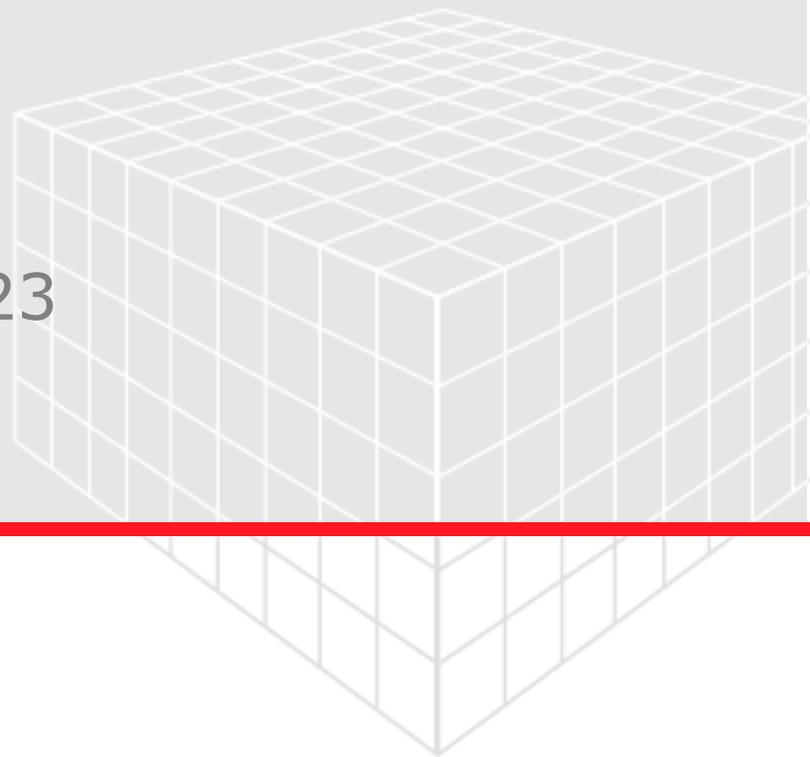


# BATTERYDICT

User Guide

GeoDict release 2023

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# GEO DICT

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# DIGITAL CHARGING & DISCHARGING OF LI-ION BATTERIES

**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 mass 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, binder, and electrolyte. Up to four different active materials can be handled for each electrode. It is also possible to perform half-cell simulations for single electrode structures, without designing the complete half-cell first.

In **GeoDict** 2023, as in previous **GeoDict** releases, it is possible to run a fully resolved simulation on the created microstructure. This very accurate solution provides results fully resolved on the micro scale. Three solvers are provided for fully resolved simulations, the LIR solver, the BEST:er-micro solver and the BESTmicro solver.

For the first time, **BatteryDict** allows now to run meso simulations with BESTmeso that are much faster than the fully resolved simulation. A simplified 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.

In **GeoDict** 2023, the functionality to compute mechanical deformations of a battery cell due to Lithium intercalation, is now available as a command in **BatteryDict** (**BatteryDict** - Degradation). 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.

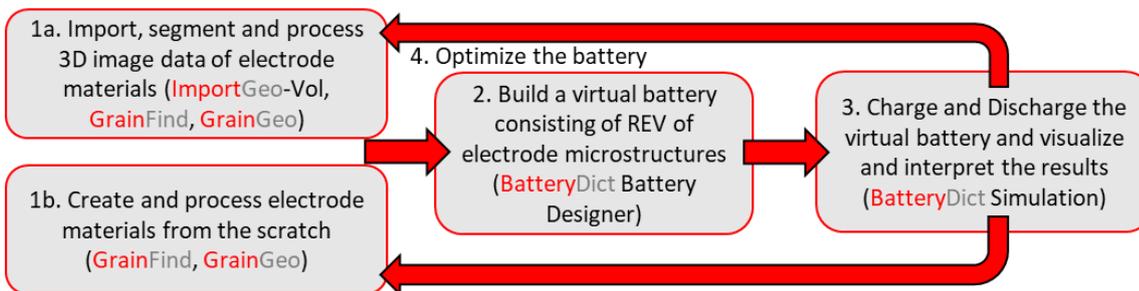
The input data for the electrode models can be either scanned data from  $\mu$ CT or FIB-SEM images of real cathode and anode materials, or realistic structures created in **GeoDict**. **BatteryDict** is capable of handling voxel-based structures, with a volume large enough (REV) to simulate the behavior 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 Basis](#). In the section [BatteryDict Computations](#), the use of the **BatteryDict** GUI and the different simulation options are outlined. The results of the simulations and their interpretation are discussed in the section [BatteryDict Computation Results](#).

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 **FlowDict**, **GrainGeo**, **GrainFind**, **PorDict**, **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 Digital Twins based on image data or realistic microstructures from scratch.

Please refer to the other handbooks of the [GeoDict User Guide](#) for more information.



## THEORETICAL BASIS

Upon charging a typical secondary Li-ion battery, the  $\text{Li}^+$  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  $\text{Li}^+$  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  $\text{Li}^+$  intercalation.

During discharging,  $\text{Li}^+$  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.

## STATE OF CHARGE (SOC)

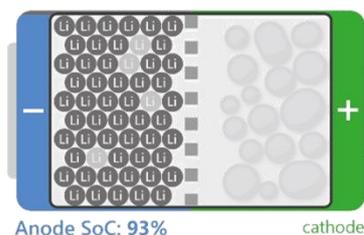
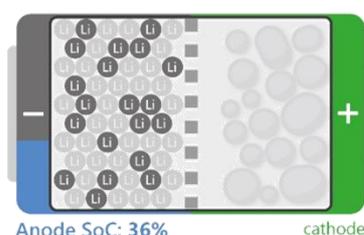
Depending on context, we distinguish different definitions of state of charge:

**Anode state of charge:** It 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.

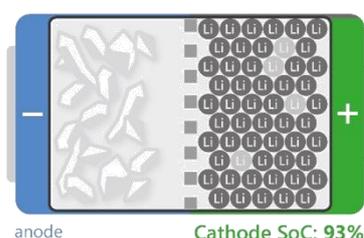
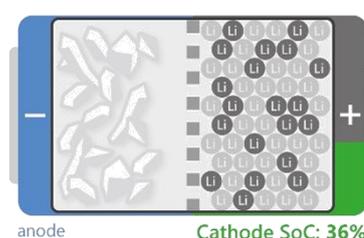
For an active material voxel, the SOC is the voxel's Li-ion concentration divided by the voxel's maximum Li-ion concentration (see page [14](#)).

The anode SOC is the mean value of the voxel SOC's of all active-material voxels within the anode.

Anode State of Charge



Cathode State of Charge

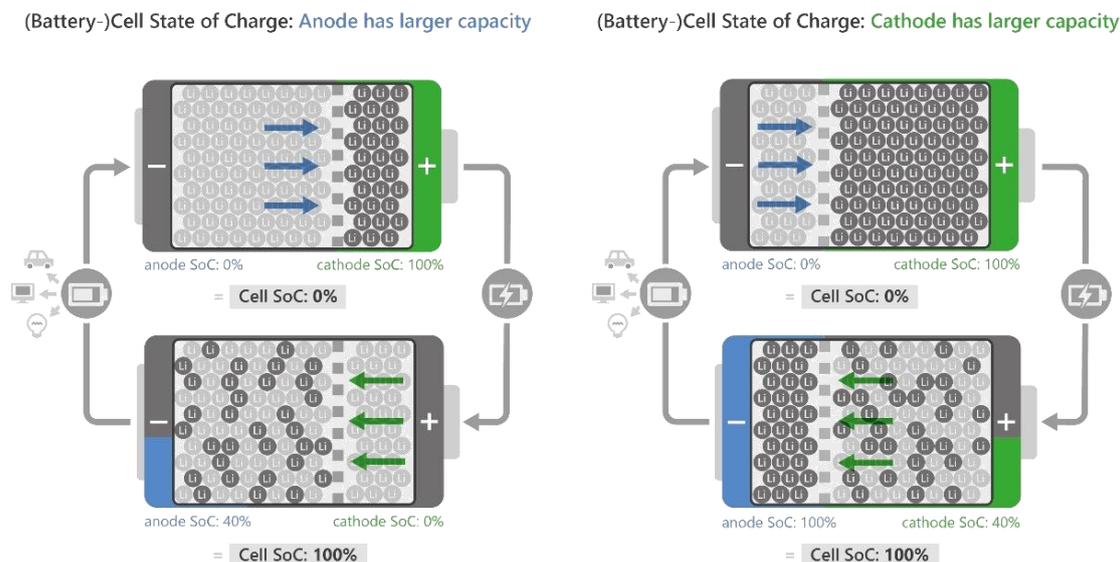


**Cathode state of charge:** It measures the Li-ion content of the cathode relative to the maximal Li-ion content of the cathode. The Li-ion content is the volume integral of the Li-ion concentration.

For an active material voxel, the SOC is the voxel's Li-ion concentration divided by the voxel's maximum Li-ion concentration (see page [14](#)).

The cathode SOC is the mean value of the voxel SOC's of all active-material voxels in the cathode.

**Cell state of charge:** It 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 page 7.

**Material state of charge (on voxel scale):** In **BatteryDict**, each voxel has a unique Material ID. 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.

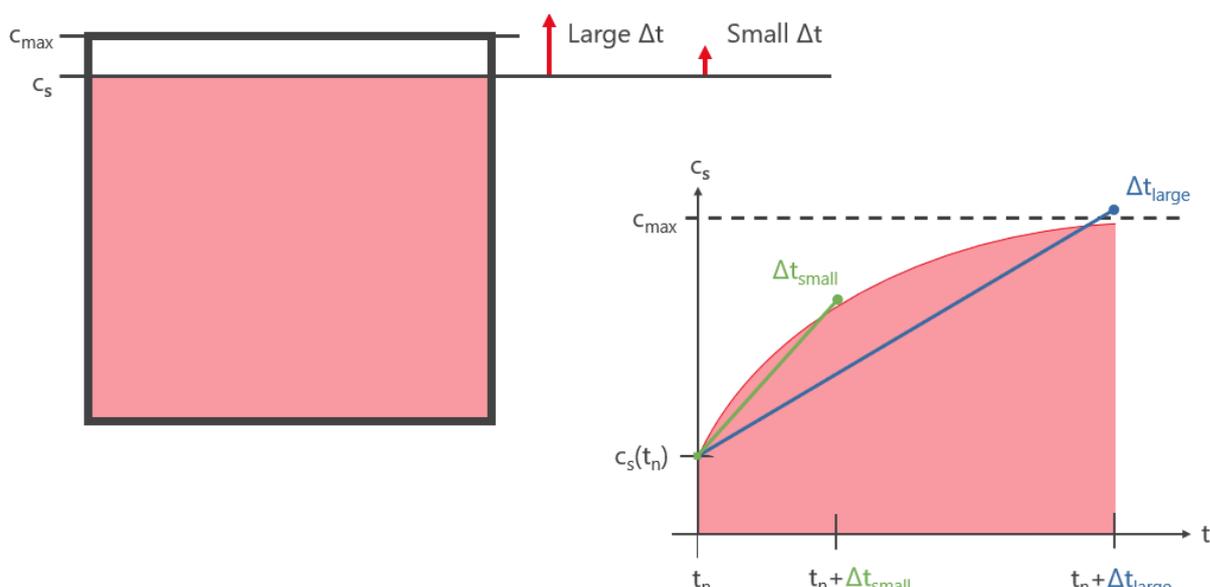
For cathode materials, the maximum lithium composition is usually the stoichiometric lithium composition (e.g.  $x=1$  for  $\text{Li}_x\text{Ni}_{0.33}\text{Mn}_{0.33}\text{Co}_{0.33}\text{O}_2$ ). The minimum lithium composition is the lithium composition where the maximal amount of lithium ions is 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 a certain "material state of charge" 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 charge is defined as

$$SOC_{material} = \frac{c_s}{c_{max}} \cdot 100\%$$

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 material SOC 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 obtain always material SOC 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 an active material 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 will usually try to solve for smaller time steps to converge to a meaningful result.

Note that the material SOC 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  $x < 1$ .

## BATTERYDICT - SIMULATION OF CHARGING AND DISCHARGING PROCESS

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 we apply a model 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:

$$\frac{\partial c}{\partial t} = -\nabla \cdot \vec{N}$$

$$0 = \nabla \cdot \vec{j}$$

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

### IN 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

$$\vec{N}_s = -D_s \nabla c_s$$

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

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

$$\vec{j}_s = -\kappa_s \nabla \varphi_s$$

where  $\kappa_s$  is the electronic conductivity and  $\varphi_s$  the electrical potential.

### 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

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

where  $\kappa_e$  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.

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

$$\vec{N}_e = -D_e \nabla c_e + \frac{t_+ \vec{J}_e}{F}$$

Further explanation about the theoretical background for the ion transport in the electrolyte can be found in [\[1\]](#).

## THE 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

$$\hat{n} \cdot \vec{N}_e = \hat{n} \cdot \vec{N}_s = i_{se}/F$$

$$\hat{n} \cdot \vec{J}_e = \hat{n} \cdot \vec{J}_s = i_{se}$$

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 current density depends on concentrations and potentials on both sides of the interface and is given by

$$i_{se} = 2k_{BV} \sqrt{c_s c_e (c_{max} - c_s)} \sinh \left[ (\varphi_s - \varphi_e - U_0(c_s)) \frac{F}{2RT} \right].$$

Here,  $k_{BV}$  is the Butler-Volmer rate constant 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  $\sqrt{c_s c_e (c_{max} - c_s)}$  in the Butler-Volmer interface current density gets 0, which can lead to numerical solver problems. As stated on page [4](#), 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 be set between 5% and 95% only in the [Charge Battery](#) and the [Charge Half Cell](#) dialog. A real battery in experimental conditions usually is set to operate in a certain voltage window (compare also the different stopping criteria, see page [10](#)) 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.

BatteryDict

**GEO**DICT

Result File Name (\*.gdr)

Constituent Materials   Experiment   Solver   Output Options   Equations & References

Charge Conservation and Electroneutrality    $0 = \nabla \cdot \vec{j}_e = -\nabla \cdot (\kappa_e \nabla \varphi_e) + \nabla \cdot \left[ \kappa_e (1 - t_+) \frac{RT}{F} \nabla \log c_e \right]$

Active Material

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

Ohm's Law    $0 = \nabla \cdot \vec{j}_s = -\nabla \cdot (\kappa_s \nabla \varphi_s)$

Interface between Electrolyte and Active Material

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

Variables and Constants

- $c_e$ : Lithium concentration in electrolyte
- $c_s$ : Lithium concentration in active material (solid)
- $j_e$ : Current density of all ionic charges in electrolyte
- $j_s$ : Effective electronic current density in active material (solid)
- $i_{se}$ : Butler-Volmer interface current density
- $\varphi_e$ : Electric potential of electrolyte
- $\varphi_s$ : Electric potential of active material (solid)
- $U_0$ : Open-circuit potential of active material vs. lithium
- $c_{max}$ : Maximum lithium concentration of active material (solid)
- $\kappa_e$ : Ionic conductivity of electrolyte
- $\kappa_s$ : Effective electronic conductivity of active material (solid)
- $D_e$ : Ionic diffusivity of electrolyte
- $D_s$ : Ionic diffusivity of active material (solid)
- $t_+$ : Lithium transference number (electrolyte)
- $k_{BV}$ : Butler-Volmer rate constant
- T: Temperature
- F: Faraday constant, 96485.33289(59) C/mol
- R: Universal gas constant, 8.3144598(48) J/(mol K)

OK   Cancel

## BOUNDARY CONDITIONS AT THE CURRENT COLLECTORS

A battery can be operated in two modes, either by prescribing the current or the voltage.

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/m<sup>2</sup>) or as 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 since [GeoDict 2022](#). In this case, 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, since [GeoDict 2022](#), it is possible to define a charging profile. This allows to simulate the charging or discharging with different boundary conditions at the current collectors one after the other.

## STOPPING CRITERIA FOR CHARGING SIMULATIONS

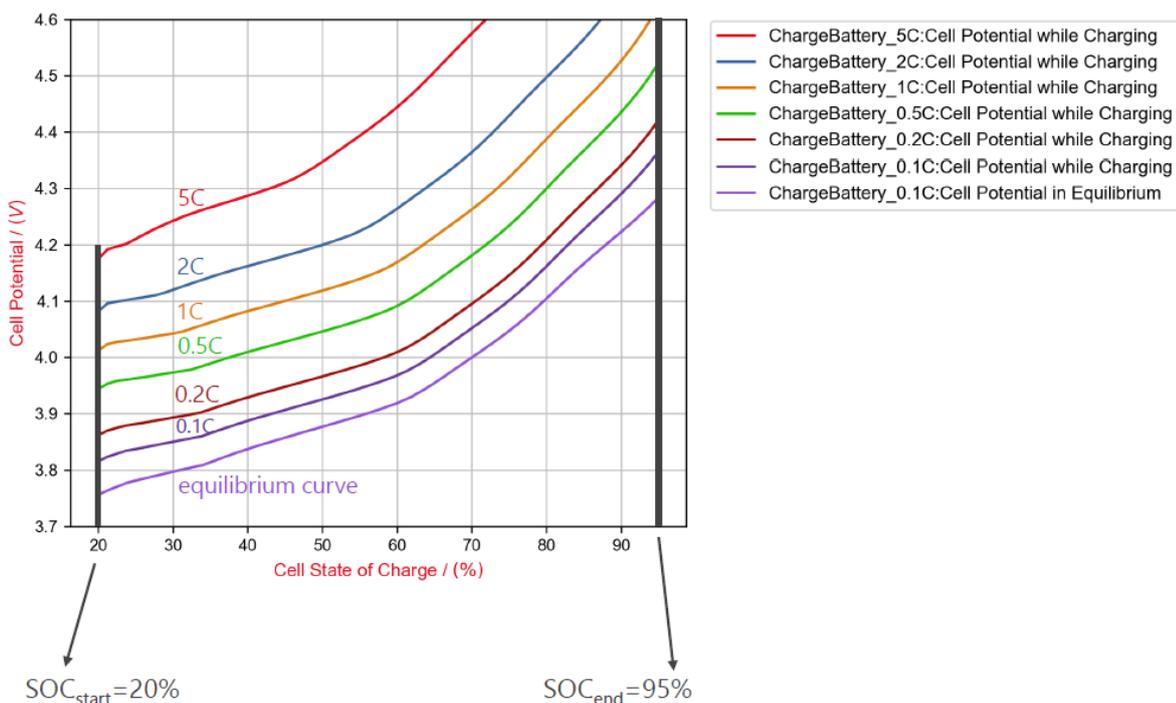
Since **GeoDict 2022**, different stopping criteria for a charging simulation can be defined. Choosing a final state-of-charge for the whole battery or for both electrodes, is the stopping criterion that was available already in previous **BatteryDict** releases.

