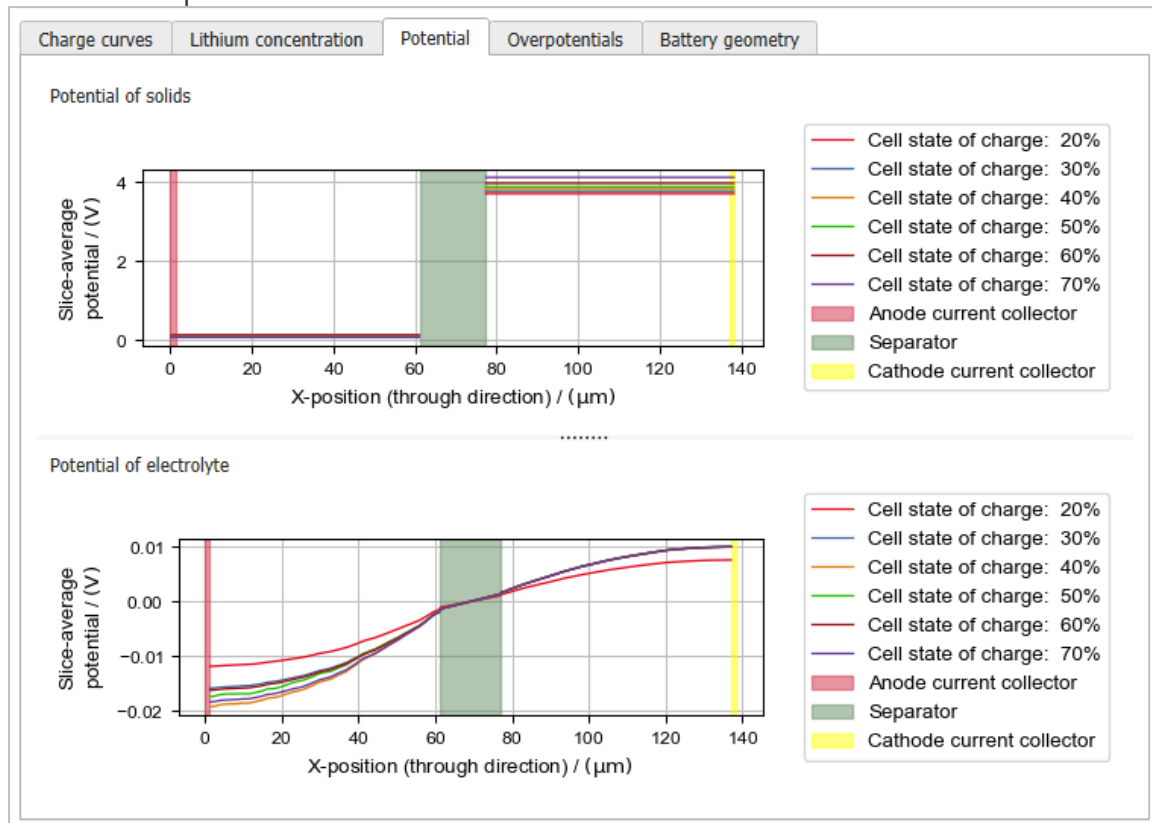
Since the diffusion of the Li-ions takes some time, the gradient of the Li-ion concentration in the electrolyte is visible in the example.



✓ Potential

The **Potential** tab shows the mean potential for each slice in y- and z-direction for the solid part of the battery, as well as for the electrolyte. All potentials are calculated with respect to an imagined lithium reference electrode in the center of the separator.

Again, for each state of charge with an intermediate result available, a separate curve is shown in the plot.



In the example shown here, for each time step, the potential in the solid is constant within each electrode. This indicates that the conductivity is high enough. If the conductivity were much smaller, the potential would exhibit a drop within one electrode.

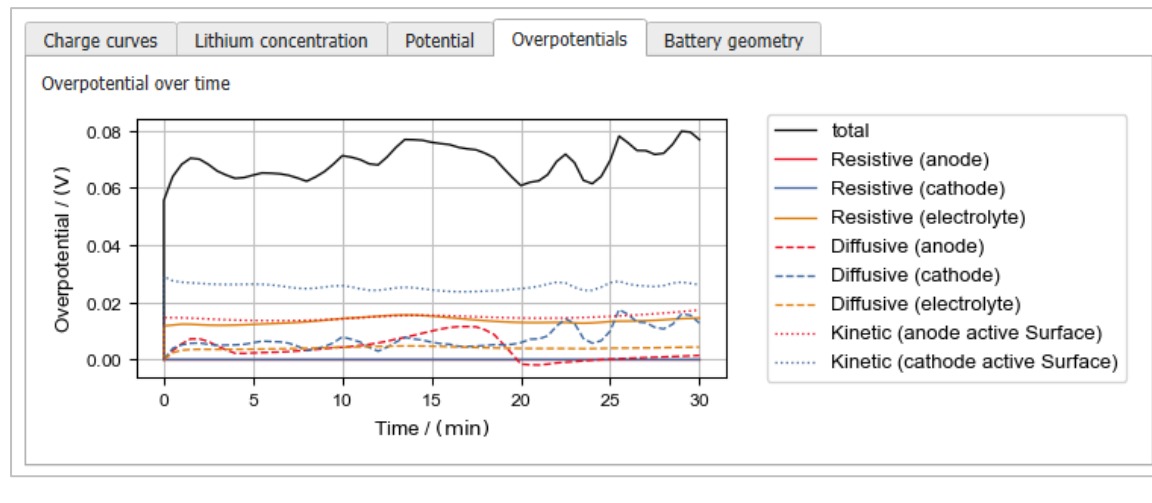
In this example, the solver calculates the battery charging by applying a constant electric current. The necessary potential difference for keeping up the current is determined from the electric current in the solids, the ionic current in the electrolyte, and the overpotentials on the boundary of electrolyte and active material.

The current is only dependent on the potential difference and not on the total potential offset. The latter can be chosen freely.

For the potential of the electrolyte, a gradient is visible between the anode current collector and the cathode current collector. This gradient increases for higher charge rates and the potential grows from left to right. This is caused by the charge current that is driven by the ions resolved in the electrolyte. The charge current leads to a growing potential in flow direction because the ionic conductivity is not zero. The lower the ionic conductivity, the stronger the growth of the electrolyte potential in flow direction.

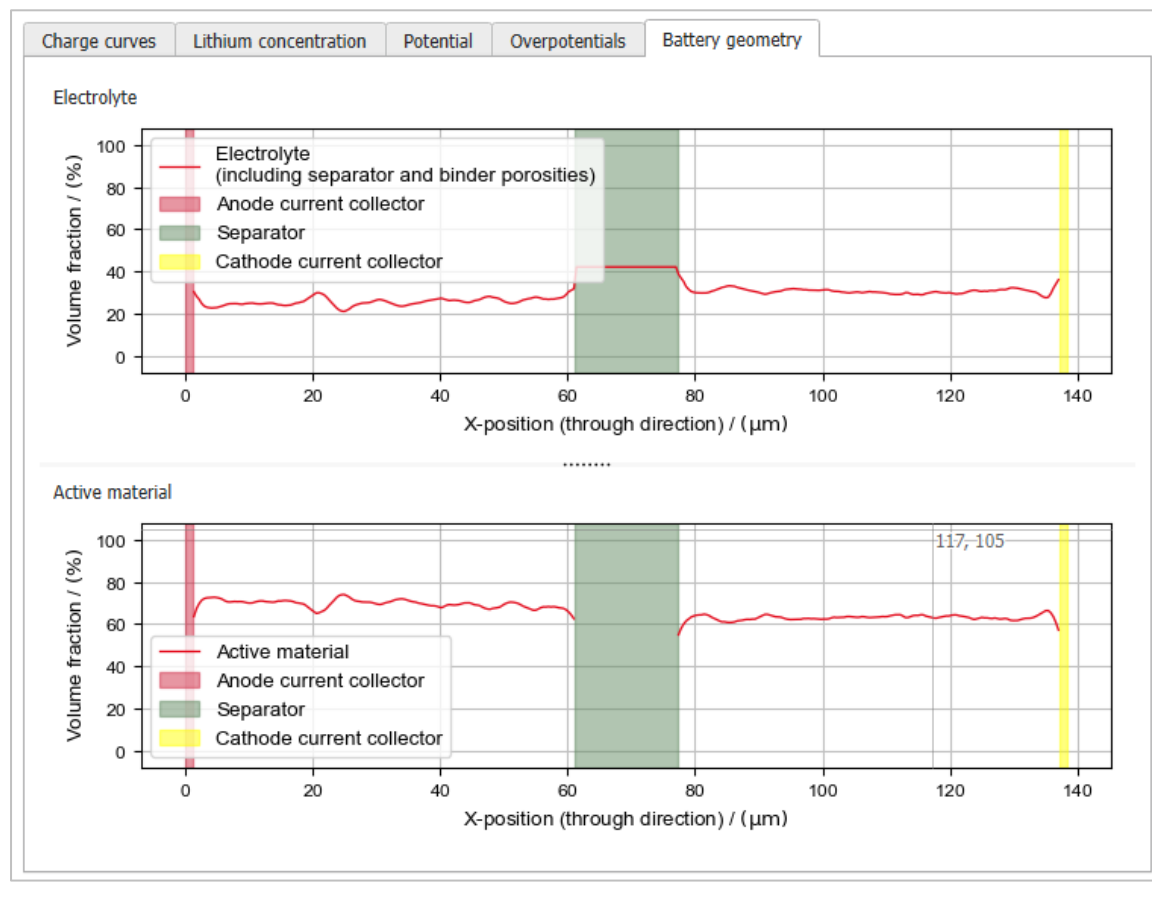
✓ Overpotentials

On the **Overpotentials** tab, the evolution of the different overpotentials over time is visualized. For an explanation of the overpotentials also see [here](#)²⁶.



✓ Battery geometry

The **Battery geometry** tab shows the mean of volume fraction of electrolyte and active material for each slice in x-direction.



Map

The **Results - Map** subtab lists all values available in the **Results - Report** subtab of the **Result Viewer** of the GeoDict result file and other information about the computation results.

Input Map Log Map Post Map Results Data Visualization Create Videos Metadata			
Report Plots Map			
Key	Unit	Value	
ErrorMessage		The simulation was successful.	
CellType		BatteryCell	
FoundGeoParameters			
Battery			
Anode			
Cathode			
EquilibriumPotential			
CellStateOfCharge	%	0, 0.5, 1, 1.5, 2, 2.5, 3, 3.5, 4, 4.5, 5, 5.5, 6, 6.5, 7, 7.5, 8, 8.5, 9, 9.5, 10, 10.5, 11, 11.5, 12, 12.5, 13...	
AnodeStateOfCharge	%	0, 0.5, 1, 1.5, 2, 2.5, 3, 3.5, 4, 4.5, 5, 5.5, 6, 6.5, 7, 7.5, 8, 8.5, 9, 9.5, 10, 10.5, 11, 11.5, 12, 12.5, 13...	
CathodeStateOfCharge	%	100, 99.51633371, 99.03266743, 98.54900114, 98.06533486, 97.58166857, 97.09800229, 96.614336, ...	
CellPotential	V	2.07784, 2.166022233, 2.259924453, 2.35620437, 2.448234115, 2.531198154, 2.606702241, 2.68520...	
AnodePotential	V	0.43667, 0.4191210135, 0.401572027, 0.3840230405, 0.3664740541, 0.3489250676, 0.3313760811, 0...	
CathodePotential	V	2.51451, 2.585143247, 2.66149648, 2.74022741, 2.814708169, 2.880123222, 2.938078322, 2.999032...	
TimeDependentValues			
Time	s	0, 0, 30, 60, 90, 120, 150, 180, 210, 240, 270, 300, 330, 360, 390, 420, 450, 480, 510, 540, 570, 600,...	
TimeStep	s	0, 30, ...	
CellPotential	V	3.527512179, 3.58374, 3.6036, 3.61473, 3.62356, 3.63074, 3.6367, 3.64191, 3.64684, 3.65175, 3.656...	
CellStateOfCharge	%	20, 20, 20.83333377, 21.66666792, 22.50000191, 23.33333618, 24.1666706, 25.00000508, 25.83333...	
AnodeStateOfCharge	%	20, 20, 20.83333545, 21.66667265, 22.50000824, 23.33334544, 24.16668284, 25.00002022, 25.8333...	
CathodeStateOfCharge	%	80.65334859, 80.65334859, 79.84723811, 79.04112768, 78.23501709, 77.42890665, 76.62279617, 75...	
TransferredCharge	Ah	0, 0, 4.167266189e-09, 8.334532378e-09, 1.250179857e-08, 1.666906476e-08, 2.083633094e-08, 2.5...	
Current	A	0, 5.000719427e-07, 5.000719427e-07, 5.000719427e-07, 5.000719427e-07, 5.000719427e-07, 5.0007...	
ProducedHeat			
Overpotentials			
TimeDependentFields			
InputStructure			

Data Visualization

Solution files can be accessed via the **Data Visualization** tab. The number of available solution files depends on the length of the interval selected for output of intermediate results in [Output Options](#) ⁹².

Input Map Log Map Post Map Results Data Visualization Create Videos Metadata

Time Steps

Choose Time Step

6: Cell SOC 70%

Time Step 6 of 6.

Cell State of Charge: 70%.

Time: 30 min.

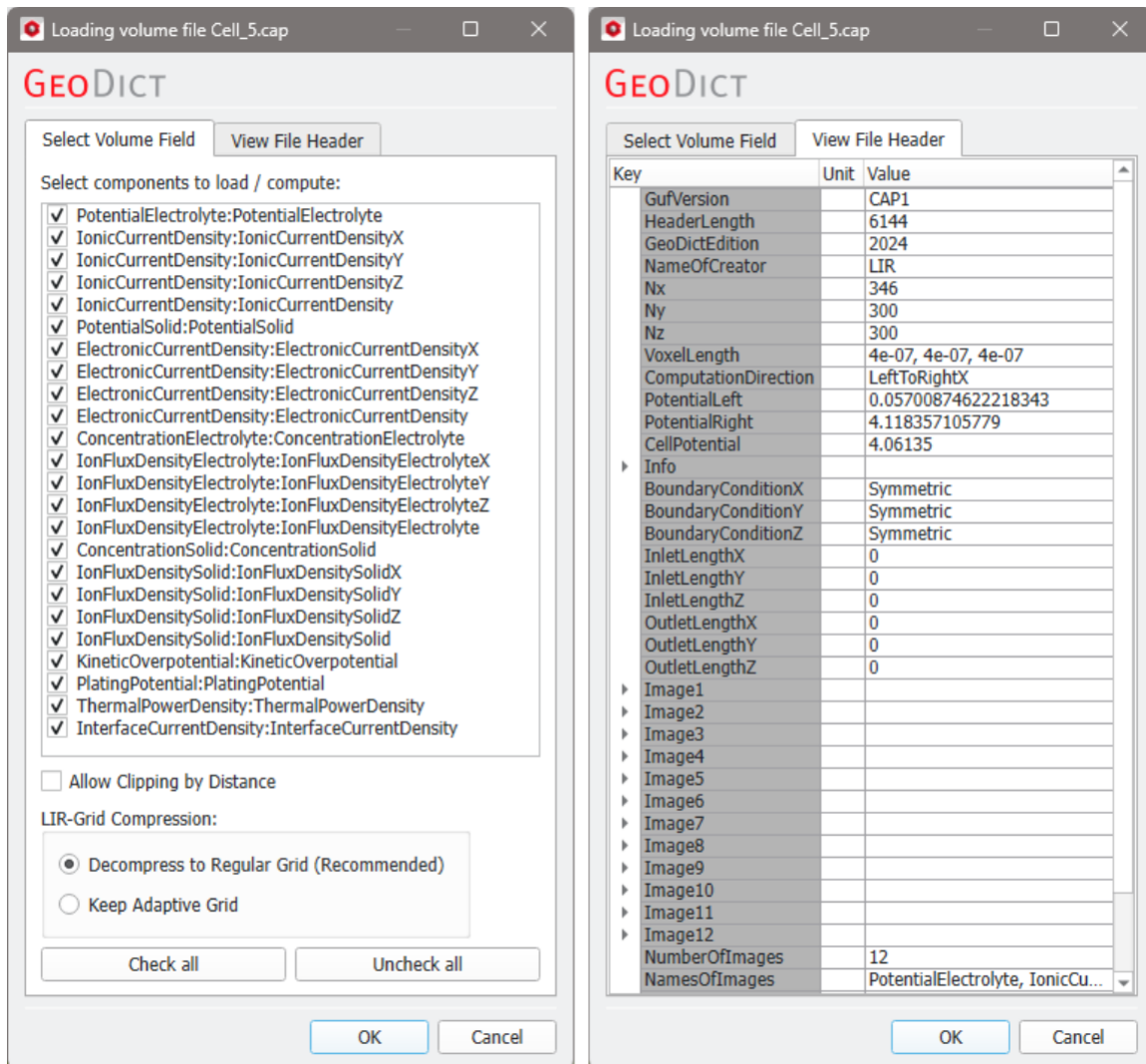
Load Solution File of Time Step 6

Load Cell_5.cap

✓ Load 3D result fields

For instance, let us select the solution file at a state of charge of 70%. For the example shown here, we just need to select time step 6 (6: Cell SOC 70%).

By clicking **Load Cell_5.cap**, the available volume fields (tab **Select Volume Fields**) of the file can be selected. Additionally, you may have a look at the file header of the result file (**View File Header**).



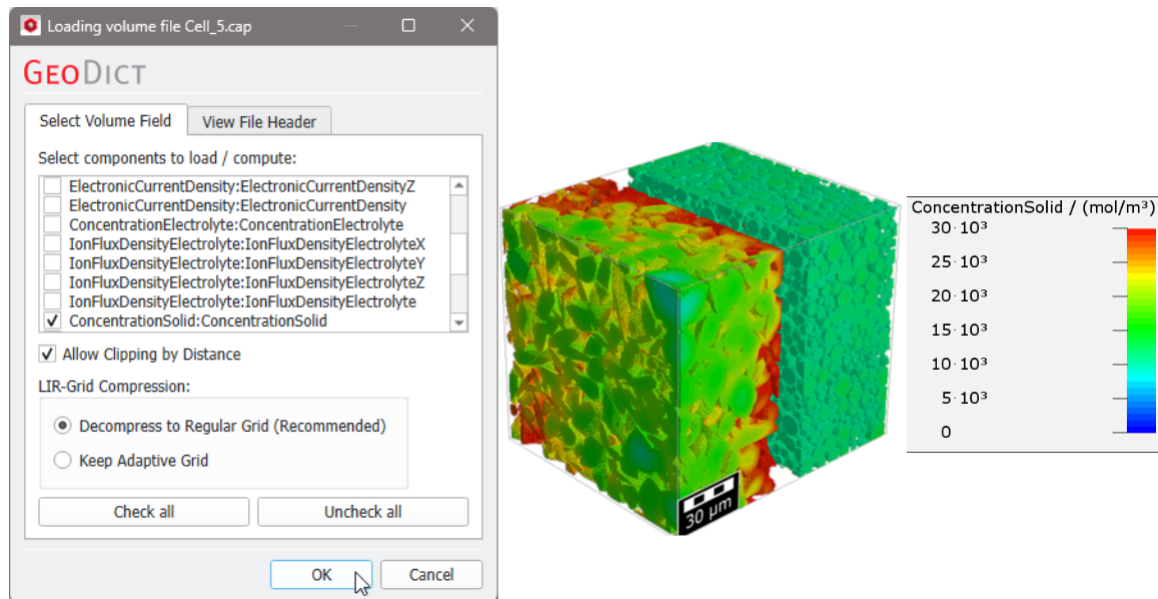
Only the fields selected under the [Output Options](#) ⁹² tab are available.

To reduce loading time, load only the desired fields. For example, you can only load the concentration in the solid part of the battery. In this case, first click **Uncheck all**.

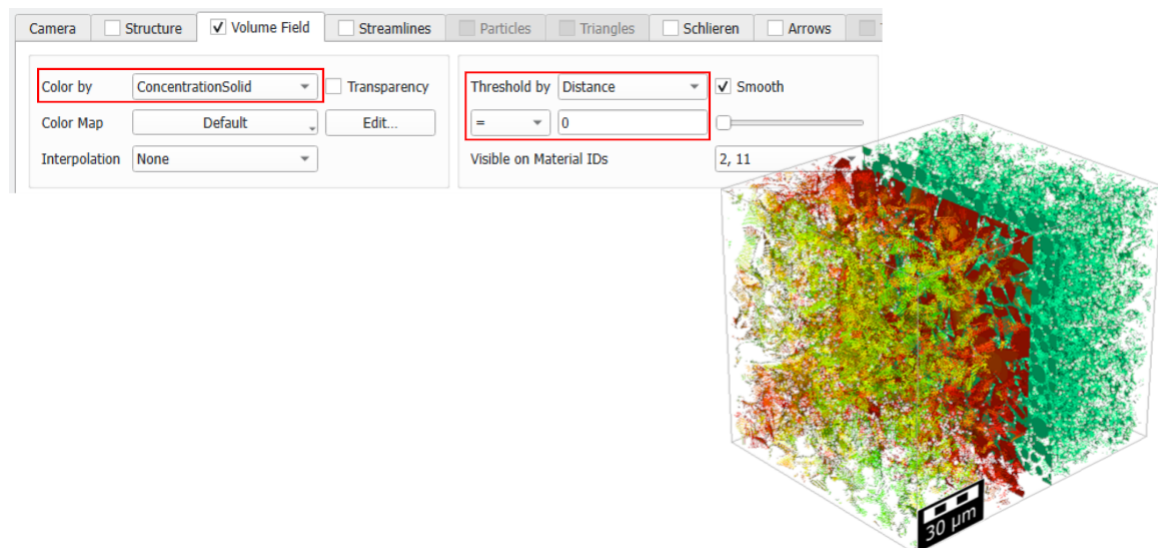
Then, select the field to visualize, in our example the **ConcentrationSolid:ConcentrationSolid**. After clicking **OK**, the selected field is loaded into the GeoDict main window.

The concentration field of lithium ions for the active materials is visualized here. Various Visualization options are available for 3D result fields.

The concentration gradient in the anode (left part of the battery) is in the example shown higher than in the cathode (right part of the battery).



Check **Allow clipping by distance** to create a distance map regarding the solid material. Its value is zero on the surface of the solid material, inside the material the values are negative and outside positive. This allows clipping any result field by its distance to the surface of the solid material. Below, the concentration solid field is thresholded by distance. Here only concentration values for the active materials are shown, when they have exactly 0 distance to the active materials, meaning only the active material surfaces. Learn more about thresholding volume fields in the Visualization chapter.

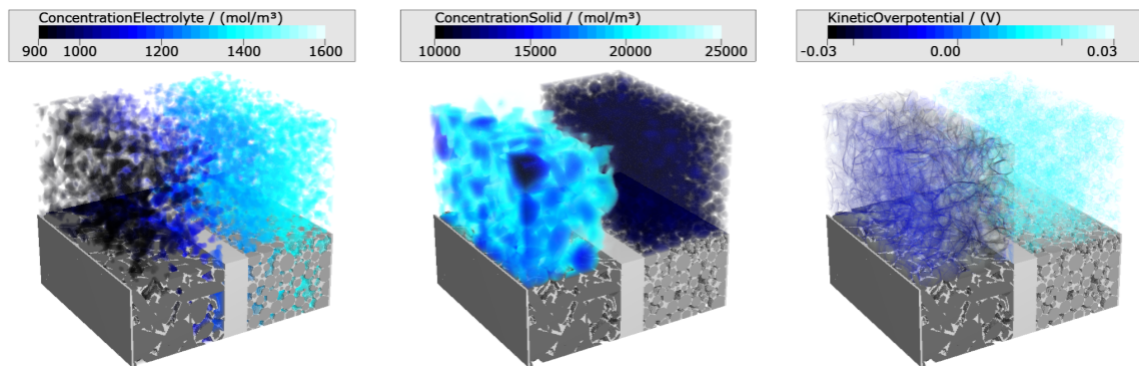


Check **Keep existing Volume Fields** if you repeat loading result fields for another time step or have other previously loaded volume fields in memory that you want to keep. If this box is not checked, previously loaded volume fields are discarded.

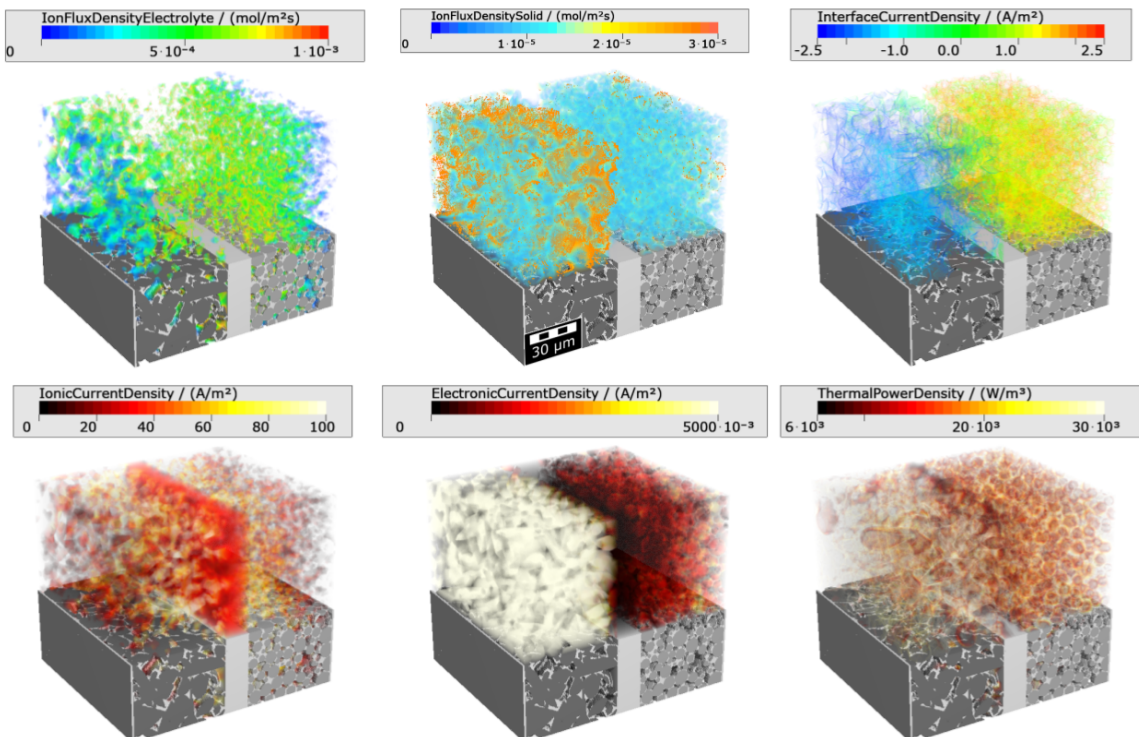
If the simulation was run with LIR solver, volume fields are stored in a compressed way. Check **Decompress fields**, to be able to use all visualization features. Uncheck the box to visualize the adaptive grid structure used for the computation. In this case, not all visualization features can be used. Learn more about grid visualization in the Visualization chapter.

✓ Available Result Fields

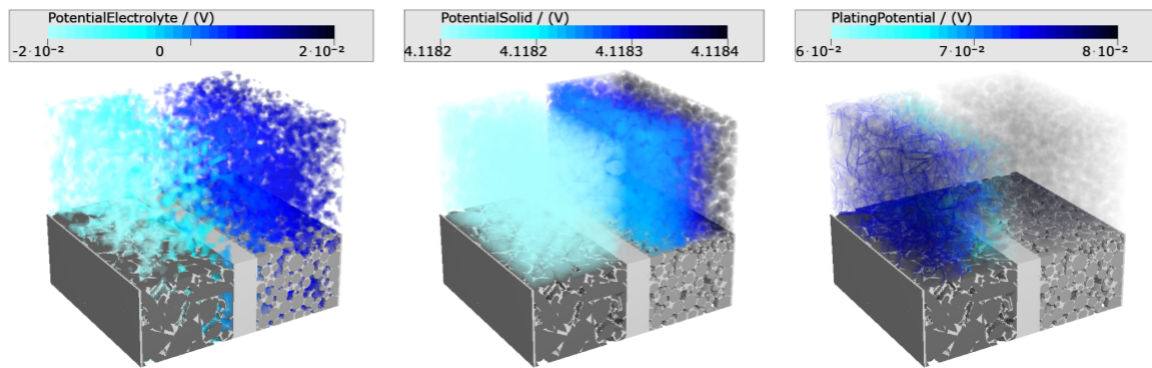
Many different 3D result fields are available. The fields in the examples below are visualized with different color maps and transparency settings. How to do that is described in the Visualization chapter. Below find the fields for concentration and kinetic overpotential:



The following density properties are available as 3D result fields:



Below find the result fields available regarding potential:



Lithium plating is a risk of battery degradation. It can occur especially at high charge rates or low operational temperatures and is indicated by values of the plating potential below 0 V. In the example above, all values are greater than 0. Thus, no plating should happen. We only visualized the anode, because plating usually does not take place in the cathode.

The plating risk is experimentally determined by measuring the potential difference between the anode and a reference lithium electrode.

In the simulation, the electrolyte potential φ_e (**PotentialElectrolyte**) is fixed in the center of the separator to 0 V. Therefore, the potential in the electrodes φ_s (**PotentialSolid**) can be interpreted as local potential difference with respect to a reference electrode.

With the volume field **PlatingPotential**, even more detailed information on the plating risk is provided: The **PlatingPotential** describes the local plating condition, given by $\varphi_s - \varphi_e$. Therefore, it provides a more exact estimation of the plating risk than **PotentialSolid** alone as it considers local variations of the electrolyte potential φ_e .

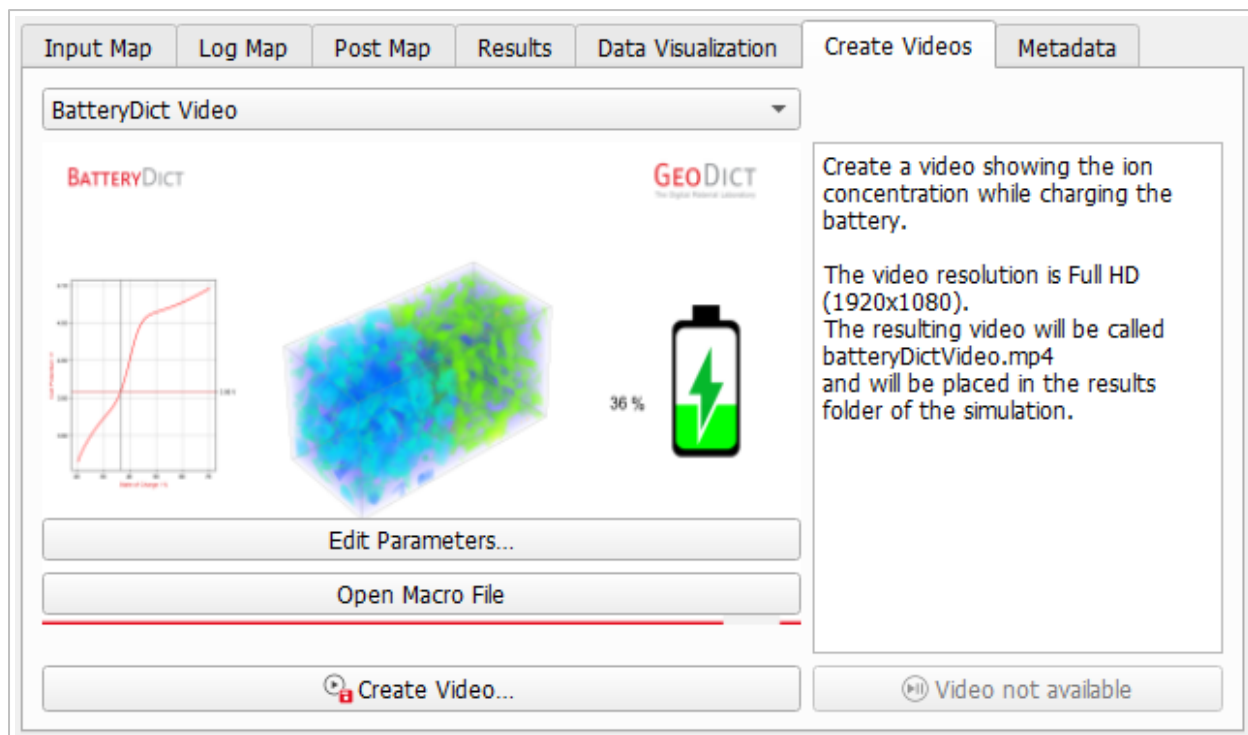
The plating potential is calculated by

$$\eta = \varphi_s - \varphi_e - U_0 \quad (60)$$

This value is written into the surface voxels of the active material. If there are multiple electrolyte voxels in the immediate vicinity, they are averaged arithmetically.

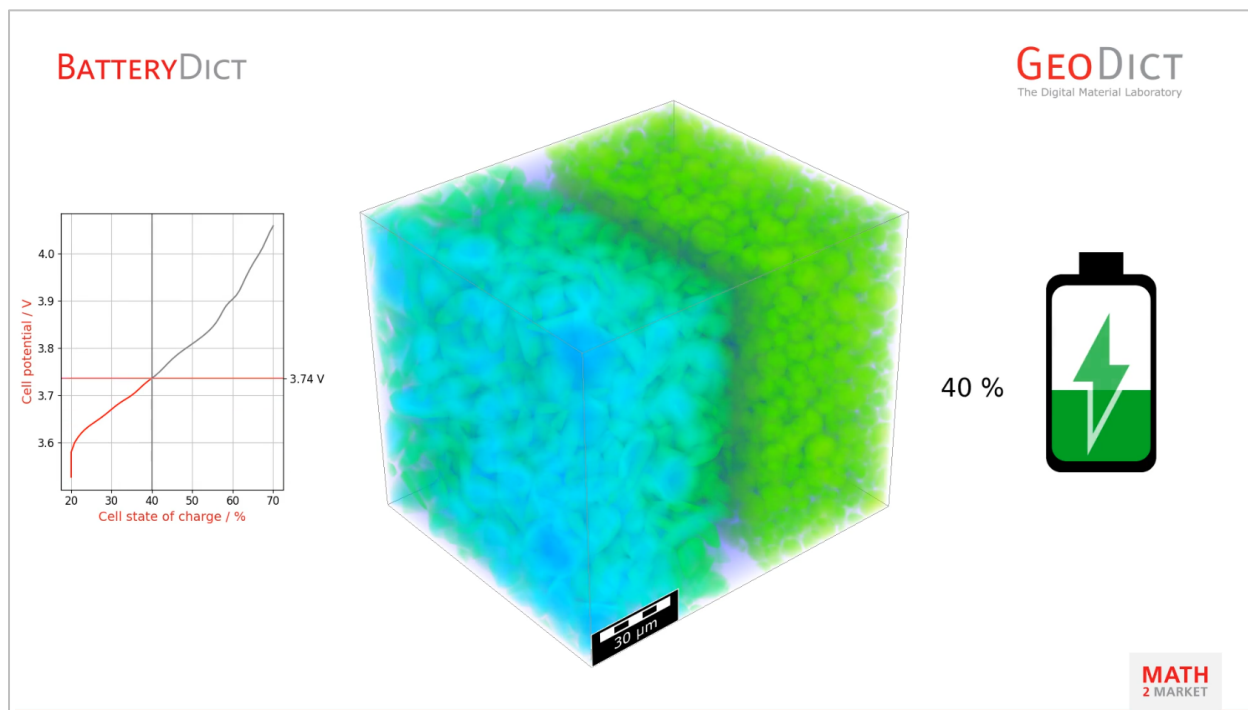
Create Video

Through the **Create Videos** tab, a video showing the ion concentration while charging or discharging of the battery can be created. The first part of the video shows the cropping of the battery structure together with the ion concentration at the start of the simulation.