Since **GeoDict 2022**, 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 on page [42](#) and [44](#).

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.

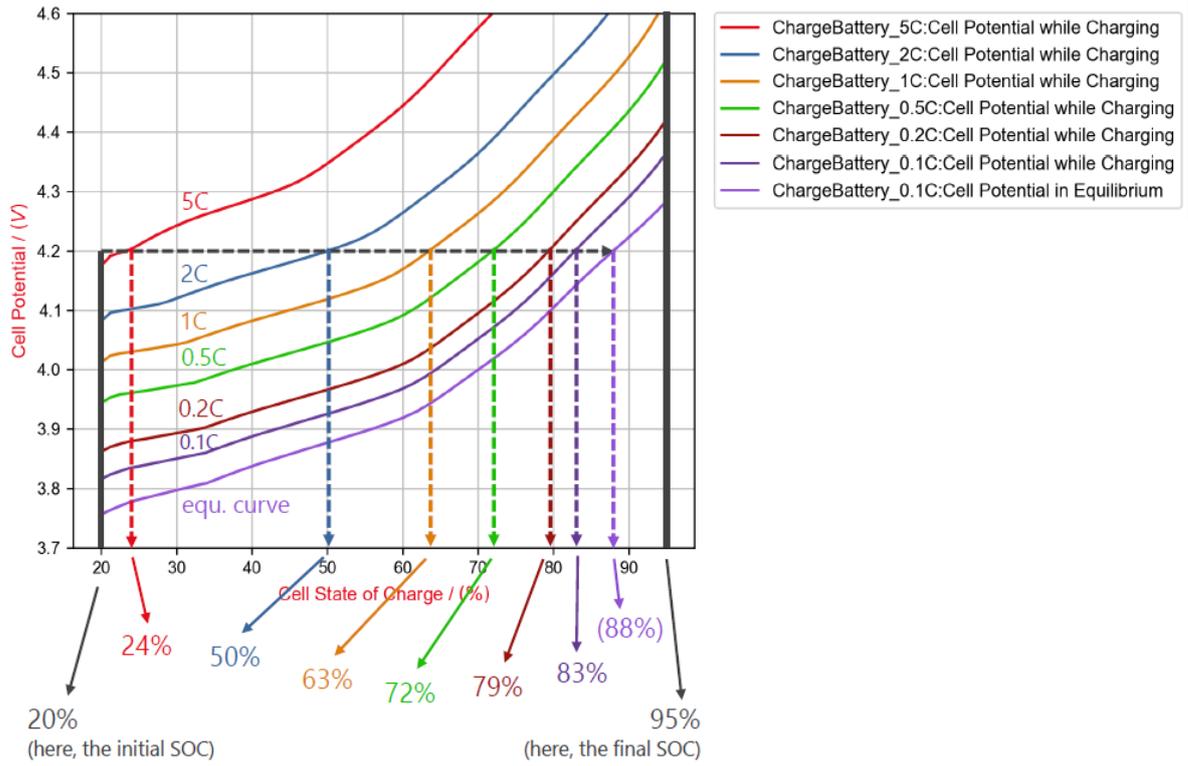
For simulations with constant charge rate, the time evolution of the cell potential depends on the charge rate selected. The higher the charge rate, the larger the deviation of the cell potential curve from the equilibrium charge curve, since the overpotentials get larger for higher charge rates (see below on page [12](#)).

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

In contrast to this, if a final potential is defined as stopping criterion, here 4.2 V, the state-of-charge reached at the end of the simulation depends on the charge rate, while the cell potential is always 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. Due to this different state-of-charge at the end of the simulation, the capacitance of the battery is different for different charge rates.



## OVERPOTENTIALS IN BATTERY CHARGING SIMULATIONS

Since **GeoDict** 2022, overpotentials of the (dis-)charging process, can be visualized for a finished simulation in the Result Viewer (see page [85](#)).

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.

In **GeoDict**, three sources of overpotential are considered:

- **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.
- **Diffusive overpotentials** result from the distribution of lithium ions in the active materials 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.

Diffusive overpotentials can even get negative in certain situations. The reason is that to compute the overpotential, the local surface concentration is compared to the concentration over the whole electrode. Two effects are therefore relevant for the diffusive overpotential, diffusion in one grain and the possible inhomogeneity in the loading of particles in the electrode.

- **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.

In the **GeoDict** Result Viewer, these three kinds of overpotentials are shown separately. Like this, it is possible to analyze for a simulation which process in the battery causes the largest amount of additional potential during charging and is responsible for the largest potential loss during discharging.

## BATTERYDICT: DEGRADATION SIMULATIONS

In **GeoDict** 2023, the simulation of one-way battery volumetric changes due to lithium intercalation of active materials is included in the module **BatteryDict** as an add-on called **BatteryDict** -Degradation.

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 (see the [ElastoDict](#) handbook of the **GeoDict** User Guide for details of the solver).

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

$$\Delta l = (C_{end} - C_{start}) \cdot \alpha \cdot l,$$

with  $\alpha$  the concentration expansion coefficient,  $C_{start}$  and  $C_{end}$  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 equivalently 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, often an expansion coefficient for volumetric changes due to lithium intercalation,  $\alpha_{vol}$ , can be found. To get the coefficient required here, use  $\alpha = \sqrt[3]{\alpha_{vol}}$ .

## SIMULATION PARAMETERS

The parameters occurring in the equations are explained in the following:

- Maximum Lithium Concentration ( $c_{max}$ ):** Maximum lithium concentration 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 the active material 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  $C_{spec,max}$  when determining the open circuit voltage potential (see below), the material density  $\rho$ , and Faraday's constant  $F$ :

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

Its unit is  $\frac{mol}{m^3}$ , i.e. the concentration is provided as amount of accessible lithium ions per volume.

- Electronic Conductivity:** Measures a materials ability to conduct electrons.
- 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, see page [38](#).
- 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 [\[4\]](#). It can also be measured by Electrochemical Impedance Measurements (EIS) [\[5\]](#). The ionic diffusion constant of an active material can depend on the material SOC, see page [4](#). **GeoDict** can consider the concentration dependence of ionic diffusion constants for electrolyte, see page [38](#).
- Butler-Volmer Rate Constant:** This 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. Experimentally, it can be determined via the exchange current density.

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 [\[5\]](#))

$$i_{se} = I_D/S = j_0 \left( \exp \left[ \frac{\alpha z F}{RT} \eta_D \right] - \exp \left[ -\frac{(1-\alpha) z F}{RT} \eta_D \right] \right), \quad (1)$$

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  $\alpha$ , the charge number  $z$  (which is  $z=1$  for a lithium-ion battery), and the overpotential  $\eta_D$ . Considering  $\alpha=1/2$ , the Butler-Volmer equation simplifies to

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

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  $\alpha=0.5$  [5]

$$j_0 = k_0 F \sqrt{c_s c_e (c_{max} - c_s)} = k_{BV} \sqrt{c_s c_e (c_{max} - c_s)} \quad (3)$$

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 (2) 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,

$$i_{se} = 2k_{BV} \sqrt{c_s c_e (c_{max} - c_s)} \sinh \left[ (\varphi_s - \varphi_e - U_0) \frac{F}{2RT} \right]. \quad (4)$$

To obtain a value of  $k_{BV}$  from the measured exchange current densities at different material SOC's (see page 4) of the electrode material, the experimental data for  $j_0(\text{SOC})$  are fit to a modified equation (3) using  $c_s = c_{max} \cdot \frac{\text{SOC}}{100\%}$ :

$$j_0(\text{SOC}) = k_{BV} \sqrt{c_e c_{max}^2 \left( \frac{\text{SOC}}{100\%} - \left( \frac{\text{SOC}}{100\%} \right)^2 \right)}$$

Note that it might be necessary to convert literature data for  $j_0$  from a function of lithium composition to a function of SOC as described in (5). The next figure shows the experimental data  $j_0$  as a function of SOC for NMC333 and a reference electrolyte (EC/DMC/EMC 1:1:1, salt  $\text{LiPF}_6$ , concentration 1 mol/L) as reported in [6] and [7].

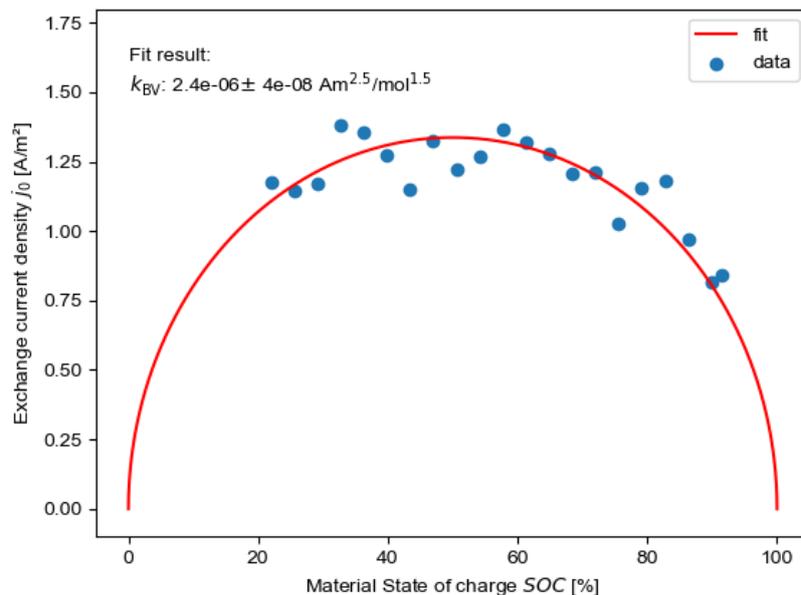


Figure 1: Measured data for  $j_0$  of NMC333 at 15°C from the Supplementary Information of [7] as a function of electrode SOC and fit to the data using the above equation. The fit results in  $k_{BV} = 2.4e-6 \text{ Am}^{2.5}/\text{mol}^{1.5}$ .

- Open-Circuit Potential (OCV) Function:** 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 SOC or a "quasi-OCV" function is measured at very low charging rates, e.g. of C/100 [6]. 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 [8]. Additionally, it depends on the charging state of the electrode and is therefore a function of the state of charge (SOC) of the material  $SOC = \frac{c_s}{c_{max}} \cdot 100\%$ , see page 4.

In literature, the OCV function is often provided as a function of the specific capacity  $C_{spec}$ , e.g. in mAh g<sup>-1</sup> against the potential vs Li/Li<sup>+</sup> [9]. The maximum experimentally accessible specific capacity of a material is denoted as  $C_{spec,max}$  and the OCV curve ends at this specific capacity. Figure 2 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  $C_{spec}$  to the material SOC by the equation:

$$SOC(C_{spec}) = \frac{C_{spec}}{C_{spec,max}} \cdot 100\%$$

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 the 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 (Li<sub>x</sub>Ni<sub>0.33</sub>Mn<sub>0.33</sub>Co<sub>0.33</sub>O<sub>2</sub>)) to the minimally reachable lithium composition  $x_{min}$ . This minimally reachable lithium composition can be calculated via the maximum experimentally accessible specific capacity  $C_{spec,max}$  and the theoretical capacity  $C_{spec,theo}$  which is calculated with the equation:

$$C_{spec,theo} = \frac{n_{Li}}{M} F$$

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  $C_{spec,max}$  to  $C_{spec,theo}$ , for instance for NMC333:

$$x_{min} = 1 - \frac{C_{spec,max}}{C_{spec,theo}} \approx 0.27$$

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

$$SOC(x) = \frac{100}{1 - x_{min}} (x - x_{min}) \quad (5)$$

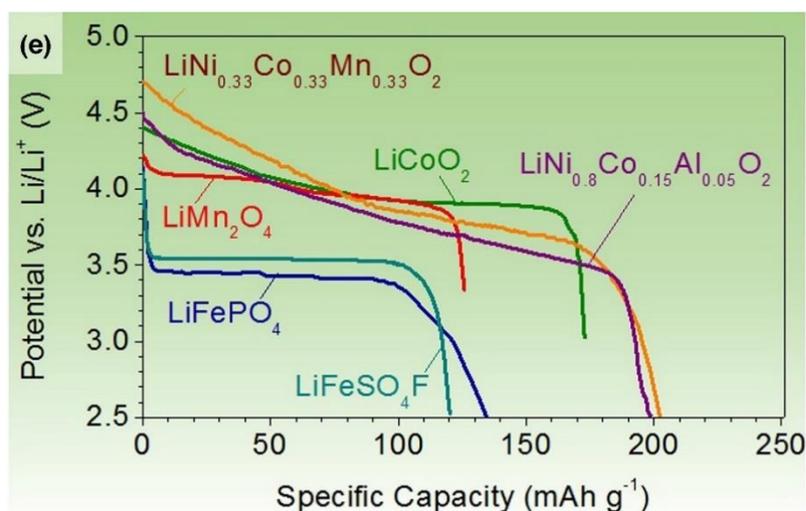


Figure 2: Typical discharge OCV potentials for intercalation cathode materials. Taken from [9].

- **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 for the electrolyte, see page [38](#).
- **Concentration Expansion Coefficient:** The concentration expansion coefficient is needed to calculate the material expansion upon lithium intercalation using [BatteryDict-Degradation](#). The expansion coefficient is calculated with the equation

$$\alpha = \frac{(1 + \Delta V)^{\frac{1}{3}} - 1}{c_{max}}$$

where  $\Delta V$  is the maximal volume change due to lithium intercalation and  $c_{max}$  is the maximum (removable) lithium concentration, [\[10\]](#).

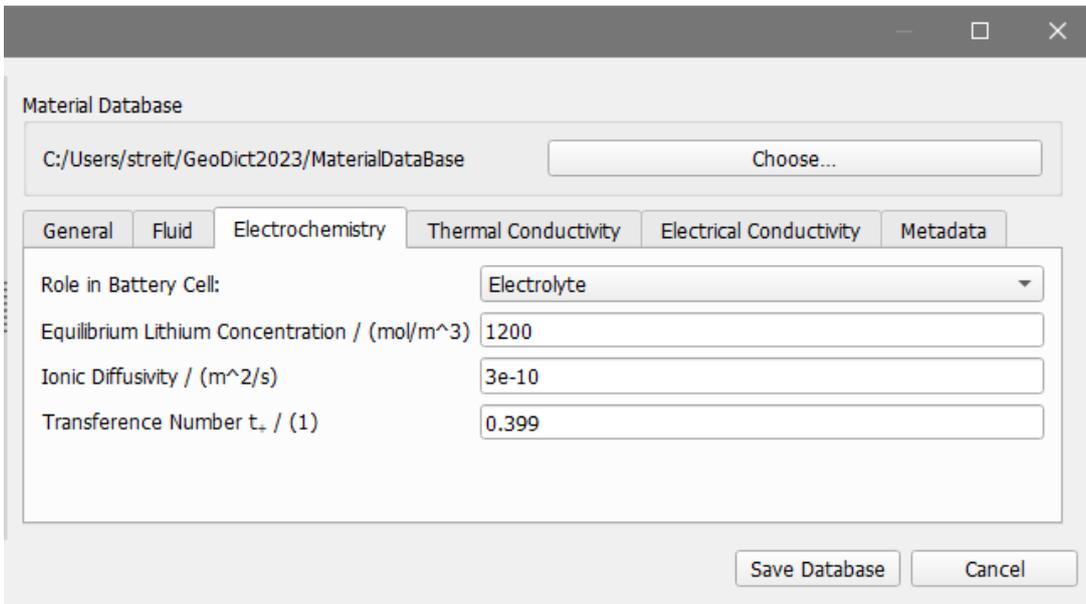
## ADDING CUSTOM ELECTROCHEMICAL MATERIALS: EXPERIMENTAL DATA NEEDED

[GeoDict](#) provides standard materials in the [GeoDict Material Database](#) for electrolyte, active materials, and binder and carbon black. For more information on the Material Database, see the [Material Database](#) handbook of the [GeoDict User Guide](#).

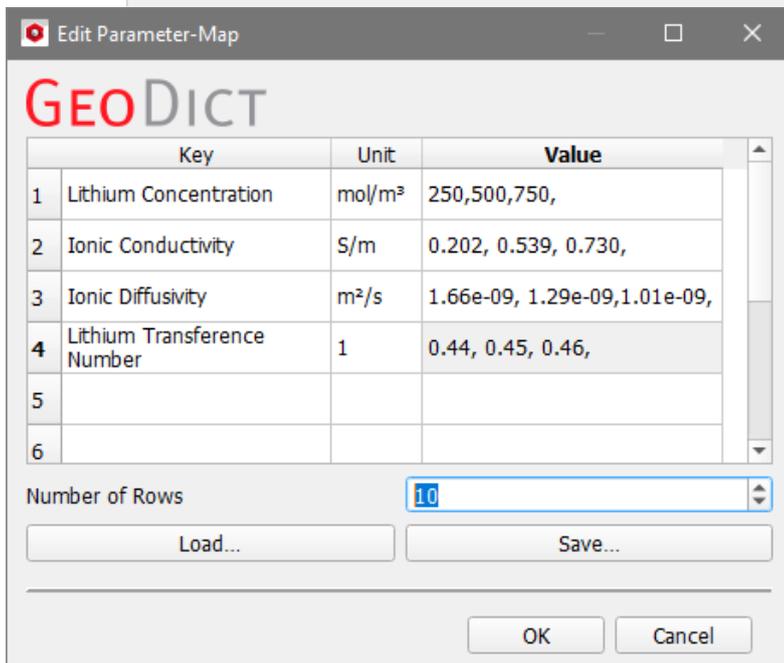
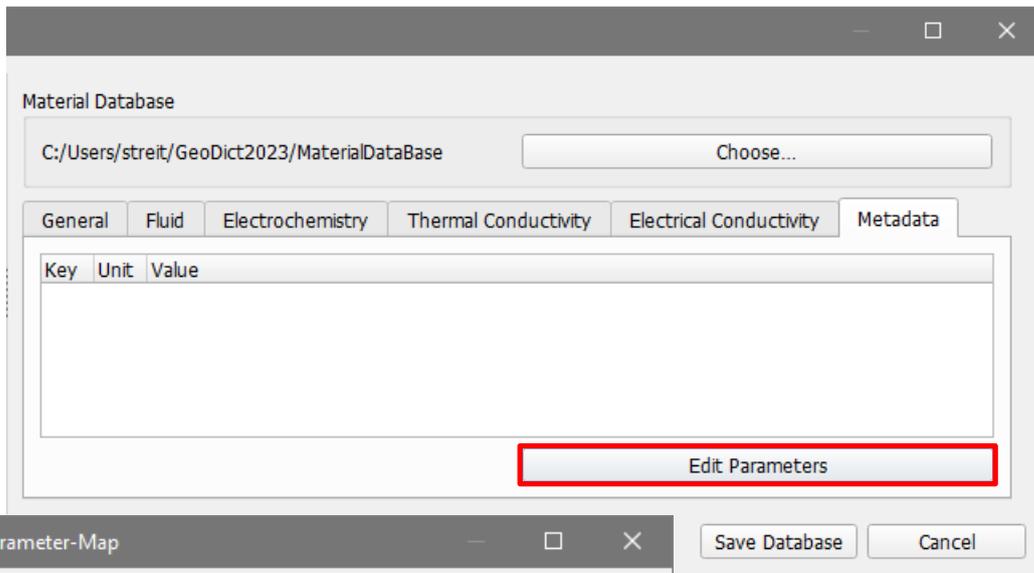
The following material parameters are required to add new materials for electrochemical simulations to the [GeoDict Material Database](#):

### Electrolyte

- Mandatory parameters:
  - Equilibrium lithium concentration
  - Ionic conductivity (effective value)
  - Ionic diffusion constant (effective value)
  - Transference number (effective value)



- 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.