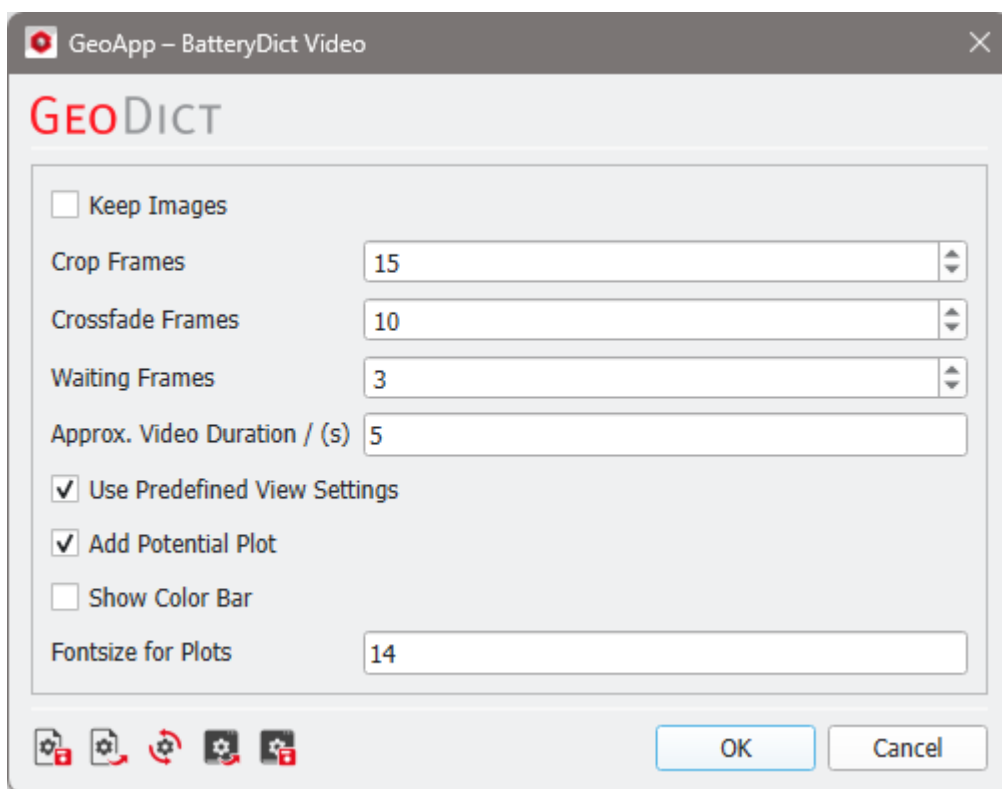
Click **Create Video** to generate the video with the default settings.

A screenshot of such a video is shown here. On the left side, you can see a graph displaying the cell potential over state of charge, with the current state of charge value indicated. In the middle, the ion concentration within the battery structure is illustrated. On the right side, a schematic representation of the current state of charge of the battery is provided.



Click **Open Macro File**, under the **Create Videos** tab, to open the GeoPy macro used to create the video, if you are interested in inspecting it with a text editor. Find out how to edit macros and automate tasks in GeoDict in the GeoPy Scripting chapter.

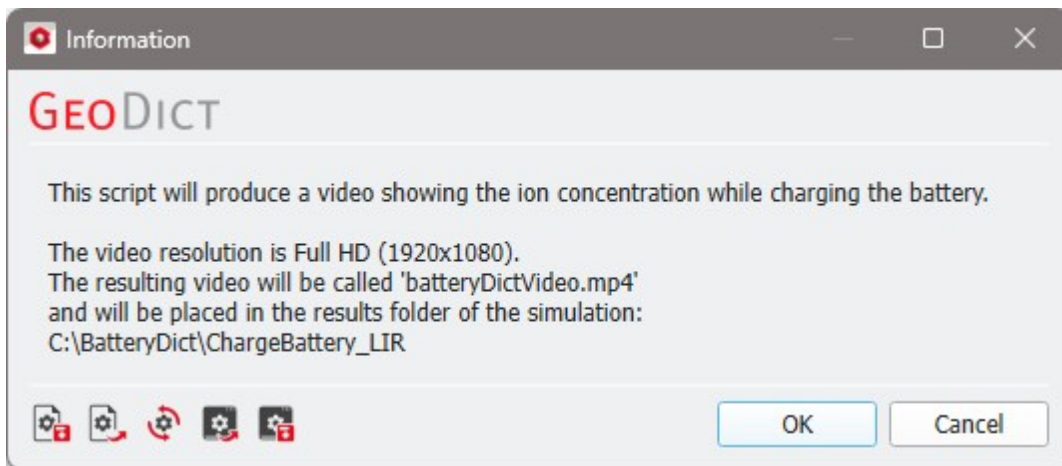
Click **Edit Parameters** to modify the default settings of the video creation.



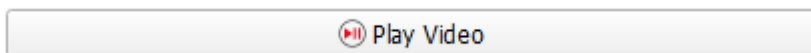
- Check **Keep Images** to save not only the video, but also the created images for the ion concentration in a separate folder.
- The number defined in **Crop Frames** defines the time for the cropping of the structure at the start of the video.
- **Crossfade Frames** defines the time for the visualization of the ion concentration field. The shorter the time defined here, the faster the charging is shown in the video.
- **Waiting Frames**: A higher number indicates a longer pause before and after charging.
- Check **Use Predefined View Settings** to use the predefined orientation of the structure for the video creation as shown in the example above. Uncheck this box to use the orientation of the structure as shown in the GeoDict Visualization Area.
- Check **Add Potential Plot** to keep the graph with the potential curve at the left of the video.
- Check **Show Color Bar** to add an additional color bar for the ion concentration below the structure.
- The font size for the potential curve graph can be set with **Fontsize for Plots**.

Click **OK** to confirm the changed settings and create the video.

A message is shown giving information about the video to save. Confirm by clicking **OK**.



If the video is created, the **Play Video** button is activated on the **Create Videos** tab.

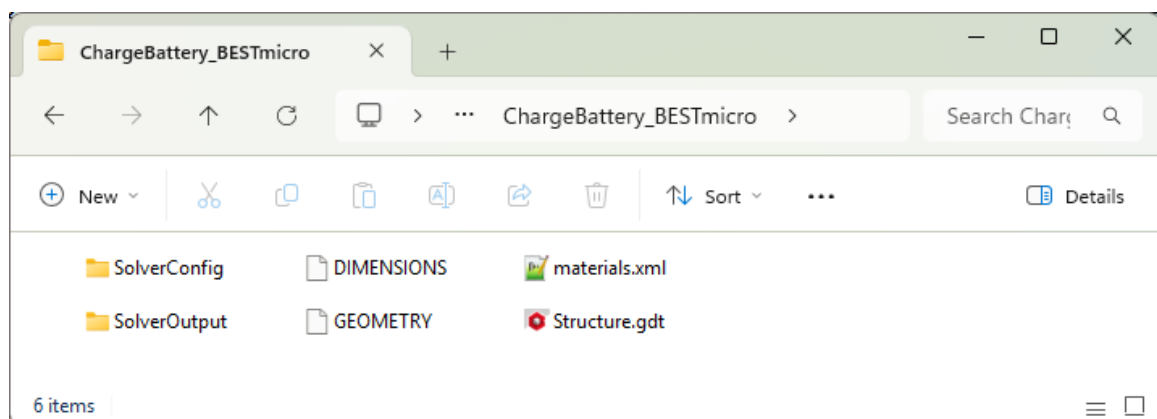


Result Folder

After the charging simulation, a GeoDict result file (.gdr) is created in the selected project folder. A subfolder with the same name as the result file contains the used battery structure (**Structure.gdt**) and several sub folders, depending on the chosen [solver](#)^[86] and on the [experiment type](#)^[141].

✓BESTmicro

After running a charging simulation with **BESTmicro**, the result folder contains the subfolders **SolverConfig** and **SolverOutput**.



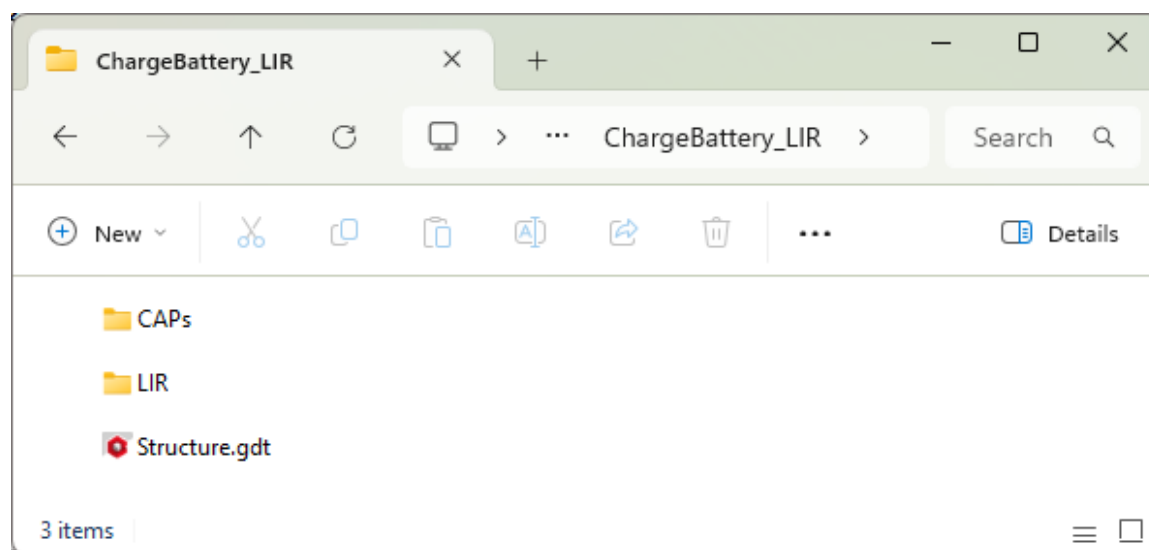
SolverConfig contains files with the input parameters for the charging simulation.

The **SolverOutput** folder contains some log-files from the solver, as well as a subfolder output with *.cap files containing volume fields. Such a *.cap file is written for the initial state, for the final state, and for each time step with intermediate output. These volume files can be loaded from the Load *.cap button under the [Data Visualization](#)^[107] tab of

the **Result Viewer** or directly from the GeoDict GUI by selecting **File - Load Volume File** in the menu bar.

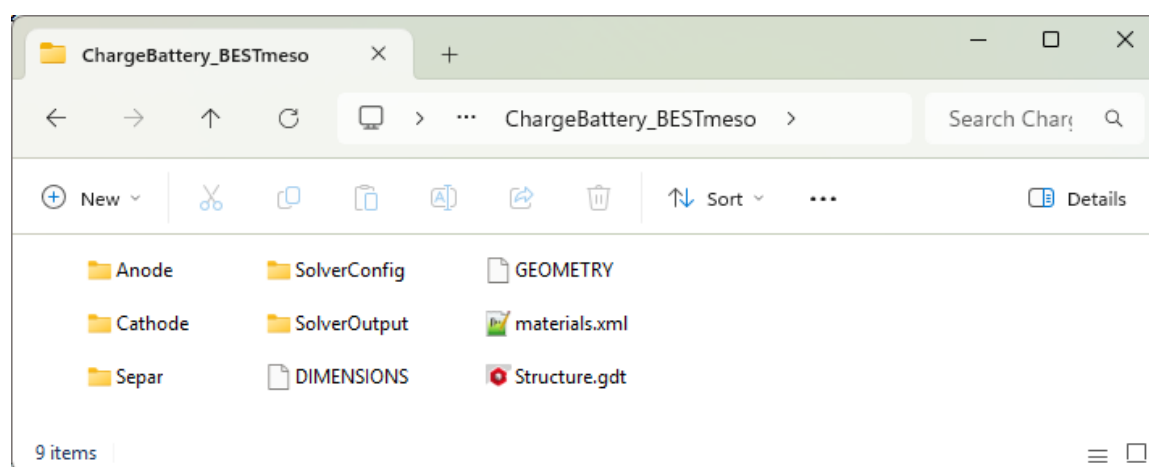
✓LIR

If the charging simulation was run with **LIR** solver, the result folder contains two subfolders. The folder **CAPs** contains the volume files for initial, final and each time step with intermediate output. The folder **LIR** contains files for each time step computed.



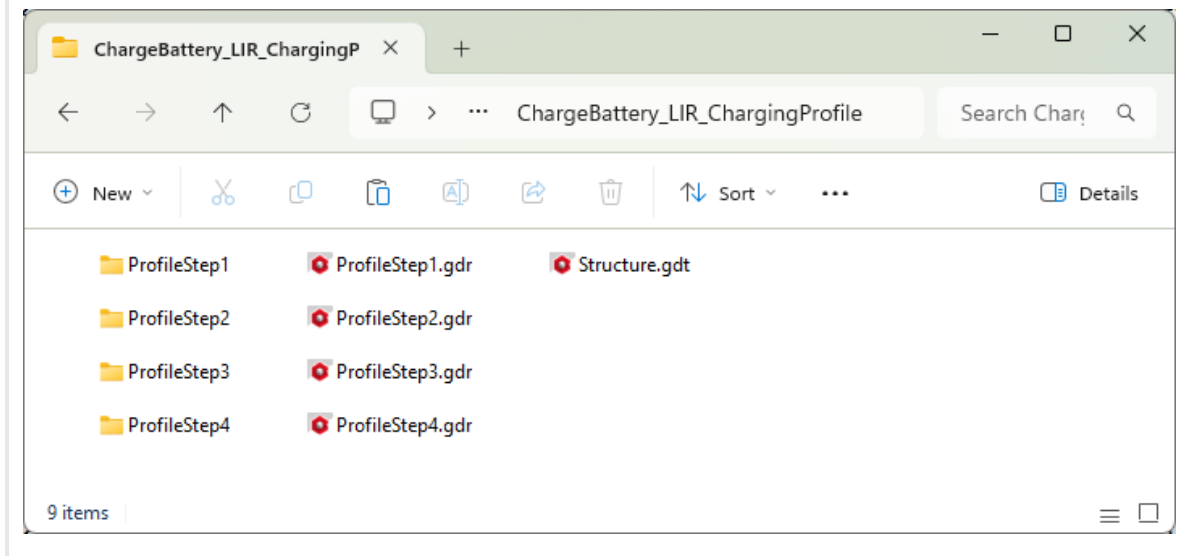
✓BESTmeso

The result folder of a homogenized simulation with **BESTmeso** contains subfolders with information about the solver configuration and output. Additionally, subfolders with the effective material parameters of electrolyte and active materials, derived from the microstructure, are available.



✓Charging Profile

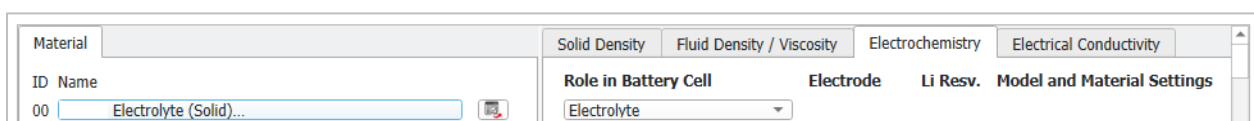
The result folder of a charging profile simulation contains the result files and corresponding result folders for each step of the charging profile additionally to the battery cell geometry (**Structure.gdt**).



All Solid State Batteries

For all solid state batteries (ASSB), the separator should be reassigned to the same material ID as the solid electrolyte using **Model - ProcessGeo - Reassign Materials & IDs**, and selecting the command **Reassign Material ID** from the ProcessGeo module. Void space in the solid state battery should be set as [Inclusion](#)^[68] as it is not taking part in the electrochemical reaction.

The **Charge Battery** dialog automatically recognizes, that a solid electrolyte is chosen, when the chosen material is **Solid** and the **Role in Battery Cell** is set to **Electrolyte** under the [Electrochemistry](#)^[68] tab under the [Constituent Materials](#)^[65] tab.



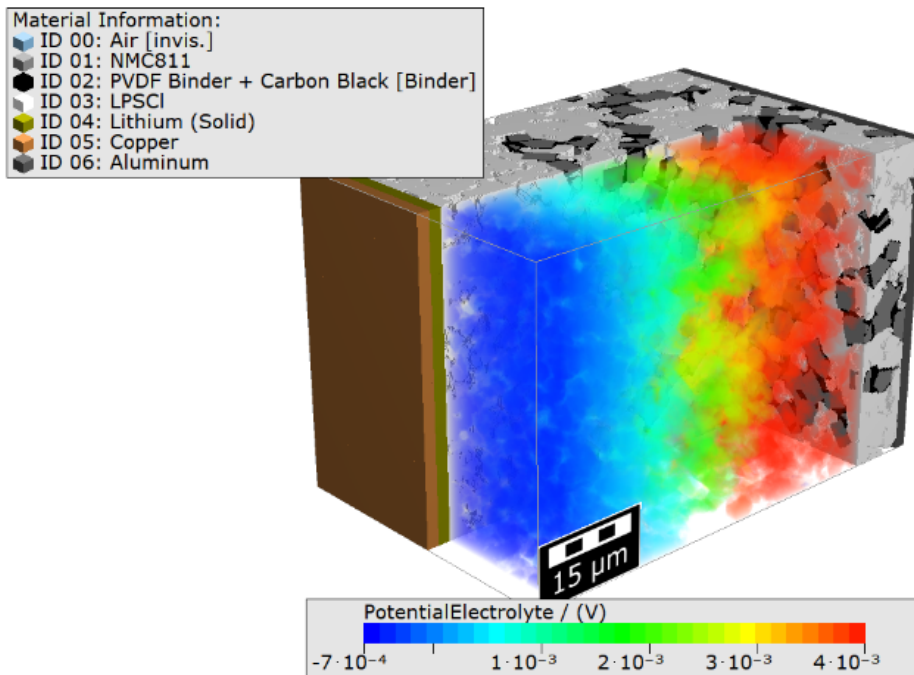
For solid electrolytes, the buttons **Edit Model** and **Edit Material** (or **View Model** and **View Material**) under the [Electrochemistry](#)^[72] tab are not available, because these parameters are only needed for fluid electrolytes. The transference number is automatically set to 1 to resemble the ion conduction in solid electrolyte. Hence, the term of electron migration due to concentration differences in [\(9\) Charge conservation and electroneutrality](#)^[14] is switched off. The only necessary parameter for the solid electrolyte is its effective ionic conductivity which can be seen in the tab [Electrical Conductivity](#)^[78].

Enter the density under the [Solid Density](#)^[67] tab instead of the **Fluid Density /Viscosity** tab.

Since a solid electrolyte cannot fill pores in the binder (or other conductive additives), any [Model Parameters](#)^[77] for binders / conductive additives are ignored, and thus are grayed out. They will always be modeled without porosity.

Remember to click [Edit Model](#)^[71] when using a Lithium Reservoir as anode to adjust the **Maximum Exchange Current Density** $i_{0,max}$ between the lithium reservoir and the solid electrolyte. We recommend to use 320 A/m² for the interface between the lithium reservoir and the solid electrolyte LPSCI, see [Fully Resolved](#)^[17] and [Singh et al., 2023](#)^[205].

If all parameters are set, click **OK** and **Charge**.



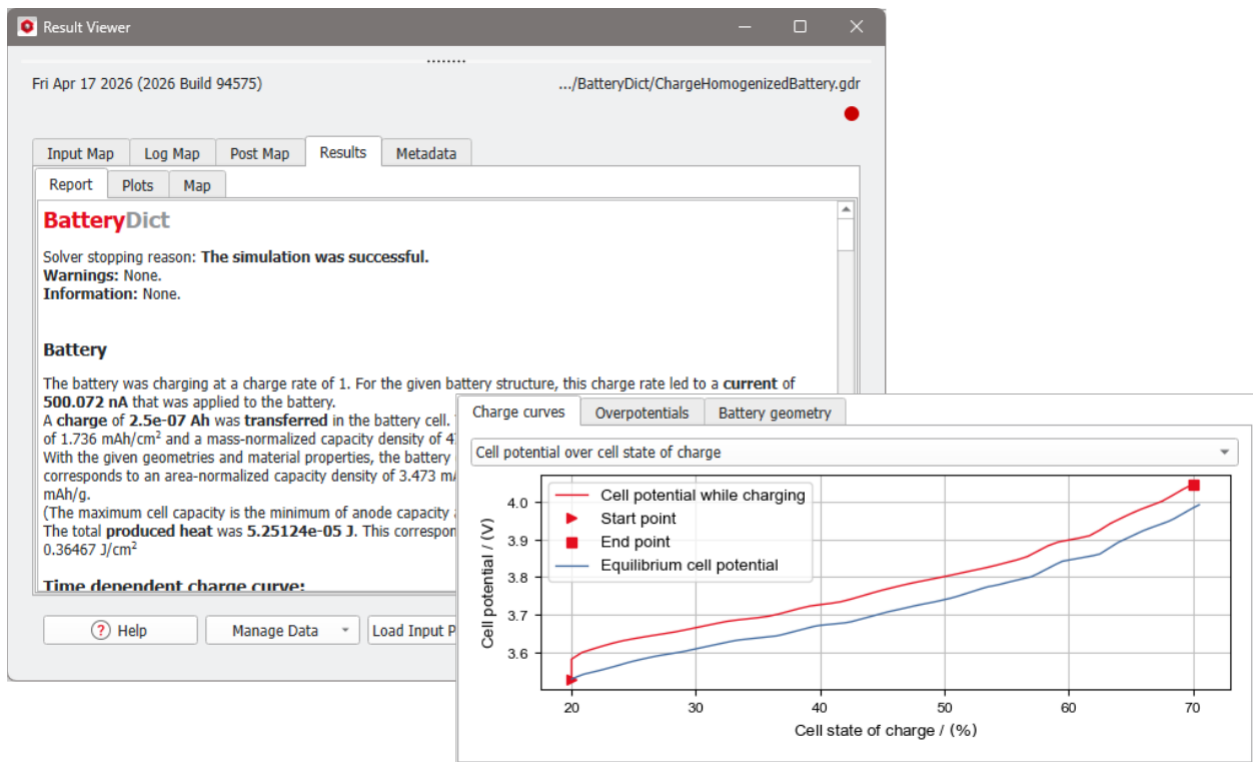
1.2.4 Charge Homogenized Battery

With the **Charge Homogenized Battery** command you can run homogenized simulations directly without providing a cell geometry. You can supply the effective parameters in two ways:

- **Pre-calculated:** Load parameters that were previously generated using the **Homogenized Simulation** option or with the new **Calculate Homogenized Parameters** option in [Charge Battery](#)^[85].
- **User-defined:** Enter the parameters manually in the dialog.

These new commands streamline the setup of parameter studies using the fast homogenized charging model.

If you want to dive deep into the underlying theory, have a look at the [Homogenized Simulation](#)^[18].

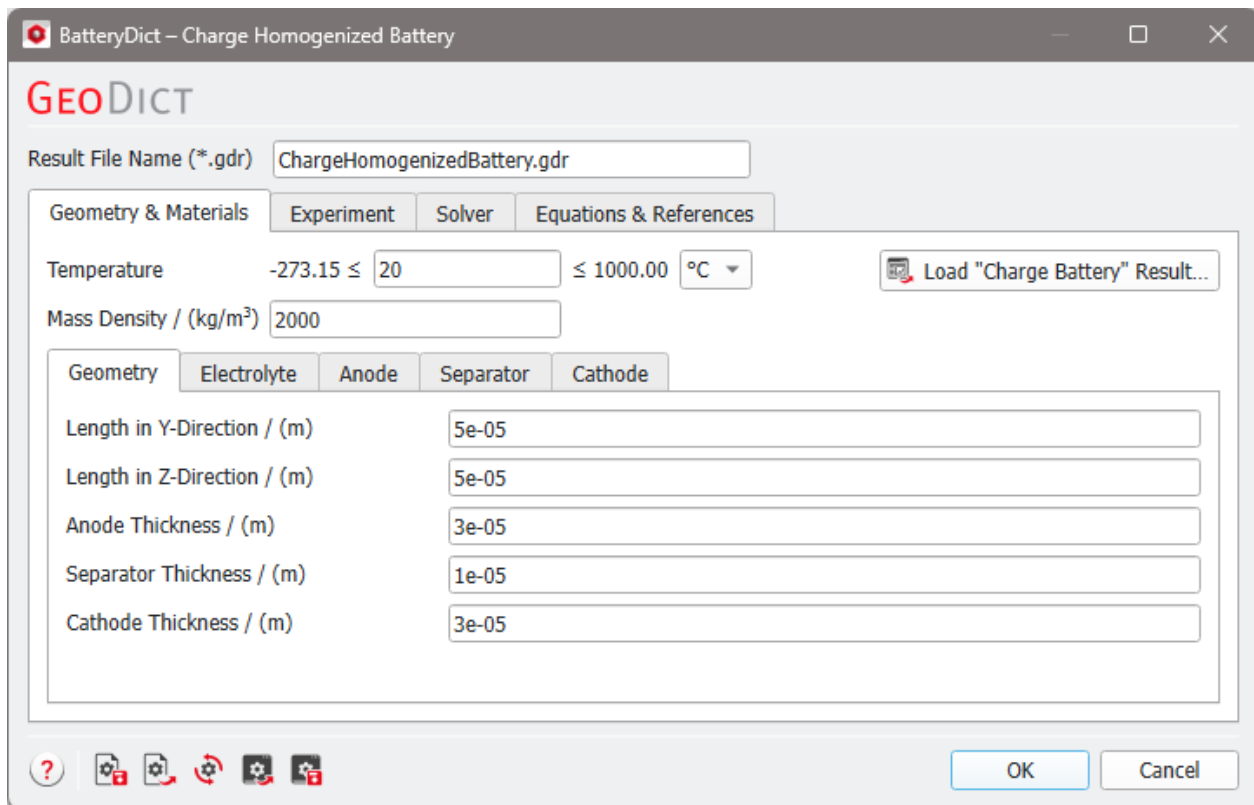


The Charge Homogenized Battery command:

- [Options](#)¹¹⁸
Define the parameters for your homogenized charging or discharging simulation.
- [Results](#)¹³³
View the results in the Result Viewer.

Options

Choose **Battery** and **Charge Homogenized Battery** from the pull-down menus in the BatteryDict section and click **Edit** to adjust the charging parameters.



Tabs of Charge Homogenized Battery:

- [Geometry & Materials](#)^[119]
Define the effective parameters of your geometry.
- [Experiment](#)^[125]
Edit the experiment parameters for charging, discharging or a charging profile.
- [Solver](#)^[130]
Define the time step and parallelization for the simulation.

Geometry & Materials

Define the effective parameters of your geometry. At the top define [temperature](#)^[120] and [mass density](#)^[120]. If you computed the effective parameters using [Charge Battery](#)^[85], click [Load \"Charge Battery\" Result](#)^[120].

Geometry & Materials

Experiment

Solver

Equations & References

Temperature

-273.15 ≤ 20 ≤ 1000.00 °C

Load "Charge Battery" Result...

Mass Density / (kg/m³)

2000

Geometry

Electrolyte

Anode

Separator

Cathode

Length in Y-Direction / (m)

5e-05

Length in Z-Direction / (m)

5e-05

Anode Thickness / (m)

3e-05

Separator Thickness / (m)

1e-05

Cathode Thickness / (m)

3e-05

✓ Load "Charge Battery" Result

If you computed the effective parameters using [Charge Battery](#)^[85], click [Load "Charge Battery" Result](#)^[120]. The parameter values will be loaded in the **Geometry & Materials** tab. The [Experiment](#)^[125] and [Solver](#)^[161] tabs are not affected by this action.

✓ Temperature

The **Temperature** defines the temperature during simulation in Kelvin (K), Celsius (°C), or Fahrenheit (°F). The material properties of active materials and electrolyte can strongly depend on the temperature.

This temperature-dependence of the material properties can currently be derived from the entries in the material database only for the electrical conductivity and density.

However, the temperature-dependent ionic diffusivity and the exchange current density are not yet available in the material database. Consequently, while the electrical conductivity values can be adjusted based on the selected temperature — provided that the temperature dependence is included in the database entry — the other material parameters must be manually modified to ensure consistency with the chosen temperature. To facilitate comparisons of simulations at different temperatures, we recommend duplicating the relevant materials in the database for each new temperature and updating the material properties accordingly.

✓ Mass Density

Specify the **Mass Density** of the structure in kg/m³. Combined with the [geometry](#)^[120] parameters, this value is used to calculate the mass-normalized cell capacity density.

✓ Geometry

Define the **Length in Y-Direction** and **Z-Direction** of your battery structure. The X-direction is the charging direction and its length is defined by the thickness of the different components of the battery: **Anode Thickness**, **Separator Thickness**, and **Cathode Thickness**.

The anode and cathode thickness do not contain the thickness of the current collectors.

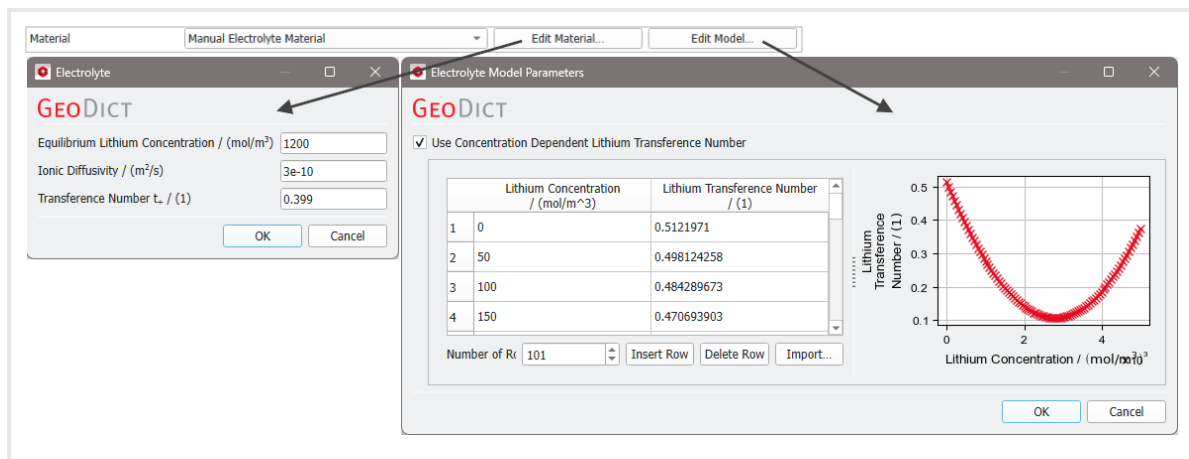
Geometry	Electrolyte	Anode	Separator	Cathode
Length in Y-Direction / (m)	0.00012			
Length in Z-Direction / (m)	0.00012			
Anode Thickness / (m)	6e-05			
Separator Thickness / (m)	1.6e-05			
Cathode Thickness / (m)	6e-05			

✓Electrolyte

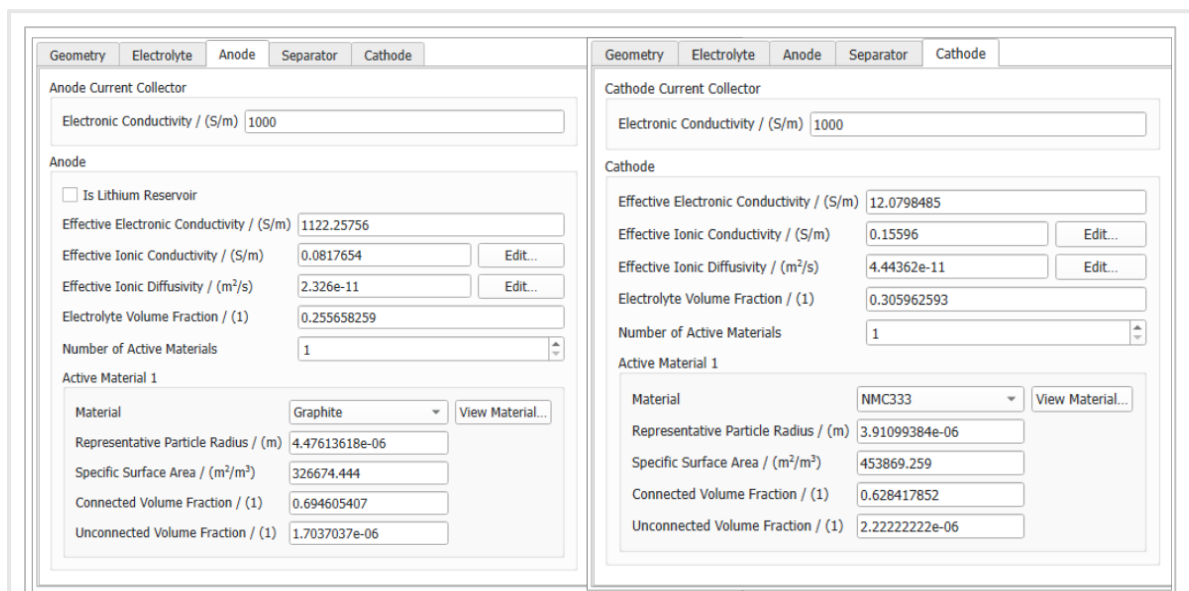
Choose a material from the pull-down menu. The material parameters button changes between **Edit Material** and **View Material** depending on whether **Manual Electrolyte Material** is selected. The material selection is generated automatically based on all materials in the GeoDict material database being assigned electrolyte as the [Role in Battery Cell](#)^[37] under the **Electrochemistry** tab. If you add your own electrolyte materials, they will also appear in the menu.

Geometry	Electrolyte	Anode	Separator	Cathode
Material	Electrolyte - Manual Electrolyte Material - Electrolyte - Electrolyte (Solvionic) - Electrolyte_LLZO - LLZO - LPSCI - h-LZSOCv2	View Material... Edit Model...		

The parameters available under [View Material / Edit Material](#)^[72] and [Edit Model](#)^[74] are similar to for the fully-resolved charging simulation. However, concentration dependent parameters are only available for the lithium transference number.



✓ Anode and Cathode



For the **Anode / Cathode Current Collector**, enter the **Electronic Conductivity** in **S/m**.

For the **Anode / Cathode**, select if the electrode should be modeled as a **Lithium Reservoir** for a half-cell simulation. Then, it will be considered as a never-ending reservoir of lithium, not limiting the battery performance. Thus, much less parameters are needed.

The **Maximum Exchange Current Density**^[32] can be defined in respect to the **Electrolyte Lithium Concentration of Exchange Current Measurement**^[35]. Define the **Effective Electronic Conductivity**^[78] and **Specific Surface Area** for the lithium reservoir. The specific surface area defines the active surface of the lithium reservoir in the anode. A larger specific surface area reduces the kinetic overpotential.

Anode

☒ Is Lithium Reservoir

Maximum Exchange Current Density / (A/m^2)

700

Electrolyte Lithium Concentration of Exchange Current Measurement / (mol/m^3)

1000

Butler-Volmer Rate Constant / ($\text{A}/(\text{m mol})^{0.5}$)

22.1359

Effective Electronic Conductivity / (S/m)

1000

Specific Surface Area / (m^2/m^3)

100000

If the electrode is not modeled as lithium reservoir, the following parameters must be set:

Define the [Effective Electronic Conductivity](#)^[78], the [Effective Ionic Conductivity](#)^[31], the **Electrolyte Volume Fraction** (relative to the electrode volume), and the **Number of Active Materials** in the electrode.

For all active materials select the **Material** from the pull-down menu.

The material selection is generated automatically based on all materials in the GeoDict material database being assigned active material as the [Role in Battery Cell](#)^[37] under the **Electrochemistry** tab. If you add your own active materials, they will also appear in the menu.

Either select a material from the database or select **Manual Active Material**.

Then, view / edit the the simulation parameters [Maximum Lithium Concentration](#)^[31], [Ionic Diffusivity](#)^[31], [Maximum Exchange Current Density](#)^[32], [Electrolyte Lithium Concentration of Exchange Current Measurement](#)^[35] and [Open-Circuit Potential Function \(OCV\) Function](#)^[35] by clicking [View Material / Edit Material](#)^[71].

Active Material

GEO DICT

Maximum Lithium Concentration / (mol/m³)

31090

Ionic Diffusivity / (m²/s)

2e-14

Maximum Exchange Current Density / (A/m²)

4

Electrolyte Lithium Concentration of Exchange Current Measurement / (mol/m³)

1000

Butler-Volmer Rate Constant / (A m⁻²/mol⁻¹/s)

8.13709e-06

Open-Circuit Potential (OCV) Function U₀

☒ Open-Circuit Potential Has Hysteresis

	Material State of Lithiation / (%)	Potential for Lithiation / (V)
1	0	0.43667
2	5.92	0.22889
3	7.427	0.21133
4	8.934	0.20978
5	10.441	0.20711
6	11.948	0.20178

Number

55

Insert Row

Delete Row

Import...

	Material State of Lithiation / (%)	Potential for Delithiation / (V)
1	0	0.43667
2	6.674	0.22778
3	8.288	0.22133
4	9.903	0.21933
5	11.625	0.218
6	13.348	0.21022

Number

53

Insert Row

Delete Row

Import...

OK

Cancel

The **Representative Particle Radius** should be a representative value for the particle size distribution in your electrode. Larger particles lead to higher [diffusive overpotentials](#)^[27].

Enter the volume of connected active material relative to the electrode volume for **Connected Volume Fraction**. The **Unconnected Volume Fraction** is then the volume of unconnected active material. The volume fractions of connected and unconnected material sum up to the total volume fraction of active material relative to the electrode volume. The sum of all volume fractions in the active material (Electrolyte, Connected Volume, and Unconnected Volume) must be not larger than 1.

✓ Separator

For the **Separator** enter the [Effective Ionic Conductivity](#)^[31], the [Effective Ionic Diffusivity](#)^[74] and the **Electrolyte Volume Fraction**. Note, that the electrolyte volume fraction needs to be given relative to the separator volume.

Geometry

Electrolyte

Anode

Separator

Cathode

Effective Ionic Conductivity / (S/m)

0.256667

Edit...

Effective Ionic Diffusivity / (m²/s)

7e-11

Edit...

Electrolyte Volume Fraction / (1)

0.42

Experiment

All parameters defining the charging simulation of the homogenized battery are defined on this tab.