Click **OK** to return to the **Metadata** tab of the Material Database.

Finally, click **Save Database**, to save the new values in your **GeoDict** Material Database folder.

Copy the values from the Metadata tab for the charging simulations to the **Charge Battery** or **Charge Half Cell** dialog, see page [38](#).

Active material:

- **Mandatory parameters:**
  - Maximum lithium concentration
  - Open-circuit potential (OCV) function curve
  - Density
  - Ionic diffusion constant
  - Electrical conductivity
  - Butler-Volmer rate Constant. This value depends not only on the active material, but also on the electrolyte. It can be therefore defined for different electrolyte materials.

Material Database

C:/Users/streit/GeoDict2023/MaterialDataBase Choose...

General Solid Mechanical Properties **Electrochemistry** Thermal Conductivity Electrical Conductivity Metadata

Role in Battery Cell: Anode Active Material

Maximum Lithium Concentration / (mol/m<sup>3</sup>) 31090

Ionic Diffusivity / (m<sup>2</sup>/s) 2e-14

Electrolyte Selection

Edit Electrolyte Default Delete Rename

Add Electrolyte Add

Butler-Volmer Rate Constant / (A m<sup>-2.5</sup>/mol<sup>1.5</sup>) 8.1e-06

Open-Circuit Potential (OCV) Function U<sub>0</sub>

Open-Circuit Potential Has Hysteresis

	Anode State of Charge / (%)	Potential / (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

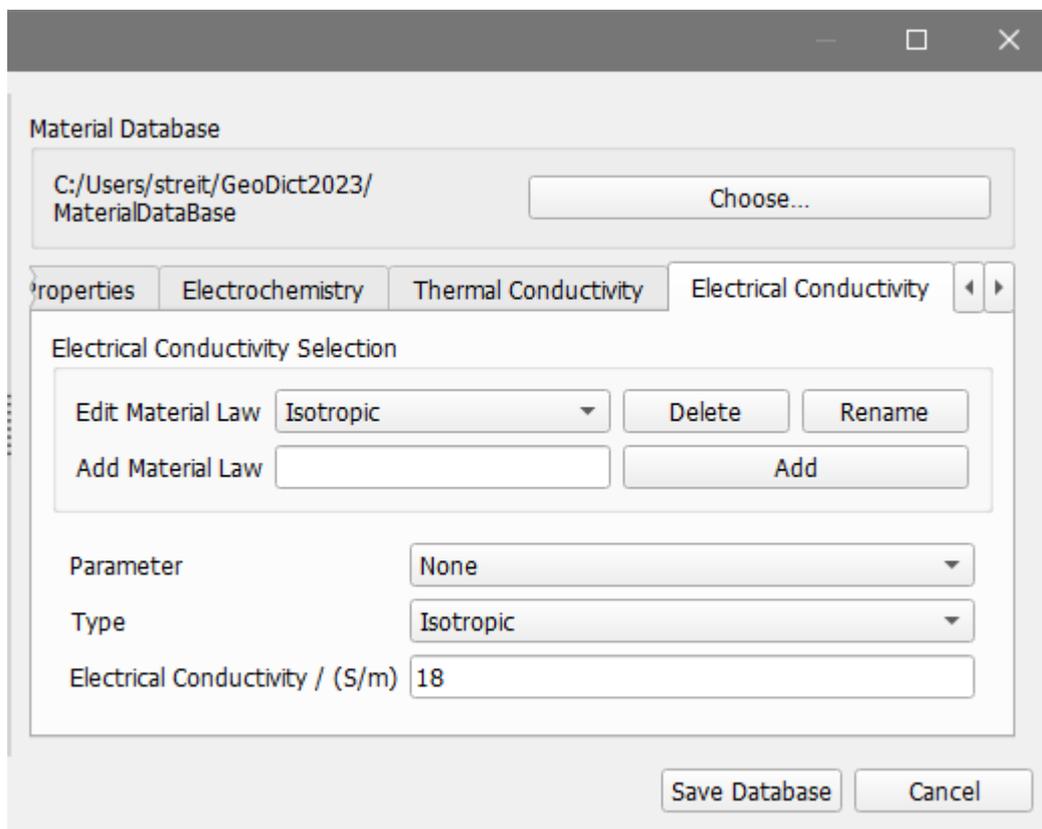
	Anode State of Charge / (%)	Potential / (V)
1	0	0.43667
2	6.674	0.22778
3	8.288	0.22133
4	9.903	0.21933
5	11.625	0.218

Save Database Cancel

- Optional parameters (see page [20](#)):
  - Lithium concentration expansion coefficient  
Used for volume expansion during lithiation with **BatteryDict-Degradation**, measured e.g. by electrochemical dilatometry.
  - Mechanical parameters for computation of mechanical deformations with **BatteryDict-Degradation**.

CBD phase (Binder+Carbon Black):

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- Mandatory parameters:
  - Effective electrical conductivity

Note that to determine temperature effects, the material parameters must also be determined at different temperatures.

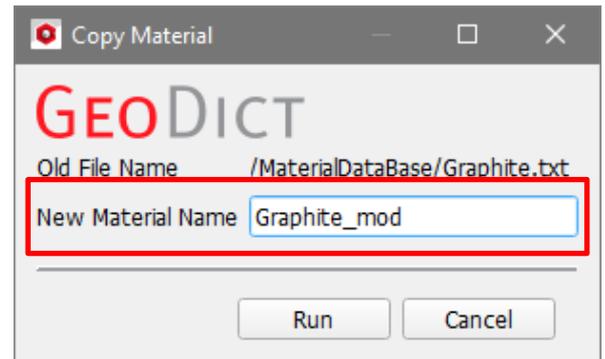
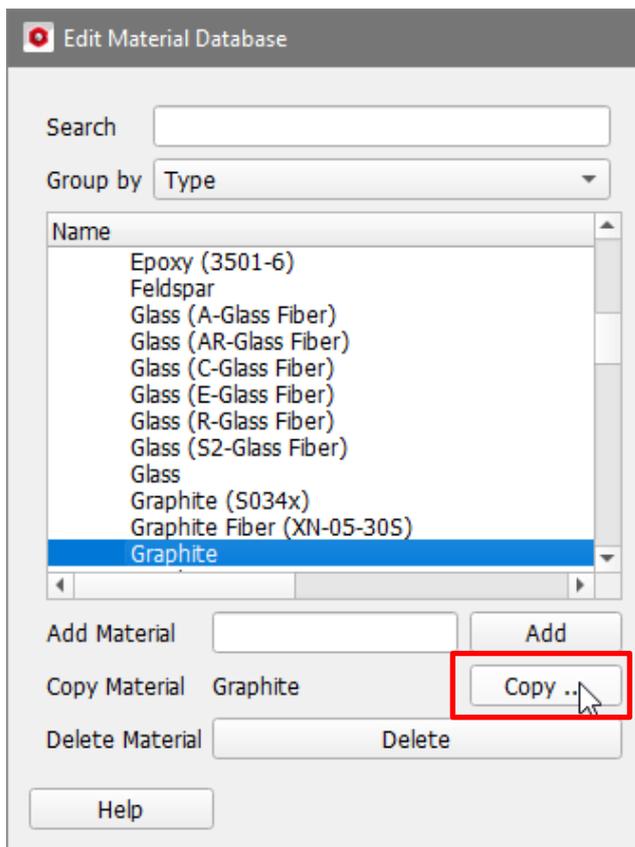
For all materials, save the changes in the material Database by clicking **Save Database**. The new material can now be used like any of the standard materials delivered with **GeoDict**.

### ADDING MATERIAL INFORMATION FOR DEGRADATION SIMULATION

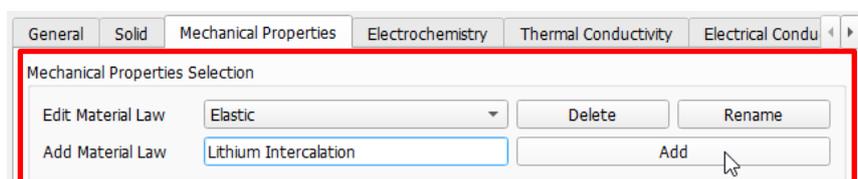
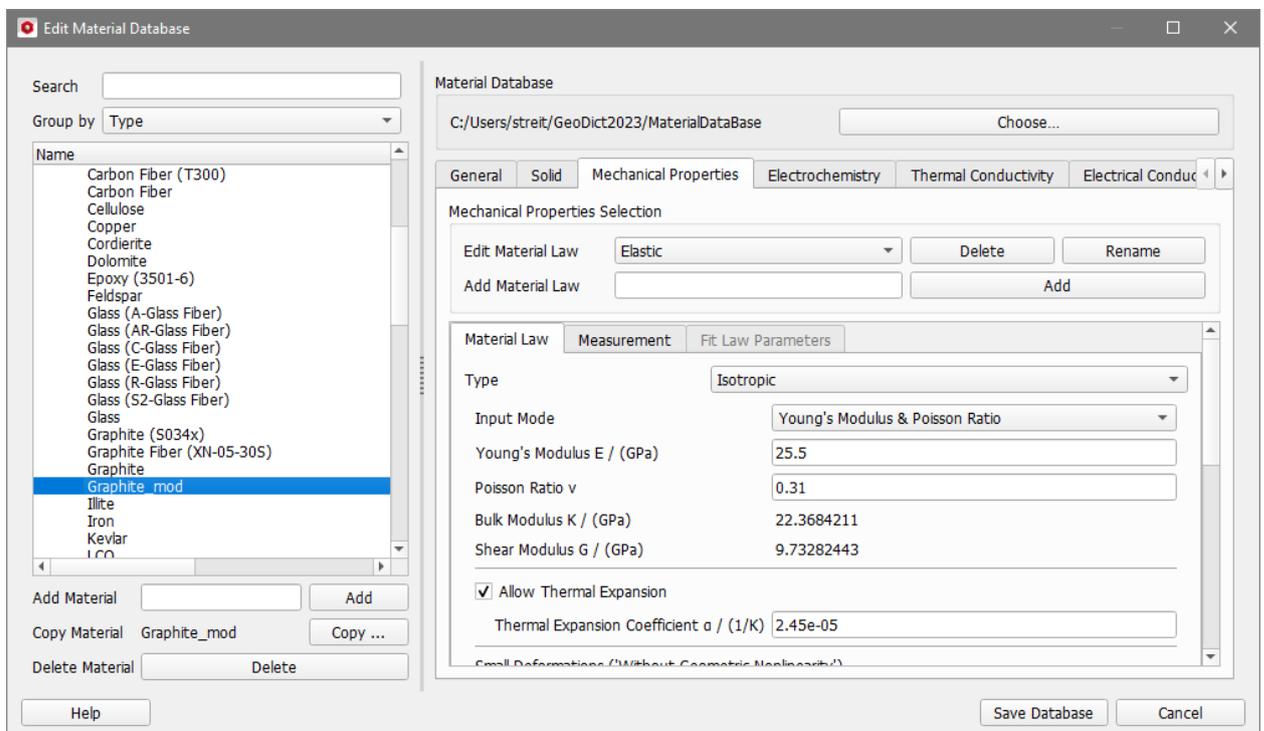
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To be able to use an active material in a degradation simulation with **BatteryDict-Degradation**, apart from the mandatory material parameters for a charging simulation (see [above](#)), the concentration expansion coefficient and the mechanical parameters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

In the **GeoDict** Material Database, select the material, e.g. Graphite in the example 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.

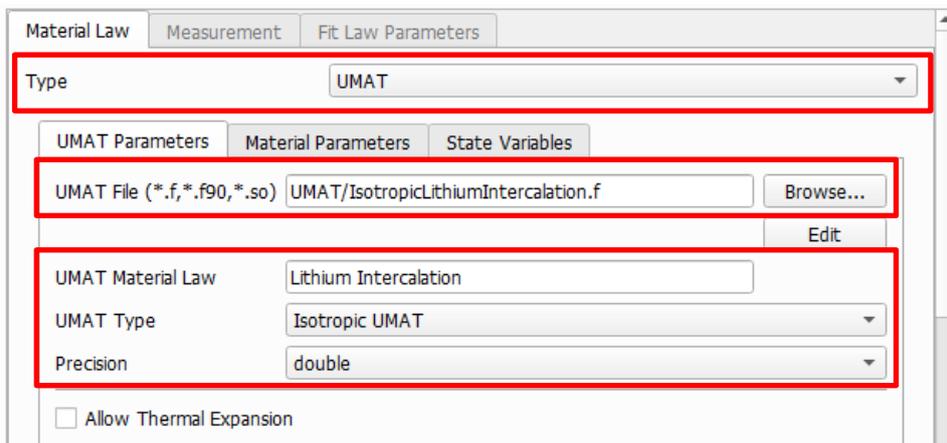


On the **Mechanical Properties** tab, add a new Material Law and call it e.g., **Lithium Intercalation**.

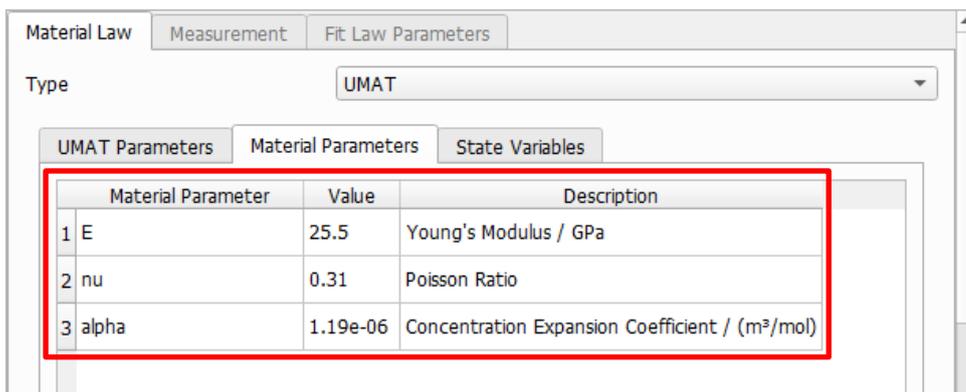


On the **Material Law** tab below, choose the Type **UMAT**. Two UMAT files for concentration dependent expansion are provided in the UMAT folder of your **GeoDict** installation. For isotropic expansion, select the file `IsotropicLithiumIntercalation.f`, for transversal isotropic expansion the file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

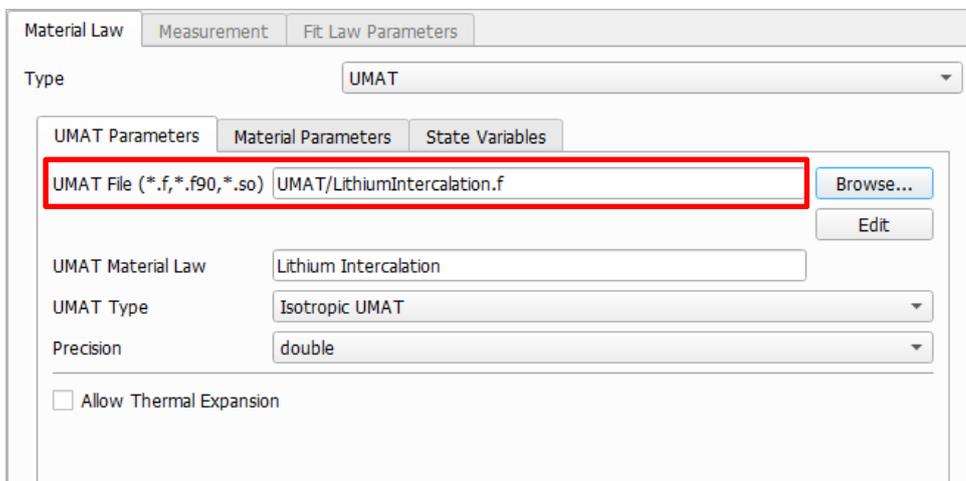
On the subtab **Material Parameters**, browse to the file you want to use. Set the appropriate **UMAT Type** and choose the **Precision** desired for the computation. We recommend using double precision.



On the subtab **Material Parameters**, define now **Young's Modulus**, **Poisson Ratio** and **Concentration Dependent Expansion Coefficient** for the isotropic case.



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 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

The [GeoDict Material Database](#) currently provides the materials Graphite, NMC333, and Silicone with these parameters.

For other materials of the battery cell (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, see page [60](#).

## 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 (see page [80](#)). The warnings help figuring out why the solver stopped and include:

1. not having enough RAM,
2. having very large particles with very low ionic diffusion at a very fast charge rate,
3. having chosen untested material parameters.

Regarding the second point above: 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 happen also, 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.

For the third reason of problems with the convergence of the solver, different tests have been carried out during the development of **BatteryDict** to identify material parameters that should lead to converging simulations.

### OVERLAPPING OCV CURVES FOR SEVERAL ACTIVE MATERIALS

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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.

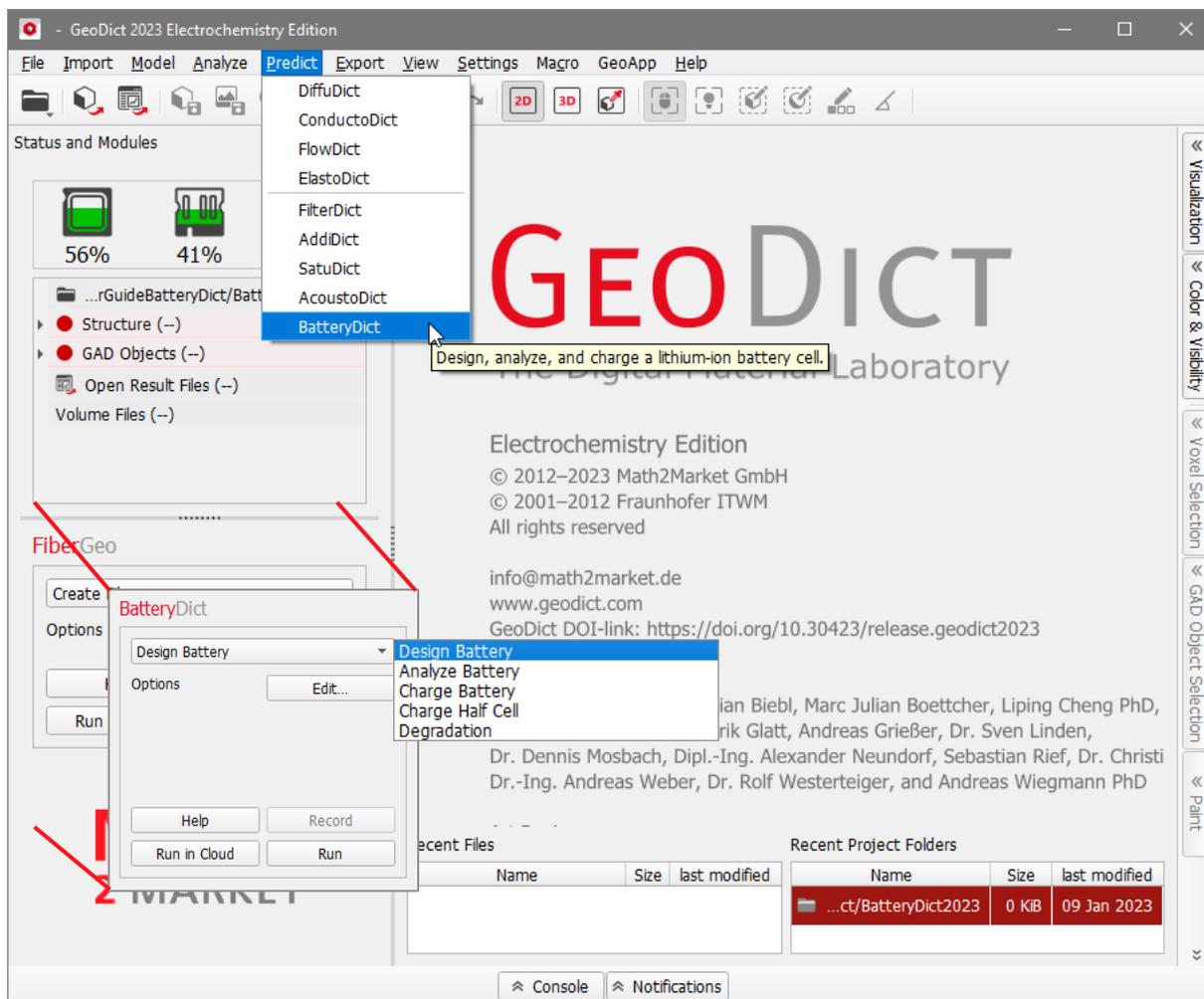
OCVs are the driving force in a battery that make lithium ions flow from materials with low OCV to materials with high OCV. If a battery is used in an electrical device and the two electrodes are conductively connected, ions flow from the negative electrode (low OCV) to the positive electrode (high OCV). 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** simulations always start from a state of equilibrium. 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.

## BATTERYDICT COMPUTATIONS

Start **BatteryDict** by selecting **Predict** → **BatteryDict** in the menu bar.



In the **BatteryDict** section, the pull-down menu includes the possibility to **Design** a **Battery**, to **Analyze** a **Battery**, to simulate the charging of a battery (**Charge Battery**) or a half-cell (**Charge Half Cell**), and to run a **Degradation** simulation.

Already in **GeoDict 2021**, the **BatteryDict** dialogs had been changed to better guide the user through the workflow of design, analyze, and charge batteries. It allows an easy change of material parameters, using materials from the **GeoDict** Material Database, and to choose the solver inside of the **Charge Battery** dialog.

In **GeoDict 2023**, the degradation simulation is now available as a command in **BatteryDict**, with a dialog like that of charging simulations.

Click **Run** to start the computation. Click **Run in Cloud** to run it in the KaleidoSim cloud, see the [High Performance Computing](#) handbook of the **GeoDict** User Guide for details.

## DESIGN BATTERY

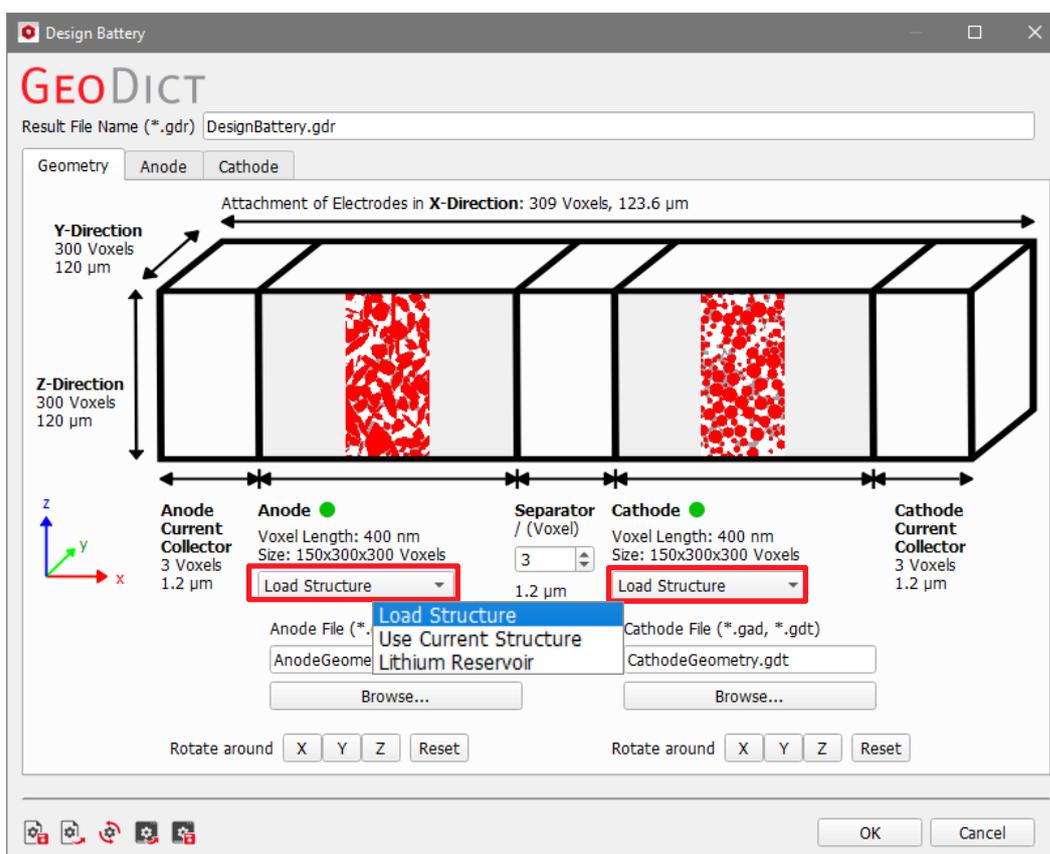
To design a battery, choose **Design Battery** from the pull-down menu and click **Edit...** to choose the options.

The **Design Battery** dialog opens, containing three tabs where to define the morphology of the battery (**Geometry** tab) and the constituent materials for anode and cathode.

## GEOMETRY

For both electrodes, either the current structure loaded in the **GeoDict** GUI can be used, a previously saved structure can be loaded, or the electrode can be modelled as a lithium reservoir.

On page 54, we show how to model a half cell structure to perform a half cell simulation with only one electrode modelled as a microstructure. Note, that since **GeoDict 2022**, it is not necessary anymore to create the geometry of the whole half-cell first. With the new functionality **Charge Half Cell** (see page 54), a half cell simulation can be started from the microstructure of a single electrode alone.

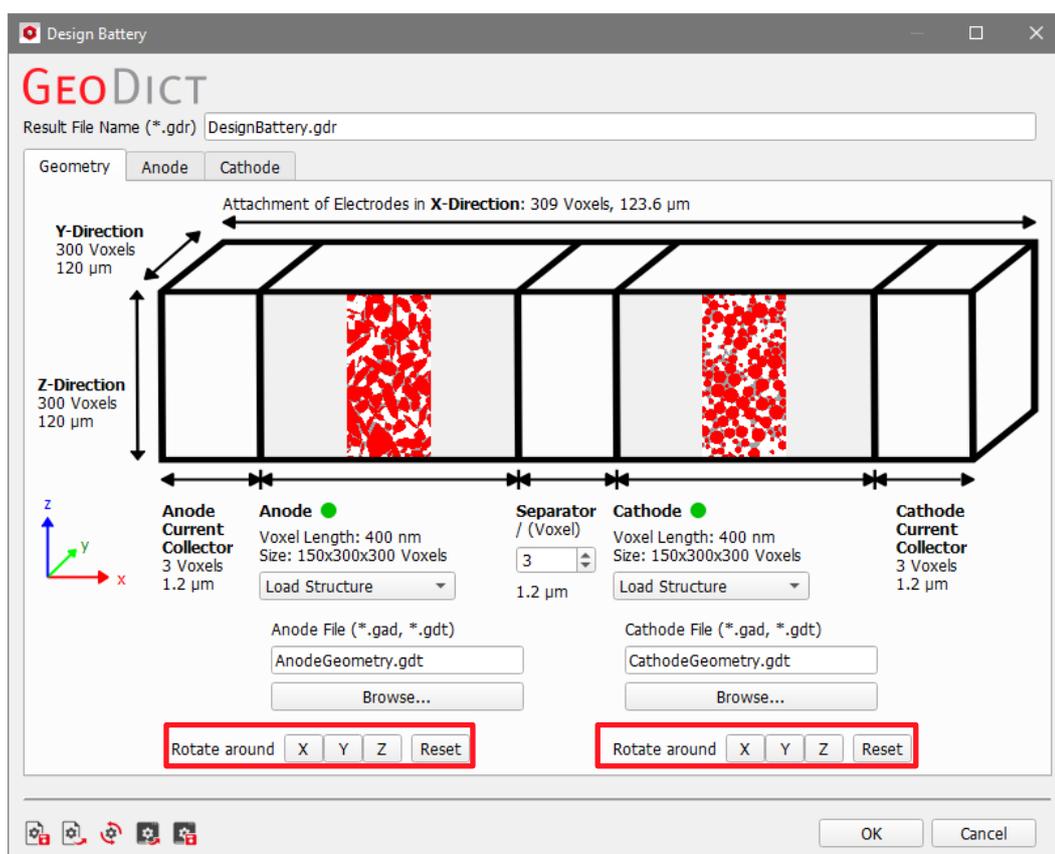


Choose **Load Structure** and use the **Browse...** buttons to select an input file for anode and cathode, in \*.gad or \*.gdt **GeoDict** formats. If the built-in default settings are used for the dialog, a default structure for anode and cathode from the BatteryDict/DesignBattery folder is loaded.

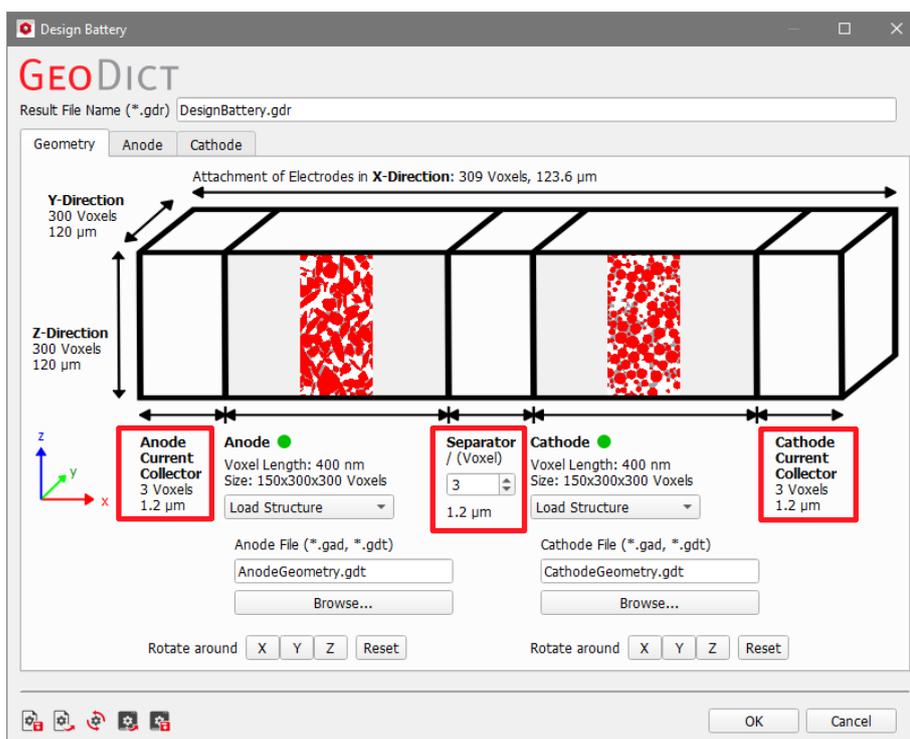
After selecting electrode files, a 2D representation of the anode and of the cathode appear in the dialog. For the example battery shown here, anode and cathode structure are created with the **GeoApps Bimodal Anode** and **Bimodal Cathode**. For details using this **GeoApps**, see the [GeoApp](#) handbook of the **GeoDict User Guide**.

- A red dot is visible for the anode and cathode, if no files are loaded at all.
- A yellow dot appears if a file is loaded but the dimensions or voxel length of the anode and the cathode do not match.
- 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.

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.



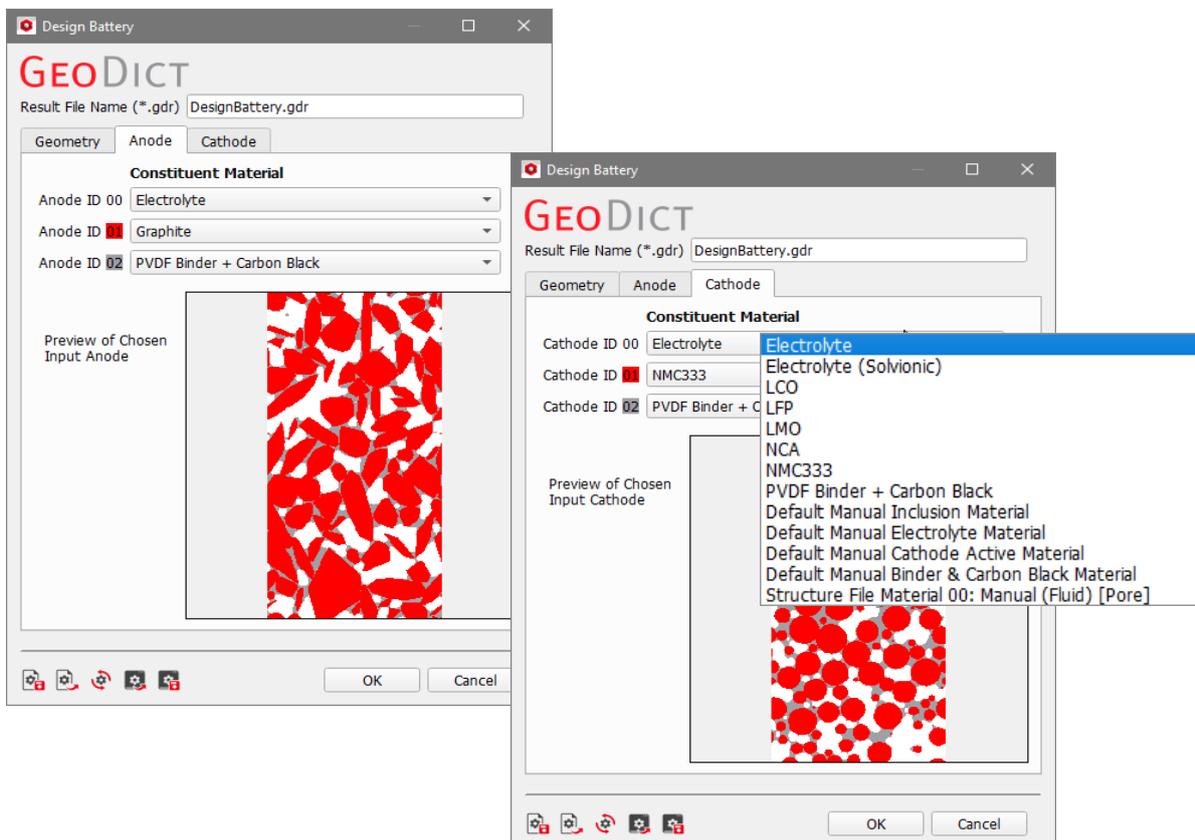
The **Rotate around X, Y and Z** buttons are used to rotate the structure 90° around the X, Y, or Z-axis. Click **Reset** to go back to the original orientation of anode and cathode in the battery structure.



The number of voxels of the separator can be defined in the GUI. The default is 3 voxels. 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, binder & carbon black, up to four different active materials per electrode, or inclusion). In the example shown here, both anode and cathode consist of 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**. Like this, no conduction is possible in this material, it has no potential, and does not contain lithium.

Click **OK** in the Design Battery dialog, to keep the parameters selected in memory, or **Cancel** to discard the parameters.

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

If the battery is created successfully, a result file with the default name DesignBattery.gdr is created in the selected project folder, as well as a structure file (\*.gdt) in the subfolder DesignBattery.

The Result Viewer of the result file opens automatically after the generation, showing the information of DesignBattery.gdr (see [Results of Design Battery](#) below).