Geometry & Materials Experiment Solver Equations & References

Experiment Type: Charge Battery Cell

Boundary Conditions in Through Direction: Charge Rate

Charge Rate / (1): 1

Start and End Condition: Minimum and Maximum Cell SOC >>> Charge >>>

Range of the Cell State of Charge / (%): 20.00 to 70.00

☐ Use Upper Cut-Off Voltage / (V): 4.3

☐ Max. Simulated Time / (s): 3600

Boundary Conditions in Tangential Direction: Symmetric

✓ Experiment Type

From the pull-down menu **Experiment Type**, select the appropriate entry to simulate the charging or discharging of the battery cell or set a charging profile. Here, a charging simulation is chosen. For the experiment types **Charge Battery Cell** and **Discharge Battery Cell** select the [Boundary Conditions in Through Direction](#)^[125] and the [Start and End Condition](#)^[126]. How to Set a **Charging Profile** is explained [here](#)^[128].

✓ Boundary Conditions in Through Direction

The **Boundary Conditions in Through Direction** can be specified by a **Charge Rate**, a **Current Density**, by defining the **Current**, by defining the **Cell Potential**, or the **Power Density**.

- With a **Charge Rate** defined, the applied current is related to the cell's maximum capacity from 0% state of charge to 100% state of charge and is a measure of the duration of the battery charging. For example, a charge rate of 1 for a battery with capacity of 1 Ah means that the battery is charged completely in 1 hour with a constant current of 1 Ampere (A). This time is unrelated to the simulation time, but instead to the time that the charging process itself requires. A charge rate of 2 means that charging the same battery with a current of 2 Ampere takes 1/2 hour.

Boundary Conditions in Through Direction: Charge Rate

Charge Rate / (1): 1

- Defining the **Current Density** instead means that the applied the applied current density (in A/m²) is defined directly.

Boundary Conditions in Through Direction: Current Density

Current Density / (A/m²): 10

- Defining the **Current** instead means that the applied current (in A) is defined directly.

Boundary Conditions in Through Direction	Current
Current / (A)	1e-11

- If **Cell Potential** is selected, the voltage is kept at a constant value during the simulation, and the current is a time-dependent value. Define a [Cut-Off Current](#)¹²⁶ as end condition.

Boundary Conditions in Through Direction	Cell Potential
Cell Potential / (V)	3.5

- Defining the **Power Density** in W/m² means that the applied current density is dynamically adjusted so that the product of cell potential and current density - i.e., the power density - remains constant throughout the simulation.

Boundary Conditions in Through Direction	Power Density
Power Density / (W/m ²)	20

✓ Start and End Condition

The **Start and End Condition** for the charging simulation can be defined in several ways:

Start and End Condition	Minimum and Maximum Cell SOC	>>> Charge >>>
Range of the Cell State of Charge / (%)	20.00	70.00
☐ Use Upper Cut-Off Voltage / (V)	4.3	
☐ Max. Simulated Time / (s)	3600	

- as minimum and maximum percentage of the [state of charge](#)⁸¹ of the whole cell (**Minimum and Maximum Cell SOC**)

Start and End Condition	Minimum and Maximum Cell SOC	>>> Charge >>>
Range of the Cell State of Charge / (%)	20.00	70.00

- for the anode SOC and cathode SOC individually (**Anode and Cathode SOC**s),

Start and End Condition	Anode and Cathode SOC	>>> Lithiate >>>
Range of the Anode State of Charge /	20.00	70.00
		<<< Delithiate <<<
Range of the Cathode State of Charge	20.00	70.00

- by selecting an initial .cap file from a previous BatteryDict simulation and defining a final SOC (**Initial *.cap File and Final Cell SOC**). This option is especially useful for simulating a charging or discharging process, starting from a non-equilibrium condition after a previous discharging or charging simulation.

Start and End Condition	Initial *.cap File and Final Cell SOC ▾	
Initial *.cap File (*.cap)		Browse...
Final Cell SOC / (%)	70	

- or, by defining an initial voltage value and a final SOC (**Initial Voltage and Final Cell SOC**). This option can be used together with **Use Upper (Lower) Cut-Off Voltage** to define a voltage window for your charging (discharging) simulation.

Start and End Condition	Initial Voltage and Final Cell SOC ▾	
Initial Equilibrium Voltage for Charging / (V)	2.8	
Final Cell SOC / (%)	70	



Important! To get a numerically stable solution, the state of charge for the whole cell as well as for anode and cathode separately can be set only between 5% and 95%, see also [Theoretical Background - Fully Resolved](#)^[15].

Depending on the selected [boundary conditions](#)^[125], it is possible to set additional an end conditions to the simulation.

- Limit the voltage in a simulation by checking **Use Upper / Lower Cut-Off Voltage**. The voltage will not exceed this limit. I.e., if the cut-off voltage is reached, the charging will end. This option is not available for the boundary condition Cell Potential.

☒ Use Upper Cut-Off Voltage / (V)	4.3
---	----------------------------------

- If Cell Potential is set as boundary condition in through direction, select the **Cut-Off Current** as an end condition to the simulation to be **Charge Rate**, **Current Density** or **Current**. For example, consider charging a battery at constant **Cell Potential**, and selecting a **Cut-Off Charge Rate**. The simulation starts with the entered SOC value and charges the battery at the provided constant cell potential, for example at 3.5 V. During the charging, the charge rate decreases with the increasing SOC. As soon as the charge rate is lower than the entered **Cut-Off Charge Rate**, the simulation stops.

Cut-Off Current	Current ▾	
Current / (A)	1e-13	Charge Rate Current Density Current

- When checking **Max. Simulated Time**, the simulation ends if the charging process exceeds the entered **Max. Simulated Time**. Note that **Max. Simulated Time** does not denote the duration given to the solver. Instead it specifies how long the simulated battery is charged or discharged. For an example, let us consider a battery that is charged from 20% state-of-charge to 70% state-of-charge at a charge rate of 1C. The battery takes 30 min to charge. If the **Max. Simulated Time** is set to 600

seconds (10 min), in this example the battery will only be charged from 20% to 36.67% state-of-charge.

☒ Max. Simulated Time / (s)

600



Note! The simulation is stopped as soon as the first of the provided end conditions is met, i.e., either the set final SOC is reached, the cut-off voltage / current is reached, or the max. simulated time is exceeded.



Know how! If a simulation diverges, it is often helpful to reduce the voltage window covered in a charging simulation.

✓ Charging Profile

Charging Profiles are a series of charging, discharging, and relaxation simulations that are performed sequentially for the same structure.

Experiment Type: Set a Charging Profile

Initial Cell Condition: Equilibrium Cell SOC

Initial Cell SOC / (%): 20

(Dis-)Charge or Relaxation?	Type of Boundary Condition	Applied BC Value	Stopping Criterion at Boundary	Stopping BC Value	Stopping Cell SOC / (%)	Stopping Time / (s)
1 Charge Battery Cell	Charge Rate / (1)	1	Cell Potential / (V)	3.8	50	☐ 1800
2 Charge Battery Cell	Cell Potential / (V)	3.8	Charge Rate / (1)	0.01	50	☒ 3600
3 Discharge Battery Cell	Charge Rate / (1)	1	Cell Potential / (V)	3.55	20	☐ 1800
4 Discharge Battery Cell	Cell Potential / (V)	3.55	Charge Rate / (1)	0.01	20	☒ 3600

Number of Rows: 4

Overall Stopping Conditions:

☐ Max. Simulated Time / (s): 3600

If **Set a Charging Profile** is selected as [Experiment Type](#)¹²⁵, the starting point for the first simulation can be defined

- as an **Equilibrium Cell SOC** (Select an initial Cell SOC between 5% and 95%, that defines the initial equilibrium state),

Experiment Type: Set a Charging Profile

Initial Cell Condition: Equilibrium Cell SOC

Initial Cell SOC / (%): 20

- as an **Equilibrium Voltage** (enter the voltage for the initial equilibrium state of the battery),

Experiment Type	Set a Charging Profile ▼
Initial Cell Condition	Equilibrium Voltage ▼
Initial Equilibrium Voltage / (V)	3.6

- or, by selecting a **.CAP File** of a previous simulation.

Experiment Type	Set a Charging Profile ▼
Initial Cell Condition	CAP File ▼
Initial *.cap File (*.cap)	InitialCAP.cap
	Browse...

The starting point for the following simulations, defined in the charging profile table, is always the final state of the previous one.

To define a charging profile, choose as many rows for the table as simulation steps desired by entering the **Number of Rows**. Select for each step, if the battery is charged, discharged, or if relaxation is simulated.

For **charging** or **discharging**, define the **Type of Boundary Condition** (BC) and the corresponding **Applied BC Value**, in the same way as for [simple charging simulations](#)¹²⁵. The same options for the boundary condition (**Charge Rate**, **Current Density**, **Current**, **Cell Potential**, and **Power Density**) are available.

For charging or discharging, next, the first stopping criterion for the selected boundary condition (**Stopping Criterion at Boundary**) is chosen for each simulation step. The available options depend on the **Type of Boundary Condition**.

- If **Charge Rate**, **Current Density**, **Current**, or **Power Density** is selected as BC, only a cut-off **Cell Potential** is possible as stopping criterion at boundary.
- For **Cell Potential** as BC, the stopping criterion at boundary can be chosen between a cut-off **Charge Rate**, **Current Density**, and **Current**.

Enter the **Stopping BC Value** for the first stopping criterion, for the second stopping criterion a stopping state-of-charge for the whole cell (**Stopping Cell SOC / %**) and for the (optional) third stopping criterion a **Stopping Time**. The computation ends for each simulation step, if the first one of the stopping criteria is reached. The next simulation step will continue from this state.

For **relaxation**, no boundary conditions need to be defined, only the stopping time as the only possible stopping criterion of the relaxation step. In a relaxation step, the return of the battery cell to an equilibrium state after charging or discharging is simulated. The solver settings, including the time step, are set by BatteryDict to optimize the simulation time required for the relaxation step.

(Dis-)Charge or Relaxation?	Type of Boundary Condition	Applied BC Value	Stopping Criterion at Boundary	Stopping BC Value	Stopping Cell SOC / (%)	Stopping Time / (s)
1 Charge Battery Cell ▾	Charge Rate / (1) ▾	1	Cell Potential / (V) ▾	3.8	50	☐ 1800
2 Charge Battery Cell ▾	Cell Potential / (V) ▾	3.8	Charge Rate / (1) ▾	0.01	50	☒ 3600
3 Discharge Battery Cell ▾	Charge Rate / (1) ▾	1	Cell Potential / (V) ▾	3.55	20	☐ 1800
4 Relaxation ▾						☒ 3600

✓ Boundary Conditions in Tangential Directions

Periodic or **Symmetric** boundary conditions can be selected for the **Boundary Conditions in Tangential Directions**.

Boundary Conditions in Tangential Direction Symmetric ▾

Periodic

Symmetric

For **periodic** boundary conditions, the structure is assumed to repeat periodically in Y- and Z-direction and for **symmetric** boundary conditions, the structure is mirrored in Y- and Z-direction and the Li⁺ ions and electrons are reflected at the boundary in Y- and Z-direction. The connected and unconnected parts of the active materials and electrolyte depend on the boundary conditions, so they are determined when the simulation begins.

Solver

Under the **Solver** tab, select the **Parallelization** and **Time Step** modes. The simulation type will always be [Homogenized Simulation](#)¹⁸ and computed with the BESTmeso solver.

Geometry & Materials Experiment **Solver** Equations & References

Simulation Type Homogenized Simulation ▾

Solver Type BESTmeso ▾

Parallelization Threads (Automatic Maximum) Edit...

Time Step

Time Step Input Mode Automatic ▾

BESTmeso

✓ Parallelization

Control how many threads are used for the computation. Parallelization is possible if your license and hardware allow it.

The **Parallelization Options** dialog opens when clicking the **Edit** button and you can choose between **Sequential**, **Parallel (Shared Memory)**, or **Automatic Maximum of Threads**.

Parallelization 12 Threads (Automatic Maximum) Edit...

Selecting **Sequential** will not apply parallelization and only one thread is used for the computation.

Parallelization Options

GEODICT

☒ Sequential

☐ Parallel (Shared Memory)

☐ Automatic Maximum of Threads

OK

Cancel

When **Parallel (Shared Memory)** is selected, the **Number of Threads** can be entered. Below, the **Number of CPU Cores** that the current machine has, the maximum number of **Licensed Threads** and the number of those licensed threads that are available (**Available Threads**) are shown in the dialog. Of course, the maximal number of parallel processes you can use, is the smallest of those three numbers.

Parallelization Options

GEODICT

☐ Sequential

☒ Parallel (Shared Memory)

☐ Automatic Maximum of Threads

Thread Parallel

Number of Threads 8

Number of CPU Cores 12

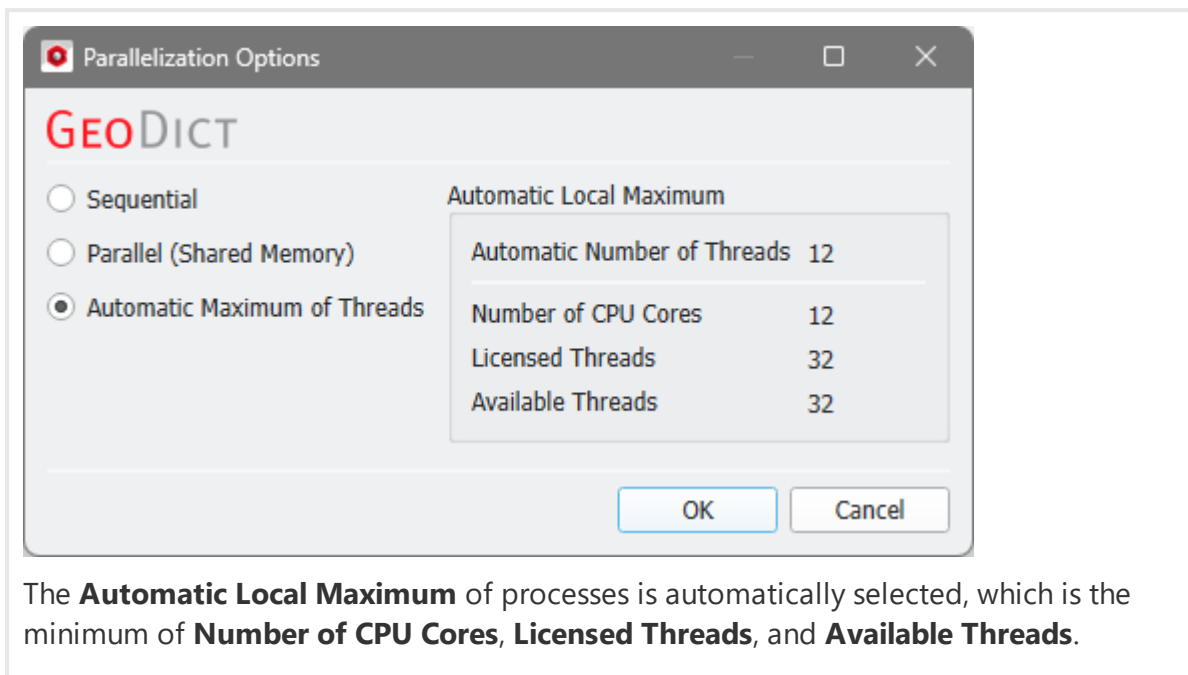
Licensed Threads 32

Available Threads 32

OK

Cancel

If **Automatic Maximum of Threads** is selected, the number of parallel processes is automatically selected for optimal speed, based on the CPU cores and licensed parallel processes.



✓ Time Step

In the **Time Step** panel an option for the **Time-Step Input Mode** may be selected.



Any of the battery solvers calculates the time evolution of the given Li-ion battery. It starts at the initial state, which has time = 0 in the [result plots](#)^[97]. It takes the time step defined as maximum time step size and tries to find the battery state at time = last time + time step by searching an equilibrium solution fulfilling the given system of differential equations. If no solution can be found for this time step size, it reduces the time step size, and the solver starts again. This procedure is repeated until an appropriate time step size is found. This time step size is used for the next steps in the simulation as well. After several successful steps with a certain time step size, the solver tries to increase this time step size again, to reduce overall computation time. With the **Time-Step Input Mode**, the maximum time-step size can be influenced. For more information on time steps see [State of Charge \(SOC\) and State of Lithiation \(SOL\)](#)^[10].

- Choosing **Automatic**, the solver selects the time-step size without restrictions.
- If a **Minimum Number of Time Steps** is defined, at least this number of points are computed for the solution and the maximum time-step size is selected accordingly. If your simulation does not produce enough points in the plots of the result file, then you might want to increase the **Minimum Number of Time Steps**.
- **Maximum Time Step Size** defines the maximum time step in seconds used in the simulation. If the size of the time step is oscillating a lot, the recommendation is to reduce this maximum value.

The time steps that were finally realized in the simulation are saved in the [Result Map](#)^[107] of the GeoDict result file (*.gdr file), created for the charging simulation, under the key **TimeDependentValues:TimeStep**.

If a new battery state is found in a simulation with a charge rate boundary condition, the solver computes the Cell-SOC step of the just found new battery state i via:

$$\Delta(SOC)_i = \Delta t_i \cdot C / (1h) \quad (61)$$

with Δt_i the time step and C the charge rate. So, it is not clear from the start which is the next computed Cell-SOC in a simulation, this depends on the time step.

Example:

- Charge Rate $C = 5$
- Time Step Size $\Delta t_i = 2.5 \text{ s}$
- Cell-SOC step $\Delta(SOC)_i = 2.5 \cdot \frac{5}{1h} = 2.5s \cdot \frac{5}{3600s} = 0.00347 = 0.347\%$

If you choose to set the current density instead of the charge rate, then the calculation of the Cell-SOC step size depends on the given current density and the cell capacity. Thereby, the cell capacity depends on the battery-geometry and the maximum lithium concentration of the active materials.

In the GeoDict result file (*.gdr file) created for the charging simulation, you can find the time-evolution of the Cell-SOCs in percent as well as the corresponding times in seconds in the [Result Map](#)^[107] under the keys

TimeDependentValues:CellStateOfCharge and **TimeDependentValues:Time**, respectively.

For simple simulations (charge rate ≤ 1 , physical domain size $\leq 5 \text{ }\mu\text{m}$, only one active material per electrode, diffusivities $\geq 1\text{e-}12 \text{ m}^2/\text{s}$, conductivities $\geq 1 \text{ S/m}$ and no warnings during the simulation), the time step size is usually the maximum time step size set. Then, also the Cell-SOC step is a constant value.

However, for more complex simulations (charge rate ≥ 10 , physical domain size $\geq 50 \text{ }\mu\text{m}$, two active materials in an electrode with different parameters, low diffusivities in the active materials and small conductivities), it might happen that the time step size may be smaller than the maximum time step size defined and not constant over the whole simulation.

Results

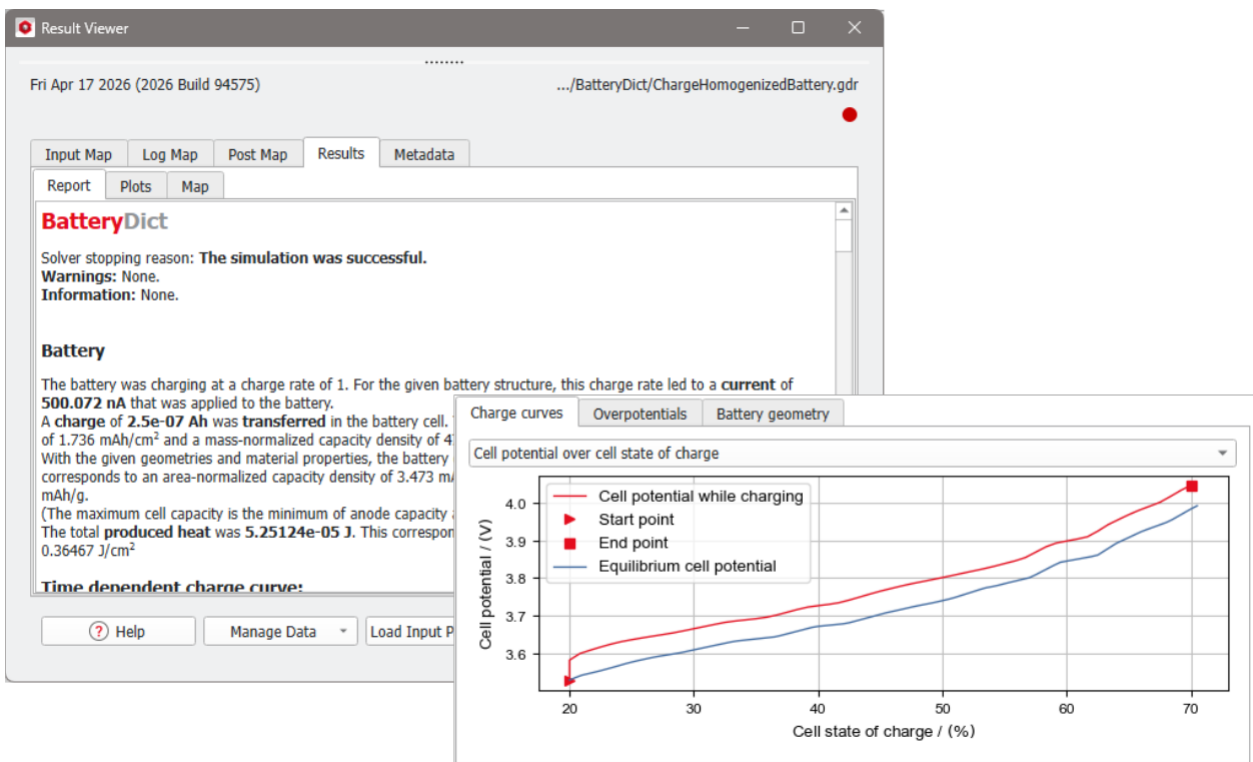
After a homogenized charging simulation has finished, a GeoDict result file (.gdr) is written and the **Result Viewer** of this result file automatically opens. The information of simulation result is shown, can be visualized, or further processed.

These results are accessible at any time by loading the .gdr file from the menu bar (**File - Open Results (*.gdr)**). No **Load Structure** button is available, since this command does not need a geometry. All effective parameters were given in the options dialog. Learn more about the general **Result Viewer** options in the Result Viewer chapter.

In the following, the results were produced using the [Calculate Homogenized Parameters](#)^[85] results from the structure used as an example for [Charge Battery](#)^[93].

The results found under the **Results** tab are the same as for a [homogenized simulation](#)^[94] using [Charge Battery](#)^[85].

The plots under the **Plots** tab are the [Charge curves](#)^[97] and [Overpotentials](#)^[105] also found for **Charge Battery** simulations. They can also be compared with **Charge Battery** results by using Combine Results.

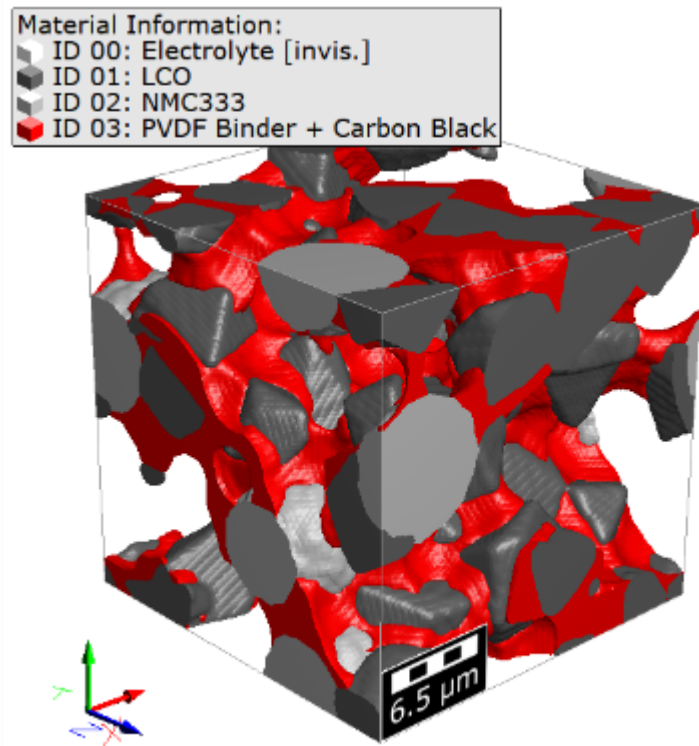


1.3 Electrode

Simulate charging or discharging of a battery only needing one electrode.

In this section only one electrode is considered. The other electrode is modeled as never-ending lithium reservoir.

Simulate lithiation and delithiation of an electrode, either [fully-resolved](#)^[12] or [homogenized](#)^[18].



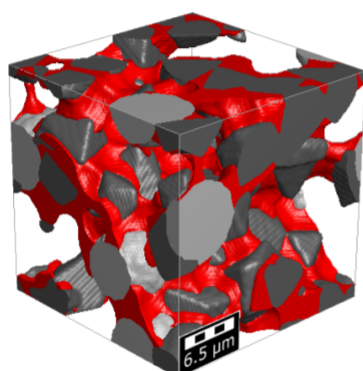
Commands available for electrode structures:

- [Charge Electrode](#)^[135]
Start a simulation lithiating or delithiating your electrode.
- [Charge Homogenized Electrode](#)^[152]
Run homogenized half-cell simulations directly without providing an electrode geometry.

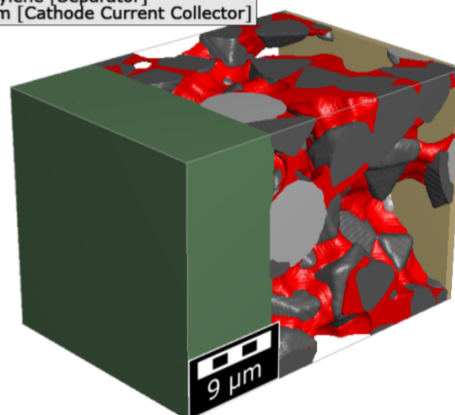
1.3.1 Charge Electrode

Use **Charge Electrode** to simulate charging discharging of a single electrode. It can be used for charging simulations of arbitrary structures loaded into GeoDict, consisting of a single electrode or an electrode together with a separator and/or a current collector as shown on the right in the image below.

Material Information:
 ID 00: Electrolyte [invis.]
 ID 01: LCO
 ID 02: NMC333
 ID 03: PVDF Binder + Carbon Black

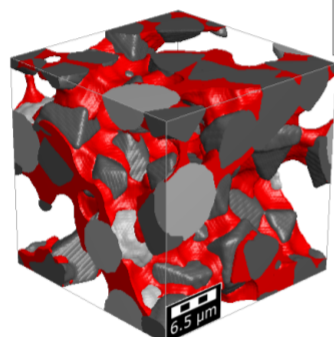


Material Information:
 ID 00: Electrolyte [invis.]
 ID 01: LCO
 ID 02: NMC333
 ID 03: PVDF Binder + Carbon Black
 ID 04: Polypropylene [Separator]
 ID 05: Aluminum [Cathode Current Collector]

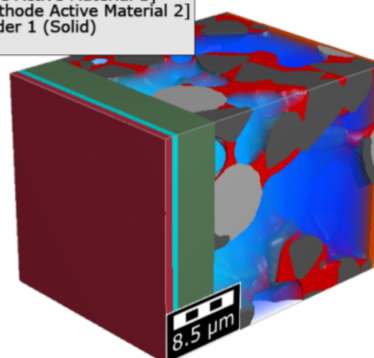


Input parameters and results are adapted here, to fit for the simulation of an electrode. The electrode can consist of any active material. Electrochemically, the lithium reservoir is always considered as the anode in the computation and the investigated electrode is considered as the cathode.

Material Information:
 ID 00: Electrolyte [invis.]
 ID 01: LCO
 ID 02: NMC333
 ID 03: PVDF Binder + Carbon Black



Material Information:
 ID 00: Electrolyte [Electrolyte] [invis.]
 ID 01: Anode Current Collector (Solid)
 ID 02: Anode Lithium Reservoir (Solid)
 ID 10: Separator (Fluid)
 ID 11: LCO [Cathode Active Material 1]
 ID 12: NMC333 [Cathode Active Material 2]
 ID 15: Cathode Binder 1 (Solid)
 ID 19: Aluminum



ConcentrationElectrolyte / (mol/m³) Plot max 1210 Plot min 1190
 1190 1200 1210

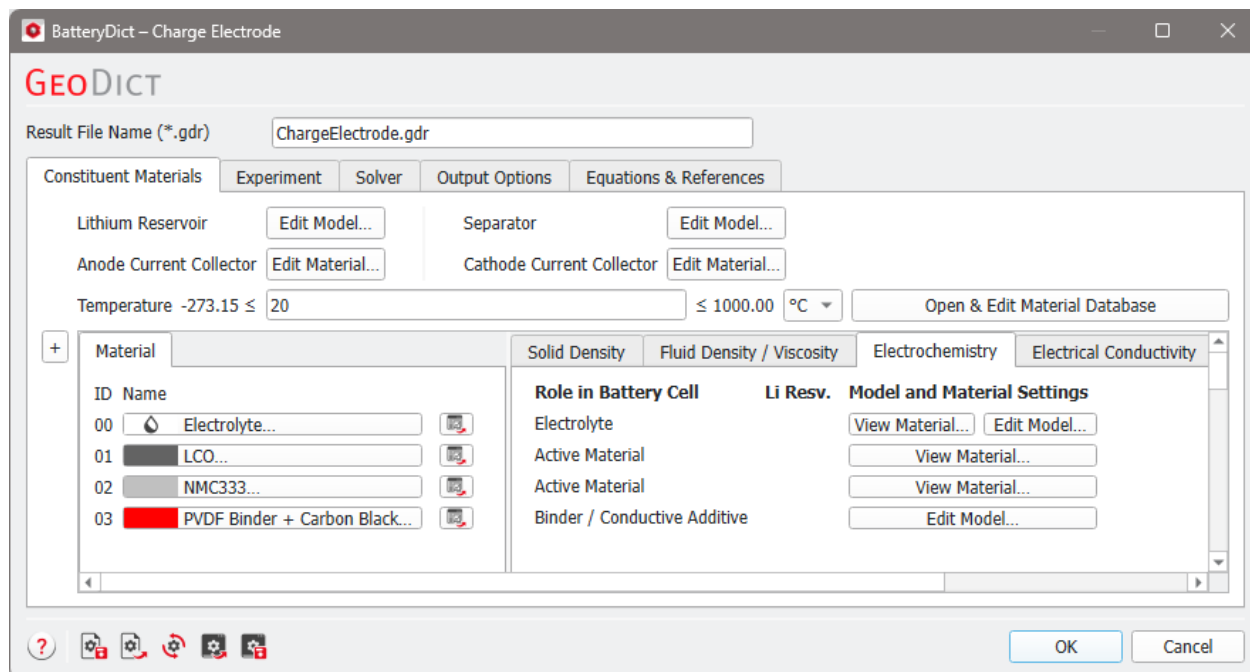
If you want to dive deep into the underlying theory, have a look at the [Theoretical Background](#) ⁷.

The Charge Electrode command:

- [Options](#) ¹³⁷
Define the parameters of your electrode lithiation or delithiation simulation.
- [Results](#) ¹⁵⁰
View the results of the simulation.

Options

Choose **Electrode** and **Charge Electrode** from the pull-down menus in the BatteryDict section and click **Edit** to adjust the charging parameters.

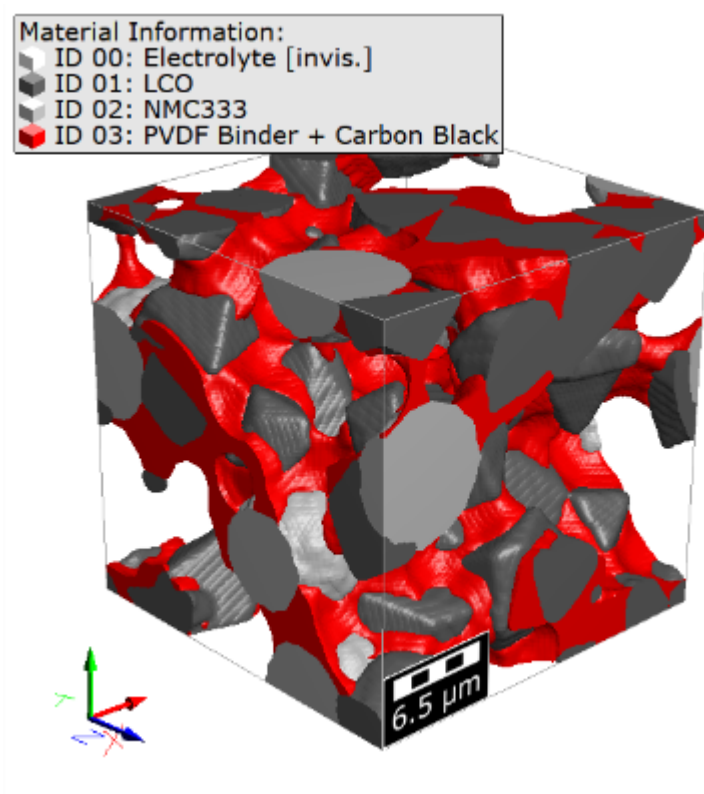


Tabs of Charge Electrode:

- [Constituent Materials](#)¹³⁷
Define the properties for all materials in the battery cell.
- [Experiment](#)¹⁴¹
Edit the experiment parameters for lithiation, delithiation or a charging profile.
- [Output Options](#)¹⁴²
Decide which 3D result fields should be saved.
- [Solver](#)¹⁴³
Define the solver and parallelization for the simulation.

Constituent Materials

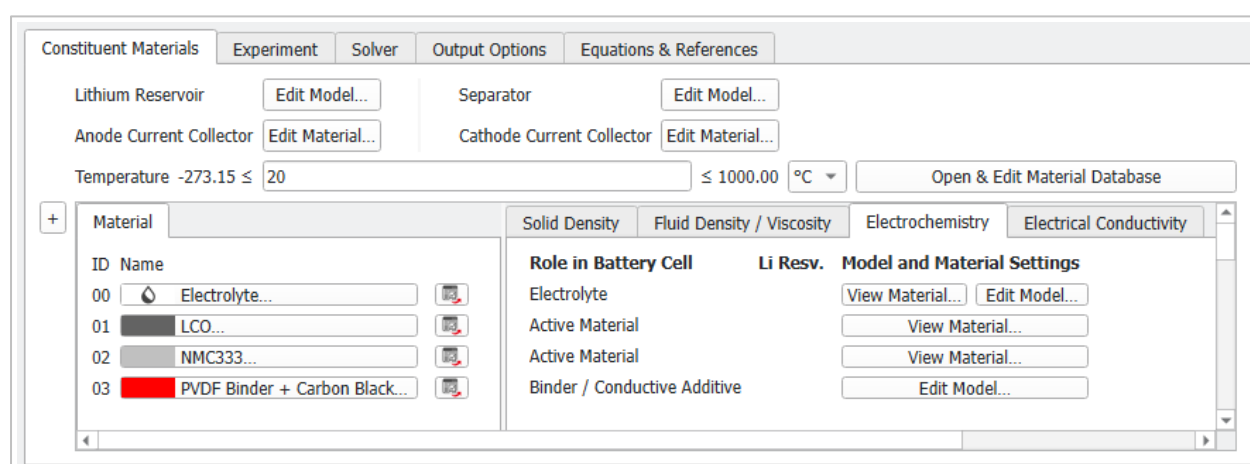
If the structure of a single electrode is loaded in GeoDict, this structure is considered as the cathode for the half cell simulation.



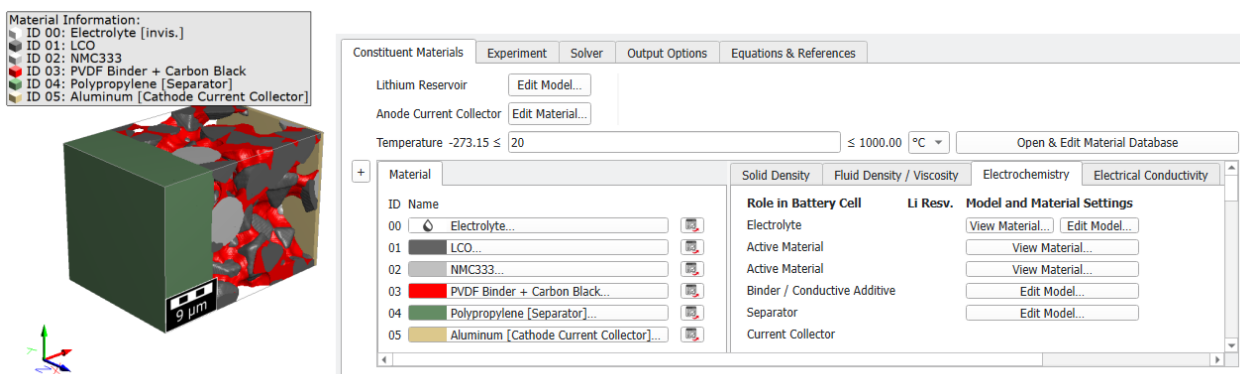
The half cell is created by attaching the electrode in X+ direction to the separator. The lithium reservoir will be attached in X- direction to the separator.