## MORE FLEXIBLE GEOMETRIES

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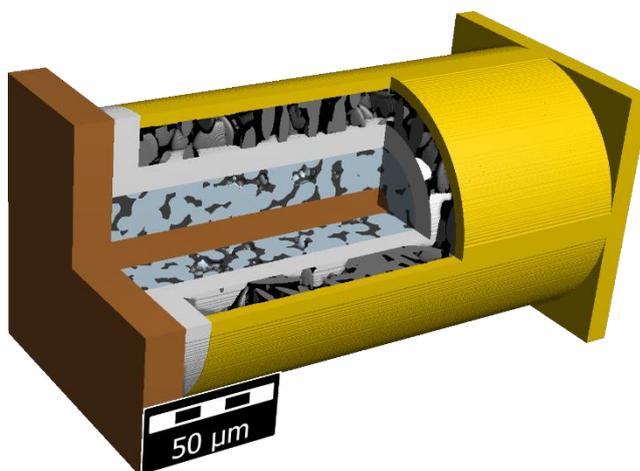
Since the **GeoDict** 2020 release, it is possible to use arbitrary battery geometries, not only cuboid ones, as shown in the **Geometry** on page [26](#).

Since **GeoDict** 2022, to use arbitrary geometries no additional expert setting is necessary for this anymore.

Regarding the current collectors of not cuboid geometries, it is necessary that they cover the whole surface of the structure in x-direction.

That is, 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.

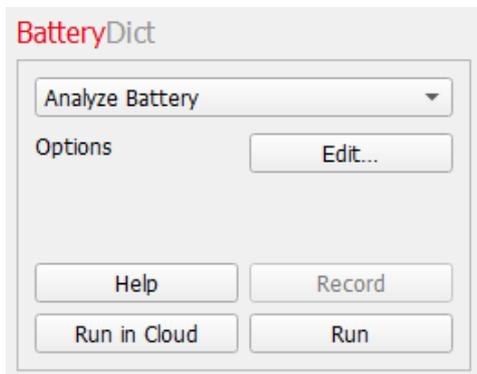
For geometries with circular cross sections, current collectors can be positioned like shown in the figure below.



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

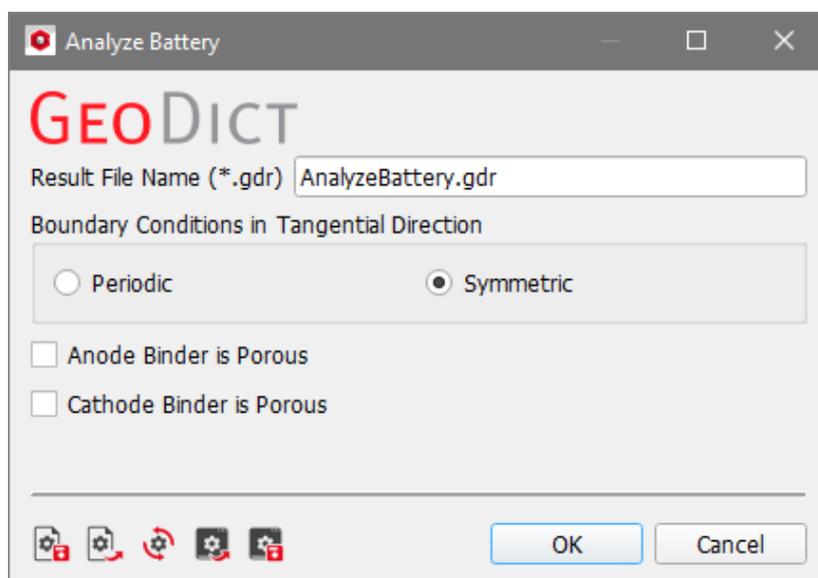
## ANALYZE BATTERY

To analyze the connection and volume of the different materials for the designed battery structure, choose **Analyze Battery** from the pull-down menu in the **BatteryDict** section.



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

First, define the result file name 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  $\text{Li}^+$  ions and electrons are reflected at the boundary in y- and z-direction.

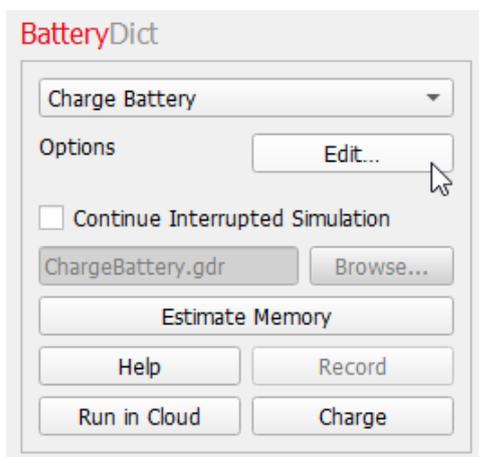
Boundary conditions are applied while identifying connected and unconnected material, since this depends on the continuation of the material in y- and z-direction. For a charging simulation, it can be chosen independent of the value selected here. Connected and unconnected material is identified again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

Check **Anode Binder is Porous** or/and **Cathode Binder is Porous** if the binder of one or both electrode(s) is a porous material with micropores that are filled with electrolyte and not resolved in the electrode structure.

Click **Run** in the **BatteryDict** section to start the analysis. If it is finished, the Result Viewer opens, see [Result of Analyze Battery](#) below.

## CHARGE BATTERY

To simulate the charging or discharging of a battery, choose **Charge Battery** from the pull-down menu in the **BatteryDict** section.

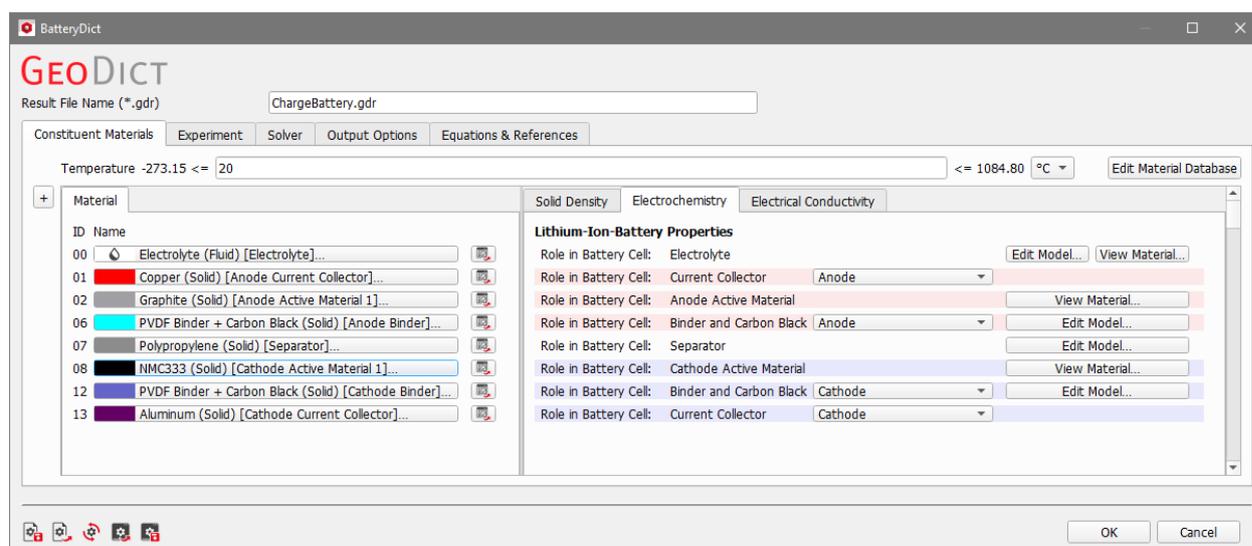


Then, click **Edit** to adjust the solver options.

The **BatteryDict** dialog opens, containing four tabs.

## 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. Because this temperature-dependence of the material parameters is not considered in the equations solved during charging or discharging, the temperature defined here needs to be consistent with the material properties defined for the materials below.

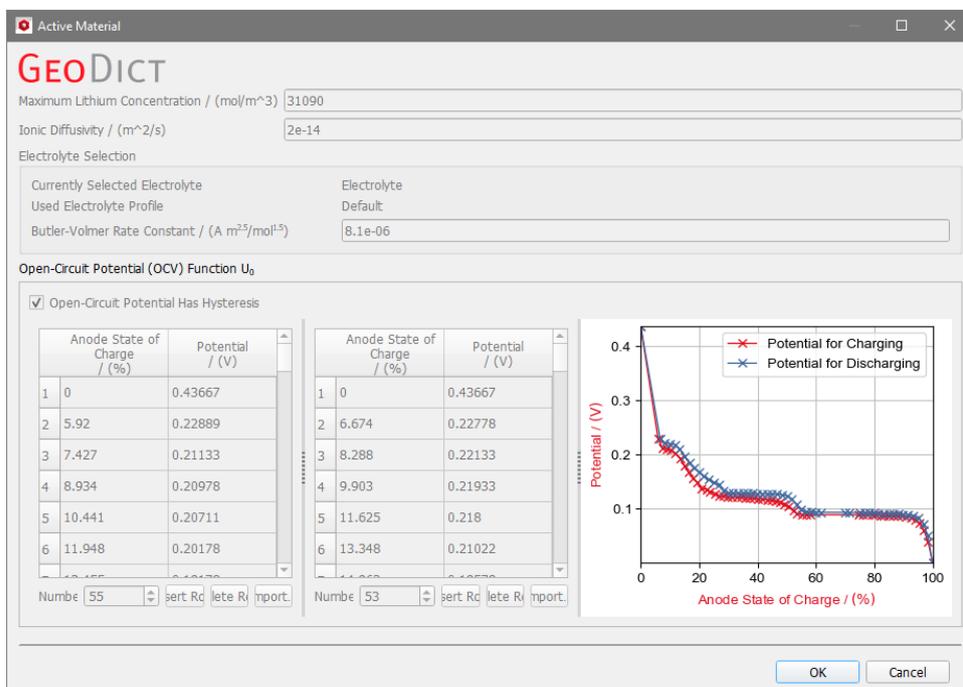
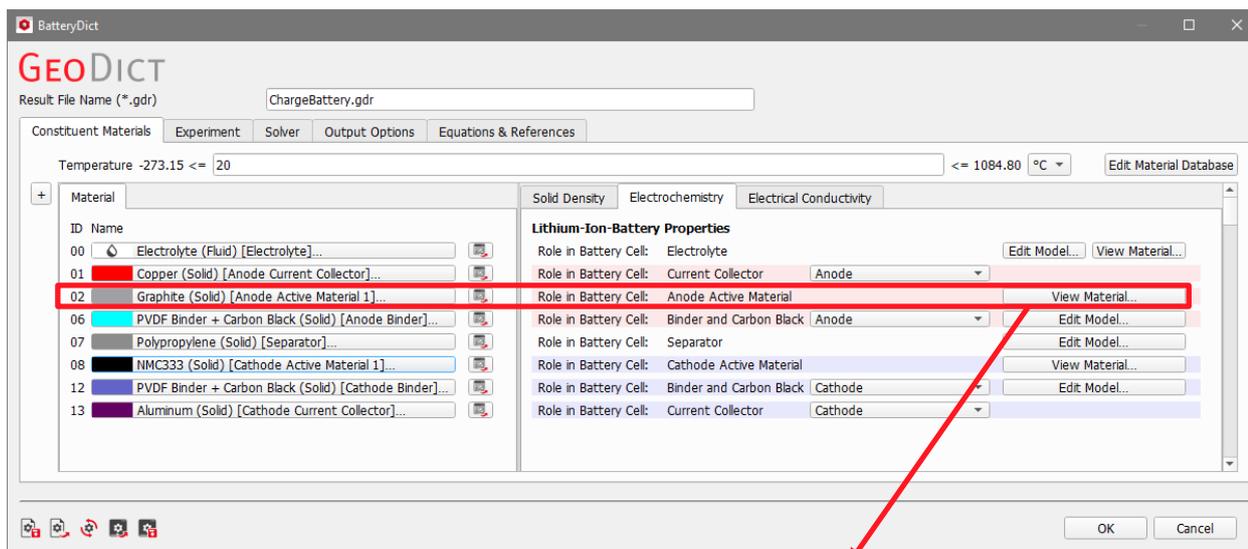
Material IDs of the structure and the assigned materials are listed on the left of the tab under **Material**.

Material properties are organized on three different subtabs on the right, **Solid Density**, **Electrochemistry** and **Electrical Conductivity**.

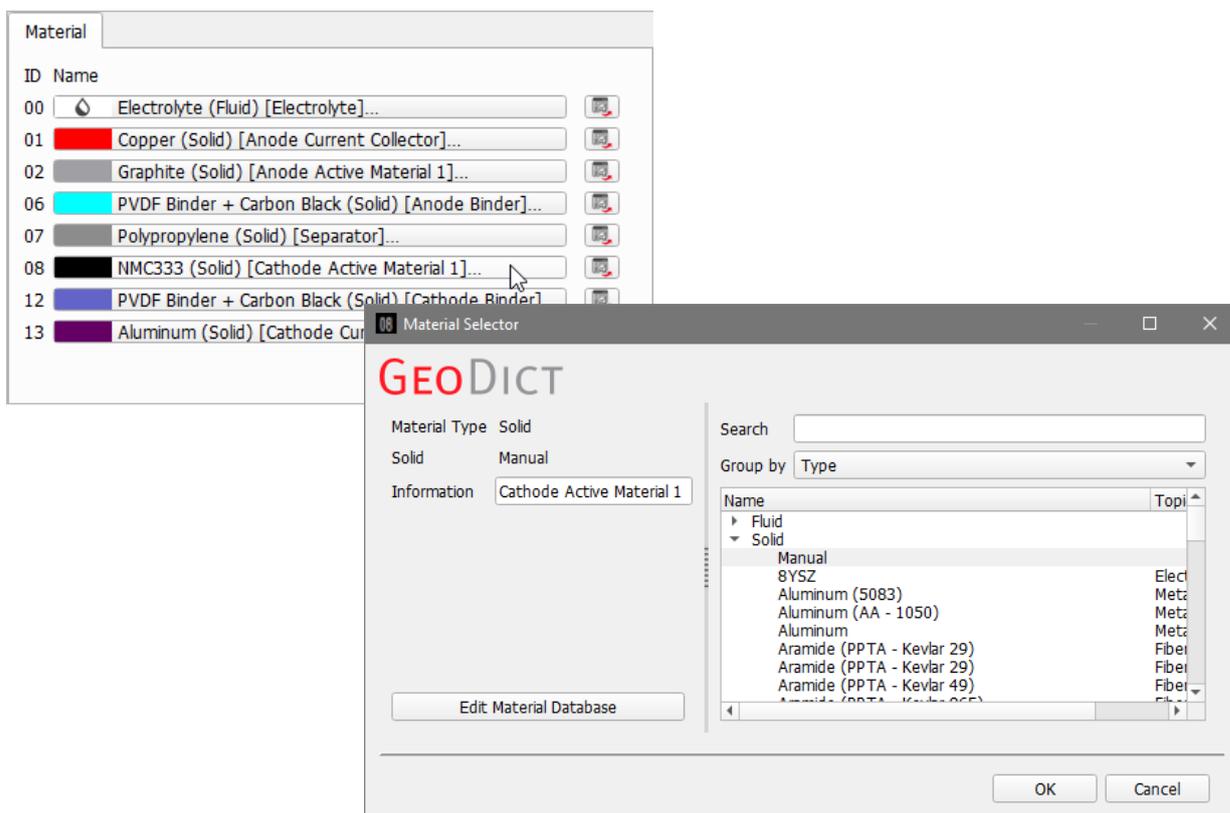
## Digital charging and discharging of Li-ion batteries

On 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.

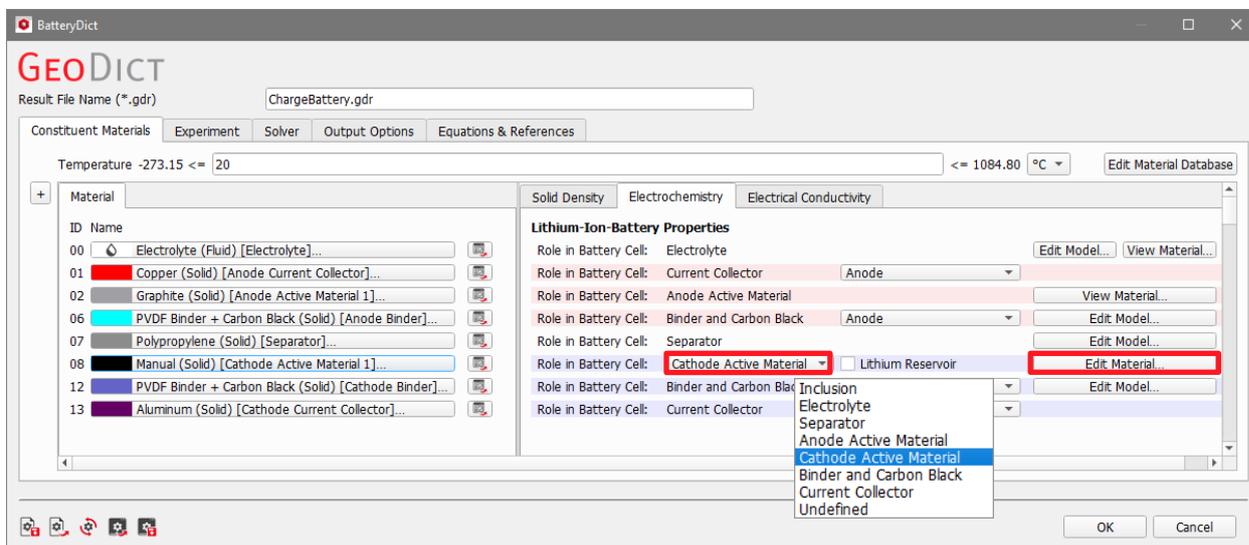
If a material from the **GeoDict** Material Database is selected for a Material ID (e.g. for ID 02 in the example shown), all parameters are set according to the database values. The electrochemical role of the material (here: Anode Active Material) is shown and the electrochemical parameters can be 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 and Electrical Conductivity are shown on the correspondent subtabs. For more details on the parameters displayed and selectable see [Parameter Dialogs section](#) below.



The assigned material 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.



Now, the electrochemical role of the material can be changed, and the electrochemical parameters can be modified.



The electrochemical roles Separator, Binder and Carbon Black for each electrode and Current Collector for each electrode, can each be selected only for one material in the structure.

The simulation cannot be started if one of the materials has the role Undefined. If one of the materials has no active role in the charging process, assign the electrochemical role Inclusion to it. No conduction is possible for a material defined as Inclusion, it has no potential, and does not contain lithium.

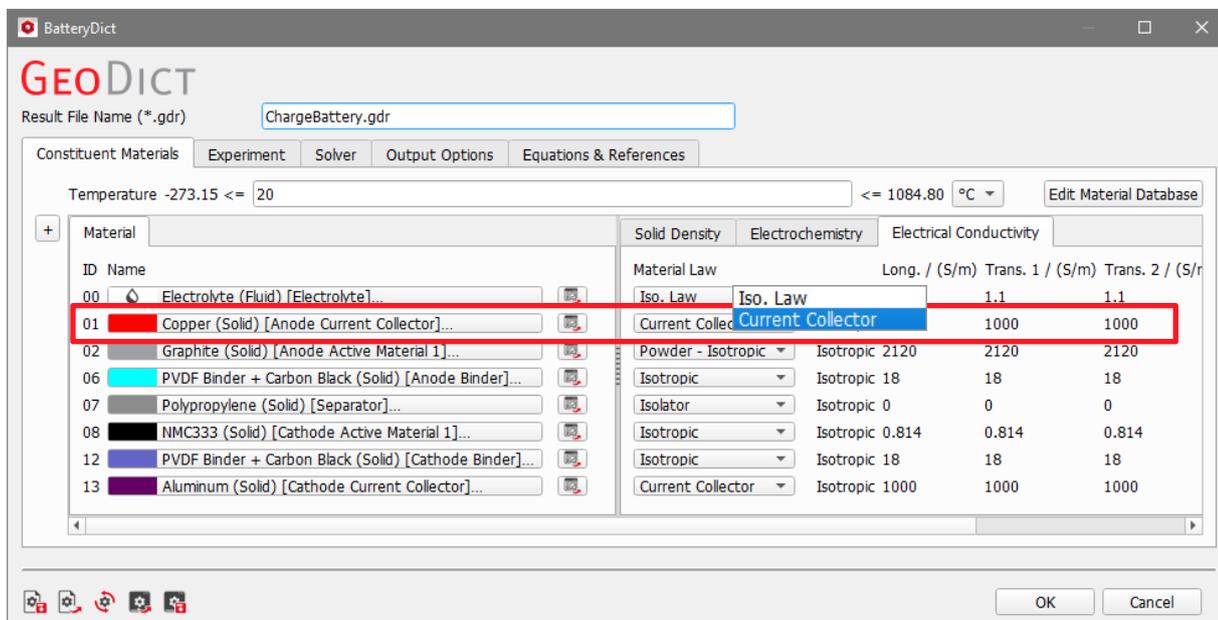
Clicking **Edit Material** opens the property dialog for active material or electrolyte for editing the values, **Edit Model** allows to change the binder and carbon black or separator model. See [Parameter Options Dialogs](#) section below for more details.

If the box **Lithium reservoir** is checked for a Cathode Active Material or an Anode Active Material, the **Edit Material** button allows to change the Butler-Volmer rate constant. The active material is then modelled 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 modelled as lithium reservoir. Note that the Lithium reservoir is modelled as a Manual material. Assigning lithium from the material database will not work to model a lithium reservoir in **BatteryDict**.

In the same way, on the other subtabs, the **Solid Density** and the **Electrical Conductivity** are shown (for materials from the Material Database) or can be selected (for Manual materials).

For numerical reasons, the electrical conductivity 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.

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 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.



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

Material

ID	Name
00	Electrolyte (Fluid) [Electrolyte]...
01	Copper (Solid) [Anode Current Collector]...
02	Graphite (Solid) [Anode Active Material 1]...
06	PVDF Binder + Carbon Black (Solid) [Anode Binder]...
07	Polypropylene (Solid) [Separator]...
08	NMC333 (Solid) [Cathode Active Material 1]...
12	PVDF Binder + Carbon Black (Solid) [Cathode Binder]...
13	Aluminum (Solid) [Cathode Current Collector]...

Report for Material with ID 08

Key	Unit	Value
Type		Solid
Name		NMC333
Information		Cathode Active Material 1
<ul style="list-style-type: none"> <li>SolidProperties                             <ul style="list-style-type: none"> <li>CurrentLaw</li> <li>NumberOfLaws</li> </ul> </li> <li>MaterialLaw1                             <ul style="list-style-type: none"> <li>Name</li> <li>Density</li> </ul> </li> <li>ElectricalConductivity                             <ul style="list-style-type: none"> <li>CurrentLaw</li> <li>NumberOfLaws</li> <li>MaterialLaw1                                     <ul style="list-style-type: none"> <li>Type</li> <li>Name</li> <li>Beta</li> </ul> </li> </ul> </li> <li>Electrochemistry                             <ul style="list-style-type: none"> <li>LiIonBattery                                     <ul style="list-style-type: none"> <li>BatteryMaterialType</li> <li>CathodeActiveMaterial   <ul style="list-style-type: none"> <li>IsLithiumReservoir</li> <li>MaxLiConcentration</li> <li>LiDiffusivity</li> <li>NumberOfElectrolytes</li> <li>Electrolyte1   <ul style="list-style-type: none"> <li>Name</li> <li>ButlerVolmerRate</li> </ul> </li> <li>OpenCircuitPotential   <ul style="list-style-type: none"> <li>HasHysteresis</li> <li>StateOfCharge</li> <li>Potential</li> </ul> </li> </ul> </li> </ul> </li> </ul> </li> </ul>		
		1
		1
		Bulk
	kg/m <sup>3</sup>	4700
		1
		1
		Isotropic
		Isotropic
	S/m	0.814
		CathodeActiveMaterial
		false
	mol/m <sup>3</sup>	35525
	m <sup>2</sup> /s	4.1e-14
		1
		Default
	A m <sup>-(2.5)</sup> /mol <sup>-(1.5)</sup>	2.4e-06
		false
	%	0, 2.368, 4.413, 6.243, 8.719, 1...
	V	4.69884, 4.63353, 4.57547, 4.52...

Close

## PARAMETER OPTIONS DIALOGS

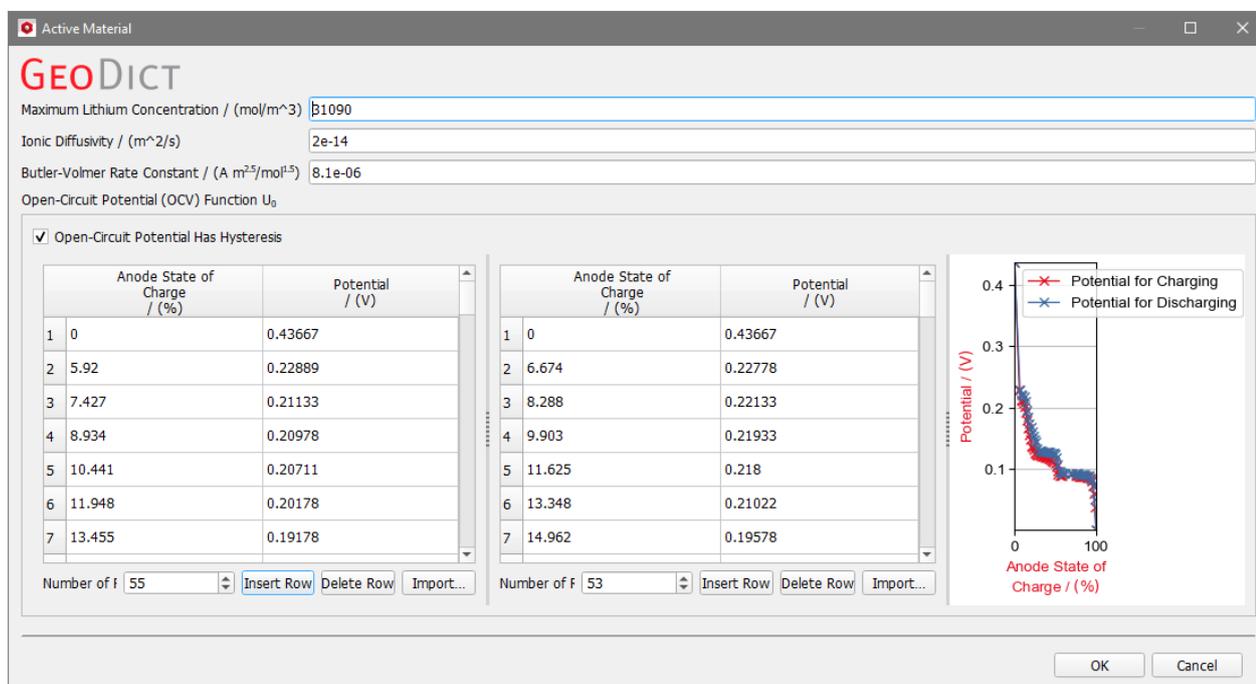
Parameter dialogs for active materials, binder and carbon black, separator and electrolyte are explained in the following. For an explanation of the meaning of the parameters, see [Simulation Parameters](#) above.

### ACTIVE MATERIAL PARAMETER DIALOG

For all active materials, the simulation parameters **Maximum Lithium Concentration**, **Ionic Diffusivity**, **Butler-Volmer Rate Constant**, and **Open-Circuit Potential Function** (OCV) need to be defined.

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.



Parameters of the material from the Material Database, that was last selected for the ID, are shown, and can be modified.

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 state of charge in percent, and the second column shows the related potential.

The chosen function is displayed as **Potential** over **Cathode/Anode State of Charge** in the plot on the right of the table.

If the Open-Circuit Potential Function is different for charging and discharging, check the box **Open-Circuit Potential Has Hysteresis** and define one OCV function for charging and a different one for discharging. Note that in **BatteryDict** the charging OCV curve is used for lithiation of the active material and the discharging OCV curve is used for delithiation of the active material.

In case the active material of an electrode is defined as Lithium reservoir, with **Edit Model ...**, the Butler-Volmer Rate Constant can be defined.



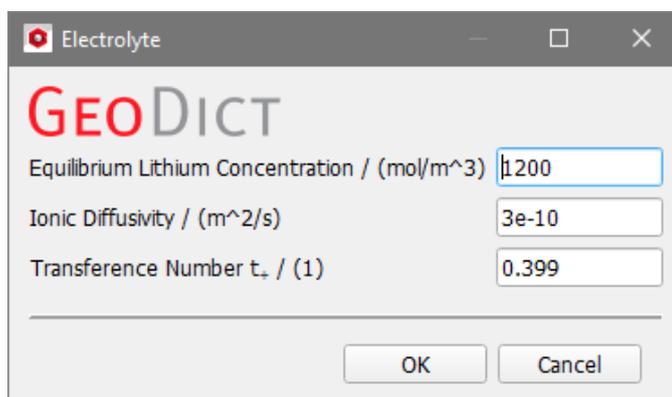
No other parameters need to be set for a lithium reservoir, since it will be considered as a never-ending reservoir of lithium, not limiting the battery performance.

### ELECTROLYTE PARAMETER DIALOG

For the electrolyte, the **Equilibrium Lithium Concentration**, **Ionic Diffusivity**, and **Transference Number** need to be defined (see [Simulation Parameters](#) above).

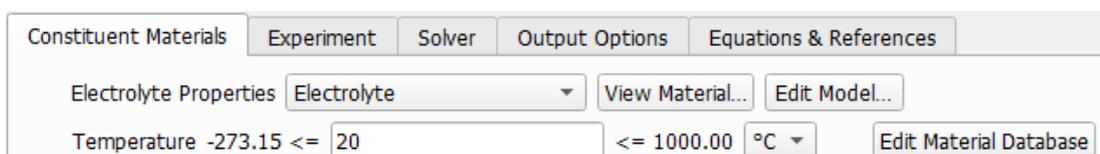
If a material from the GeoDict Material Database is selected for the electrolyte, values are shown in the **Electrolyte** dialog, but cannot be changed.

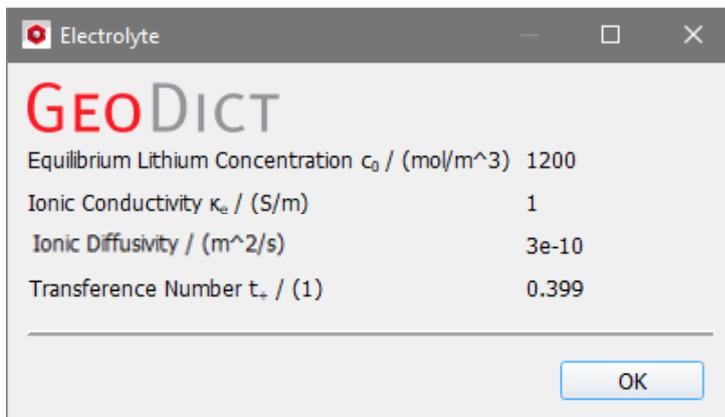
Set the electrolyte to **Manual (Fluid)** or **Manual (Solid)** and click **Edit Material** to modify the parameters.



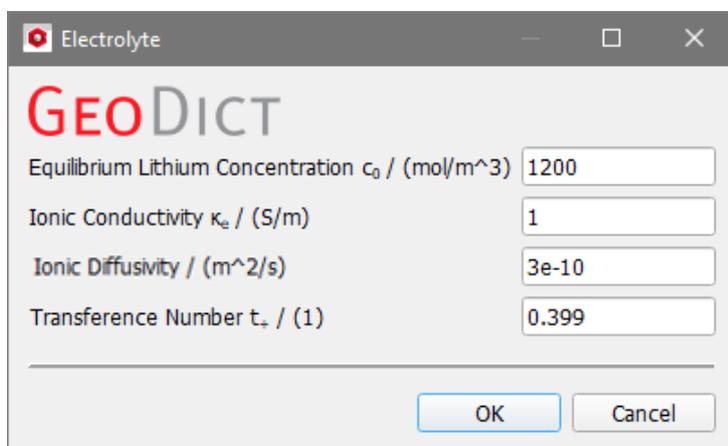
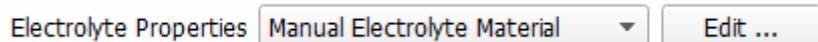
The ionic conductivity of the electrolyte is the value for the electrical conductivity defined on the **Electrical Conductivity** tab. In the case of electrolyte materials, the electrical conductivity corresponds to the ionic conductivity, since they have no electronic conductivity.

If no material ID with material defined as electrolyte exists, the electrolyte can be defined in the upper part of the Constituent Materials tab. In this case, no electrolyte exists in both electrodes, but only in the separator.



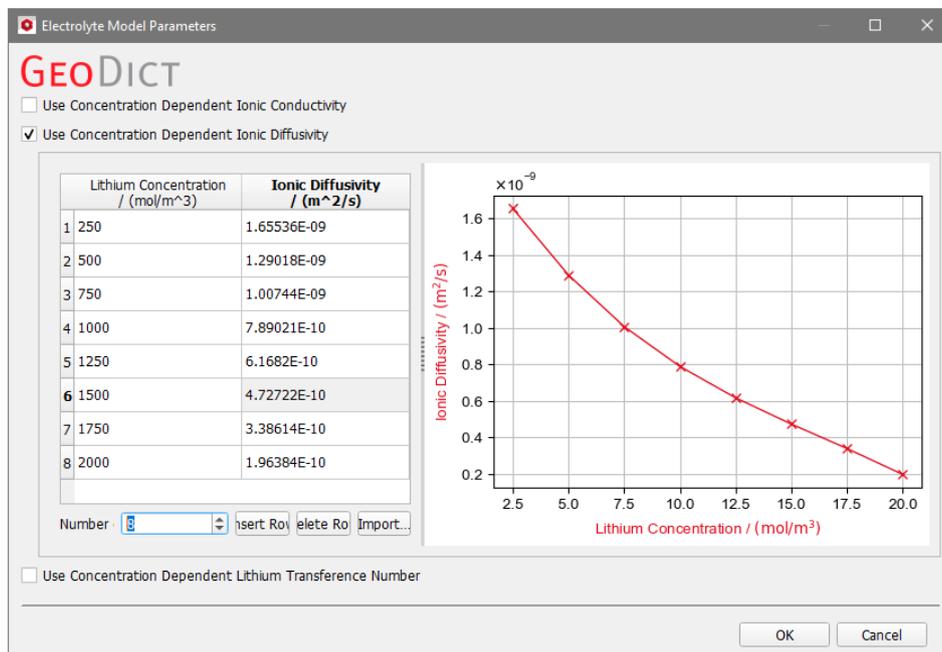


In this case, the ionic conductivity is shown additionally in the Electrolyte dialog, and can be set here, like the other parameters, if Manual Electrolyte Material is selected.



In GeoDict 2023, electrolyte parameters can be modelled depending on the lithium concentration.

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



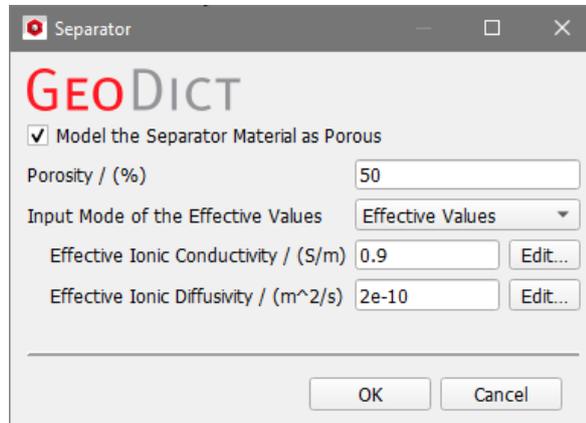
Note that concentration dependent parameters are not yet available for the LIR solver. Therefore, if the LIR solver is selected, you will find an exclamation mark on a yellow triangle on the **Edit Model** button.  Edit Model...

## SEPARATOR PARAMETER DIALOG

If the box **Model the Separator Material as Porous** is unchecked, the separator gets the same properties as the electrolyte. Since it is filled with electrolyte, this assumption is reasonable if the properties are not influenced by the microstructure of the separator.

If this assumption does not hold, 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 in this case necessary.