If a material ID for the separator is provided, it must adhere to the rule that the half cell is assembled in the X-direction.

On top of the tab, the parameters for anode current collector and lithium reservoir can be modified. If not specified by a separate material ID in the structure, the parameters for the separator and the cathode current collector can also be defined.



If the structure is created with separate material IDs for cathode current collector and separator, these roles can be defined for the materials on the **Electrochemistry** subtab. In this case, the buttons for modifying the corresponding properties disappear from the top of the dialog.



✓ Lithium Reservoir Parameters

For the lithium reservoir, choose **Edit Model** to enter the parameters for the simulation.

Define the **Lithium Reservoir Width** in number of voxels.

The [Maximum Exchange Current Density](#)^[32] and the corresponding [Electrolyte Lithium Concentration of Exchange Current Measurement](#)^[35]. The **Butler-Volmer Rate Constant** is automatically computed.

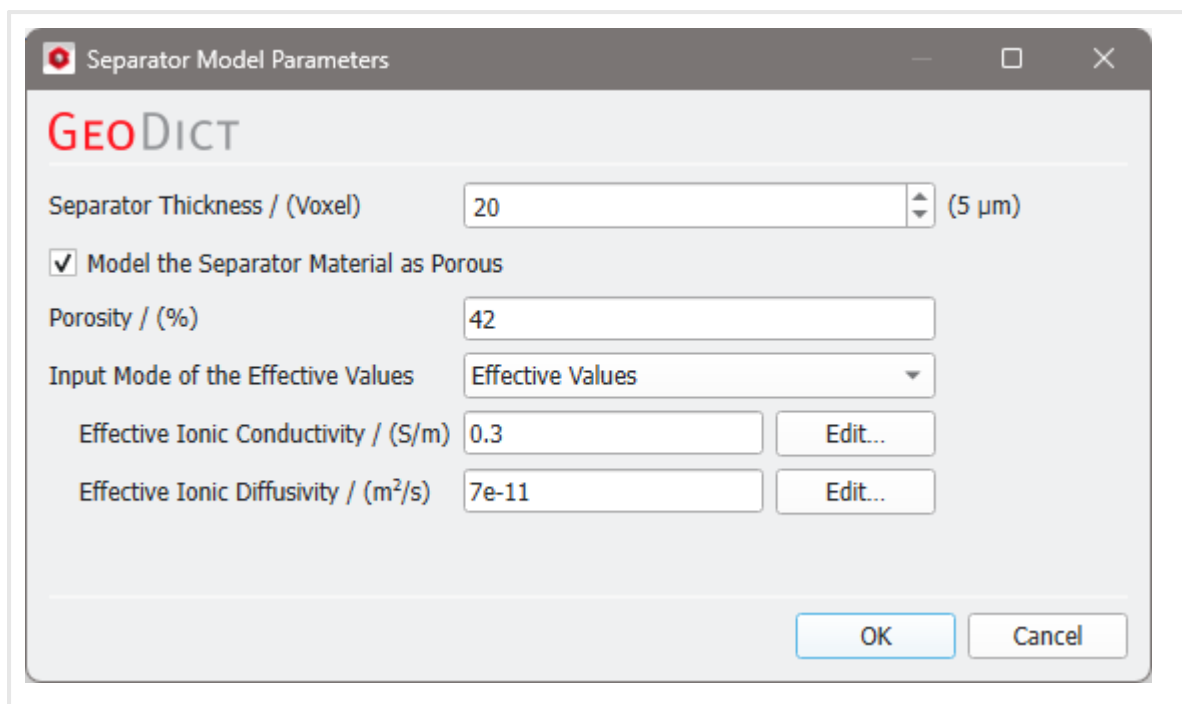
The last parameter is the [Effective Electronic Conductivity](#)^[31].

Parameter	Value	Unit
Lithium Reservoir Width / (Voxel)	3	(750 nm)
Maximum Exchange Current Density / (A/m ²)	700	
Electrolyte Lithium Concentration of Exchange Current Measurement / (mol/m ³)	1000	
Butler-Volmer Rate Constant / (A/(m mol) ^{0.5})	22.1359	
Effective Electronic Conductivity / (S/m)	1000	

OK Cancel

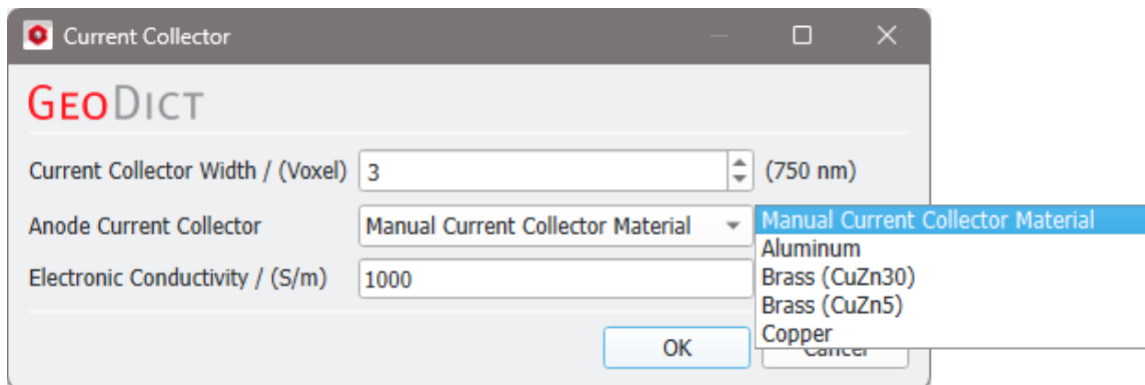
✓ Separator Parameters

For the separator, with **Edit Model** the **Separator Width** can be selected in number of voxels. Additionally, as already explained for the [Charge Battery](#)^[74] simulation, the ionic conductivity and ionic diffusivity of the electrolyte can be selected, or effective values can be defined. If **Model the Separator Material as Porous** is unchecked, the separator will have the same properties as the electrolyte for the simulation. When using a [solid electrolyte](#)^[116] in an all-solid-state electrode, porous separator (and porous Binder / Conductive Additive) is always unchecked.



✓ Current Collector Parameters

Width, material, and electronic conductivity of the current collectors can be defined with the corresponding **Edit Material** buttons.



Important! Even for materials from the GeoDict material database, the [effective electronic conductivity](#)^[31] needs to be defined in the dialog. It is recommended that the value defined is not higher than 1000 S/m to avoid numerical problems of the solver (see [Electrical Conductivity](#)^[78] for more details).

✓ Temperature

The **Temperature** defines the temperature during simulation in Kelvin (K), Celsius (°C), or Fahrenheit (°F). The material properties of active materials and electrolyte can

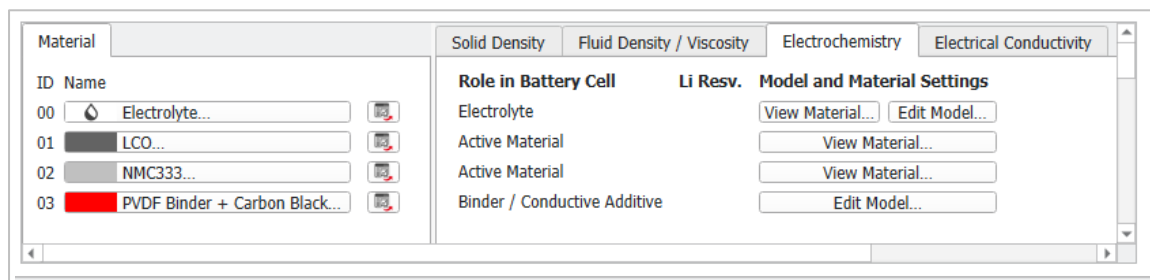
strongly depend on the temperature.

This temperature-dependence of the material properties can currently be derived from the entries in the material database only for the electrical conductivity and density.

However, the temperature-dependent ionic diffusivity and the exchange current density are not yet available in the material database. Consequently, while the electrical conductivity values can be adjusted based on the selected temperature — provided that the temperature dependence is included in the database entry — the other material parameters must be manually modified to ensure consistency with the chosen temperature. To facilitate comparisons of simulations at different temperatures, we recommend duplicating the relevant materials in the database for each new temperature and updating the material properties accordingly.

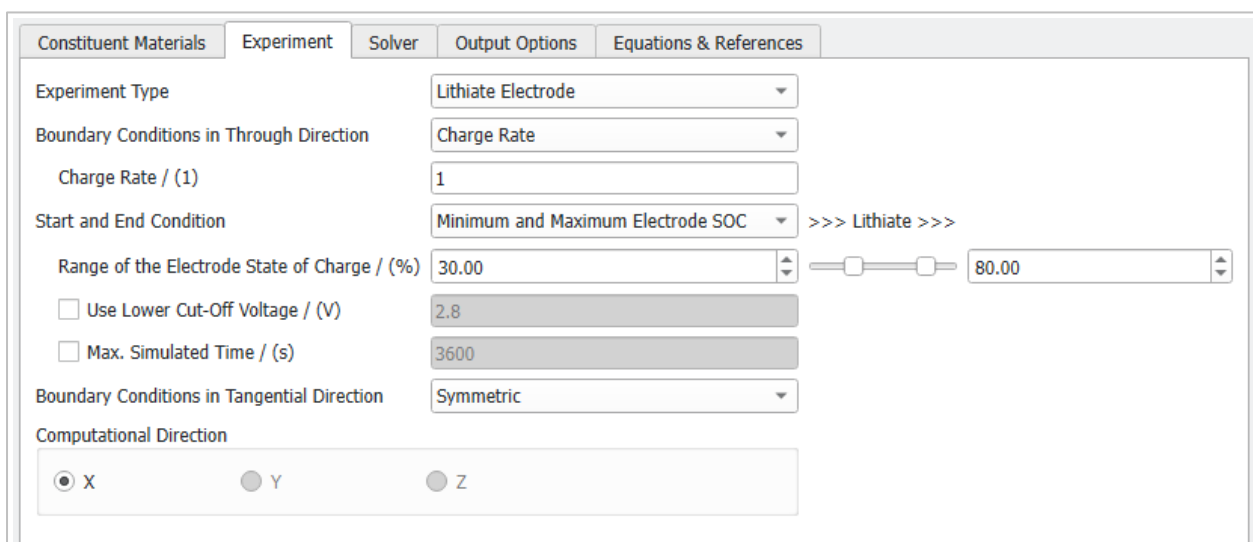
✓ Electrode Material Parameters

In the **Material** tab, the constituent materials of the electrode are shown. In the same way as for [battery charging](#)⁶⁵, the parameters of the materials can be shown or modified in the tabs on the right.



Experiment

For the charging simulation of an electrode, the parameters that need to be selected on the **Experiment** tab, are nearly the same as for the simulation of a [whole battery](#)⁷⁹.



Differences arise because, in a half cell simulation, only the state of charge (SOC) of the electrode being studied needs to be taken into account. The other electrode is modeled as a never-ending lithium reservoir.

Therefore, the available experiment types, **Lithiate Electrode** and **Delithiate Electrode**, simulate the lithiation or delithiation of the investigated electrode versus the lithium reservoir. The **Start and End Condition** for the simulation are defined by selecting **Minimum and Maximum Electrode SOC**.

The screenshot shows a software interface for setting simulation conditions. It features a dropdown menu labeled 'Start and End Condition' with the selected option 'Minimum and Maximum Electrode SOC'. To the right of the dropdown is a button labeled '>>> Lithiate >>>'. Below the dropdown is a label 'Range of the Electrode State of Charge' followed by a numerical input field containing '30.00'. To the right of this field is a slider control with a range from 30.00 to 80.00, indicated by a horizontal line with a double-headed arrow and numerical labels at both ends.

To start the simulation from a lithium concentration in the electrode, resulting from a previous simulation, select **Initial *.cap File and Final Electrode SOC**. Choose a .cap file as starting point of the simulation, and define the final SOC of the electrode that is not modeled as the lithium reservoir.

The screenshot shows a software interface for setting simulation conditions. It features a dropdown menu labeled 'Start and End Condition' with the selected option 'Initial *.cap File and Final Electrode SOC'. Below the dropdown is a label 'Initial *.cap File (*.cap)' followed by a text input field. To the right of the input field is a button labeled 'Browse...'.

The **Computational Direction** is fixed in X direction. If you need to rotate your structure to make the X-direction the charging direction, use the **Permute, Rotate & Mirror** command in **ProcessGeo**.

The screenshot shows a software interface for selecting the computational direction. It features a label 'Computational Direction' above three radio button options: 'X', 'Y', and 'Z'. The 'X' option is selected, indicated by a filled circle next to the label.

Output Options

Several options can be defined under the output options tab.

Constituent Materials Experiment Solver **Output Options** Equations & References

Electrode SOC Interval of Result Output / (%)

Write Fields into *.cap Files

- ☒ Concentration
- ☒ Potential
- ☒ Ion Flux Density
- ☒ Electric Current Density
- ☒ Kinetic Overpotential
- ☒ Plating Potential
- ☒ Produced Heat
- ☒ Interface Current Density

✓ Electrode SOC Interval of Result Output

The **Electrode SOC interval of result output** defines the interval for the export of intermediate result files in percent of the cell state of charge.

✓ Write Fields into *.cap Files

Select which fields to write into the 3D result files (*.cap).

The lithium ion **Concentration** and the **Potential** are always written.

For the other fields, decide which ones you need. Deselecting fields saves disc space.

For a visualization of all result fields see [here](#)^[110].

Solver

Under the **Solver** tab, select the type of simulation to run and the solver to use when solving the system of partial differential equations, as well as the solver options.

Constituent Materials Experiment **Solver** Output Options Equations & References

Simulation Type

Solver Type

Parallelization 16 Threads

Time Step

Time Step Input Mode

LIR BESTmicro BESTmeso

☒ Error Bound

☐ Maximum Iterations

☐ Maximum Run Time / (h)

▶ Advanced Options

✓ Simulation Type

Select the **Simulation Type** to one of the following:

- The **Fully Resolved Simulation**^[12] runs directly on the voxels of the battery structure. It is therefore very accurate, and, in addition to charge curves, also provides solution files with results resolved on the voxel scale and slice mean plots.
- The **Homogenized Simulation**^[18] is much faster than the fully resolved simulation. It uses an advanced pseudo 2D-Newman-model (DFN-model) which is a simplified model, that is created from the given structure. The effective parameters for this simulation are computed in GeoDict. It returns a charge curve as well, but no solution fields resolved on the voxel scale.
- The **Calculate Homogenized Parameters** option does not run a charging simulation. Instead it only computes the effective parameters from the structure that are needed for a pseudo-2D Newman model (DFN-model) simulation. The **Experiment**^[79] and **Output Options**^[92] tabs are grayed out. These parameters can be loaded into the **Charge Homogenized Electrode**^[155] dialog for fast simulations on an already homogenized electrode.
- The last option is to **Calculate Equilibrium Potential Curve**. The **Experiment**^[79] and **Output Options**^[92] tabs are grayed out, because the full simulation is not performed. The cell potential in equilibrium is determined considering only geometry and material information.

✓ Solver Type

For a **Fully Resolved Simulation**, select **LIR** or **BESTmicro** for **Solver Type**.

For the **Homogenized Simulation**, only the **BESTmeso** solver is available.

If using any of the other two simulation types none of the solvers are used.

For the **LIR** solver, [additional parameters](#)^[148] for the computation can be defined.

✓ Parallelization

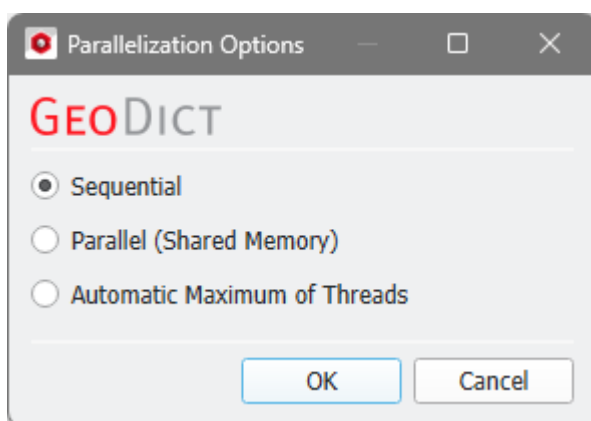
Control how many threads are used for the computation. Parallelization is possible if your license and hardware allow it.

The **Parallelization Options** dialog opens when clicking the **Edit** button and you can choose between **Sequential**, **Parallel (Shared Memory)**, or **Automatic Maximum of Threads**.

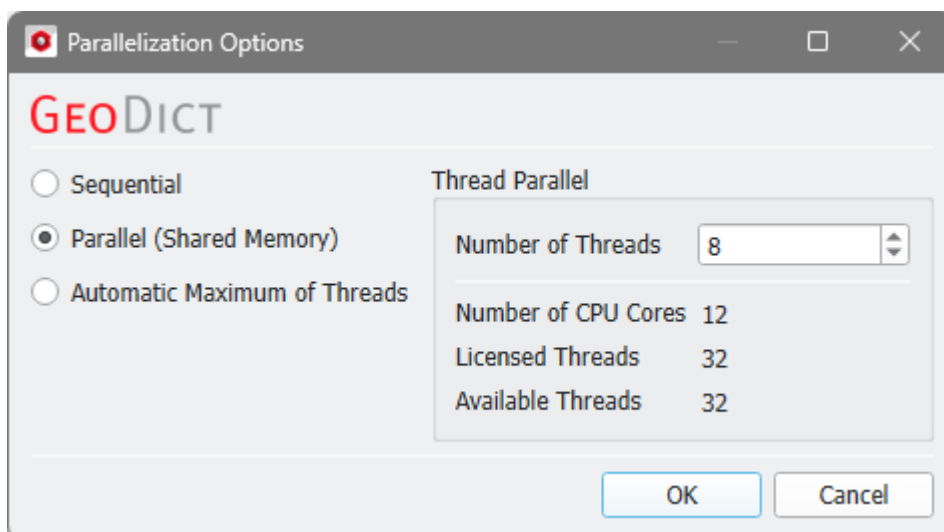
Parallelization 12 Threads (Automatic Maximum)

Edit...

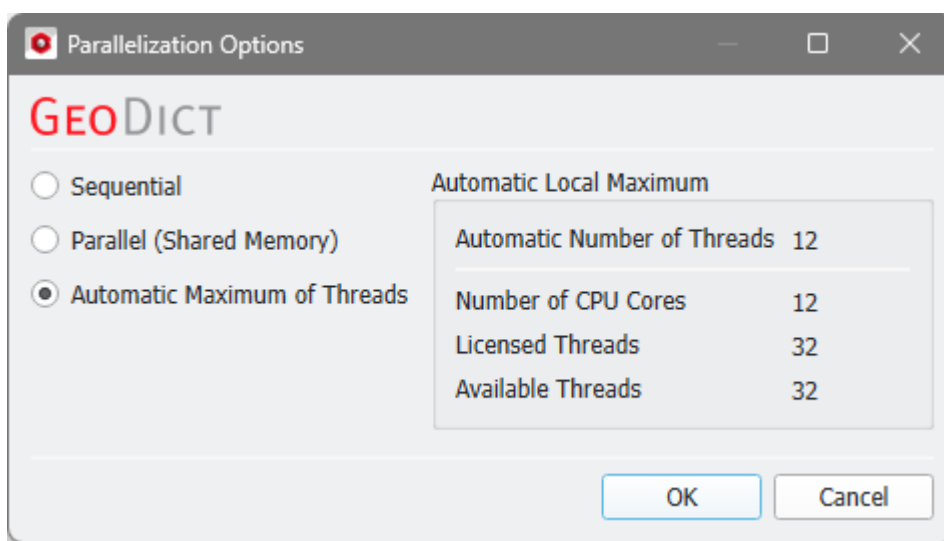
Selecting **Sequential** will not apply parallelization and only one thread is used for the computation.



When **Parallel (Shared Memory)** is selected, the **Number of Threads** can be entered. Below, the **Number of CPU Cores** that the current machine has, the maximum number of **Licensed Threads** and the number of those licensed threads that are available (**Available Threads**) are shown in the dialog. Of course, the maximal number of parallel processes you can use, is the smallest of those three numbers.



If **Automatic Maximum of Threads** is selected, the number of parallel processes is automatically selected for optimal speed, based on the CPU cores and licensed parallel processes.

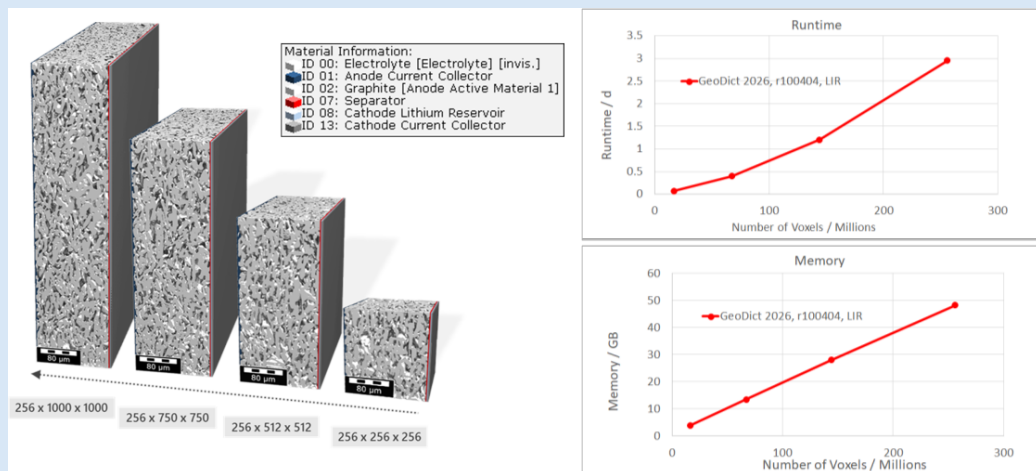


The **Automatic Local Maximum** of processes is automatically selected, which is the minimum of **Number of CPU Cores**, **Licensed Threads**, and **Available Threads**.

i Parallelization Benchmark Results

A half cell consisting of a graphite electrode and a lithium reservoir is simulated. The graphite electrode is charged from 5% to 91%. The simulation is run for increasing structure size to account for inhomogeneities or for battery aging simulations.

The simulation is run with LIR solver. The necessary memory for the computation is increasing linearly with the number of voxels simulated. Even a simulation with 250 million voxels can be run in less than 3 days, with only 50 GB RAM required.



✓ Time Step

In the **Time Step** panel an option for the **Time-Step Input Mode** may be selected.

Time Step	
Time Step Input Mode	Automatic
	Automatic Minimum Number of Time Steps Maximum Time Step Size

Any of the electrode solvers calculates the time evolution of the given Li-ion electrode. It starts at the initial state, which has time = 0 in the [result plots](#)^[97]. It takes the time step defined as maximum time step size and tries to find the electrode state at time = last time + time step by searching an equilibrium solution fulfilling the given system of differential equations. If no solution can be found for this time step size, it reduces the time step size, and the solver starts again. This procedure is repeated until an appropriate time step size is found. This time step size is used for the next steps in the simulation as well. After several successful steps with a certain time step size, the solver tries to increase this time step size again, to reduce overall computation time. With the **Time-Step Input Mode**, the maximum time-step size can be influenced. For more information on time steps see [State of Charge \(SOC\) and State of Lithiation \(SOL\)](#)^[10].

- Choosing **Automatic**, the solver selects the time-step size without restrictions.
- If a **Minimum Number of Time Steps** is defined, at least this number of points are computed for the solution and the maximum time-step size is selected accordingly. If your simulation does not produce enough points in the plots of the result file, then you might want to increase the **Minimum Number of Time Steps**.
- **Maximum Time Step Size** defines the maximum time step in seconds used in the simulation. If the size of the time step is oscillating a lot, the recommendation is to reduce this maximum value.

The time steps that were finally realized in the simulation are saved in the [Result Map](#)^[107] of the GeoDict result file (*.gdr file), created for the charging simulation, under the key **TimeDependentValues:TimeStep**.

If a new battery state is found in a simulation with a charge rate boundary condition, the solver computes the Electrode-SOC step of the just found new battery state i via:

$$\Delta(SOC)_i = \Delta t_i \cdot C / (1h) \quad (62)$$

with Δt_i the time step and C the charge rate. So, it is not clear from the start which is the next computed Electrode-SOC in a simulation, this depends on the time step.

Example:

- Charge Rate $C = 5$
- Time Step Size $\Delta t_i = 2.5 \text{ s}$
- Electrode-SOC step $\Delta(SOC)_i = 2.5 \cdot \frac{5}{1h} = 2.5s \cdot \frac{5}{3600s} = 0.00347 = 0.347\%$

If you choose to set the current density instead of the charge rate, then the calculation of the Electrode-SOC step size depends on the given current density and the cell

capacity. Thereby, the cell capacity depends on the electrode-geometry and the maximum lithium concentration of the active materials.

In the GeoDict result file (*.gdr file) created for the charging simulation, you can find the time-evolution of the Electrode-SOCs in percent as well as the corresponding times in seconds in the [Result Map](#)^[107] under the keys

TimeDependentValues:ElectrodeStateOfCharge and **TimeDependentValues:Time**, respectively.

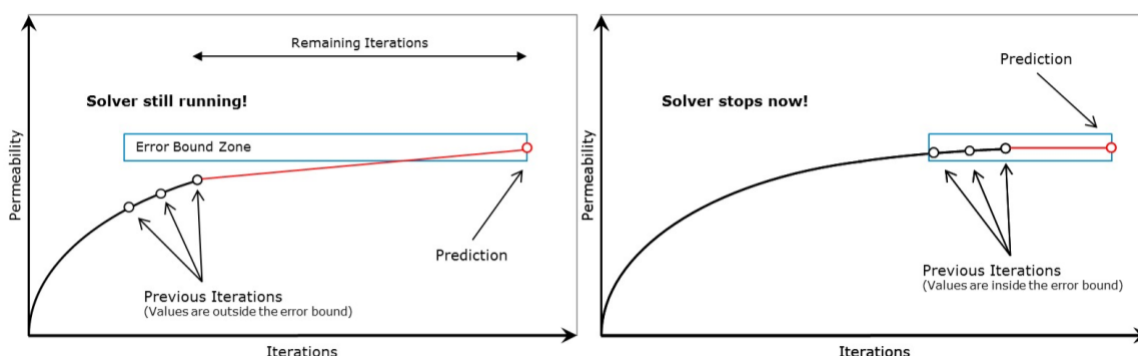
For simple simulations (charge rate ≤ 1 , physical domain size $\leq 5 \mu\text{m}$, only one active material per electrode, diffusivities $\geq 1\text{e-}12 \text{ m}^2/\text{s}$, conductivities $\geq 1 \text{ S/m}$ and no warnings during the simulation), the time step size is usually the maximum time step size set. Then, also the Electrode-SOC step is a constant value.

However, for more complex simulations (charge rate ≥ 10 , physical domain size $\geq 50 \mu\text{m}$, two active materials in an electrode with different parameters, low diffusivities in the active materials and small conductivities), it might happen that the time step size may be smaller than the maximum time step size defined and not constant over the whole simulation.

✓ LIR Solver Options

With the LIR solver, the partial differential equations of each time step are solved iteratively with an adaptive tree structure. Several solver options can be chosen in the panel on the right.

The stopping criterion **Error Bound** uses the result of previous iterations, and predicts the final solution based on linear and quadratic extrapolation. The solver stops if the relative difference between computed and predicted solution is smaller than the specified error bound. The stopping criterion recognizes oscillations in the convergence behavior and prevents premature stopping at local minima or maxima. A damped convergence curve is fit through the oscillating curve and the solver stops then regarding the damped convergence curve.



If the Krylov method (under LIR - Advanced Options) is activated, which is always the case in BatteryDict, the definition of **Error Bound** is somewhat different. Here, no prediction is made, instead the continuity between neighboring cells and the conservation of mass is checked. The maximal value is normalized by the mean flow and if this value is smaller than the **Error Bound** the simulation stops.

Use the **Maximum Iterations** value or the **Maximum Run Time (h)** stopping criteria causes the solver to stop if the maximal number of iterations and/or the maximal runtime (in hours) is exceeded.

When the solver stops because one of these criteria has been reached, no guarantee on the quality of solution can be given. In this case, a warning is printed into the report. The following possibilities might help:

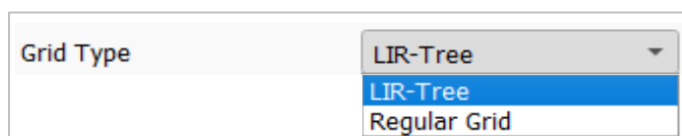
- Check the corresponding .log file to see how large the residual values and the computed values are. If the computed values are in reasonable range and they do not have changed during the last iterations, you may decide to use the current result.
- Double-check the structure and parameter values. Unphysical parameters or too rough resolution of the structure (leading, e.g., to artificial unconnected components) can cause an iterative solver to fail.



Important! Note that all stopping criteria selected are applied for each time step separately. Thus, the maximal run time defined is not the maximal run time for the whole charging simulation, but for each time step.

Unfold **Advanced Options** to gain access to several advanced solver options.

The **Grid Type** decides what kind of tree structure is used for the simulation.



The default option is **LIR-Tree** and should always be used. The solver uses an adaptive grid structure called LIR-tree and needs up to 10 times less runtime and memory compared to the **Regular Grid** option.

The solver can analyze the result field during the computation and improves the adaptive grid in places where more accuracy is needed. The LIR solver splits cells where a high gradient occurs.

Depending on the material parameters and geometry of the structure, the underlying mathematical problem can vary in complexity, thus influencing the behavior of the solver. The more complex the problem is, the more stable the solver settings should be.

Relaxation	1
------------	--------------------------------

With the **Relaxation** number, the solver is adjusted from **Stable** (which results in higher number of iterations, slower time stepping, and longer solver run times), to **Fast**, which makes the solver run less iterations but implies the risk that the solver does not converge. The **Relaxation** is a parameter of the [SOR method](#) and must be between 0 and 2 to ensure convergence. For relaxation values smaller than one (<1.0), the simulation is more stable. For relaxation values larger than one (>1.0), the simulation converges faster.

The **LIR** solver can **Optimize for Speed** or **Memory**.

Optimize for	Speed Memory Speed
--------------	---

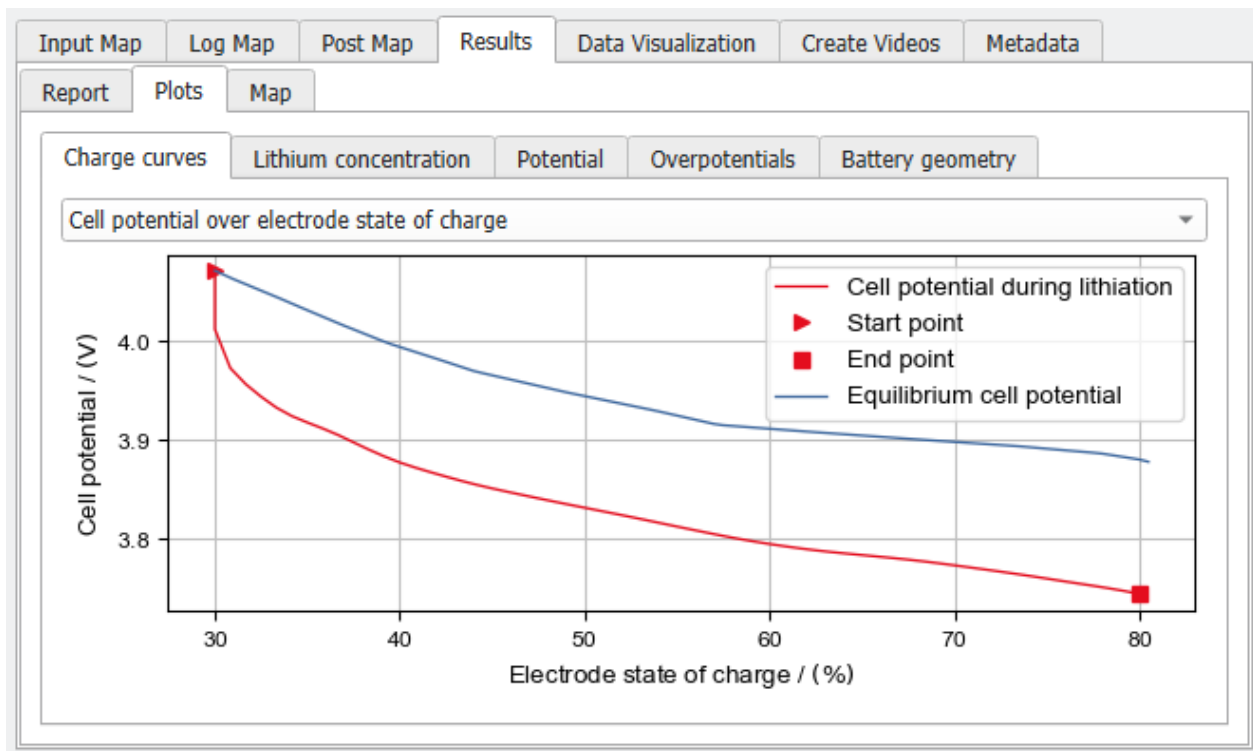
- If **Speed** is chosen, the solver constructs additional optimization structures. The runtime is decreased by up to 30% but requires up to 50% more memory compared to the other option.
- If **Memory** is chosen, the runtime is increased by up to 40% but the solver requires up to 50% less memory.

Results

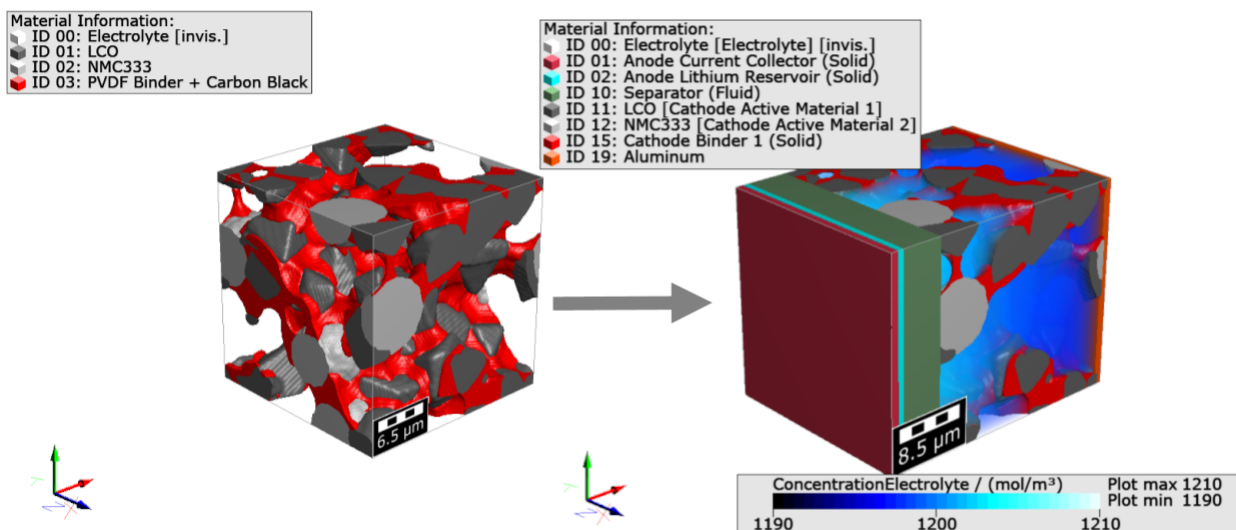
When the simulation of charging the electrode has finished, a GeoDict result file (.gdr) is available in the project folder and the **Result Viewer** of this result file automatically opens. Learn more about the general **Result Viewer** options in the Result Viewer chapter.

For the charging simulation of a single electrode, the same information as for charging a whole battery is available in this result file. It is shown, can be visualized, or further processed in the [same way](#) ⁹³.

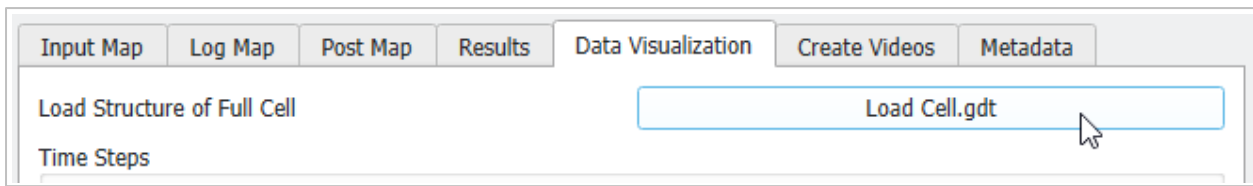
Note that for the charging simulation of a half cell, the modeled electrode is electrochemically always considered as the cathode. Lithiating the cathode, i.e., increasing the electrode state of charge, means discharging the half cell. On the **Results -Plots – Charge curves** subtab, the cell potential is shown over the electrode state of charge and is therefore decreasing during the charging simulation of the half cell.