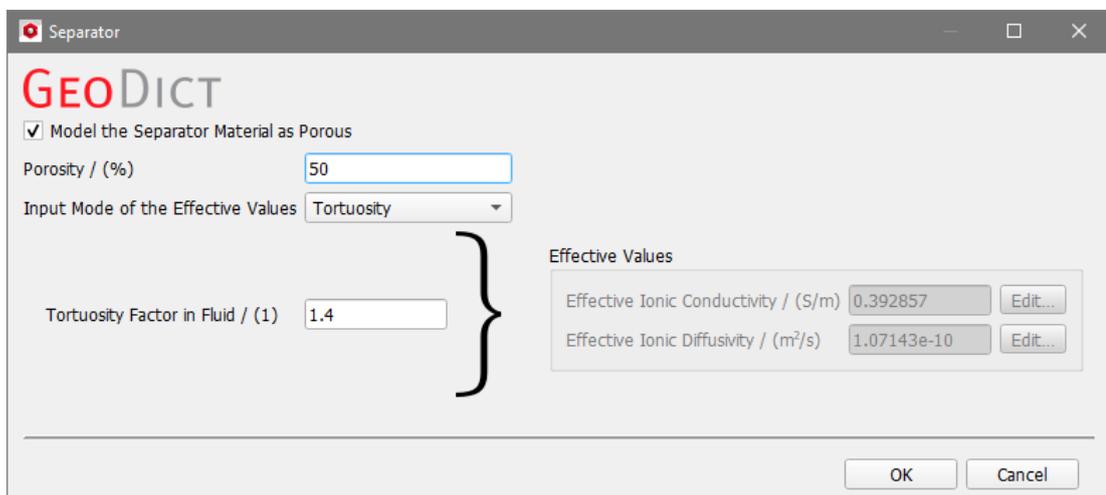
To define the effective values directly, choose **Effective Values** as **Input Mode of the Effective Values**.



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

$$D_{eff} = \frac{\varepsilon}{\kappa_{fluid}} \cdot D_0$$

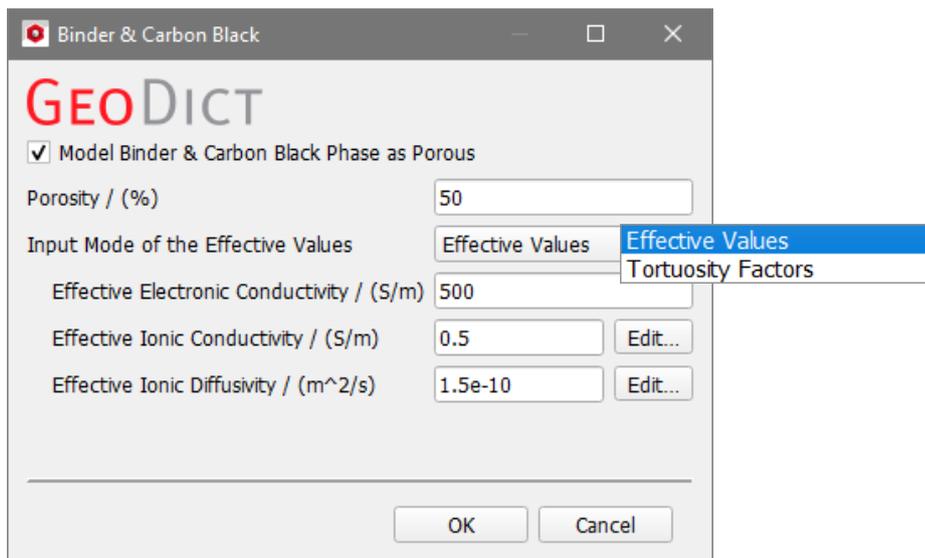
where  $\varepsilon$  is the porosity,  $\kappa_{fluid}$  the tortuosity factor in the fluid, and  $D_0$  the diffusivity of the electrolyte (see also the [GeoApp handbook of the User Guide](#) in the section Compute Tortuosity).



**BINDER & CARBON BLACK PARAMETER DIALOG**

If the binder is modelled as solid material, leave the box **Model Binder & Carbon Black Phase as Porous** unchecked. In this case, only the electronic conductivity of the binder and carbon black material is used for the simulation. This value is defined by the electrical conductivity on the **Electrical Conductivity** tab. For binder and carbon black material, with no ionic conductivity, electrical and electronic conductivity are equivalent.

To model binder and carbon black with unresolved electrolyte pores in the simulation, check **Model Binder & Carbon Black Phase as Porous**. In this case, define the **Porosity** of the binder and carbon black 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**:

- Select **Effective Values** to define the properties directly.
- Or 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. They cannot be changed there.

The effective electronic conductivity  $\sigma_{eff}$  is calculated by the equation

$$\sigma_{eff} = \frac{1 - \varepsilon}{\kappa_{solid}} \cdot \sigma_0$$

where  $\varepsilon$  is the porosity,  $\kappa_{solid}$  the tortuosity factor in the Solid, and  $\sigma_0$  the electronic conductivity of the (non-porous) Binder & Carbon Black 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 [GeoApp](#) handbook of the User Guide in the section *Compute Tortuosity*.

Binder & Carbon Black

# GEO DICT

Model Binder & Carbon Black Phase as Porous

Porosity / (%)

Input Mode of the Effective Values

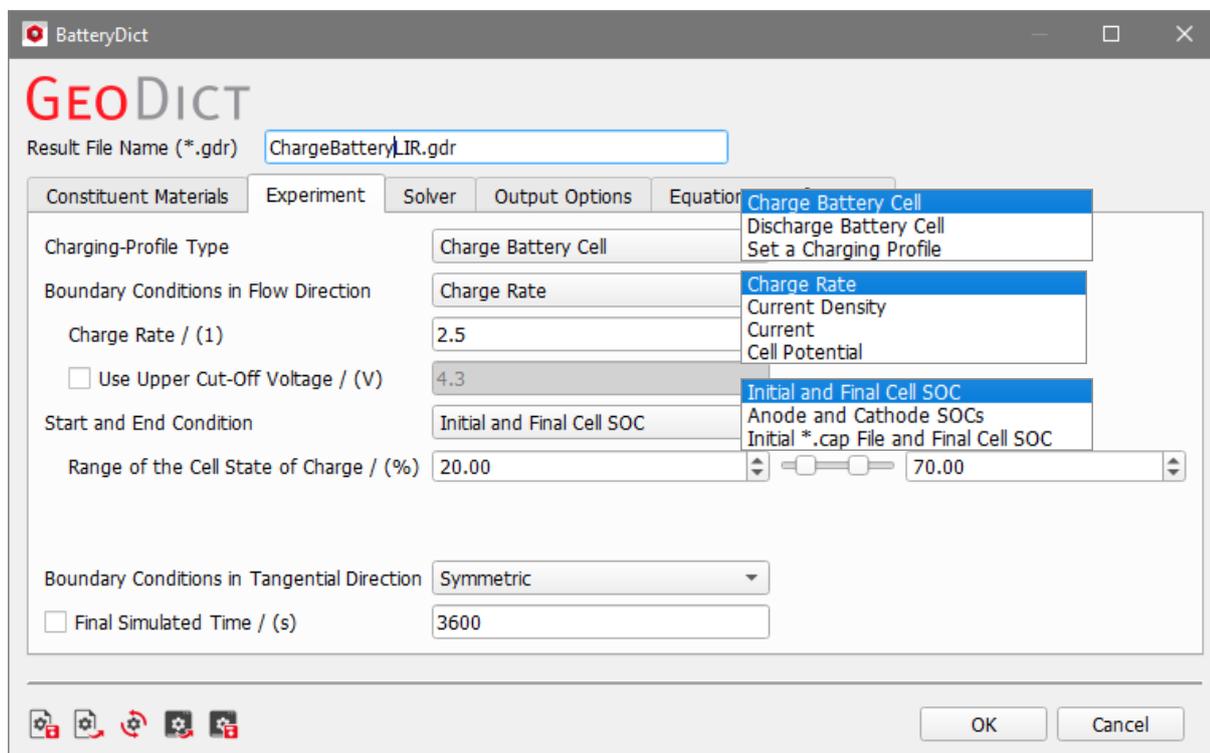
Tortuosity Factor in Solid / (1)	<input type="text" value="1.4"/>	}
Tortuosity Factor in Fluid / (1)	<input type="text" value="1.4"/>	

**Effective Values**

Effective Electronic Conductivity / (S/m)	<input type="text" value="6.42857"/>	<input type="button" value="Edit..."/>
Effective Ionic Conductivity / (S/m)	<input type="text" value="0.392857"/>	<input type="button" value="Edit..."/>
Effective Ionic Diffusivity / (m <sup>2</sup> /s)	<input type="text" value="1.07143e-10"/>	<input type="button" value="Edit..."/>

## EXPERIMENT

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



From the pull-down menu **Charging Profile Type**, select to simulate the charging or discharging of the battery or to set a charging profile. Here, a charging simulation is chosen. Charging profiles will be explained below, see page [44](#).

The **Boundary Conditions in Flow Direction** can be specified by a **Charge Rate**, a **Charge Density**, by defining the **Current** in Ampère (A) or by defining the **Cell Potential**.

With a **Charge Rate** defined, the applied current is related to the cells capacity 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 loaded 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 ½ hour.

Defining the **Current** or the **Current Density** instead means that the applied current (in A) or the current density (in A/m<sup>2</sup>) is defined directly.

If **Cell Potential** is selected, the voltage is kept at a constant value during the simulation, and the current is a time-dependent value instead.

Check **Use Upper Cut-Off Voltage** to limit the voltage in a simulation with defined charge rate, current, or current density. The voltage will not rise above this limit. I.e., if the maximum voltage is reached, the charging will not continue with the charge rate, current, or current density defined above, but with a smaller one.

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

- as percentage of the state of charge (SOC, see [State of Charge](#) above) of the whole cell

Start and End Condition: Initial and Final Cell SOC

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

- for the anode SOC and cathode SOC individually, or

State-of-Charge Input Mode: Anode and Cathode SOC's

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

Range of the Cathode State of Charge / (%): 30.00 to 75.00

- by selecting an initial .cap file from a previous BatteryDict simulation and defining a final SOC.

This option is especially useful for simulating a charging or discharging process,

Start and End Condition: Initial \*.cap File and Final Cell SOC

Initial \*.cap File (\*.cap): ChargeBattery/CAPs/Cell\_1.cap

Final Cell SOC / (%): 70

starting from a non-equilibrium condition after a previous discharging or charging simulation.

Note that 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 page [7](#).

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

For periodic boundary conditions, the structure is assumed to repeat periodically in y- and z-direction and for symmetric boundary conditions, the Li<sup>+</sup> ions and electrons are reflected at the boundary in y- and z-direction. Connected and unconnected parts of the active materials and of the electrolyte are dependent on the boundary conditions, and are, therefore, identified when the simulation is started.

Boundary Conditions in Tangential Direction: Symmetric

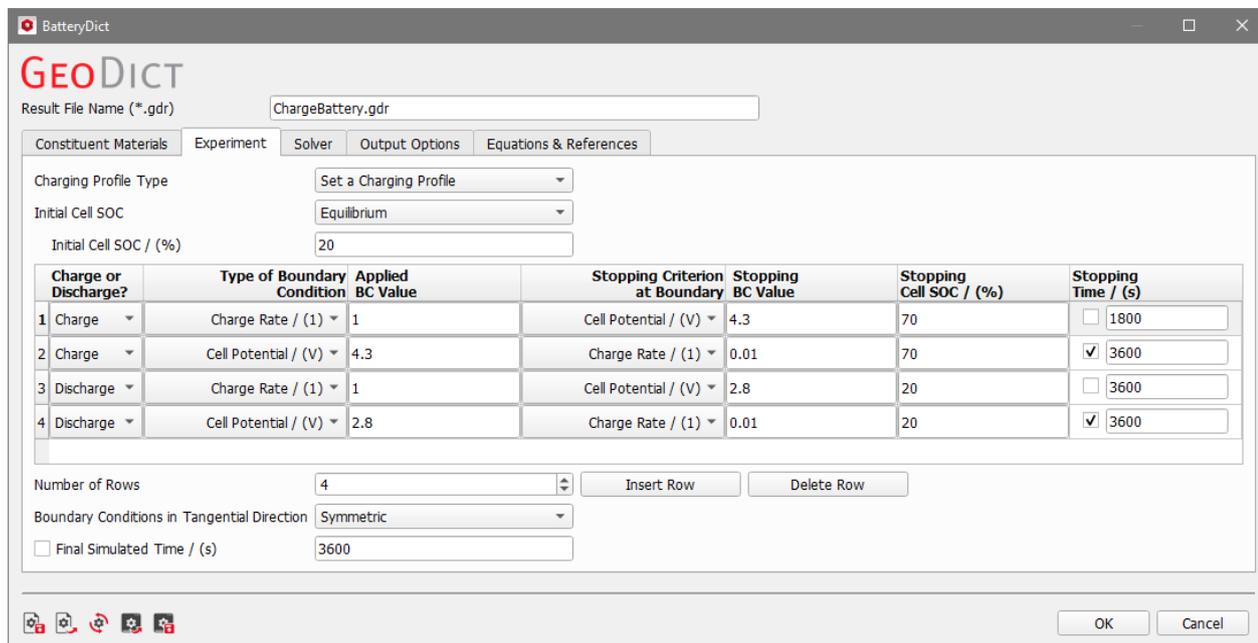
Final Simulated Time / (s): 3600

Checking **Final Simulated Time**, the total time that the battery will be charged can be defined. The simulation ends if the charging process exceeds the **Final Simulated Time** even if the final state of charge for the simulation is not reached. Note that the **Final Simulated Time** is not the time that the solver is given for its computation, but it is the time, the simulated battery is given for charging or discharging.

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 **Final Simulated Time** is set to 600 seconds (10 min), then in this example, the battery will only be charged from 20% to 36.67% state-of-charge.

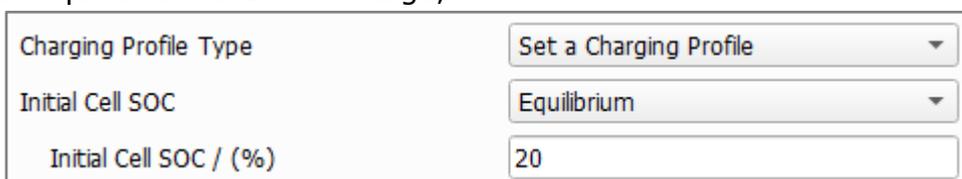
**DEFINE CHARGING PROFILES**

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



If **Set a Charging Profile** is selected as **Charging Profile Type**, the starting point for the first simulation can be defined

- as an equilibrium state of charge,



- or, by selecting a .cap file of a previous simulation.



The starting point for the following simulations 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. Select, if the battery is charged or discharged, the type of boundary condition and the corresponding value for the boundary condition, in the same way as for simple charging simulations, see page 42. The same options for the boundary condition (Charge Rate, Current Density, Current, and Cell Potential) are available.

Next, the stopping criterion for the selected boundary condition is chosen for each simulation step. The available options depend on the type of boundary condition (BC). If Charge Rate, Current Density, or Current is selected as BC, only Cell Potential is

possible as stopping criterion. For Cell Potential as BC, the Stopping Criterion can be chosen between Charge Rate, Current Density, and Current.

	Charge or Discharge?	Type of Boundary Condition	Applied BC Value	Stopping Criterion at Boundary	Stopping BC Value	Stopping Cell SOC / (%)	Stopping Time / (s)
1	Charge ▾	Charge Rate / (1) ▾	1	Cell Potential / (V) ▾	4.3	70	<input type="checkbox"/> 1800
2	Charge ▾	Cell Potential / (V) ▾	4.3	Charge Rate / (1) ▾	0.01	70	<input checked="" type="checkbox"/> 3600
3	Discharge ▾	Charge Rate / (1) ▾	1	Cell Potential / (V) ▾	2.8	20	<input type="checkbox"/> 3600
4	Discharge ▾	Cell Potential / (V) ▾	2.8	Charge Rate / (1) ▾	0.01	20	<input checked="" type="checkbox"/> 3600

Number of Rows

Boundary Conditions in Tangential Direction

Final Simulated Time / (s)

Enter the **Stopping BC Value** for the **Stopping Criterion**, a stopping state-of-charge for the whole cell (**Stopping Cell SOC / %**) and (optionally) a stopping time. For each simulation step, the computation will end, if the first one of the stopping criteria is reached. The next simulation step will continue from this state.

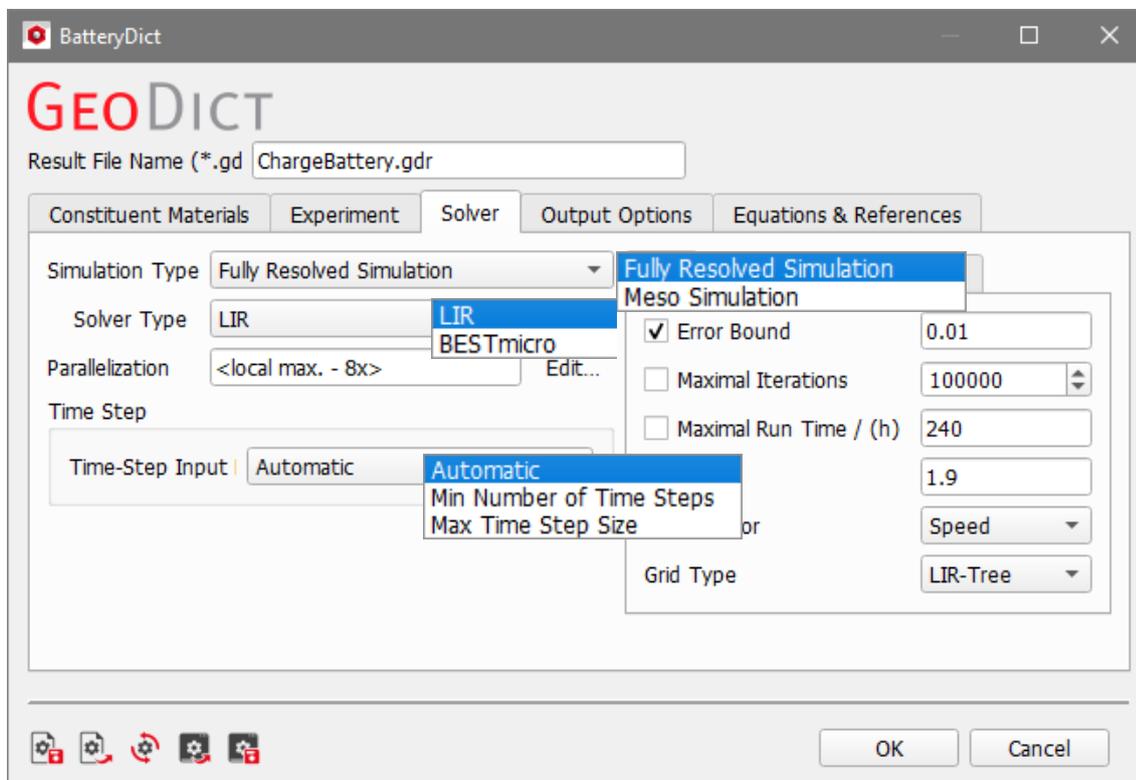
## SOLVER

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

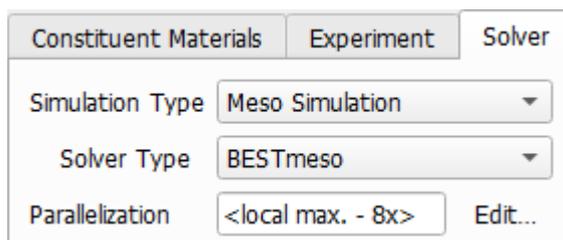
Select the **Simulation Type Fully Resolved Simulation** or **Meso Simulation**.