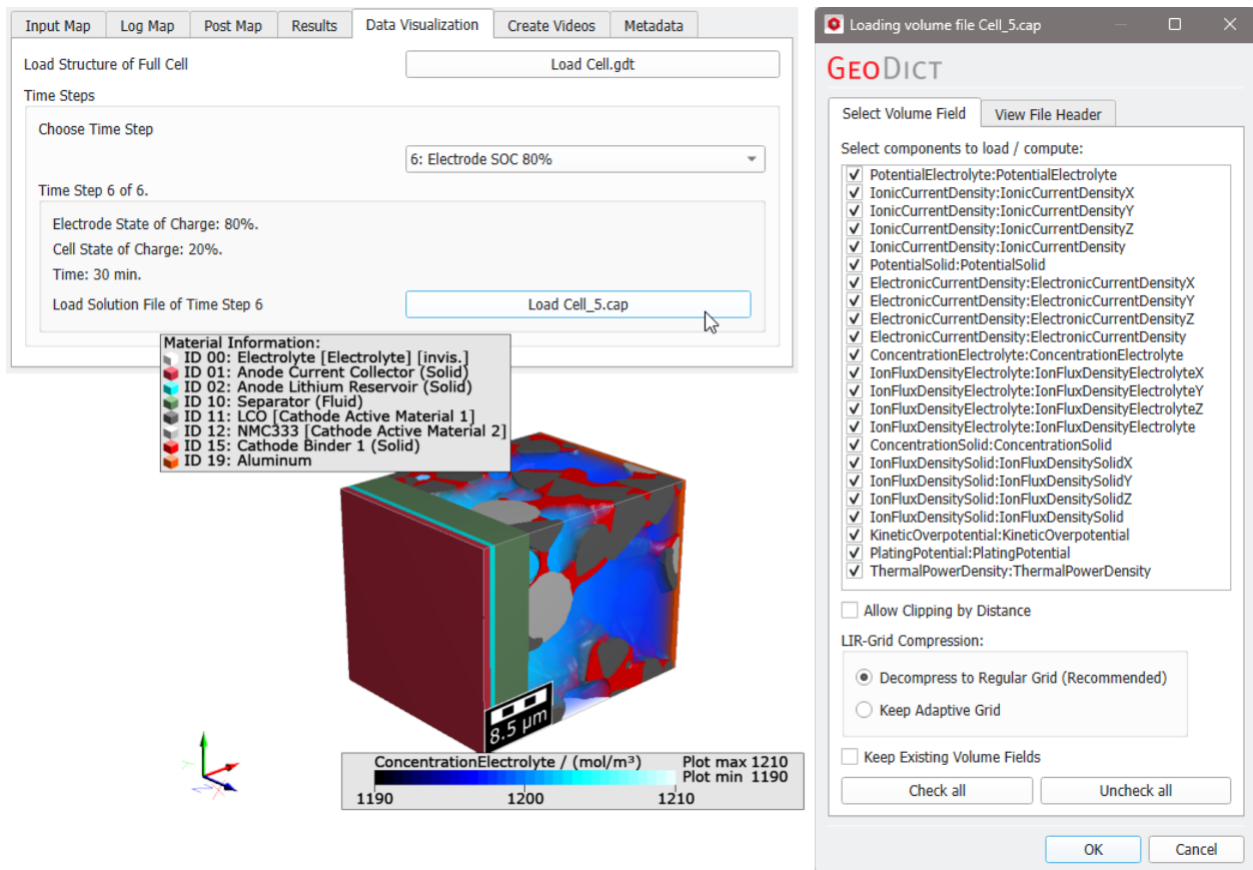
It is important to note that in the volume files of simulation (*.cap files), the result fields are stored for the entire half cell structure (including the electrode, both current collectors, separator, and lithium reservoir), rather than just the electrode alone. If the structure used as input for the simulation (and shown in the Visualization area of the main GUI) does not contain all components of the half cell, the size of the volume fields therefore does not fit to the structure size. Therefore, when loading one of the volume fields, the complete cell structure containing also the missing half cell components is loaded automatically



Choose **Load Cell.gdt** on the **Data Visualization** tab to load only the structure of the whole half cell without additional volume fields.



Select a **Time Step** and click **Load Cell_#.cap** to load the complete cell structure and the desired volume fields of this time step to the visualization area.



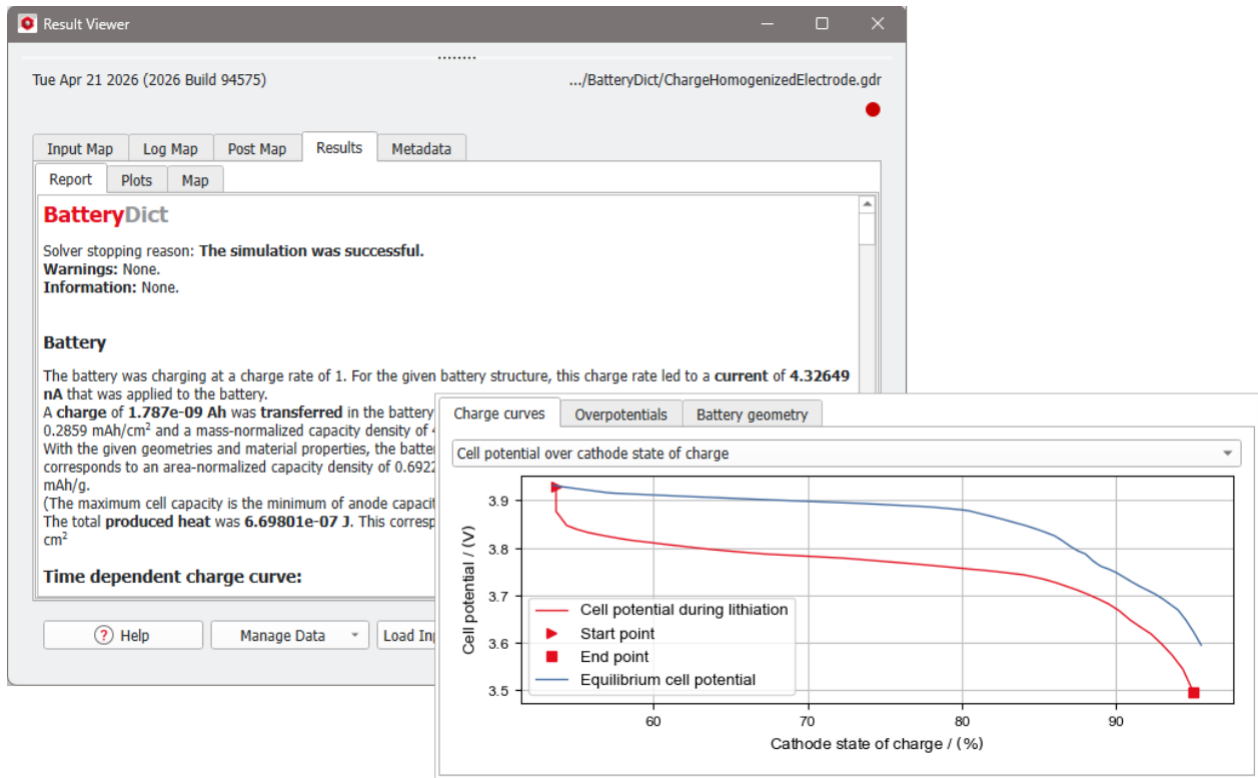
1.3.2 Charge Homogenized Electrode

With the **Charge Homogenized Electrode** command you can run homogenized half-cell simulations directly without providing an electrode geometry. You can supply the effective parameters in two ways:

- **Pre-calculated:** Load parameters that were previously generated using the **Homogenized Simulation** option or with the new **Calculate Homogenized Parameters** option in [Charge Electrode](#)^[143].
- **User-defined:** Enter the parameters manually in the dialog.

These new commands streamline the setup of parameter studies using the fast homogenized charging model.

If you want to dive deep into the underlying theory, have a look at the [Homogenized Simulation](#)^[18].



The Charge Homogenized Electrode command:

- [Options](#) ¹⁵³
Define the parameters for your homogenized charging or discharging simulation.
- [Results](#) ¹⁶⁴
View the results in the Result Viewer.

Options

Choose **Electrode** and **Charge Homogenized Electrode** from the pull-down menus in the BatteryDict section and click **Edit** to adjust the charging parameters.

BatteryDict – Charge Homogenized Electrode

GEODICT

Result File Name (*.gdr)

Geometry & Materials Experiment Solver Equations & References

Temperature -273.15 ≤ ≤ 1000.00 °C

Mass Density / (kg/m³)

Geometry Electrolyte Anode Separator Cathode

Length in Y-Direction / (m)

Length in Z-Direction / (m)

Anode Thickness / (m)

Separator Thickness / (m)

Cathode Thickness / (m)

? [Save] [Load] [Undo] [Redo] [Zoom] OK Cancel

Tabs of Charge Homogenized Electrode:

- [Geometry & Materials](#)^[154]
Define the effective parameters of your geometry.
- [Experiment](#)^[159]
Edit the experiment parameters for lithiation, delithiation or a charging profile.
- [Solver](#)^[161]
Define the time step and parallelization for the simulation.

Geometry & Materials

Define the effective parameters of your geometry. At the top define [temperature](#)^[155] and [mass density](#)^[155]. If you computed the effective parameters using [Charge Electrode](#)^[143], click [Load "Charge Electrode" Result](#)^[155].

Geometry & Materials
Experiment
Solver
Equations & References

Temperature
-273.15 ≤ 20 ≤ 1000.00 °C
Load "Charge Electrode" Result...

Mass Density / (kg/m³)
1000

Geometry
Electrolyte
Anode
Separator
Cathode

Length in Y-Direction / (m)
5e-05

Length in Z-Direction / (m)
5e-05

Anode Thickness / (m)
3e-05

Separator Thickness / (m)
1e-05

Cathode Thickness / (m)
3e-05

✓ Load "Charge Electrode" Result

If you computed the effective parameters using [Charge Electrode](#)^[143], click **Load "Charge Electrode" Result**. The parameter values will be loaded in the **Geometry & Materials** tab. The [Experiment](#)^[125] and [Solver](#)^[161] tabs are not affected by this action.

✓ Temperature

The **Temperature** defines the temperature during simulation in Kelvin (K), Celsius (°C), or Fahrenheit (°F). The material properties of active materials and electrolyte can strongly depend on the temperature.

This temperature-dependence of the material properties can currently be derived from the entries in the material database only for the electrical conductivity and density.

However, the temperature-dependent ionic diffusivity and the exchange current density are not yet available in the material database. Consequently, while the electrical conductivity values can be adjusted based on the selected temperature — provided that the temperature dependence is included in the database entry — the other material parameters must be manually modified to ensure consistency with the chosen temperature. To facilitate comparisons of simulations at different temperatures, we recommend duplicating the relevant materials in the database for each new temperature and updating the material properties accordingly.

✓ Mass Density

Specify the **Mass Density** of the structure in kg/m³. Combined with the [geometry](#)^[155] parameters, this value is used to calculate the mass-normalized cell capacity density.

✓ Geometry

Define the **Length in Y-Direction** and **Z-Direction** of your battery structure. The X-direction is the charging direction and its length is defined by the thickness of the different components of the battery: **Anode Thickness**, **Separator Thickness**, and **Cathode Thickness**.

The anode and cathode thickness do not contain the thickness of the current collectors.

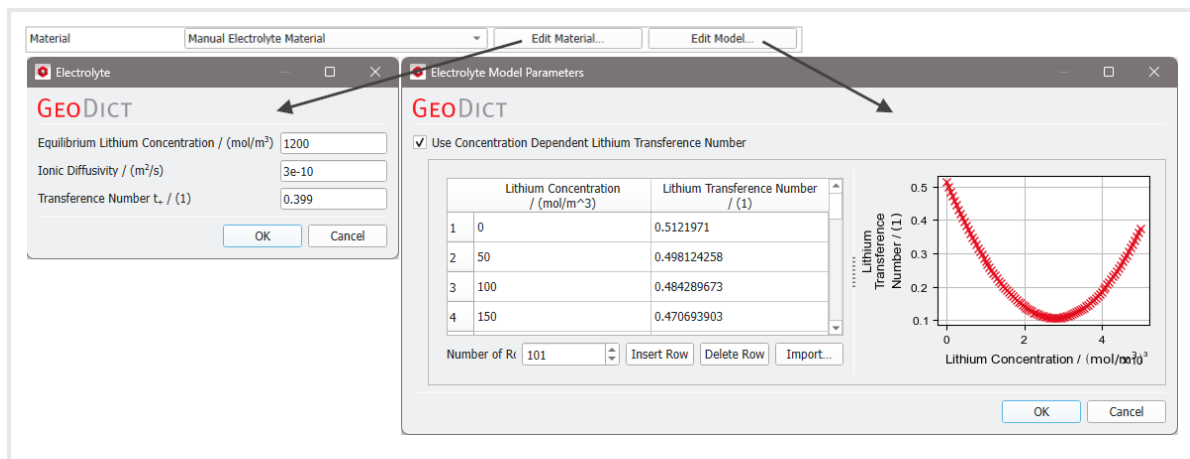
Geometry	Electrolyte	Anode	Separator	Cathode
Length in Y-Direction / (m)	0.00012			
Length in Z-Direction / (m)	0.00012			
Anode Thickness / (m)	6e-05			
Separator Thickness / (m)	1.6e-05			
Cathode Thickness / (m)	6e-05			

✓ Electrolyte

Choose a material from the pull-down menu. The material parameters button changes between **Edit Material** and **View Material** depending on whether **Manual Electrolyte Material** is selected. The material selection is generated automatically based on all materials in the GeoDict material database being assigned electrolyte as the [Role in Battery Cell](#)^[37] under the **Electrochemistry** tab. If you add your own electrolyte materials, they will also appear in the menu.

Geometry	Electrolyte	Anode	Separator	Cathode
Material	Electrolyte - Manual Electrolyte Material Electrolyte - Electrolyte (Solvionic) - Electrolyte_LLZO - LLZO - LPSCI - h-LZSOCv2	View Material... Edit Model...		

The parameters available under [View Material / Edit Material](#)^[72] and [Edit Model](#)^[74] are similar to for the fully-resolved charging simulation. However, concentration dependent parameters are only available for the lithium transference number.



✓ Anode

For the **Anode Current Collector** enter the **Electronic Conductivity** in **S/m**.

For **Charge Homogenized Electrode** the anode is always modeled as a **Lithium Reservoir** for an half-cell simulation and will be considered as a never-ending reservoir of lithium, not limiting the battery performance.

The **Maximum Exchange Current Density**^[32] can be defined in respect to the **Electrolyte Lithium Concentration of Exchange Current Measurement**^[35]. Define the **Effective Electronic Conductivity**^[78] and **Specific Surface Area** for the lithium reservoir. The specific surface area defines the active surface of the lithium reservoir in the anode. A larger specific surface area reduces the kinetic overpotential.

Geometry	Electrolyte	Anode	Separator	Cathode
Anode Current Collector Electronic Conductivity / (S/m) 1000				
Lithium Reservoir Maximum Exchange Current Density / (A/m²) 700 Electrolyte Lithium Concentration of Exchange Current Measurement / (mol/m³) 1000 Butler-Volmer Rate Constant / (A/(m mol)⁰.⁵) 22.1359 Effective Electronic Conductivity / (S/m) 1000 Specific Surface Area / (m²/m³) 100000				

✓ Separator

For the **Separator** enter the **Effective Ionic Conductivity**^[31], the **Effective Ionic Diffusivity**^[74] and the **Electrolyte Volume Fraction**. Note, that the electrolyte volume fraction needs to be given relative to the separator volume.

Geometry	Electrolyte	Anode	Separator	Cathode	
Effective Ionic Conductivity / (S/m)				0.256667	Edit...
Effective Ionic Diffusivity / (m ² /s)				7e-11	Edit...
Electrolyte Volume Fraction / (1)				0.42	

✓Cathode

For the **Cathode Current Collector** enter the **Electronic Conductivity** in S/m.

Geometry	Electrolyte	Anode	Separator	Cathode	
Cathode Current Collector					
Electronic Conductivity / (S/m)				1000	
Cathode					
Effective Electronic Conductivity / (S/m)				12.0798485	
Effective Ionic Conductivity / (S/m)				0.15596	Edit...
Effective Ionic Diffusivity / (m ² /s)				4.44362e-11	Edit...
Electrolyte Volume Fraction / (1)				0.305962593	
Number of Active Materials				1	
Active Material 1					
Material		NMC333	View Material...		
Representative Particle Radius / (m)		3.91099384e-06			
Specific Surface Area / (m ² /m ³)		453869.259			
Connected Volume Fraction / (1)		0.628417852			
Unconnected Volume Fraction / (1)		2.22222222e-06			

For the **Cathode** the following parameters need to be defined:

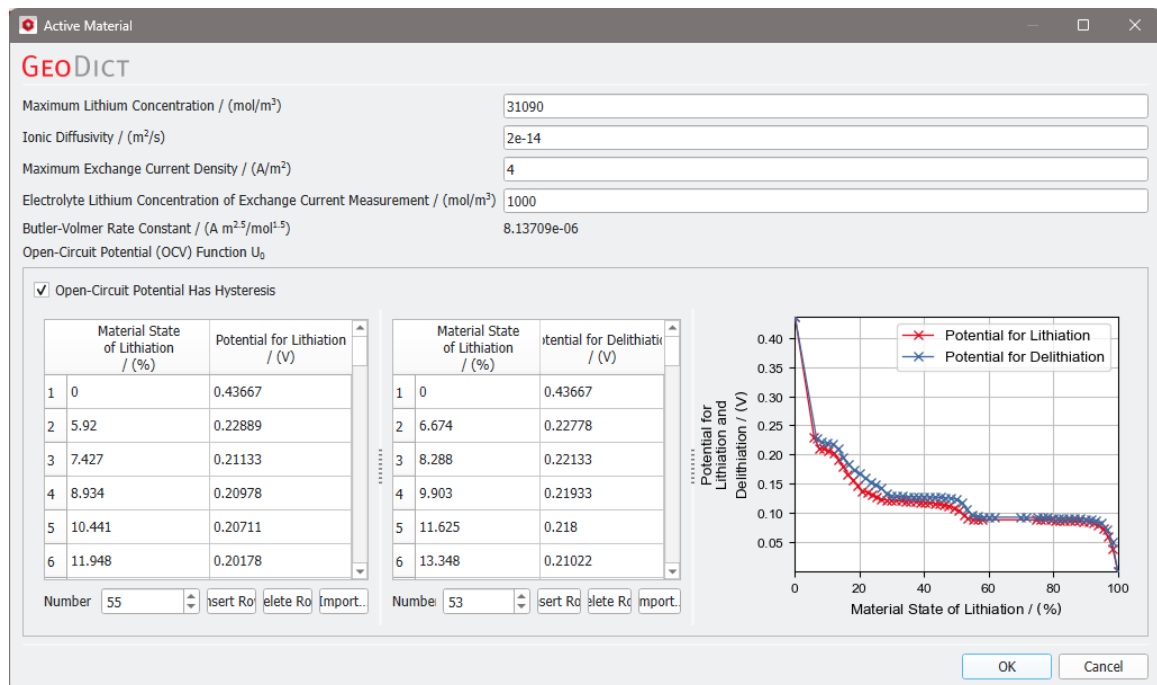
Define the [Effective Electronic Conductivity](#)^[78], the [Effective Ionic Conductivity](#)^[31], the **Electrolyte Volume Fraction** (relative to the electrode volume), and the **Number of Active Materials** in the electrode.

For all active materials select the **Material** from the pull-down menu.

The material selection is generated automatically based on all materials in the GeoDict material database being assigned active material as the [Role in Battery Cell](#)^[37] under the **Electrochemistry** tab. If you add your own active materials, they will also appear in the menu.

Either select a material from the database or select **Manual Active Material**.

Then, view / edit the the simulation parameters [Maximum Lithium Concentration](#)^[31], [Ionic Diffusivity](#)^[31], [Maximum Exchange Current Density](#)^[32], [Electrolyte Lithium Concentration of Exchange Current Measurement](#)^[35] and [Open-Circuit Potential Function \(OCV\) Function](#)^[35] by clicking [View Material / Edit Material](#)^[71].



The **Representative Particle Radius** should be a representative value for the particle size distribution in your electrode. Larger particles lead to higher [diffusive overpotentials](#)^[27].

Enter the volume of connected active material relative to the electrode volume for **Connected Volume Fraction**. The **Unconnected Volume Fraction** is then the volume of unconnected active material. The volume fractions of connected and unconnected material sum up to the total volume fraction of active material relative to the electrode volume. The sum of all volume fractions in the active material (Electrolyte, Connected Volume, and Unconnected Volume) must be not larger than 1.

Experiment

For the charging simulation of an electrode, the parameters that need to be selected on the **Experiment** tab are nearly the same as for the simulation of a [whole battery](#)^[79].

Geometry & Materials	Experiment	Solver	Equations & References
Experiment Type		Lithiate Electrode	
Boundary Conditions in Through Direction		Charge Rate	
Charge Rate / (1)		1	
Start and End Condition		Initial Voltage and Final Electrode SOC	
Initial Equilibrium Voltage for Lithiation / (V)		3.93	
Final Electrode SOC / (%)		95	
☒ Use Lower Cut-Off Voltage / (V)		2.8	
☐ Max. Simulated Time / (s)		3600	
Boundary Conditions in Tangential Direction		Symmetric	
Computational Direction			
☒ X ☐ Y ☐ Z			

Differences arise because, in a half cell simulation, only the state of charge (SOC) of the electrode being studied needs to be taken into account. The other electrode is modeled as a never-ending lithium reservoir.

Therefore, the available experiment types, **Lithiate Electrode** and **Delithiate Electrode**, simulate the lithiation or delithiation of the investigated electrode versus the lithium reservoir. The **Start and End Condition** for the simulation are defined by selecting **Minimum and Maximum Electrode SOC**.

Start and End Condition	Minimum and Maximum Electrode SOC	>>> Lithiate >>>
Range of the Electrode State of Charge	30.00	80.00

To start the simulation from a lithium concentration in the electrode, resulting from a previous simulation, select **Initial *.cap File and Final Electrode SOC**. Choose a .cap file as starting point of the simulation, and define the final SOC of the electrode that is not modeled as the lithium reservoir.

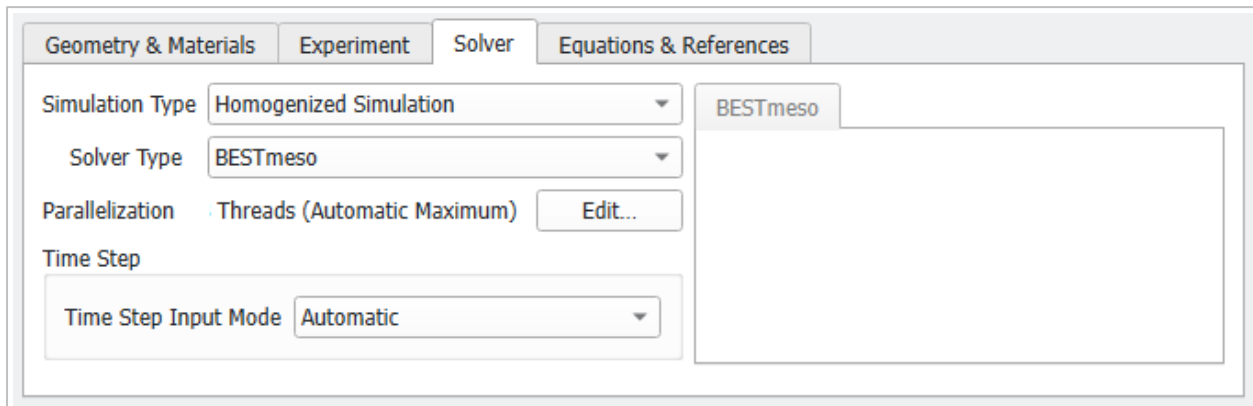
Start and End Condition	Initial *.cap File and Final Electrode SOC
Initial *.cap File (*.cap)	Browse...

The **Computational Direction** is fixed in X direction. If you need to rotate your structure to make the X-direction the charging direction, use the **Permute, Rotate & Mirror** command in **ProcessGeo**.

Computational Direction
☒ X ☐ Y ☐ Z

Solver

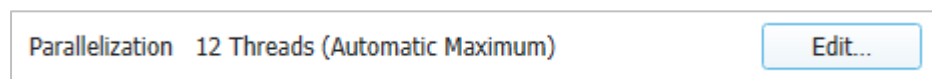
Under the **Solver** tab, select the **Parallelization** and **Time Step** modes. The simulation type will always be [Homogenized Simulation](#)¹⁸ and computed with the BESTmeso solver.



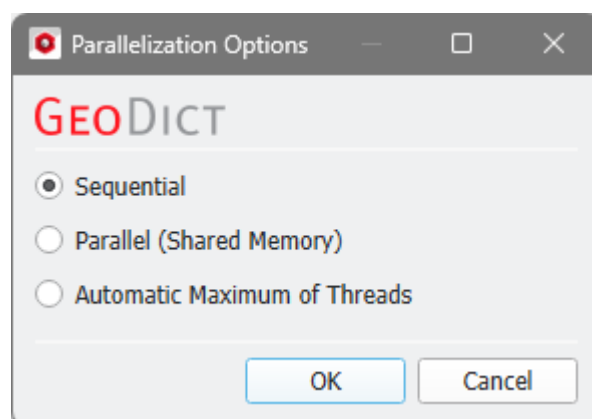
✓ Parallelization

Control how many threads are used for the computation. Parallelization is possible if your license and hardware allow it.

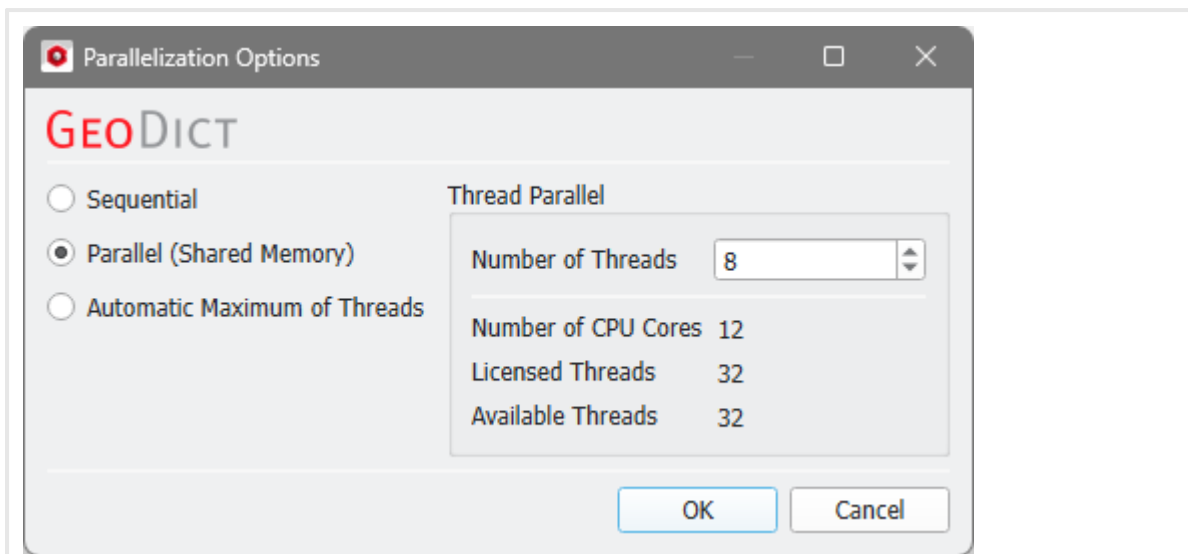
The **Parallelization Options** dialog opens when clicking the **Edit** button and you can choose between **Sequential**, **Parallel (Shared Memory)**, or **Automatic Maximum of Threads**.



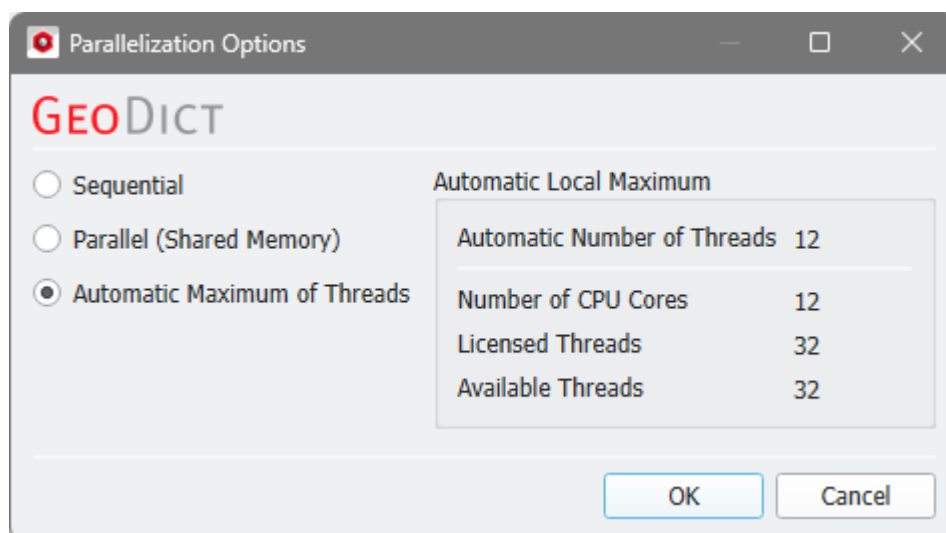
Selecting **Sequential** will not apply parallelization and only one thread is used for the computation.



When **Parallel (Shared Memory)** is selected, the **Number of Threads** can be entered. Below, the **Number of CPU Cores** that the current machine has, the maximum number of **Licensed Threads** and the number of those licensed threads that are available (**Available Threads**) are shown in the dialog. Of course, the maximal number of parallel processes you can use, is the smallest of those three numbers.



If **Automatic Maximum of Threads** is selected, the number of parallel processes is automatically selected for optimal speed, based on the CPU cores and licensed parallel processes.



The **Automatic Local Maximum** of processes is automatically selected, which is the minimum of **Number of CPU Cores**, **Licensed Threads**, and **Available Threads**.

✓ Time Step

In the **Time Step** panel an option for the **Time-Step Input Mode** may be selected.



Any of the electrode solvers calculates the time evolution of the given Li-ion electrode. It starts at the initial state, which has time = 0 in the [result plots](#)⁹⁷. It takes the time step defined as maximum time step size and tries to find the electrode state at time =

last time + time step by searching an equilibrium solution fulfilling the given system of differential equations. If no solution can be found for this time step size, it reduces the time step size, and the solver starts again. This procedure is repeated until an appropriate time step size is found. This time step size is used for the next steps in the simulation as well. After several successful steps with a certain time step size, the solver tries to increase this time step size again, to reduce overall computation time. With the **Time-Step Input Mode**, the maximum time-step size can be influenced. For more information on time steps see [State of Charge \(SOC\) and State of Lithiation \(SOL\)](#)^[107].

- Choosing **Automatic**, the solver selects the time-step size without restrictions.
- If a **Minimum Number of Time Steps** is defined, at least this number of points are computed for the solution and the maximum time-step size is selected accordingly. If your simulation does not produce enough points in the plots of the result file, then you might want to increase the **Minimum Number of Time Steps**.
- **Maximum Time Step Size** defines the maximum time step in seconds used in the simulation. If the size of the time step is oscillating a lot, the recommendation is to reduce this maximum value.

The time steps that were finally realized in the simulation are saved in the [Result Map](#)^[107] of the GeoDict result file (*.gdr file), created for the charging simulation, under the key **TimeDependentValues:TimeStep**.

If a new battery state is found in a simulation with a charge rate boundary condition, the solver computes the Electrode-SOC step of the just found new battery state i via:

$$\Delta(SOC)_i = \Delta t_i \cdot C / (1h) \quad (63)$$

with Δt_i the time step and C the charge rate. So, it is not clear from the start which is the next computed Electrode-SOC in a simulation, this depends on the time step.

Example:

- Charge Rate $C = 5$
- Time Step Size $\Delta t_i = 2.5 \text{ s}$
- Electrode-SOC step $\Delta(SOC)_i = 2.5 \cdot \frac{5}{1h} = 2.5 \cdot \frac{5}{3600s} = 0.00347 = 0.347\%$

If you choose to set the current density instead of the charge rate, then the calculation of the Electrode-SOC step size depends on the given current density and the cell capacity. Thereby, the cell capacity depends on the electrode-geometry and the maximum lithium concentration of the active materials.

In the GeoDict result file (*.gdr file) created for the charging simulation, you can find the time-evolution of the Electrode-SOCs in percent as well as the corresponding times in seconds in the [Result Map](#)^[107] under the keys

TimeDependentValues:ElectrodeStateOfCharge and **TimeDependentValues:Time**,

respectively.

For simple simulations (charge rate ≤ 1 , physical domain size $\leq 5 \mu\text{m}$, only one active material per electrode, diffusivities $\geq 1\text{e-}12 \text{ m}^2/\text{s}$, conductivities $\geq 1 \text{ S/m}$ and no warnings during the simulation), the time step size is usually the maximum time step size set. Then, also the Electrode-SOC step is a constant value.

However, for more complex simulations (charge rate ≥ 10 , physical domain size $\geq 50 \mu\text{m}$, two active materials in an electrode with different parameters, low diffusivities in the active materials and small conductivities), it might happen that the time step size may be smaller than the maximum time step size defined and not constant over the whole simulation.

Results

After a homogenized charging simulation has finished, a GeoDict result file (.gdr) is written and the **Result Viewer** of this result file automatically opens. The information of simulation result is shown, can be visualized, or further processed.

These results are accessible at any time by loading the .gdr file from the menu bar (**File - Open Results (*.gdr)**). No **Load Structure** button is available, since this command does not need a geometry. All effective parameters were given in the options dialog. Learn more about the general **Result Viewer** options in the Result Viewer chapter.

In the following, the results were produced using the [Calculate Homogenized Parameters](#)^[143] results from the structure used as an example for [Charge Electrode](#)^[150].

The results found under the **Results** tab are the same as for a [homogenized simulation](#)^[94] using [Charge Electrode](#)^[143].

The plots under the **Plots** tab are the [Charge Curves](#)^[97] and [Overpotentials](#)^[105] also found for **Charge Electrode** simulations. They can also be compared with **Charge Electrode** results by using Combine Results.

Result Viewer

Tue Apr 21 2026 (2026 Build 94575)

.../BatteryDict/ChargeHomogenizedElectrode.gdr

Input Map

Log Map

Post Map

Results

Metadata

Report

Plots

Map

BatteryDict

Solver stopping reason: **The simulation was successful.**

Warnings: None.

Information: None.

Battery

The battery was charging at a charge rate of 1. For the given battery structure, this charge rate led to a **current of 4.32649 nA** that was applied to the battery.

A **charge of 1.787e-09 Ah** was transferred in the battery.

0.2859 mAh/cm² and a mass-normalized capacity density of 4.0 mAh/g.

With the given geometries and material properties, the battery corresponds to an area-normalized capacity density of 0.6922 mAh/g.

(The maximum cell capacity is the minimum of anode capacity and cathode capacity.)

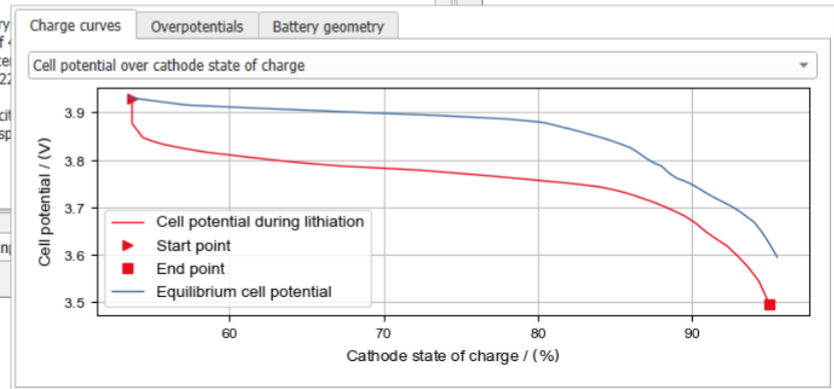
The total **produced heat** was **6.69801e-07 J**. This corresponds to a heat production of 0.0001775 mW/cm².

Time dependent charge curve:

Help

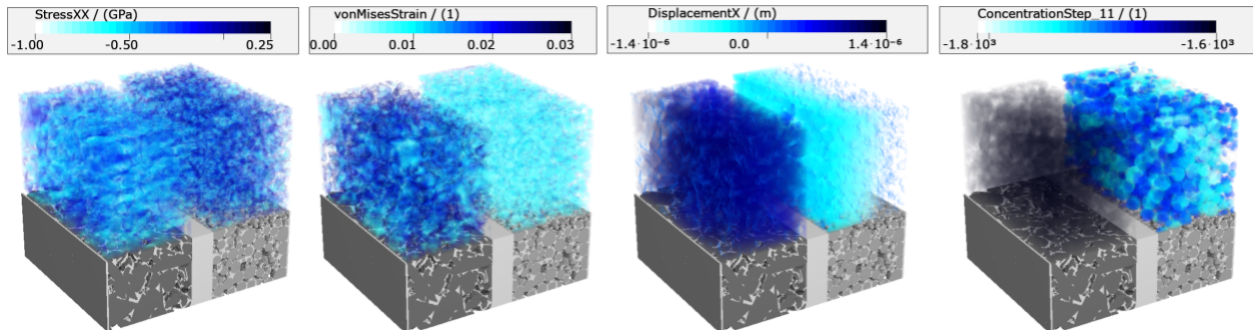
Manage Data

Load In



1.4 Degradation

Compute mechanical deformations of a battery cell due to lithium intercalation after running a charging simulation with [Charge Battery](#)⁶² or [Charge Electrode](#)¹³⁵.



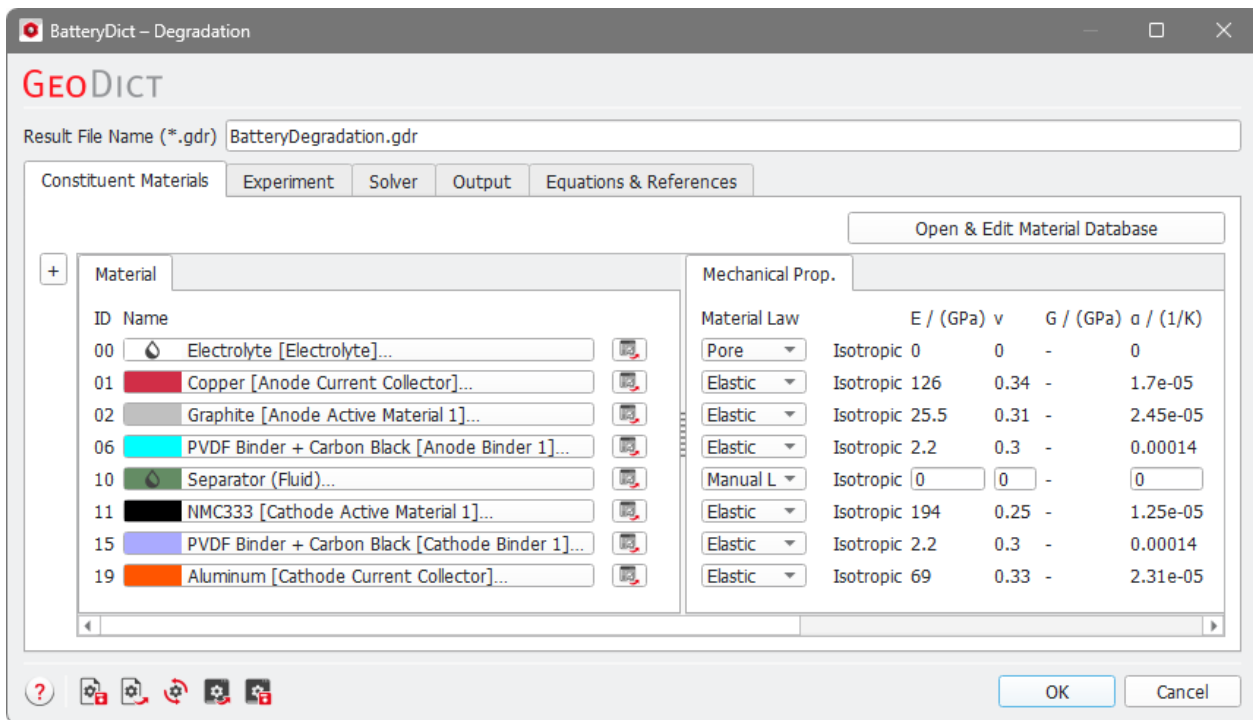
Important! If the lithium concentration fields have been calculated with [Charge Electrode](#)¹³⁵, it is required to use the cell geometry of the simulation for **Degradation**, see [Charge Electrode - Results](#)¹⁵¹.

The Degradation command:

- [Options](#)¹⁶⁶
Define the parameters for your degradation simulation.
- [Results](#)¹⁸⁰
View the results of the degradation simulation.

1.4.1 Options

Select **Degradation** in the BatteryDict section and click **Edit** to open the options dialog for the simulation.

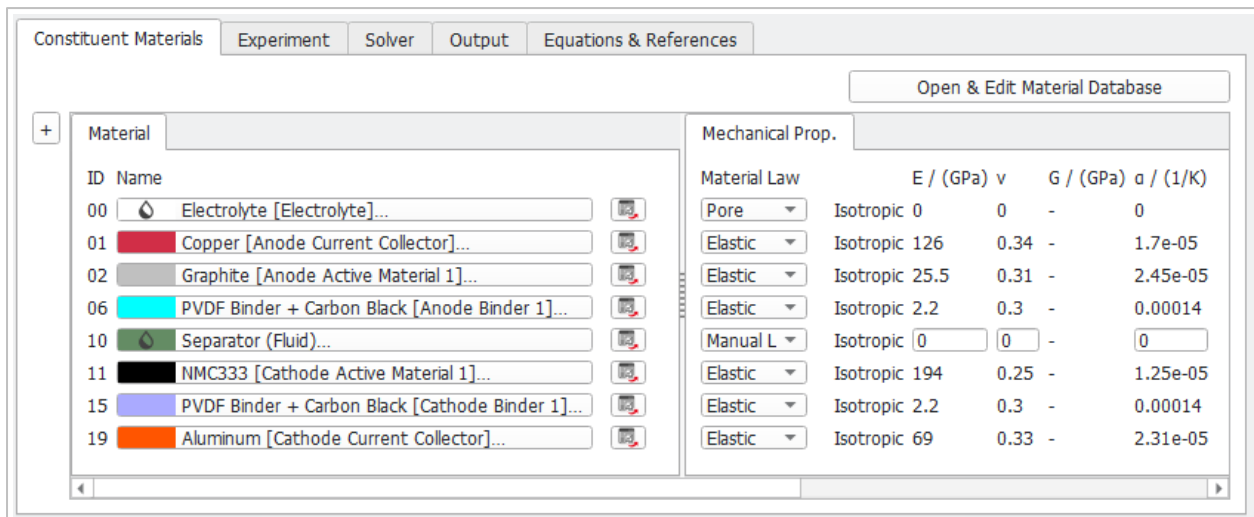


Tabs of Degradation:

- [Constituent Materials](#)¹⁶⁷
Define the properties for all materials in the battery cell.
- [Experiment](#)¹⁶⁹
Edit the experiment parameters for the degradation simulation.
- [Solver](#)¹⁷²
Define the stopping criteria and parallelization for the simulation.
- [Output](#)¹⁷⁸
Decide which 3D result fields and geometries should be saved.

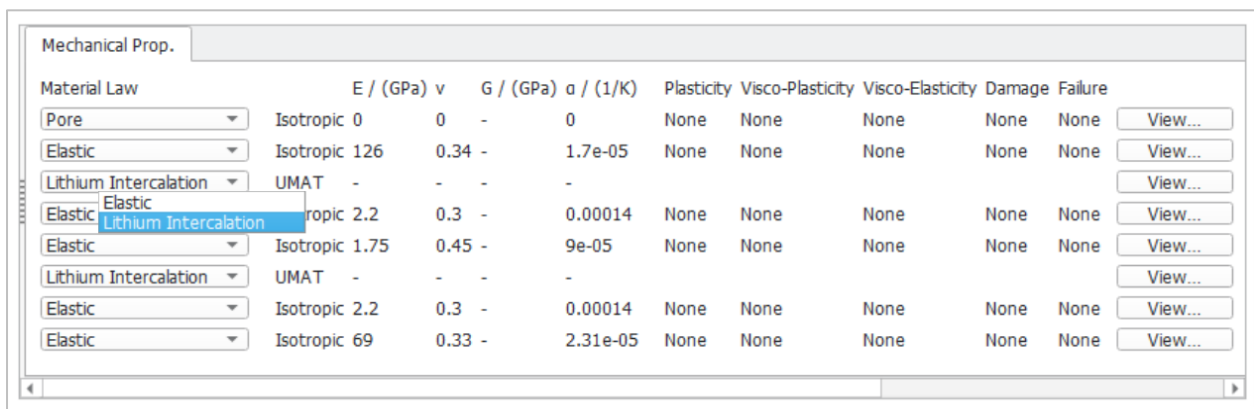
Constituent Materials

In the **Constituent Materials** tab, the mechanical properties of all materials are defined for the deformation simulation. Select the appropriate materials.



Mechanical Properties

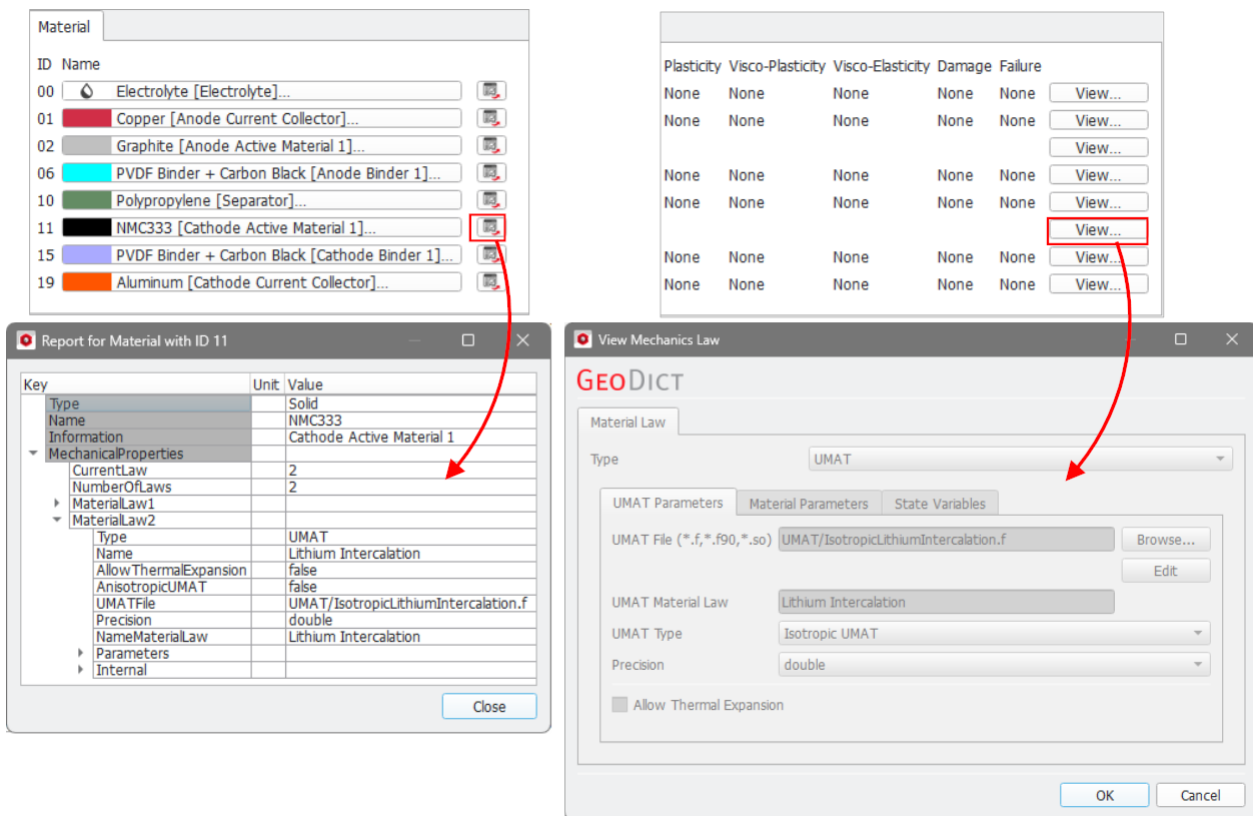
For all active materials of the battery cell, choose the **Material Law Lithium Intercalation** to account for expansion of the material due to changes in the local lithium concentration. The GeoDict material database currently provides the materials Graphite, NMC333, NMC532, NMC622, NMC811, LNO, LCO, LFP, LMO, LTO, NCA, and Silicon with the Material Law Lithium Intercalation.



For all other solid materials, mechanical properties (Young's modulus and Poisson ratio) need to be defined for the simulation. All **Material Laws** that are available in ElastoDict, can be used in a degradation simulation as well. Click **View**, on the right of the mechanical properties shown, to see the parameters defined in the layout of the material database or click the icon



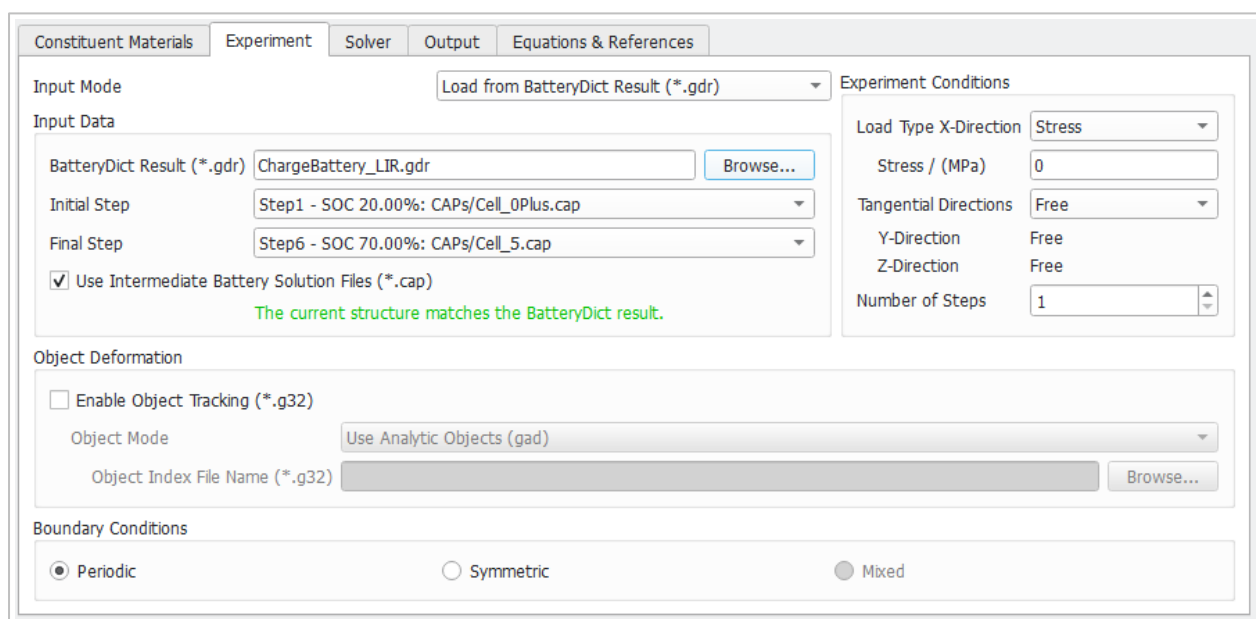
to see the parameters as a report.



For **Manual** materials you can add and remove material laws via the **+** and **-** icons. This is useful, if you run different simulations one after the other using different mechanical properties for one of the materials. Click **Edit** and set the **Type** to **UMAT**. Edit the parameters as described [here](#)⁴².

Experiment

On the **Experiment** tab, define the parameters for the simulation itself.



✓ Input Mode and Input Data

The input for a degradation simulation is the lithium concentration at the start and the end of a charging simulation. A previously run charging simulation with [Charge Battery](#)^[62] or [Charge Electrode](#)^[135] is therefore required before a degradation simulation can be run. With the **Input Mode**, define how the results of the charging simulation are provided for the expansion simulation.

Select **Load from BatteryDict Results (*.gdr)** to choose a charging simulation result file. Browse to the result file and choose the simulation step that you want to use as initial and final step for the degradation simulation.

Input Mode

Load from BatteryDict Result (*.gdr) ▼

Input Data

BatteryDict Result (*.gdr)

ChargeBattery_LIR.gdr

Browse...

Initial Step

Step1 - SOC 20.00%: CAPs/Cell_0Plus.cap ▼

Final Step

Step6 - SOC 70.00%: CAPs/Cell_5.cap ▼

☒ Use Intermediate Battery Solution Files (*.cap)

The current structure matches the BatteryDict result.

GeoDict verifies if the battery currently in memory matches the selected result file. If a match is found, it will be displayed in green below the .cap files chosen as the initial and final steps. If a different structure is currently loaded, a warning is displayed in red.

The current structure does not match the BatteryDict result.

Check **Use intermediate Battery solution files (*.cap)** to use all intermediate *.cap files between initial step and final step in the simulation.

Select **Choose *.cap Files** as **Input Mode** to define the .cap file directly. Browse to the .cap file with the lithium concentration for initial and final step of the expansion simulation. Make sure that the structure currently in memory fits to the selected .cap files.

Input Mode

Choose *.cap Files ▼

Input Data

Initial Step (*.cap)

ChargeBattery_LIR/CAPs/Cell_1.cap

Browse...

Final Step (*.cap)

ChargeBattery_LIR/CAPs/Cell_5.cap

Browse...

✓ Experiment Conditions

In the upper right part of the dialog, choose the **Experiment Conditions**.

Experiment Conditions

Load Type X-Direction	Stress
Stress / (MPa)	0
Tangential Directions	Free
Y-Direction	Free
Z-Direction	Free
Number of Steps	1

You can simulate external mechanical load in the charging direction. This is useful for solid state batteries, which are always operated under an external stack pressure or for cells confined in a battery pack. Select the **Load Type X-Direction** to be **Stress** or **Strain**. Then prescribe the compressive **Stress** in MPa (megapascal) or the applied **Strain** in % in X-direction, which is the charging direction. Note that applying stress of 0 MPa is equivalent with setting the load type in X-direction to free in previous GeoDict releases. For confined boundary conditions in X-direction set the **Strain** to 0%.

Load Type X-Direction	Strain	Load Type X-Direction	Stress
Strain / (%)	0	Stress / (MPa)	0

For the tangential coordinate directions, define if the cell can expand **Free** in these coordinate directions, or if it cannot expand at all (**Confined**). Chose **Mixed**, when the cell can only expand in one direction.

Tangential Directions	Free	Tangential Directions	Confined	Tangential Directions	Mixed
Y-Direction	Free	Y-Direction	Confined	Y-Direction	Free
Z-Direction	Free	Z-Direction	Confined	Z-Direction	Confined

Additionally, define the **Number of Steps** for the simulation. The number of steps defines the number of intermediate steps in the computation of the expansion. Either the whole concentration difference between initial and final step is applied in one step, or it is divided linearly and applied in several steps. If **Use intermediate Battery solution files (*.cap)** is checked, the number of steps defined is applied between all intermediate .cap files available.

✓ Object Deformation

Enable Object Tracking to keep object indices in the deformation simulation. This allows for the identification of the deformation of each individual object in the simulation. If the structure considered contains analytic object information, the .g32 file with object indices can be created from this analytic information,

Object Deformation

☒ Enable Object Tracking (*.g32)

Object Mode Use Analytic Objects (gad)

Object Index File Name (*.g32) Browse...

or a previously created *.g32 file can be selected.

Object Deformation

☒ Enable Object Tracking (*.g32)

Object Mode Load Object Information from File (*.g32)

Object Index File Name (*.g32) Browse...

✓ Boundary Conditions

Finally, select the boundary conditions for the structure in the simulation. Use **Periodic** if the structure is periodic in all coordinate directions, **Symmetric** if it is not. Mixed boundary conditions are not available so far in BatteryDict-Degradation.

Boundary Conditions

☒ Periodic ☐ Symmetric ☐ Mixed

Solver

On the **Solver** tab, specify the settings for the **FeelMath** solver.

Constituent Materials Experiment **Solver** Output Equations & References

Simulation Stopping Criterion

Tolerance 0.0001

☐ Maximum Iterations 1000

☐ Maximum Run Time / (h) 240

Method Intermediate (Memory Efficient Conjugate Gradient)

Parallelization 32 Threads (Automatic Maximum) Edit...

Orientation Mode for Anisotropic Materials Use Orientation from Analytic Objects (gad)

Orientation File Name (*.gof) Browse...

☐ Write Deformation Data to File (slower but less memory)

Simulation Stopping Criterion

The equations are solved by an iterative approach.



Iterative Solver

The basic idea of an iterative method is to

1. Start with some initial guess for the unknown values
2. Improve the current values in each iterative step
3. Repeat the iterative process until one of the stopping criteria is reached.

The iterative process is controlled by setting the values and activation for **Tolerance**, **Maximal Iterations**, and **Maximal Run Time (h)**. The stopping criteria apply for each computational direction individually.

If multiple stopping criteria are selected, the first criterion that is reached causes the solver to stop.

The stopping criterion that has been reached can be viewed in the Result Viewer of the GeoDict result file (*.gdr) under the **Results Report** tab.

✓ Tolerance

The **Tolerance** stopping criterion looks for stagnation of the method when the process becomes stationary, i.e., the improvement in the computed value becomes extremely small from iteration to iteration.

In each iteration, the solver checks for the current computed value x_c against the values x_{c-i} of the last 100 iterations if there are any changes.

$$\max_{i \in [1, 100]} \frac{x_c - x_{c-i}}{x_{c-i}} < \text{tolerance} \quad (64)$$

The computation is stopped if the maximal relative change is smaller than the value entered for **Tolerance**. When there is doubt about the quality of the solution, decrease the **Tolerance** value by a factor of ten. The drawback of this criterion is that the solver sometimes might stop too early in case of slow convergence rate or at local extrema of oscillatory convergence curves.

✓ Maximum Iterations and Maximum Runtime

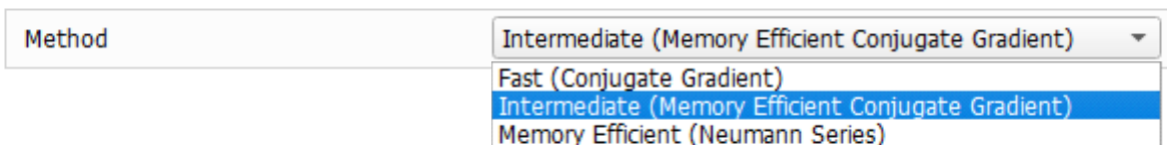
Use the **Maximum Iterations** value or the **Maximum Run Time (h)** stopping criteria causes the solver to stop if the maximal number of iterations and/or the maximal runtime (in hours) is exceeded.

When the solver stops because one of these criteria has been reached, no guarantee on the quality of solution can be given. In this case, a warning is printed into the report. The following possibilities might help:

- Check the corresponding .log file to see how large the residual values and the computed values are. If the computed values are in reasonable range and they do not have changed during the last iterations, you may decide to use the current result.
- Double-check the structure and parameter values. Unphysical parameters or too rough resolution of the structure (leading, e.g., to artificial unconnected components) can cause an iterative solver to fail.

Method

For the **FeelMath-Deformations** solver, three different iterative methods are available: **Fast (Conjugate Gradient)**, **Intermediate (Memory Efficient Conjugate Gradient)**, and **Memory Efficient (Neumann Series)**.



The **Fast** method converges faster, especially for strongly varying material parameters and nonlinear material laws (as, e.g., plasticity or damage), but needs about four times as much memory as the **Memory Efficient** method.

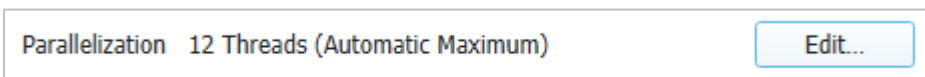
The **Intermediate Method** needs approximately 40 % less memory than the **Fast** method but is slower. The **Estimate Memory** button in the ElastoDict section can be used to decide which method is applicable for the current structure on the available computer.

In general, it is recommended to use the default (**Memory Efficient Conjugate Gradient**) or the **Conjugate Gradient** method. The **Neumann Series** method should only be used if the memory is not sufficient for the other methods.

Parallelization

Control how many threads are used for the computation. Parallelization is possible if your license and hardware allow it.

The **Parallelization Options** dialog opens when clicking the **Edit** button and you can choose between **Sequential**, **Parallel (Shared Memory)**, **Automatic Maximum of Threads**, or **Cluster** (only available if EJ, SimpleFFT, or FeelMath were selected as solver).



The parallelization of the solvers is done with two technical methods: **MPI Parallelization** or

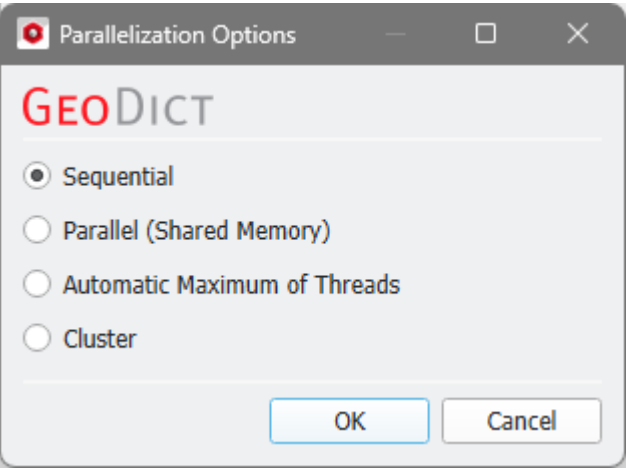
Thread parallelization. The following table shows the support of both parallelization methods:

Solver	Parallelization method	
	MPI Parallel	Thread Parallel
EJ	✓	✗
SimpleFFT	✓	✗
LIR	✗	✓
FeelMath	✓	✓
BEST	✗	✓

Depending on the used parallelization method, the **Number of Processes** (MPI parallel) or the **Number of Threads** (thread parallel) can be entered.

✓ **Sequential**

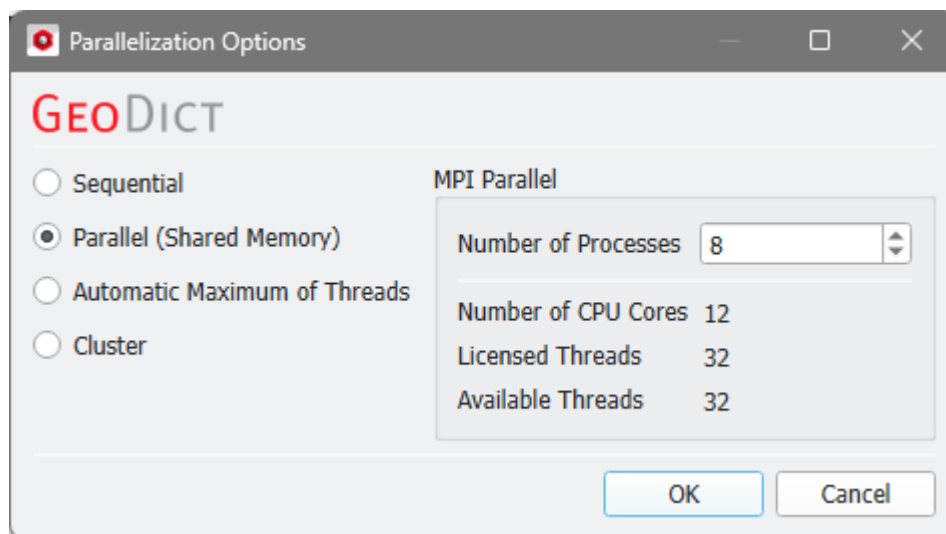
Selecting **Sequential** will not apply parallelization and only one thread is used for the computation.



✓ **Parallel (Shared Memory)**

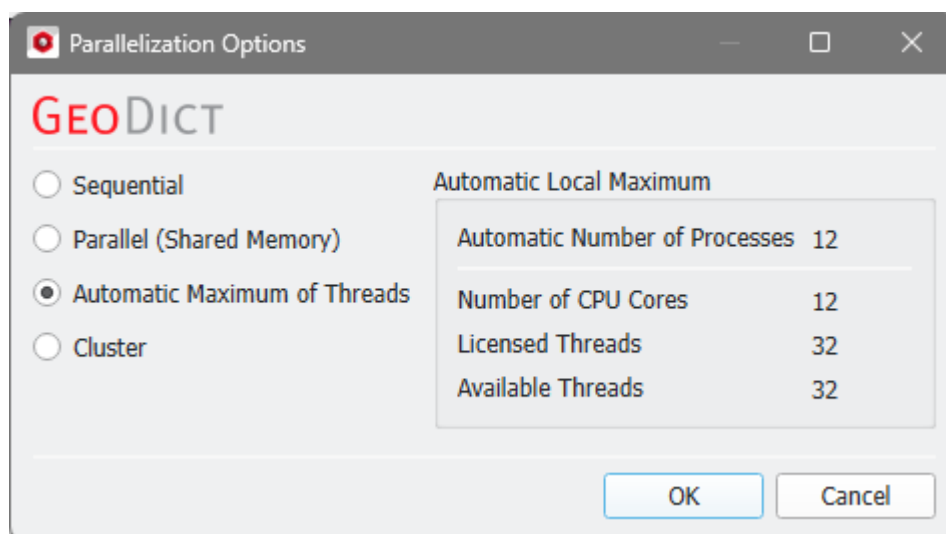
When **Parallel (Shared Memory)** is selected, the **Number of Processes** or **Number of Threads** can be entered. Below, the **Number of CPU Cores** that the current machine has, the maximum number of **Licensed Threads** and the number of those licensed threads that are available (**Available Threads**) are shown in the dialog. Of course, the maximal number of parallel processes you can use, is the smallest of those three

numbers.



✓ Automatic Maximum of Threads

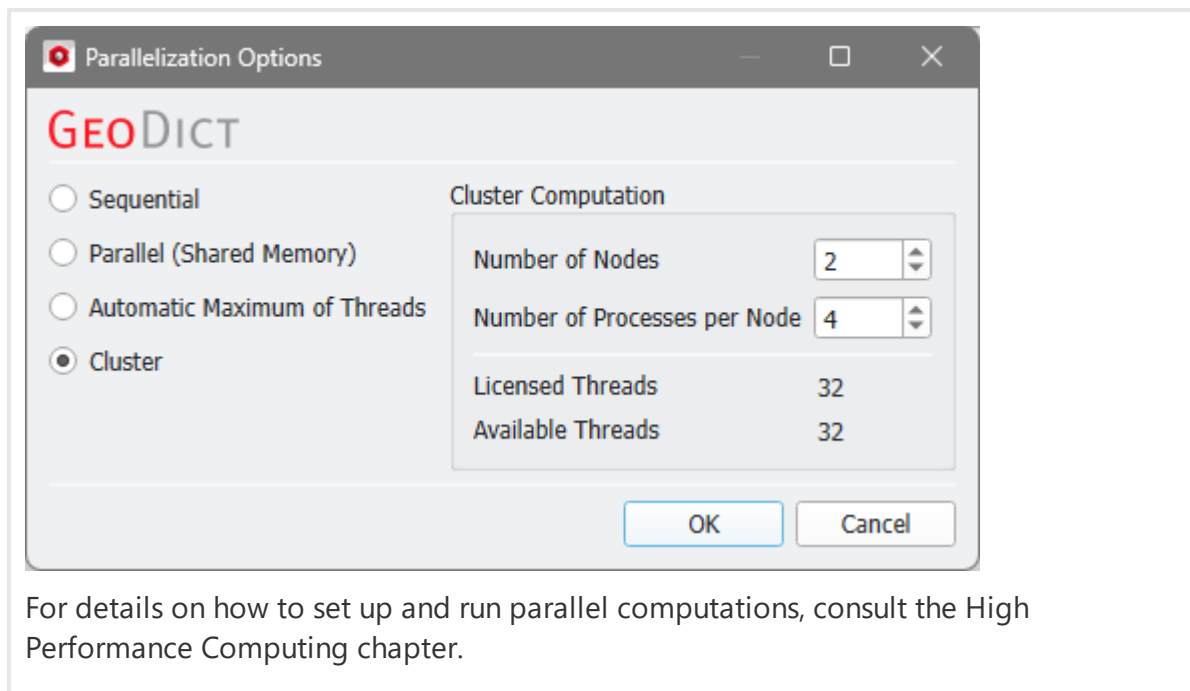
If **Automatic Maximum of Threads** is selected, the number of parallel processes is automatically selected for optimal speed, based on the CPU cores and licensed parallel processes.



The **Automatic Local Maximum** of processes is automatically selected, which is the minimum of **Number of CPU Cores**, **Licensed Threads**, and **Available Threads**.

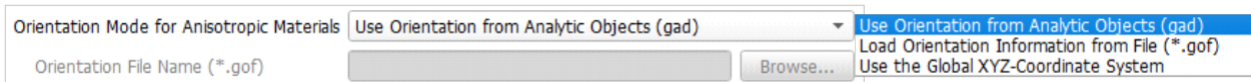
✓ Cluster

The **Cluster** parallelization requires that the solver supports the **MPI Parallelization** method. Moreover, the choice of **Cluster** is for users of Linux systems only.



Orientation Mode for Anisotropic Materials

BatteryDict-Degradation can handle non-isotropic constituent materials. For these materials, an orientation must be additionally specified. If the analyzed structure consists of analytical objects (gad data), the orientation of these objects is used when **Use Orientation from Analytic Objects (gad)** is selected.



Alternatively, with **Load Orientation Information from File (*.gof)**, orientation information can be loaded from a file. Such a file can be generated for example with GrainFind for granular structures. The third option, **Use the Global XYZ-Coordinate System**, allows to use anisotropic materials even if no orientation information for the structure is available. This makes sense only if the grains are all oriented directly according to the coordinate axis, which is usually not the case.

Write Deformation Data to File

For the computation of the deformed structures, intermediate data is computed which describes the displacement for each voxel. Before this computation, it is not clear how large this data will be, since a voxel in the original structure might be partially moved in multiple voxels in the deformed structure. Therefore, this data might not fit in the main memory of the computer. Due to this, it is possible to write the deformation data to a file on the hard disk by checking **Write Deformation Data to File**.

☐ Write Deformation Data to File (slower but less memory)

But note that writing and loading data from the hard drive is many times slower than writing and loading data in the main memory (even if the drive is an SSD). This causes a bottleneck, which can slow down the simulation.

If the data exceeds available RAM, you can store the deformation data on disk by enabling "Write Deformation Data to File. We recommend keeping this setting, and to select **Write Deformation Data to File** only if the simulation fails because the data does not fit into the RAM.

Output

The options available in the **Output** tab define which information is written to the hard disk during the computation.

The screenshot shows the 'Output' tab of a software interface. It contains two main sections: 'Deformed Geometry' and 'Write Volume Field'.

Deformed Geometry

- ☒ Write Deformed Geometry
- ☒ Write Volume Fields for Deformed Geometry
- ☐ Write Volume Fractions for Deformed Geometry
- ☐ Write Deformed Fields for Final *.cap File

Write Volume Field

Displacement

- ☐ X
- ☐ Y
- ☐ Z
-
-

Stress

- ☒ XX
- ☒ YY
- ☒ ZZ
- ☒ YZ
- ☒ XZ
- ☒ XY
- ☒ Von Mises Stress

Strain

- ☒ XX
- ☒ YY
- ☒ ZZ
- ☒ YZ
- ☒ XZ
- ☒ XY
- ☒ Von Mises Strain

☒ Material State Variables

☐ Export VTK File (*.vti)

✓ Deformed Geometry

In the **Deformed Geometry** panel, select which information is exported for the deformed geometry.

Deformed Geometry

- ☒ Write Deformed Geometry
 - ☒ Write Volume Fields for Deformed Geometry
 - ☐ Write Volume Fractions for Deformed Geometry
 - ☐ Write Deformed Fields for Final *.cap File

When **Write Deformed Geometry** is chosen, a geometry with the current displacements is resampled and saved after each step.

With **Write Volume Fields for Deformed Geometry**, also the result fields are resampled with the current displacements so that they match the deformed geometries. A GeoDict *.das file is created for this volume fields.

With **Write Volume Fractions for Deformed Geometry**, the volume fractions for each material ID in each voxel after the deformation are additionally written to the *.das files. This information is used for the computation of the deformed geometries. In general, it is not necessary to save this information. However, it is required for the export of the deformed fields for the final .cap file.

If **Write Deformed Fields for Final *.cap File** is checked, the fields of the final .cap file are resampled to match the final geometry and exported to the .das file as well. This is necessary if the deformed geometry of the degradation simulation should be used as starting point for a new charging or discharging simulation.

✓ Write Volume Field

Under **Write Volume Field**, checking or un-checking the boxes for **Displacement**, **Stress**, and **Strain** determines whether these result outputs are available for visualization and post-processing after the run of the FeelMath solver.

Write Volume Field

Displacement

☐ X☐ Y☐ ZCheck AllUncheck All

Stress

☒ XX☒ YY☒ ZZ☒ YZ☒ XZ☒ XY☒ Von Mises Stress

Strain

☒ XX☒ YY☒ ZZ☒ YZ☒ XZ☒ XY☒ Von Mises Strain☒ Material State Variables

Different from ElastoDict, the stress and strain tensor itself (XX, YY, ...) is currently always exported in BatteryDict-Degradation, but **Von Mises Stress** and **Strain** can be checked or unchecked.

✓ Export VTK File (*.vti)

Besides using GeoDict's own visualization tools, it is possible to export the solution in the commonly used VTK (Visualization Toolkit) format (see: <https://vtk.org/> and <https://www.paraview.org/>) by checking Export VTK File (*.vti).

☐ Export VTK File (*.vti)

1.4.2 Results

If the degradation simulation finished successfully, the GeoDict Result Viewer opens for the result file (*.gdr file created).

Learn more about the general **Result Viewer** options in the Result Viewer chapter.

The screenshot shows the 'Result Viewer' window for a simulation named 'BatteryDict:ChargeBattery'. The window displays various tabs including 'Input Map', 'Log Map', 'Post Map', 'Results', 'Strain/Stress Visualization', 'Create Videos', and 'Metadata'. The 'Results' tab is active, showing a table of 'Average strain' and 'Average stress' data for two steps (0 and 1) at different states of charge (20.00% and 70.00%).

BatteryDegradation
This simulation is based on the **BatteryDict:ChargeBattery** result file **ChargeBattery_LIR.gdr**.

Average strain

Step	State of charge / (%)	XX / (%)	YY / (%)	ZZ / (%)	YZ / (%)	XZ / (%)	XY / (%)	VonMises / (%)	Hydrostatic / (%)
0	20.00	0	0	0	0	0	0	0	0
1	70.00	-0.77229	-0.033897	-0.038945	0.017708	0.034977	-0.012197	0.73931	0.28171

Average stress

Step	State of charge / (%)	XX / (MPa)	YY / (MPa)	ZZ / (MPa)	YZ / (MPa)	XZ / (MPa)	XY / (MPa)	VonMises / (MPa)	Hydrostatic / (MPa)
0	20.00	0	0	0	0	0	0	0	0
1	70.00	0.00016294	3.0657e-05	3.2322e-05	-0.76521	4.0208	0.71578	7.1967	-7.5307e-05

References:
[Nils Wenzler, Sebastian Rief et al; 2023; 3D electrochemical-mechanical battery simulation tool: implementation with full cell simulations and verification with operando x-ray tomography; Journal of the Electrochemical Society 170, 020511.](#)

Total runtime: 02:00:37, Total memory usage: 31.675 GiB

Buttons at the bottom: ? Help, Manage Data, Load Input Parameters, Export, Close

✓ Report

The **Results - Report** subtab shows the average strain and stress tensor, as well as the average Von Mises and hydrostatic strain and stress for each computation step.

Input Map
Log Map
Post Map
Results
Strain/Stress Visualization
Create Videos
Metadata

Report
Plots
Map

BatteryDegradation

This simulation is based on the **BatteryDict:ChargeBattery** result file **ChargeBattery_LIR.gdr**.

Average strain

Step	State of charge / (%)	XX / (%)	YY / (%)	ZZ / (%)	YZ / (%)	XZ / (%)	XY / (%)	VonMises / (%)	Hydrostatic / (%)
0	20.00	0	0	0	0	0	0	0	0
1	70.00	-0.77229	-0.033897	-0.038945	0.017708	0.034977	-0.012197	0.73931	0.28171

Average stress

Step	State of charge / (%)	XX / (MPa)	YY / (MPa)	ZZ / (MPa)	YZ / (MPa)	XZ / (MPa)	XY / (MPa)	VonMises / (MPa)	Hydrostatic / (MPa)
0	20.00	0	0	0	0	0	0	0	0
1	70.00	0.00016294	3.0657e-05	3.2322e-05	-0.76521	4.0208	0.71578	7.1967	-7.5307e-05

References:

[Nils Wenzler, Sebastian Rief et al; 2023; 3D electrochemical-mechanical battery simulation tool: implementation with full cell simulations and verification with operando x-ray tomography; Journal of the Electrochemical Society 170, 020511.](#)

If an [external strain or stress](#)¹⁷⁰ was defined, the entered value also appears in the result file in the third column of the respective table. For instance, if a strain of 2% was applied, the XX column for the **Average Strain** table will consistently show a value of 2%. In the example below additionally [Use Intermediate Battery Solution Files](#)¹⁶⁹ was checked leading to more rows in the table, one row for each solution file.

Average strain									
Step	State of charge / (%)	XX / (%)	YY / (%)	ZZ / (%)	YZ / (%)	XZ / (%)	XY / (%)	VonMises / (%)	Hydrostatic / (%)
0	20.00	0	0	0	0	0	0	0	0
1	20.00	2	-0.32856	-0.34382	0.034302	-0.047766	-0.063853	2.3411	-0.44254
2	25.00	2	-0.34407	-0.3601	0.039303	-0.051626	-0.067857	2.3577	-0.43194
3	30.00	2	-0.35952	-0.37634	0.044306	-0.05551	-0.07187	2.3744	-0.42138
4	35.00	2	-0.37552	-0.39314	0.049612	-0.059939	-0.07522	2.3917	-0.41045
5	40.00	2	-0.39152	-0.40996	0.05492	-0.064359	-0.078566	2.4091	-0.39951
6	45.00	2	-0.4086	-0.42739	0.060005	-0.067657	-0.081512	2.4272	-0.388
7	50.00	2	-0.42567	-0.44482	0.065089	-0.070955	-0.08446	2.4454	-0.3765
8	55.00	2	-0.44098	-0.46058	0.070312	-0.073307	-0.087652	2.4618	-0.36615
9	60.00	2	-0.45628	-0.47633	0.075536	-0.075669	-0.090847	2.4783	-0.3558
10	65.00	2	-0.47157	-0.49243	0.080925	-0.079755	-0.094147	2.4952	-0.34534
11	70.00	2	-0.48685	-0.50852	0.086317	-0.08384	-0.097447	2.5121	-0.33488

On the left, find the post processing panel where to define the **Load Sign Definition**, **Report Settings** and **Plot Settings**. The plot settings are explained [below](#)¹⁸³.

Input Map
Log Map
Post Map
Results
Strain/Stress Visualization
Create Videos
Metadata

Load Sign Definition
Compression is Positive

Report Settings

Report Stress Unit
MPa

Report Strain Unit
%

Plot Settings

X-Axis
State of Charge

Y-Axis
Von Mises Stress

Apply

☒ Back-up result file

Plot Options

Decide whether the **Compression is Positive** or the **Tension is Positive**. This changes the sign for the tensor values. This setting also changes the plot under the [Plots](#) ¹⁸³ tab.

Average strain									
Load Sign Definition									
Compression is Positive									
Step	State of charge / (%)	XX / (%)	YY / (%)	ZZ / (%)	YZ / (%)	XZ / (%)	XY / (%)	VonMises / (%)	Hydrostatic / (%)
0	20.00	0	0	0	0	0	0	0	0
1	70.00	-0.77229	-0.033897	-0.038945	0.017708	0.034977	-0.012197	0.73931	0.28171

Average stress									
Load Sign Definition									
Compression is Positive									
Step	State of charge / (%)	XX / (MPa)	YY / (MPa)	ZZ / (MPa)	YZ / (MPa)	XZ / (MPa)	XY / (MPa)	VonMises / (MPa)	Hydrostatic / (MPa)
0	20.00	0	0	0	0	0	0	0	0
1	70.00	0.00016294	3.0657e-05	3.2322e-05	-0.76521	4.0208	0.71578	7.1967	-7.5307e-05

Average strain									
Load Sign Definition									
Tension is Positive									
Step	State of charge / (%)	XX / (%)	YY / (%)	ZZ / (%)	YZ / (%)	XZ / (%)	XY / (%)	VonMises / (%)	Hydrostatic / (%)
0	20.00	0	0	0	0	0	0	0	0
1	70.00	0.77229	0.033897	0.038945	-0.017708	-0.034977	0.012197	0.73931	0.28171

Average stress									
Load Sign Definition									
Tension is Positive									
Step	State of charge / (%)	XX / (MPa)	YY / (MPa)	ZZ / (MPa)	YZ / (MPa)	XZ / (MPa)	XY / (MPa)	VonMises / (MPa)	Hydrostatic / (MPa)
0	20.00	0	0	0	0	0	0	0	0
1	70.00	-0.00016294	-3.0657e-05	-3.2322e-05	0.76521	-4.0208	-0.71578	7.1967	-7.5307e-05

Under the **Report Settings** change the **Report Stress Unit** (GPa, MPa or KPa) and the **Report Strain Unit** (% or 1), for example:

Report Settings
 Report Stress Unit: GPa
 Report Strain Unit: 1

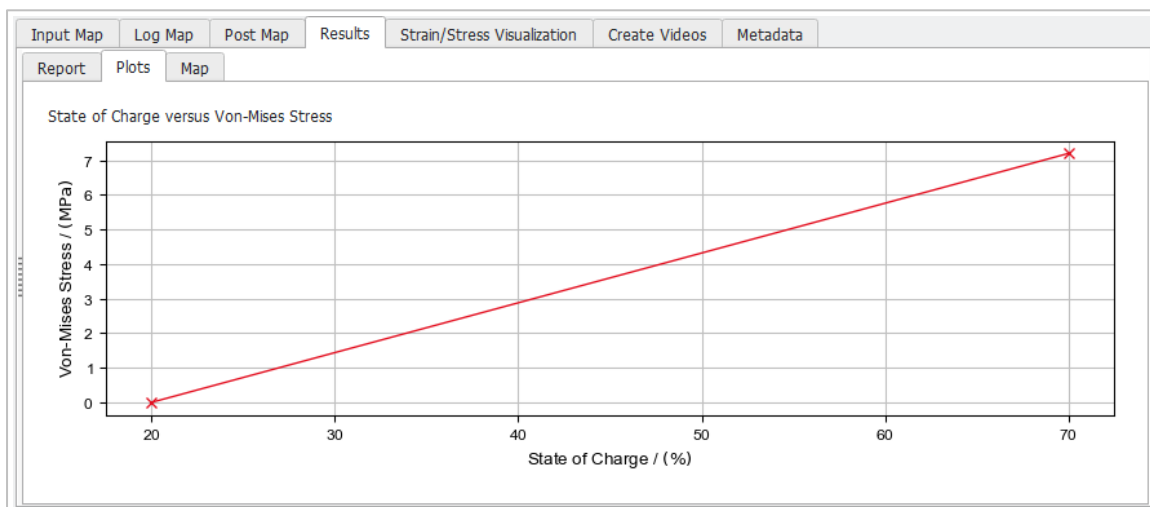
Step	State of charge / (%)	XX / (1)	YY / (1)	ZZ / (1)	YZ / (1)	XZ / (1)	XY / (1)	VonMises / (1)	Hydrostatic / (1)
0	20.00	0	0	0	0	0	0	0	0
1	70.00	-0.0077229	-0.00033897	-0.00038945	0.00017708	0.00034977	-0.00012197	0.0073931	0.0028171

Step	State of charge / (%)	XX / (GPa)	YY / (GPa)	ZZ / (GPa)	YZ / (GPa)	XZ / (GPa)	XY / (GPa)	VonMises / (GPa)	Hydrostatic / (GPa)
0	20.00	0	0	0	0	0	0	0	0
1	70.00	1.6294e-07	3.0657e-08	3.2322e-08	-0.00076521	0.0040208	0.00071578	0.0071968	-7.5307e-08

After the settings are as desired, click **Apply** to change the report. If **Back-up result file** is checked, the original result file is saved inside the result folder as described in the Result Viewer chapter.

✓ Plots

Under the **Plots** tab the plot shows the **State of Charge versus Von-Mises Stress**, by default.



Use the **Post-Processing** panel on the left to show other plots. Under **Plot Settings**, choose the parameters to plot from the pull-down menus for **X-Axis** and **Y-Axis**. Click **Apply** to load the new plot. If **Back-up result file** is checked, the original result file is saved inside the result folder as described in the Result Viewer chapter.

The pull-down menu **Plot Options** contains the options to edit the axis settings and the graph styles, which are also available when right-clicking in the plot. They are described in the Result Viewer chapter.

✓ Strain / Stress Visualization

On the **Strain/Stress Visualization** tab, the volume fields for each **Simulation Step** can be loaded by selecting it from the pull-down menu and clicking **Load** for **Solution File (*.das)**.

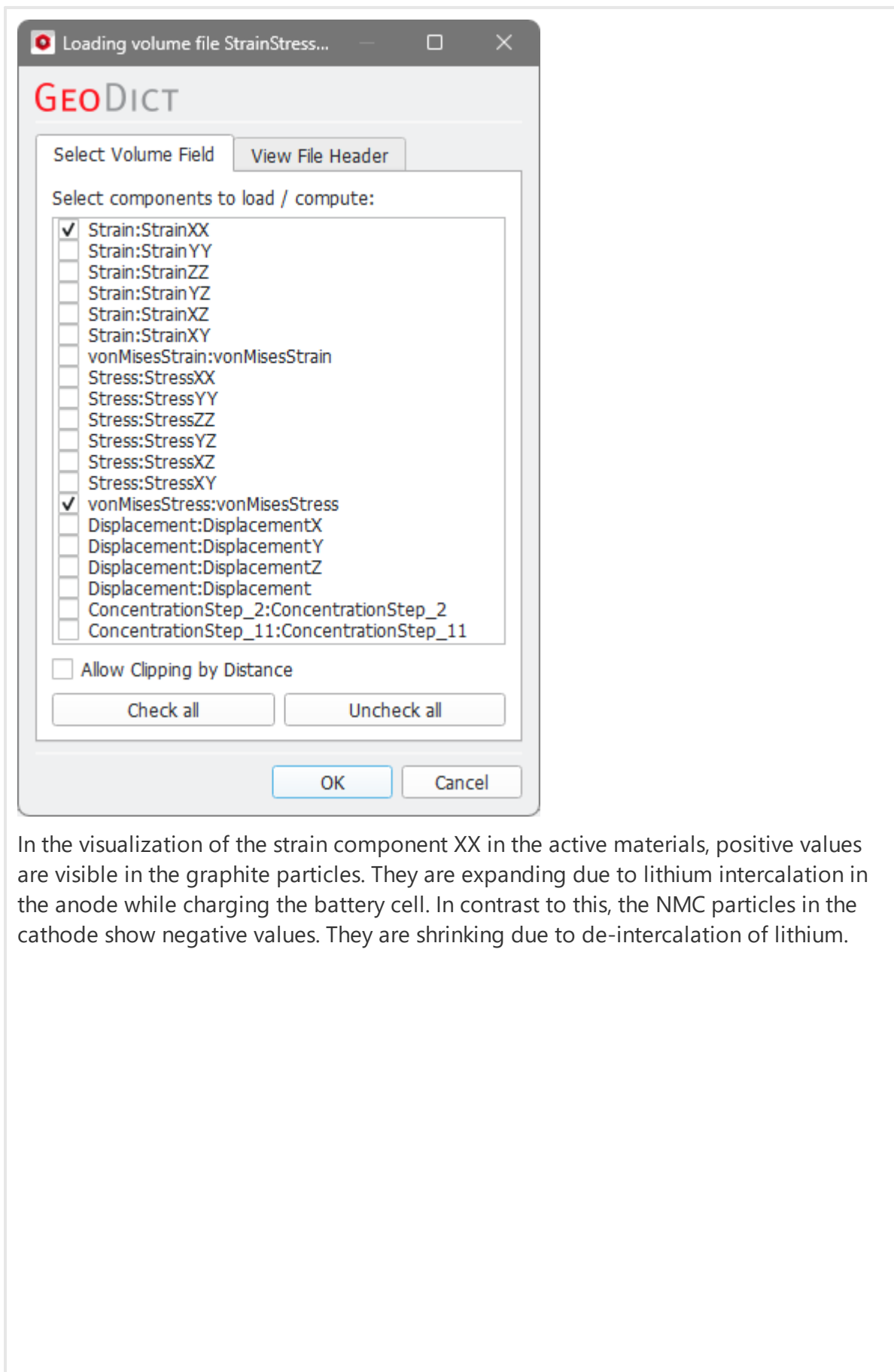
The screenshot shows the 'Strain/Stress Visualization' tab in the BatteryDict software interface. At the top, there are several tabs: 'Input Map', 'Log Map', 'Post Map', 'Results', 'Strain/Stress Visualization' (which is active), 'Create Videos', and 'Metadata'. Below these tabs, there is a 'Simulation Step' dropdown menu currently set to '10'. Underneath, the text 'Step 10' is displayed. A table-like structure follows with three rows, each representing a different data type and its corresponding 'Load' button:

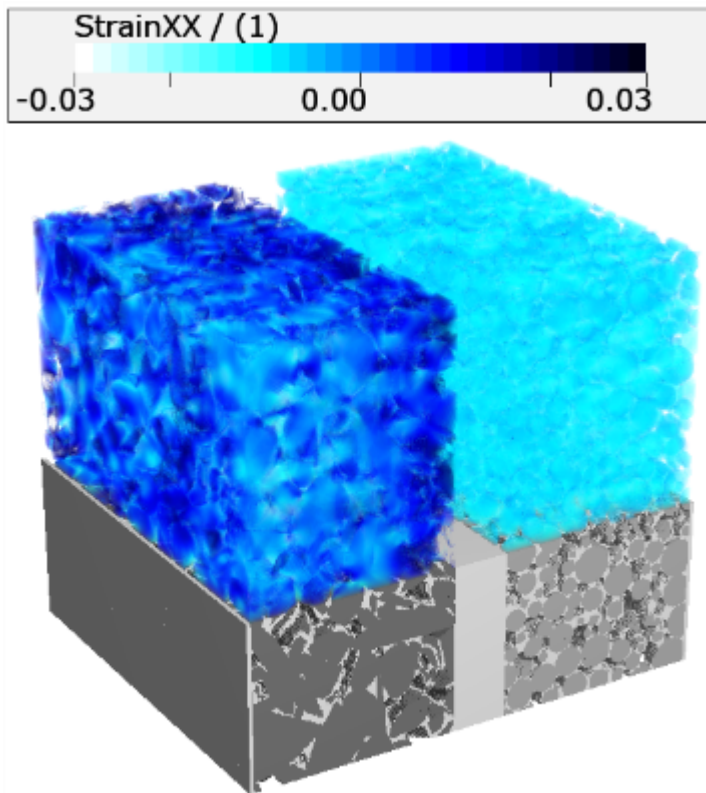
Data Type	Action
Deformed Geometry (*.gdt)	Load
Deformed Solution File (*.das)	Load
Solution File (*.das)	Load

A mouse cursor is pointing at the 'Load' button for the 'Solution File (*.das)' row. At the bottom of the window, there is a button labeled 'Load deformed battery solution file (*.cap)'.

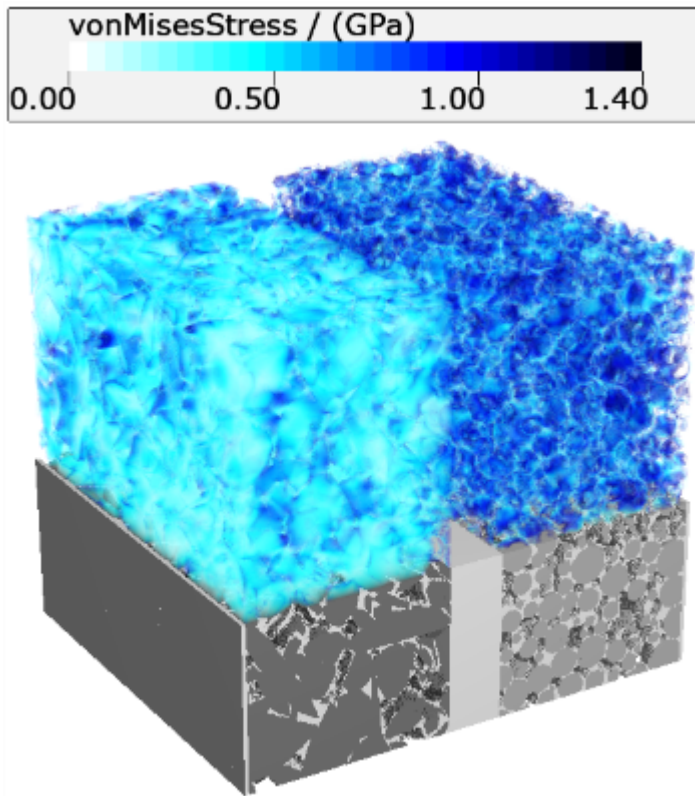
If the deformed geometry and the volume fields for the deformed geometry are written to the hard disk (see [Output tab](#)¹⁷⁸), they can be loaded for visualization here as well. For details on the (deformed) solution files, we refer to the ElastoDict chapter.

Visualize, e.g., the von **Mises Stress** and the strain component XX in the battery after expansion, by loading the **Solution File (*.das)**, selecting the volume fields to load and clicking **OK**.

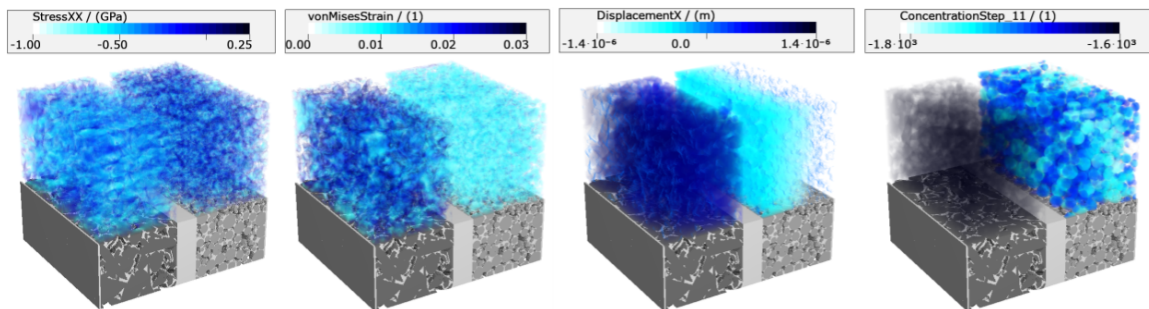




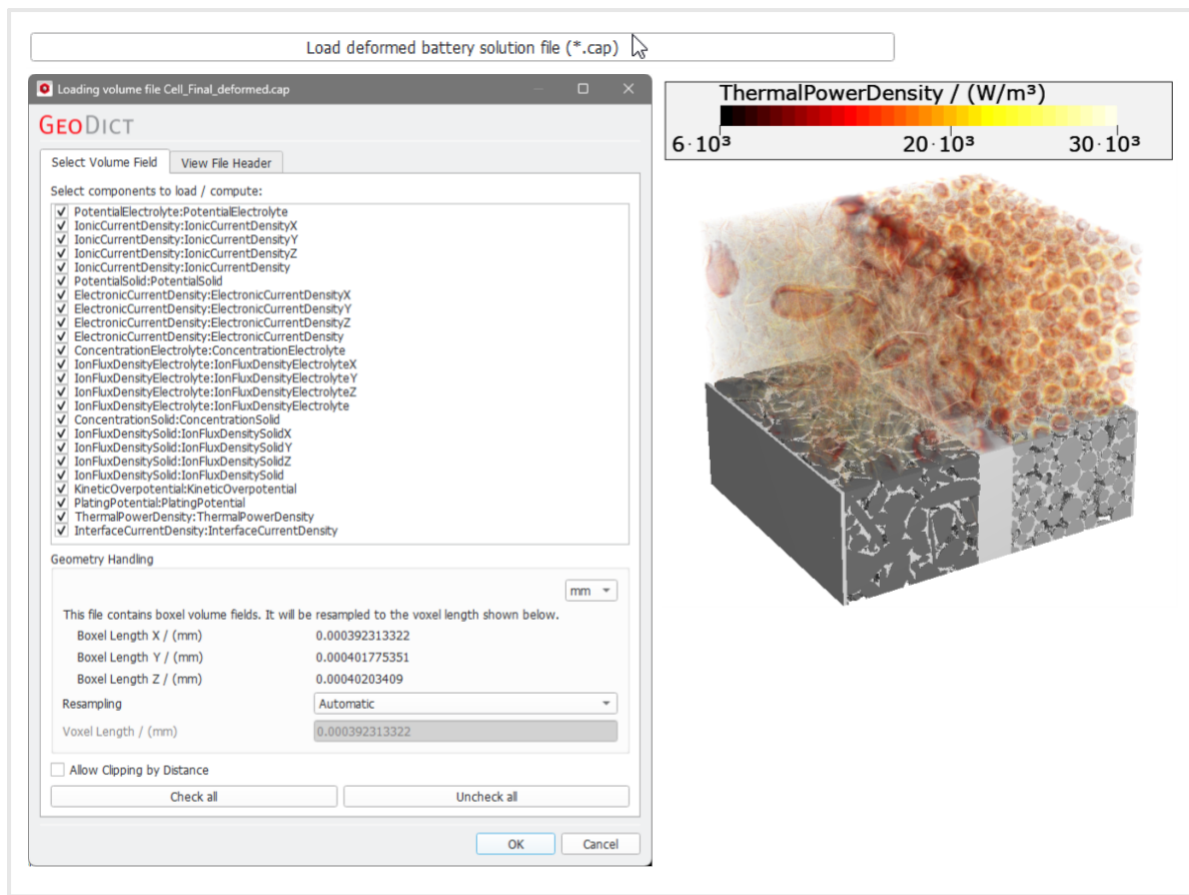
The **von Mises Stress** in the cathode shows its highest values at the boundary of the NMC grains where they are in contact with neighboring grains. This is reasonable since contact detachment during shrinking of the active material is not yet possible in BatteryDict-Degradation.



The solution file additionally also contains the different stress components, for example the StressXX shown below, the vonMisesStrain, the different Displacement components, and the concentration for the first and the last step.

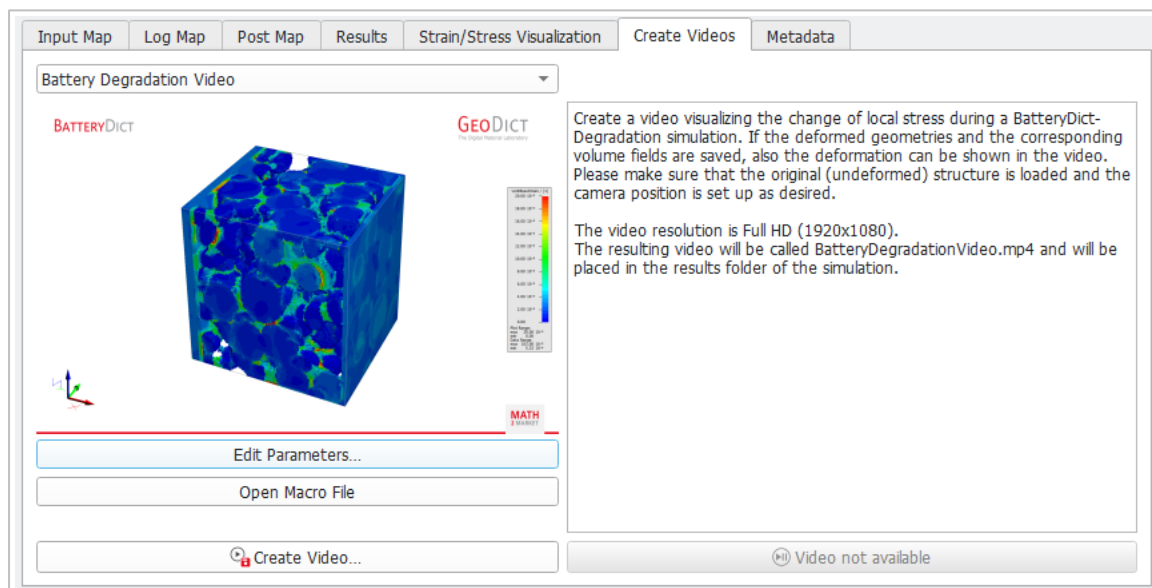


It is also possible to load the deformed battery solution file. Afterward, load the deformed geometry, such that the volume dimensions of volume file and structure match. The result fields are the same as those for the [Charge Battery](#)₁₁₀ command, but they have been resampled to match the deformed geometry.



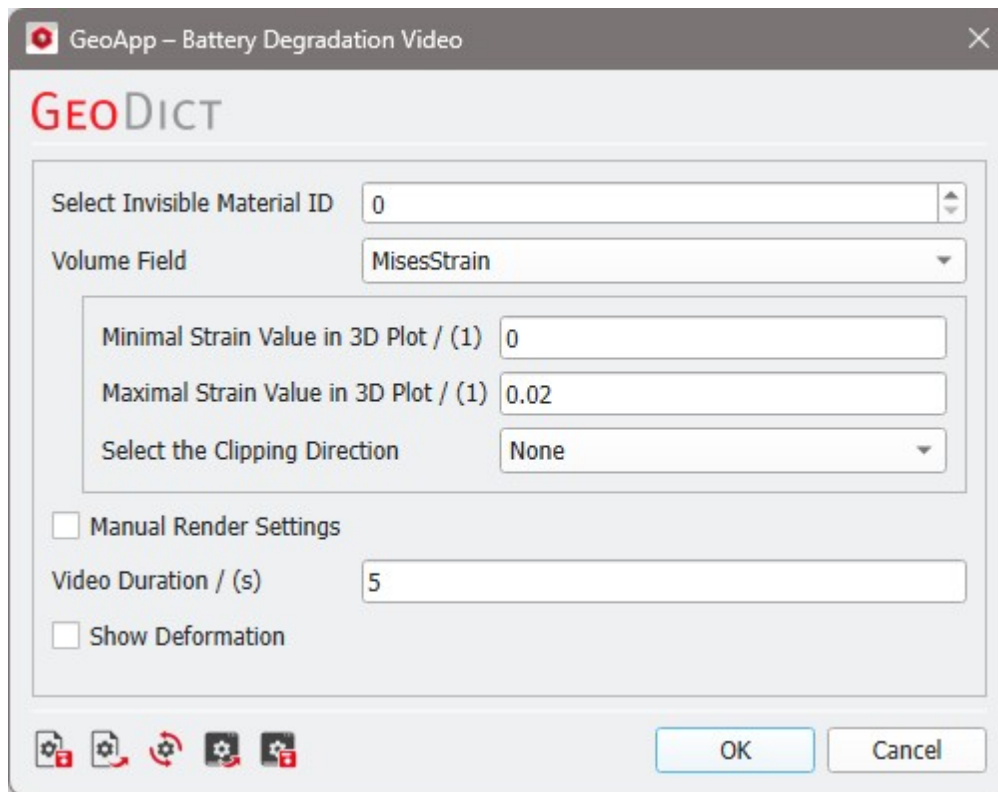
✓ Create Videos

On the **Create Videos** tab, a video visualizing the change of one of the volume fields during a BatteryDict-Degradation simulation can be visualized.



Click **Create Video** to generate the video with the default settings. Once the video is created successfully, the button **Play Video** gets active.

Select **Edit Parameters** to modify the settings for the video generation.

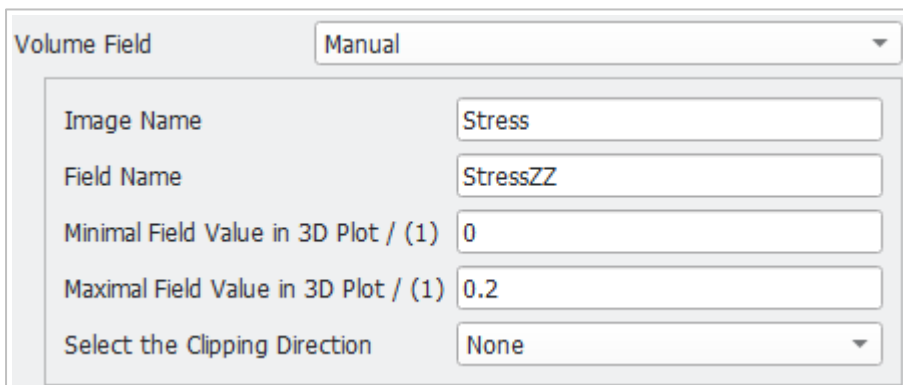


With **Select Invisible Material ID** one material can be selected to be invisible in the video. This can be, e.g., the pore material.

Choose the **Volume Field** to be shown in the plot. Dependent on the selection here, additional parameters need to be defined.

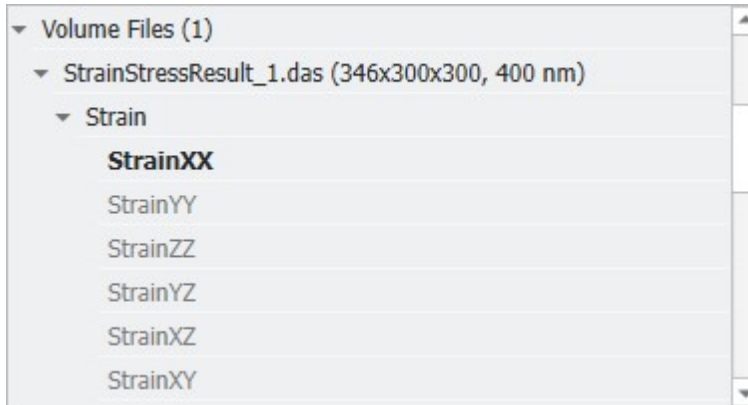
If **Mises Stress** or **Mises Strain** is selected, the minimal and maximal stress or strain values can be set for the color map.

Select **Manual** to choose another volume field available for the visualization. Additional to minimum and maximum value, the name of the image respectively field needs to be chosen as well.



For scalar fields like von Mises Strain, image and field names are the same. For vector and tensor fields, the field name uses the direction as suffix. In the example shown here,

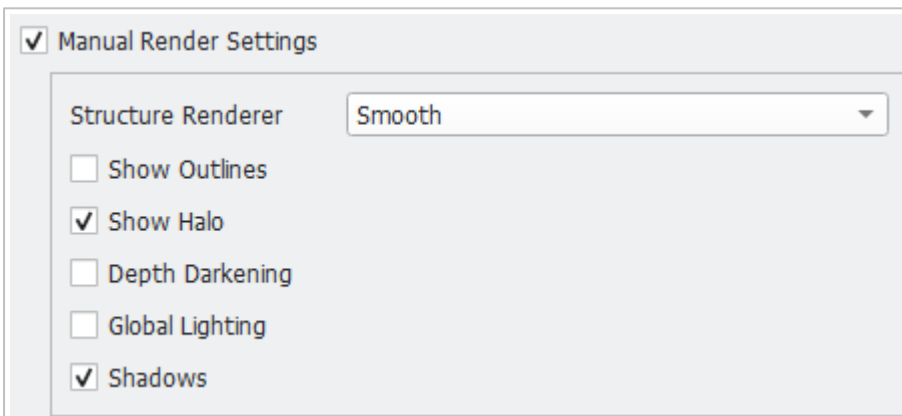
the image name is Strain, the field name StrainXX. If the volume field is loaded into the visualization area, image and field names are visible, e.g., under Volume Files on the left of the Visualization area.



Choose **None**, if no volume field at all should be visualized.

If volume fields should be visualized together with the structure **Select the Clipping Direction** for the structure.

Check **Manual Render Settings** to change the options of the structure renderer. More about these settings can be found in the Visualization chapter.



The value in **Video Duration** defines the overall length of the video in seconds.

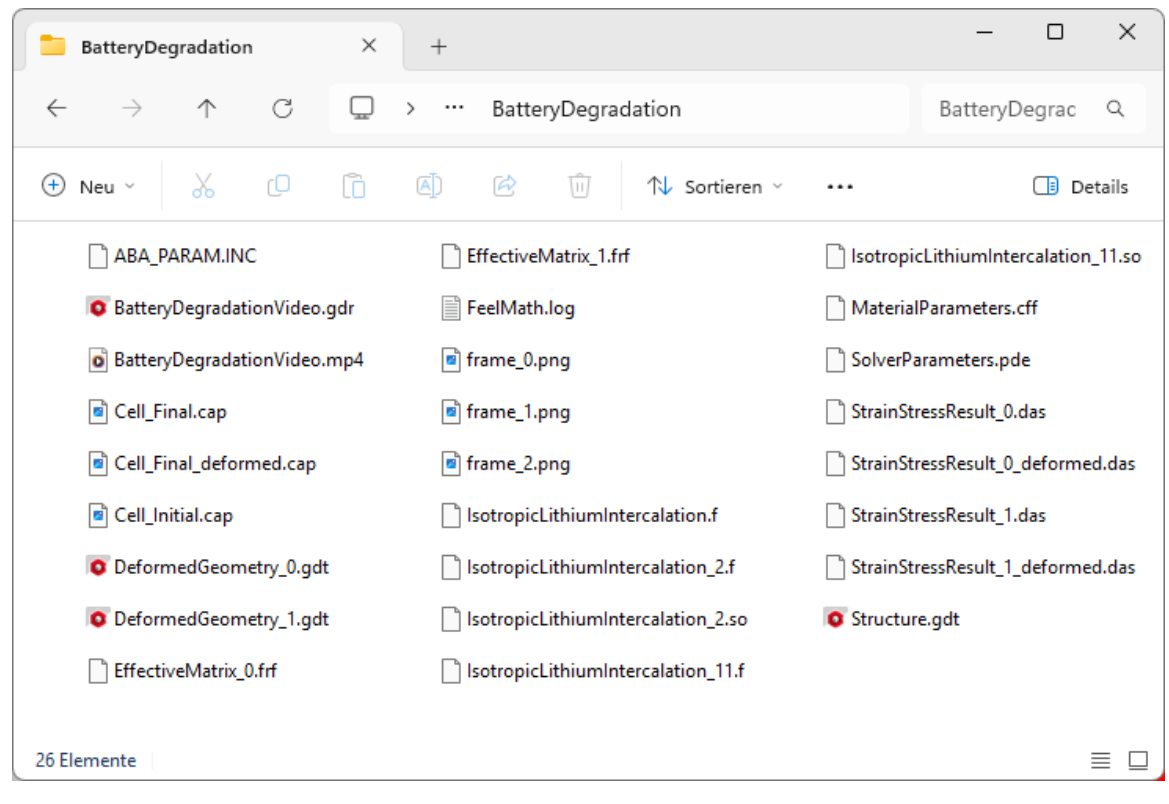
If **Show Deformation** is checked, the video is based on the deformed geometries and volume fields. Otherwise, it shows the values of the volume fields in the undeformed geometry.

✓ Result Folder

The result folder of a degradation simulation contains the initial and final .cap file of the previously run charging simulation and the *.das files with the volume fields created in the mechanical simulation for the undeformed geometry.

If selected on the [Output](#)¹⁷⁸ tab, it contains additionally the deformed geometry and the *.das files for the deformed geometry for each step.

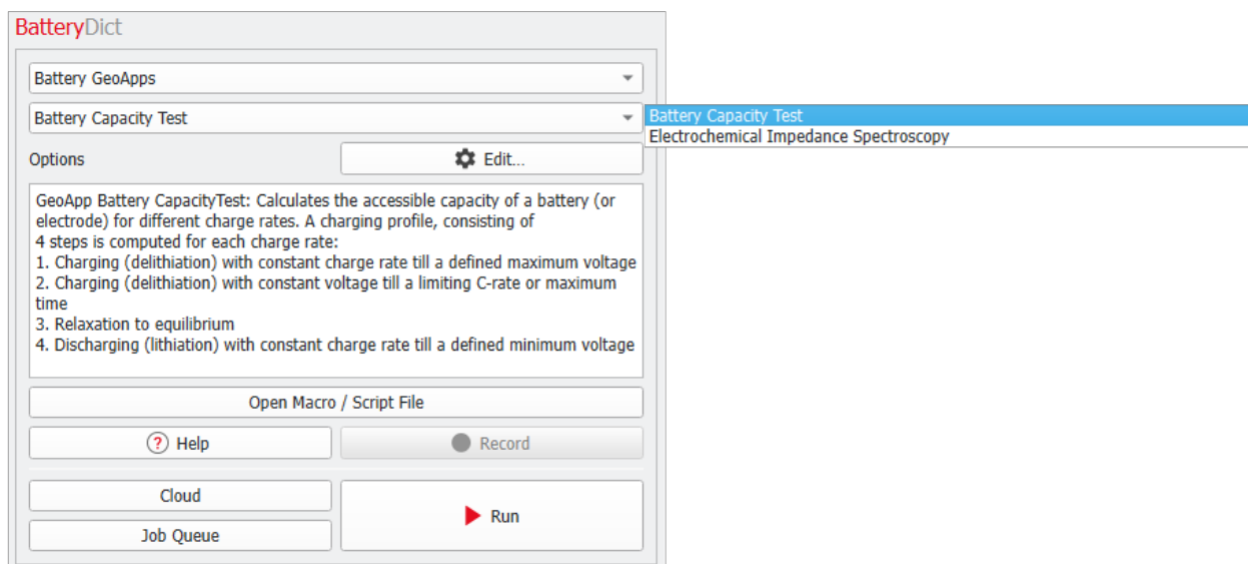
The other files are needed internally for running the mechanical simulation.



1.5 Battery GeoApps

Select **Battery GeoApps** to access pre-defined macros included in GeoDict which are useful for battery simulations.

Two macros are included in the standard installation package. Additional macros can be placed there by the system administrator as described in the GeoApps section and would then be available for all users.



They can be opened and inspected with a standard text editor. To open the corresponding *.py file for a predefined macro, click the **Open Macro / Script File** button.

To use a predefined macro, select it from the pull-down menu, click the **Edit ...** button to set the parameters, and then the **Run** button to run the simulation.

The following GeoApps are available in the BatteryDict section:

- [Battery Capacity Test](#)^[192]
Fast charging of batteries reduces the accessible cell capacity. The GeoApp Battery Capacity Test allows prediction of accessible cell capacity for different charge rates.
- [Electrochemical Impedance Spectroscopy](#)^[200]
Calculate the complex-valued resistance called "impedance".

1.5.1 Battery Capacity Test

Fast charging of batteries reduces the accessible cell capacity. The GeoApp **Battery Capacity Test** allows prediction and easy comparison of accessible cell capacity for different charge rates. A voltage window can be defined in the same way as it is defined in experiments for a battery or electrode.

A [charging profile](#)^[83], consisting of 4 steps is computed for each charge rate:

1. Charging (delithiation) with constant charge rate until a defined maximum voltage
2. Charging (delithiation) with constant voltage until a limiting C-rate or maximum time

3. Relaxation to equilibrium
4. Discharging (lithiation) with constant charge rate until a defined minimum voltage



Needed Modules:

BatteryDict



Note! Also have a look at our [website](#) for more information.

Parameters

Clicking **Edit...** opens the **Battery Capacity Test** dialog. At the top, define a **Result File Name** for the result file and the result folder containing the generated structure and volume fields.

GeoApp – Battery Capacity Test

GEODICT

Result File Name (*.gdr)

Structure, Materials and Simulation Settings

Result File of a Charge Battery Simulation (*.gdr)

Minimum Voltage / (V)

Maximum Voltage / (V)

Step 1 and 4, Charging/Delithiation and Discharging/Lithiation with Constant Current

Boundary Conditions in Through Direction

Charging/Discharging Type

Constant Current: Charge Rates

Charge Rates Charging/Delithiation and Discharging/Lithiation / (1)	
1	

Step 2, Charging with Constant Voltage

☒ Run Step 2, Charging with Constant Voltage

Constant Voltage: Stopping Criterion at Boundary

Charge Rate Limit / (1)

Constant Voltage: Time Limit / (s)

Step 3, Relaxation

☒ Use Perfect Relaxation



✓ Structure, Materials and Simulation Settings

Browse for the **Result File of a Charge Battery Simulation**. This result file is created by successfully running the BatteryDict commands [Charge Battery](#)^[62] or [Charge Electrode](#)^[135]. It contains all the necessary parameters. The parameters from the

[Constituent Materials](#)^[65], [Solver](#)^[85] and [Output Options](#)^[92] tab as well as the Boundary Conditions in Tangential Directions defined under the [Experiment](#)^[79] tab are used for the simulations in the GeoApp Battery Capacity Test. The other settings under the Experiment tab are replaced by a charging profile set according to the input parameters defined in the GeoApp dialog.

Define the voltage range for the battery capacity test by entering **Minimum Voltage** and **Maximum Voltage**. Below the settings for the [example](#)^[197] are entered.

Structure, Materials and Simulation Settings

Result File of a Charge Battery Simulation (*.gdr)

Minimum Voltage / (V)

Maximum Voltage / (V)

✓ Step 1 and 4, Charging / Delithiation and Discharging / Lithiation with Constant Current

Choose the **Boundary Conditions in Through Direction**.

- **Charge Rate:** Specify a charge rate. The necessary current density for the given charge rate will be calculated by the solver.
- **Current Density:** Specify a current density.
- **Current:** Specify a current. Please note, that the current in the microstructure is very small.

Below, the settings for the [example](#)^[197] are entered.

Step 1 and 4, Charging/Delithiation and Discharging/Lithiation with Constant Current

Boundary Conditions in Through Direction

Charging/Discharging Type

Constant Current: Charge Rates

Charge Rates Charging/Delithiation and Discharging/Lithiation / (1)	
1	1
2	3
3	5
4	7

Decide whether the values for the selected **Charging / Discharging Type** should be the same for both processes or different. Enter the values in the table. As soon, as you enter a value, another row appears in the table. Fill in as many rows as desired. A simulation will be run for each row, and the accessible capacities for all simulations will be compared in the GeoApp's [Result File](#)¹⁹⁷.

✓ Step 2, Charging with Constant Voltage

Uncheck **Run Step 2, Charging with Constant Voltage**, if this step should be omitted.

If checked, select which **Stopping Criterion at Boundary** should be used and enter the respective limiting value for the second simulation step.

You can provide a **Time Limit** that defines the simulated-time-threshold after which the step will end, regardless of whether previous stopping criteria were reached.

Below the settings for the [example](#)¹⁹⁷ are entered.

Step 2, Charging with Constant Voltage

☒ Run Step 2, Charging with Constant Voltage

Constant Voltage: Stopping Criterion at Boundary CRate

Charge Rate Limit / (1) 0.1

Constant Voltage: Time Limit / (s) 1800

✓ Step 3, Relaxation

Check **Use Perfect Relaxation**, if a perfect relaxation to equilibrium after charging/delithiation should be assumed.

Step 3, Relaxation

☒ Use Perfect Relaxation

Otherwise, define a **Relaxation Time** for defining the time after that the relaxation of the cell is stopped.

Below, the settings for the [example](#)¹⁹⁷ are entered.

Step 3, Relaxation

☐ Use Perfect Relaxation

Relaxation Time / (s)

1000

Results

After successfully running the command, the result file created is opened in the GeoDict Result Viewer.

Under the **Results-Report** subtab, the file names of all simulations run, and saved in the project folder, are listed. The accessible area-normalized and mass-normalized cell capacities are shown in separate tables for the charging/delithiation and discharging/lithiation.

Input MapLog MapPost MapResultsMetadata

ReportPlotsMap

Battery Capacity Test Results

4 simulations were run successfully. 10 result plots were created.

Results were created using the following files:

Battery_C_1.0.gdr

Battery_C_3.0.gdr

Battery_C_5.0.gdr

Battery_C_7.0.gdr

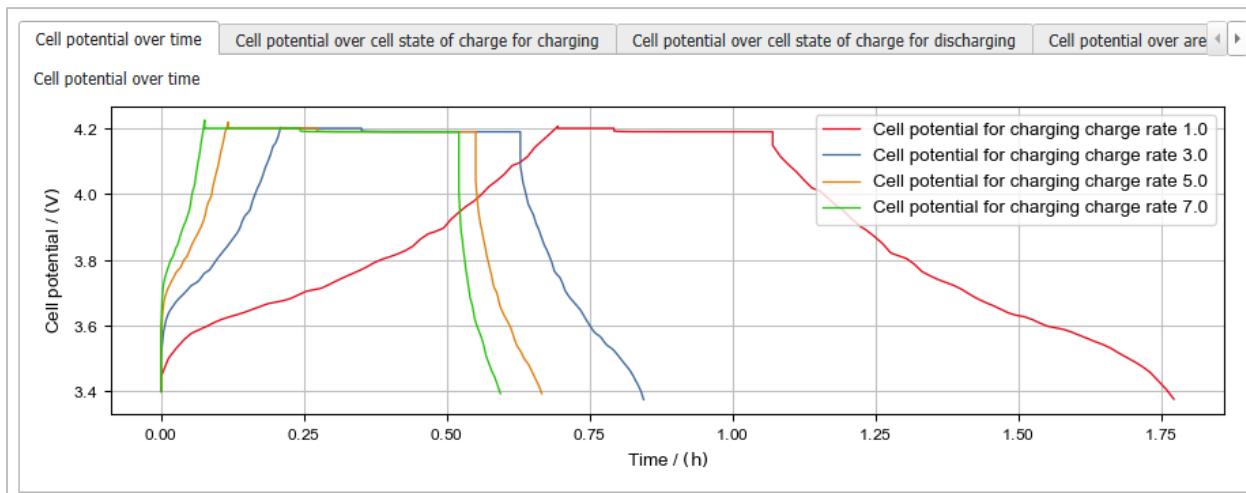
Accessible cell capacity for charging

ChargeRate	Accessible area-normalized cell capacity for charging with constant current / (mAh/cm ²)	Accessible area-normalized cell capacity for charging with constant current and constant voltage / (mAh/cm ²)	Accessible mass-normalized cell capacity for charging with constant current / (mAh/g)	Accessible mass-normalized cell capacity for charging with constant current and constant voltage / (mAh/g)
1.0	1.553	1.627	65.37	68.46
3.0	1.404	1.627	59.08	68.45
5.0	1.314	1.627	55.31	68.44
7.0	1.195	1.626	50.28	68.44

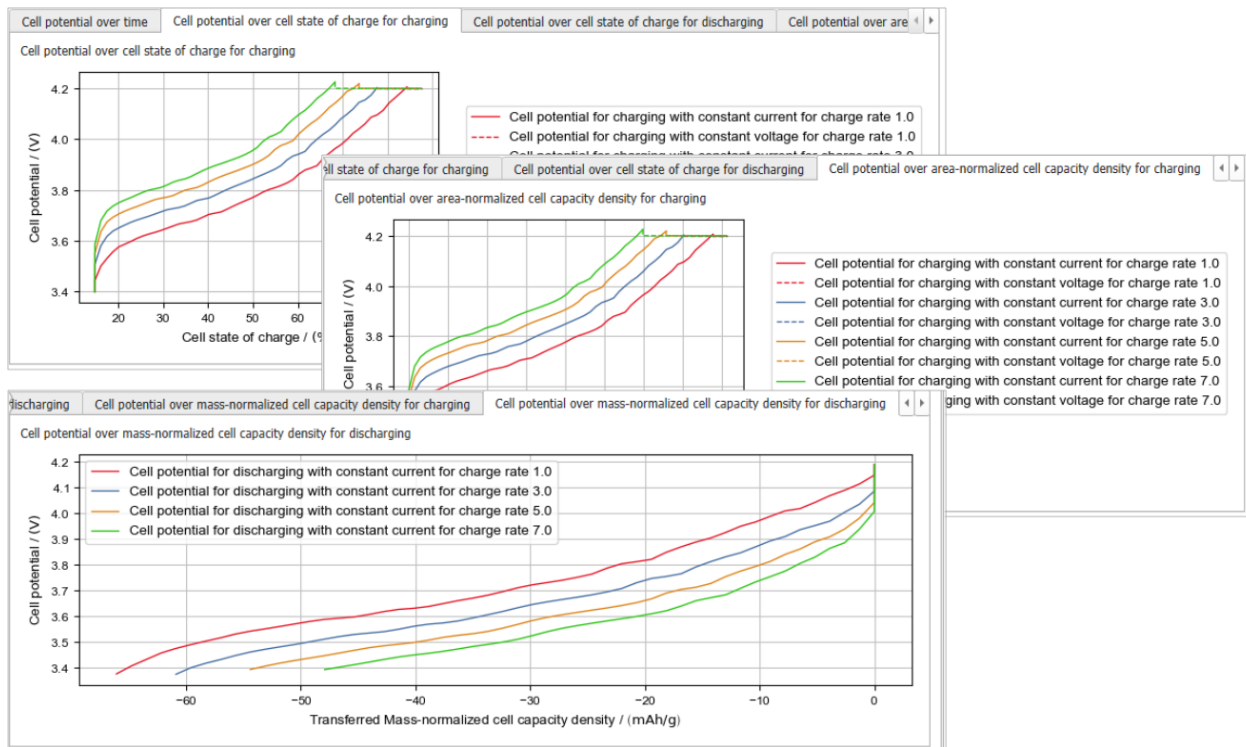
Accessible cell capacity for discharging

ChargeRate	Accessible area-normalized cell capacity for discharging with constant current / (mAh/cm ²)	Accessible mass-normalized cell capacity for discharging with constant current / (mAh/g)
1.0	1.57	66.08
3.0	1.447	60.89
5.0	1.293	54.4
7.0	1.139	47.92

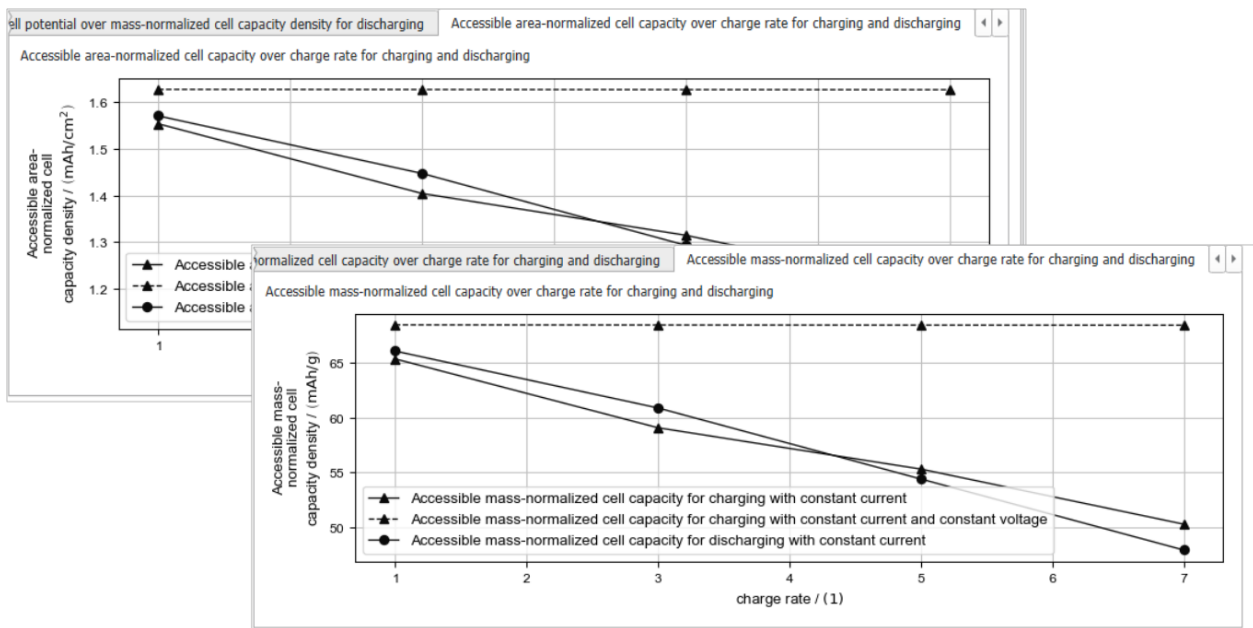
Under the **Results - Plots** subtab, the results of the simulations are compared in different ways. The whole charge curve for all simulations is shown as **Cell potential over time**.



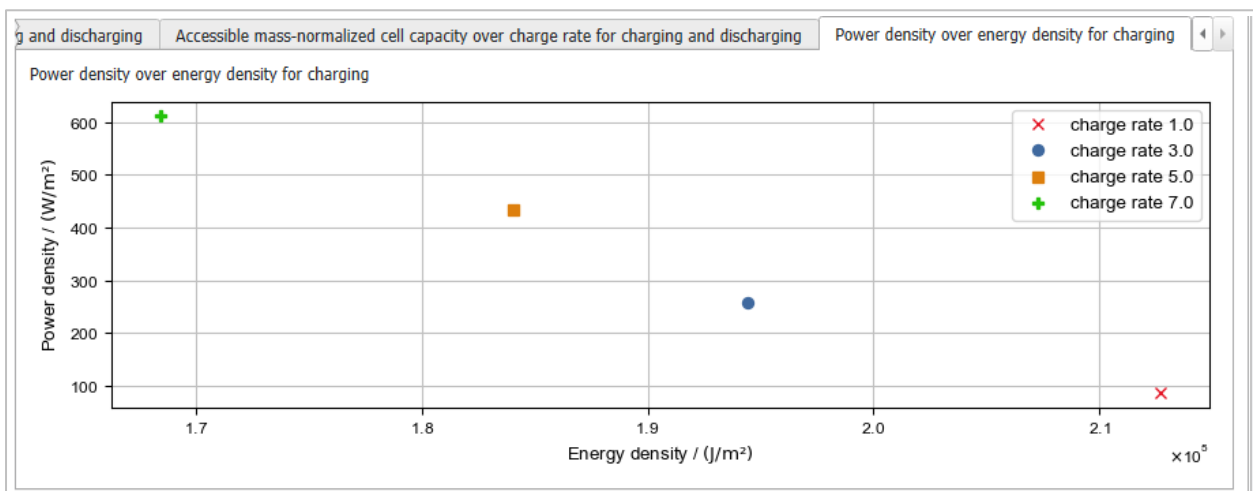
Under the following tabs, the cell potential of all simulations is shown for charging / delithiation and discharging / lithiation separately. First as **cell potential over the cell state of charge**, and then over the **area-normalized** and **mass-normalized cell capacity density**.



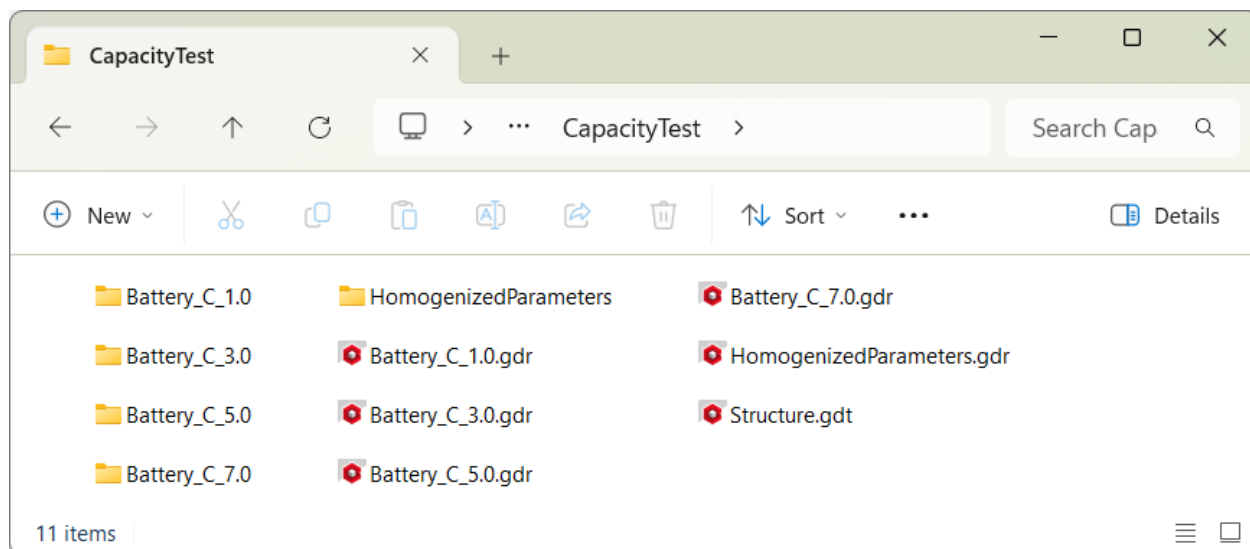
The two tabs **Accessible area-normalized cell capacity** and **Accessible mass-normalized cell capacity over charge rate for charging and discharging**, compare the accessible capacities for the different simulations. These values are also listed in the **Report**.



Finally, the plot under the last tab shows the **Power density over the energy density** computed for the charging step 1, charging with constant charge rate.



In the **Result Folder** find the intermediate results from the charging simulations for the different charging steps:



1.5.2 Electrochemical Impedance Spectroscopy

Calculate the complex-valued resistance called "impedance" that many battery developers and scientists use to understand the behavior of electrical components like resistors, capacitors, inductors and batteries.

Technically, this GeoApp sets expert settings for Electrochemical Impedance Spectroscopy (EIS) simulation and runs a charging simulation using the current settings in [Charge Battery](#)^[62], [Charge Electrode](#)^[135], [Charge Homogenized Battery](#)^[117], or [Charge Homogenized Electrode](#)^[152] in BatteryDict.



Needed Modules:

BatteryDict, BatteryDict-BEST, BatteryDict-EIS

Theoretical Background

Performing an EIS simulation is currently only possible with the [BEST solvers](#)^[85]. The simulation by itself does not modify the underlying model equations, it only activates an additional double layer model for the [interface active material - electrolyte](#)^[15].

The electrochemical double layer describes an effect at the interface of liquid electrolytes and active materials. Due to the polarization of the electrodes, the ions in the electrolyte arrange in a layered structure close to the active material surface, which imposes charge separation and acts as a capacitor. This takes place on the molecular scale. The double layer stores charges based on the voltage at the interface, releasing charges as the voltage drops or accumulating them as voltage increases, similar to a capacitor. Since the capacity of the double layer is comparatively small relative to the overall cell capacity, it equilibrates fast with voltage changes and has minimal impact during regular cell operation in the field. Only when studying

higher frequency dynamics, the double layer becomes crucial to consider. An example for this is the characteristic semi-circle in EIS, which is the result of the intercalation and double layer acting similar to a resistor-capacitor pair.

The double layer model is based on Hein, 2020 and introduces an additional interface current density between active material and electrolyte that is connected in parallel with the intercalation model resulting in a total interface current $i_{se,EIS}$ of

$$i_{se,EIS} = i_{se} + i_{DL} \quad (65)$$

where i_{se} is the Butler-Volmer interface current and i_{DL} is the double layer current.

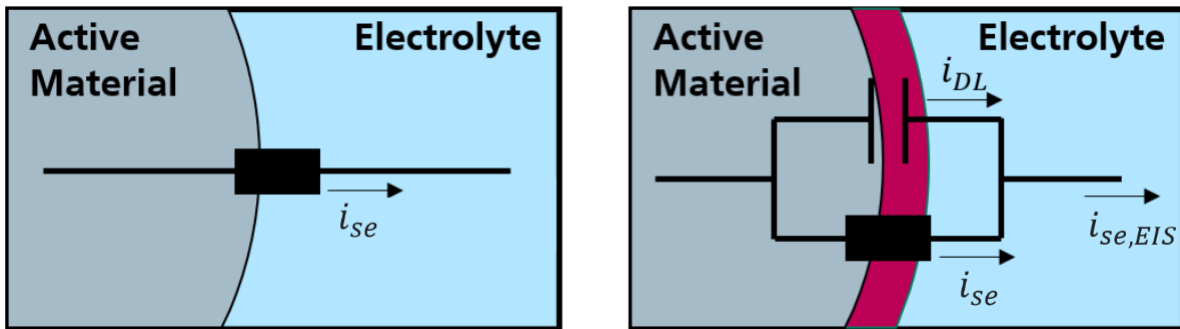
For a comparison the usual equations for the interface between electrolyte and active material are given in the [Fully Resolved Simulation](#)^[15] and [Homogenized Simulation](#)^[19] topics of the BatteryDict User Guide.

The double layer is modeled as an effective interface property between active material and electrolyte acting as ideal capacitor. The current density flowing across the double layer is given by

$$i_{DL} = C_{DL} \frac{\partial}{\partial t} (\varphi_s - \varphi_e) \quad (66)$$

using the areal capacitance C_{DL} , the local Maxwell potential of the electrode φ_s , and the local electrochemical potential in the electrolyte φ_e .

The figure below shows the different configurations that can be achieved with the intercalation and double layer model. It visualizes the different settings that are considered with the double layer model. The circuit drawings provide some information on how these settings would translate if the interface conditions of the continuum scale modeling approach would be transferred to an equivalent circuit model. On the left, the active material-electrolyte interface as modeled in [Charge Battery](#)^[62] and [Charge Electrode](#)^[135] is shown. Only the Butler-Volmer exchange current density is considered, resulting in an interface resistance. On the right, the model used in EIS-simulations is shown. Double layer and intercalation kinetics are both active and connected in parallel acting as a resistor-capacitor pair.



Finally, a specific predefined voltage operation protocol with Amplitude 10mV is executed including the double layer model to get the time transient current response of the cell.

Afterward, the time, current and voltage information can be post-processed to translate the information to the frequency domain and evaluate the complex impedance.

Parameters

Clicking **Edit...** opens the **Electrochemical Impedance Spectroscopy** dialog. At the top, define a **Result File Name** for the result file and the result folder containing the BatteryDict charging simulation run with the EIS plots.

To automatically add the suffix "_EIS" to this result file name, check **Add Suffix _EIS to BatteryDict Result File**.

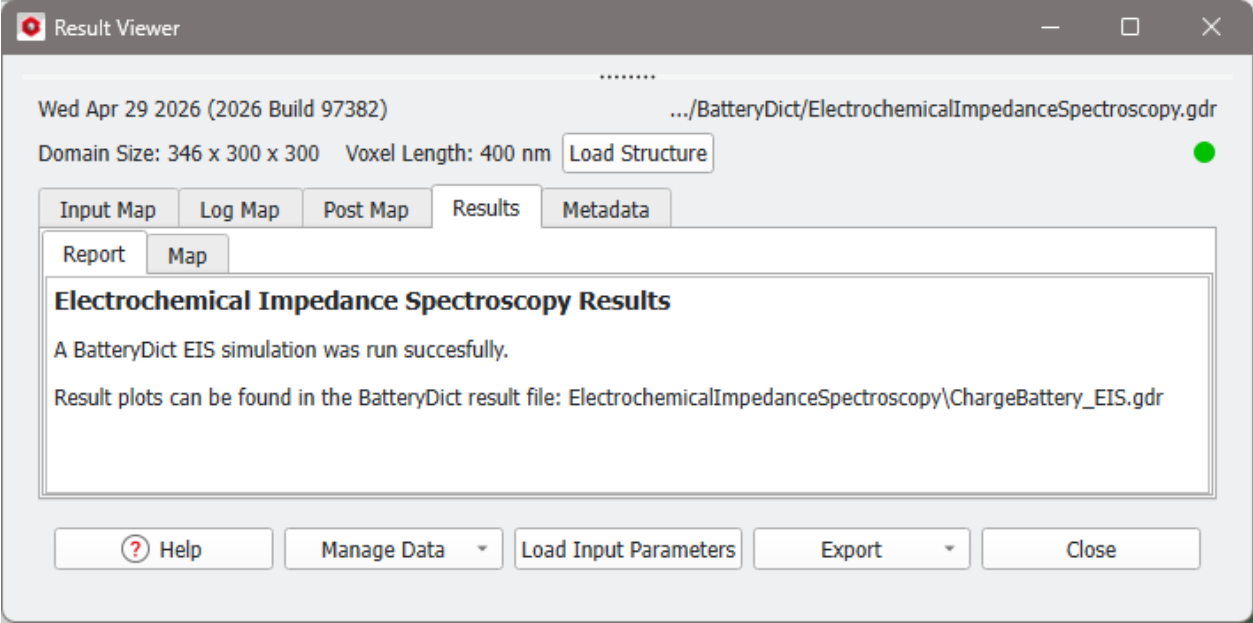
Choose the experiment type ([Charge Battery](#)^[62], [Charge Electrode](#)^[135], [Charge Homogenized Battery](#)^[117] or [Charge Homogenized Electrode](#)^[152]) and optionally the custom double layer capacities of the active materials.

Subsequently, when choosing Charge Battery or Charge Electrode for the simulation, you can use either BESTmeso (homogenized simulation) or BESTmicro (fully resolved simulation) as a [solver](#)^[85]. Charge Homogenized Battery or Charge Homogenized Electrode are always run with the BESTmeso solver.

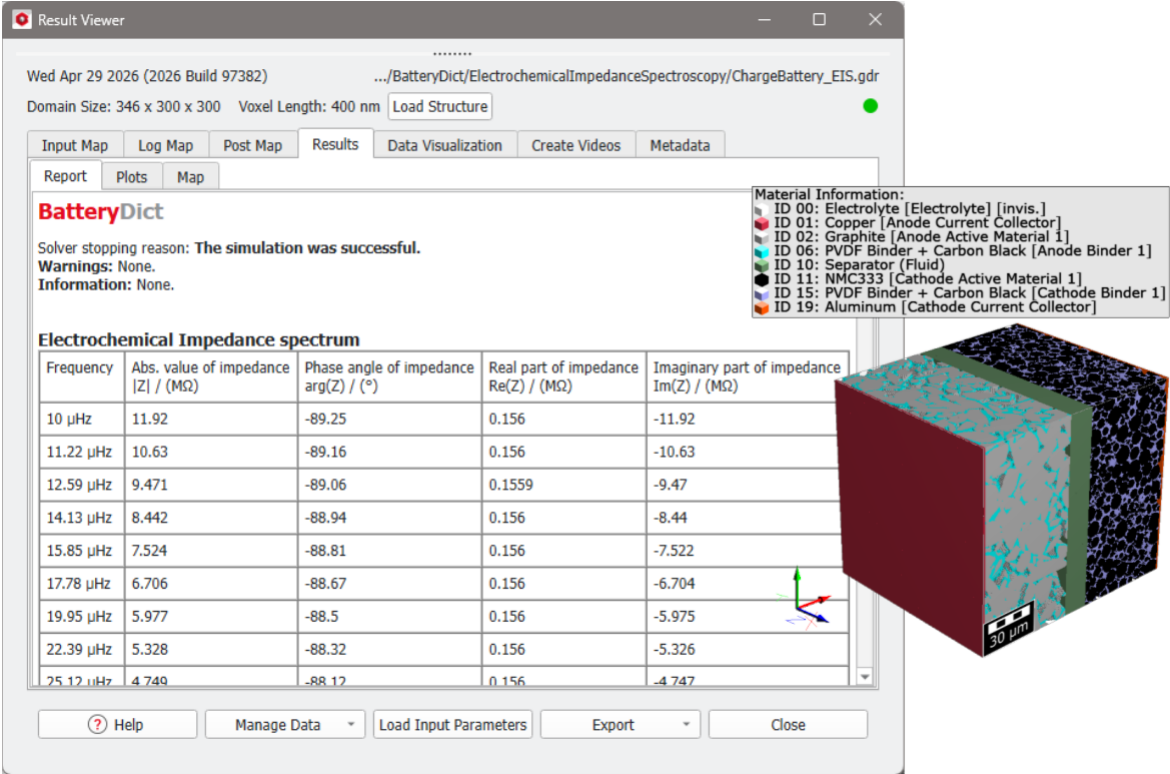
The start condition of the [Experiment](#)^[79] tab of the selected experiment type will be used. However, instead of a (dis)charging / (de)lithiation experiment, the EIS experiment at this start condition is simulated.

Results

After the BatteryDict simulation is finished the result file is opened in the Result Viewer.

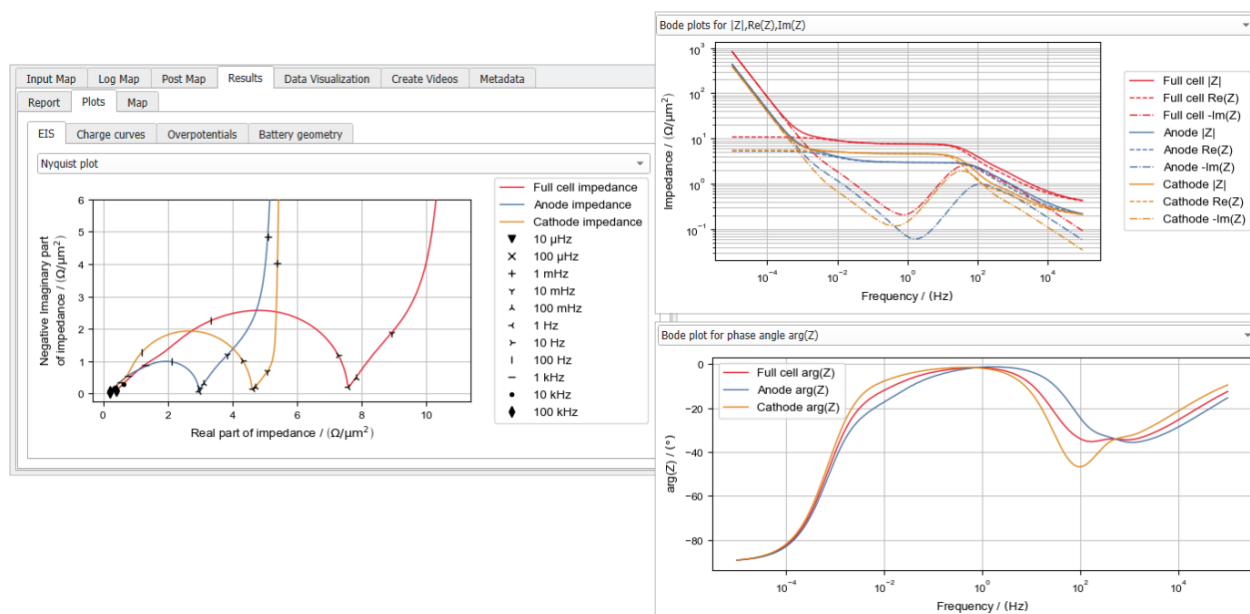


The report tells you where to look for the results. Load the BatteryDict result file from the result folder (**File** → **Open Results (*.gdr)**) Additionally to the usual [BatteryDict results](#)^[93], the report shows the **Electrochemical impedance spectrum** table. In the example, we used [Charge Battery](#)^[62] with the [BESTmeso](#)^[86] solver.



Under the **Plots** tab you find three **EIS** plots selectable from the pull-down menu: One Nyquist plot and two Bode plots.

The Bode plots visualize the real and imaginary part of the frequency response as well as the phase angle. All plots are shown for the full cell as well as for cathode and anode separately.



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