The fully resolved simulation 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 meso simulation is much faster than the fully resolved simulation. It uses a simplified model (an advanced 1D-Newman-model) that is created from the given battery 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.

For a **Fully Resolved Simulation**, the **Solver Type LIR** or **BESTmicro** can be selected.



For **Meso Simulation**, the **BESTmeso** solver is available.



Dependent on the choice of simulation and solver, the parameters for the computation need to be defined.

### FULLY RESOLVED SIMULATION - LIR SOLVER

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

Stopping criteria **Error Bound**, **Maximal Iterations**, and **Maximal Run Time** can be selected. The stopping criteria **Error Bound** stops the solver if the relative difference between computed and predicted solution is smaller than the error bound defined.

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

The balance between stable and fast simulation is managed for the LIR solver through the **Relaxation** value, that must be positive and should not be larger than 2: For a relaxation value smaller than 1, the simulation is more stable. For a value larger than 1 it is faster.

The LIR solver can **Optimize for** speed or memory.

- If **Speed** is chosen, the solver constructs additional optimization structures. The runtime is decreased but it requires more memory compared to the **Memory** option.
- If **Memory** is chosen, the runtime is increased but the solver requires less memory.

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 tree 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.

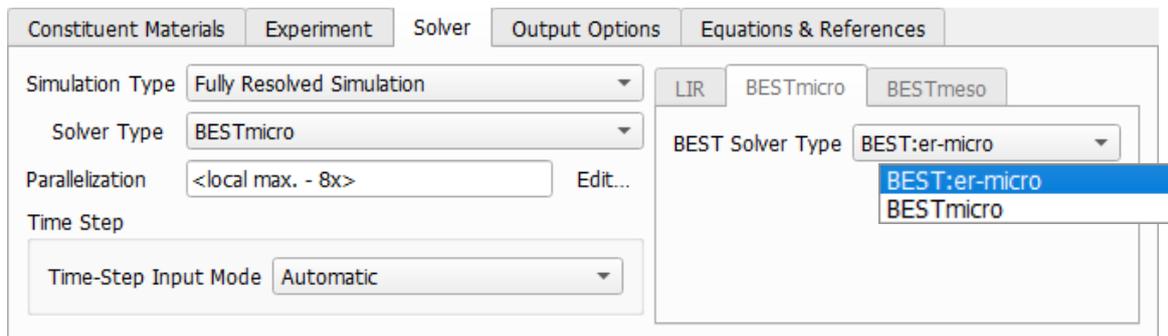
### FULLY RESOLVED SIMULATION - BESTMICRO SOLVER

The BESTmicro solver uses algebraic multigrid methods to solve the system of partial differential equations of the battery charging process. Two implementations are available for the BESTmicro solver from the Battery and Electrochemistry Simulation Tools of Fraunhofer ITWM:

## Digital charging and discharging of Li-ion batteries

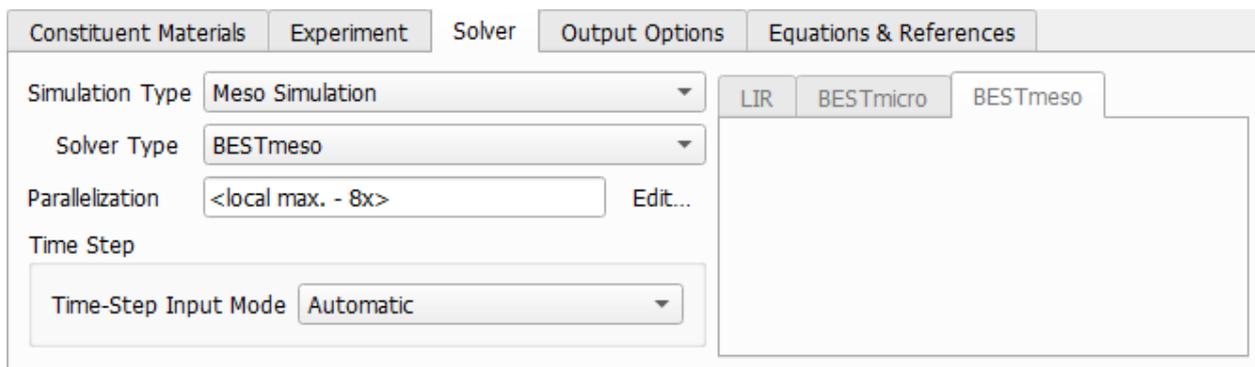
- **BESTmicro**: Implementation of BESTmicro solver available in GeoDict since GeoDict 2018. This implementation is very robust, with more than a decade of experience. However, it needs a lot of memory.
- **BEST:er-micro**: Reimplementation of BESTmicro, newly available in GeoDict 2023. It is faster than BESTmicro and needs less memory.

For both implementations, apart from the parallelization and the Time-Step Input Mode, no additional solver options need to be defined on the panel on the right for this solver.



## MESO SIMULATION – BESTMESO SOLVER

For the BESTmeso solver, only the parallelization and the Time-Step Input Mode need to be chosen, no further solver options need to be defined.



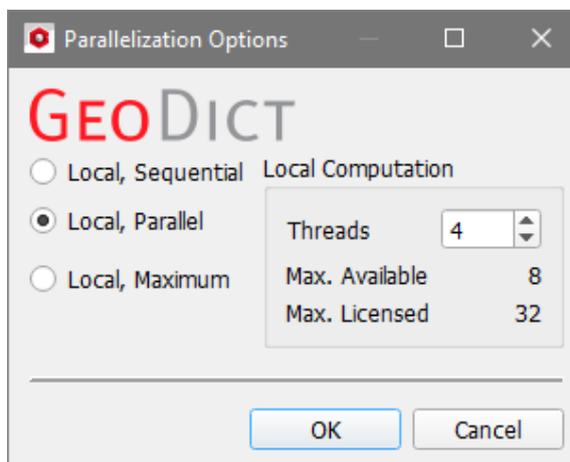
## PARALLELIZATION AND TIME-STEP

The **Parallelization Options** dialog box opens when clicking the **Edit ...** button, to choose between **Local, Sequential**, **Local, Parallel**, or **Local, Maximum**.

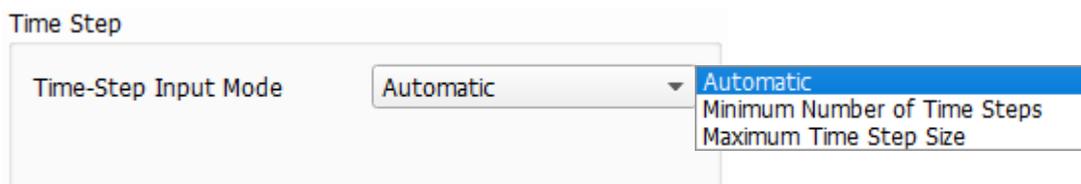
If **Local, Maximum** is selected, the maximum number of parallel processes is used. The maximum number depends on the available hardware and on the maximum number of processes licensed.

If **Local, Parallel** is selected, the number of threads can be selected. The maximum thread number available and licensed is shown.

With **Local, Sequential**, only one thread is used and no parallel computation is done.



Finally, 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 (see page [77](#)). 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, 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.

- Choosing **Automatic**, the solver selects the time-step size without restrictions of the user.
- 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 of the **GeoDict** result file (\*.gdr file), created for the charging simulation, under the key **TimeDependentValues:TimeStep**. If a new battery state is found, the solver computes the Cell-SOC of the just found battery state via: Cell-SOC step = time step \* charge rate / (1 hour). 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 = 5
- Time Step Size = 2.5 s
- Cell-SOC step =  $2.5 \text{ s} * 5 / (1 \text{ h}) = 2.5 \text{ s} * 5 / (3600 \text{ s}) = 0.00347 = 0.347 \%$

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 cell-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 under the keys **TimeDependentValues:CellStateOfCharge** and **TimeDependentValues:Time**, respectively (see page [79](#)).

For simple simulations (charge rate  $\leq 1$ , 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 Cell-SOC step is a constant value.

However, for more complex simulations (charge rate  $\geq 10$ , 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.

### PARALLELIZATION BENCHMARK RESULTS

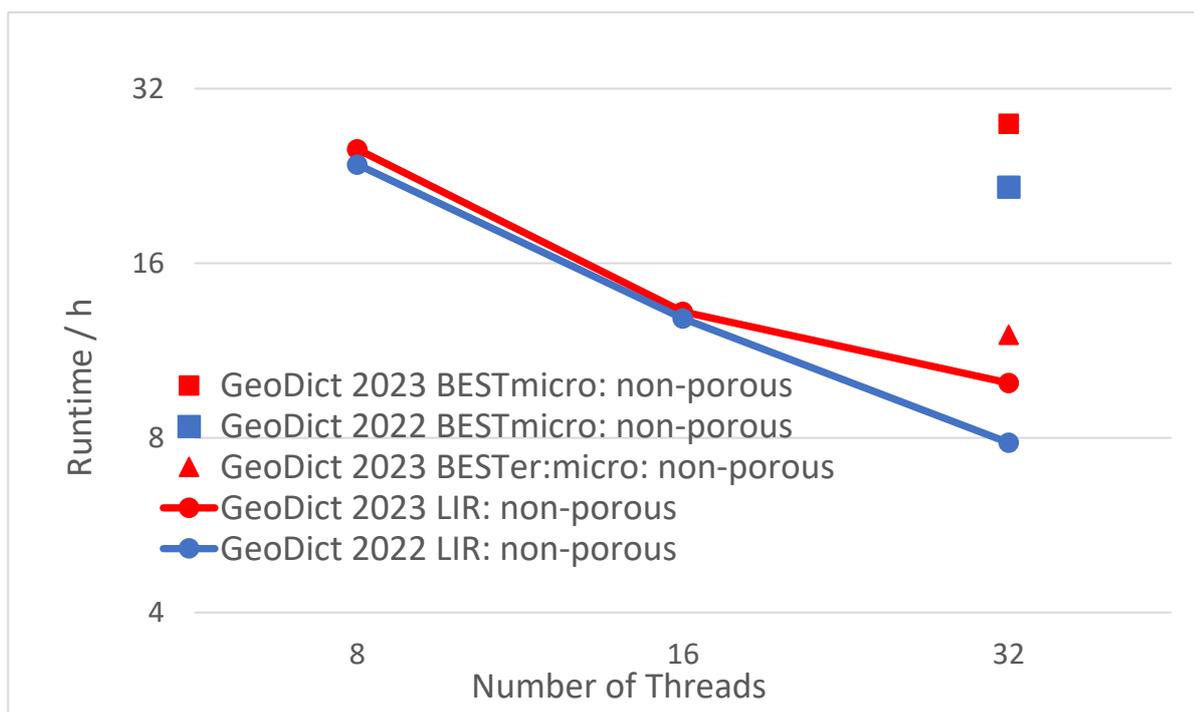
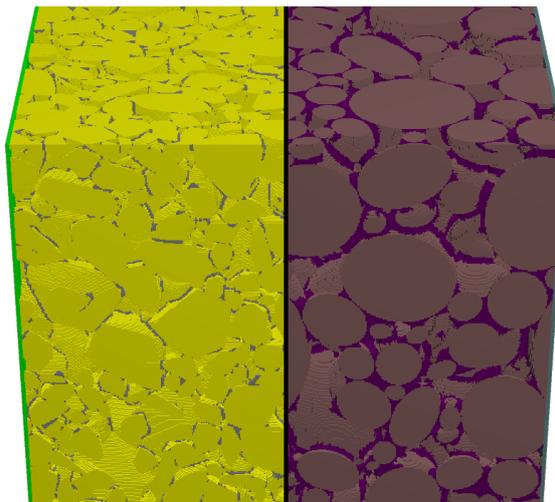
As an example for the parallelization, a full battery structure of size  $409 \times 400 \times 400$  voxels with  $200 \text{ nm}$  voxel length is used to simulate the charging from the cell state of charge 20% till 70%. The computation is run on a server with 2 x Intel E5-2697A v4 processors with 16 cores each, running with a maximum of  $3.60 \text{ GHz}$ , and  $1 \text{ TB}$  RAM.

The simulations are computed with GeoDict 2023, Service Pack 2.

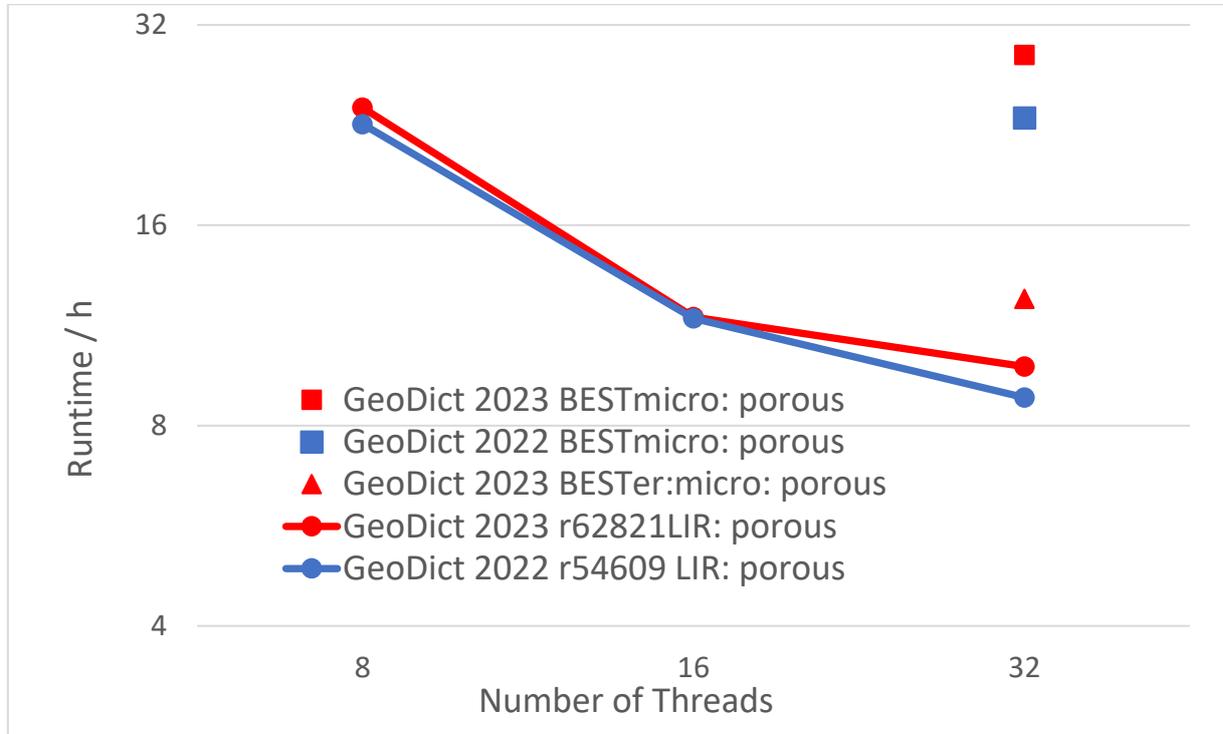
When the binder is considered as solid, the LIR solver needs only  $1/3$  of the runtime compared to BESTmicro with GeoDict 2023.

In GeoDict 2023, with the LIR solver, the runtime is almost the same with in GeoDict 2022. Also, in GeoDict 2023 the BEST:er-micro solver is added and it takes only 43% of runtime of BESTmicro.

The LIR solver needs only  $14 \text{ GB}$  of RAM which is 5% of the memory required by BESTmicro and 10% of the memory required by BEST:er-micro. The speedup for LIR solver is nearly optimal.

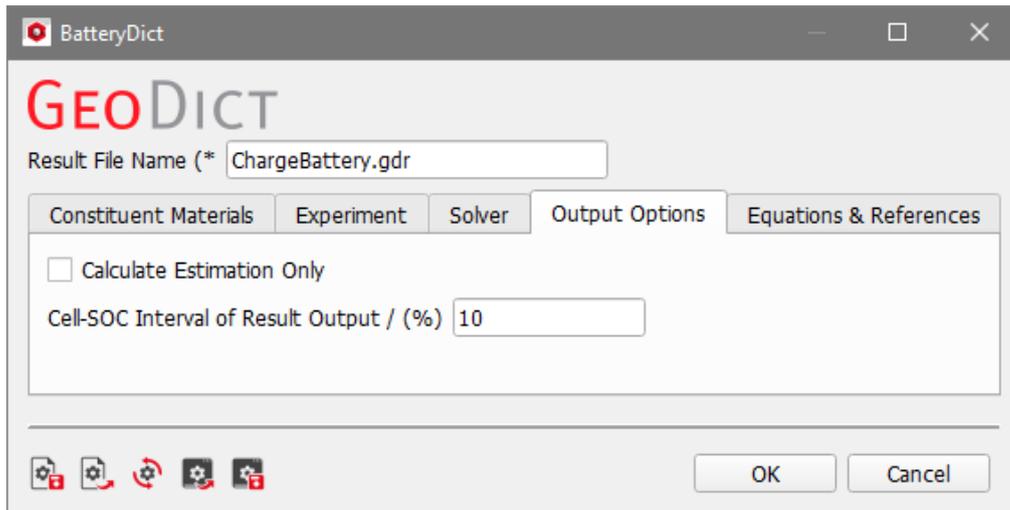


When the binder is considered as porous, since GeoDict 2022, LIR can also solve the porous case. The LIR solver needs 15 GB of RAM, only 4.3% of the memory required by BESTmicro, 346 GB and 10% of the memory required by BEST:er-micro. The runtimes of LIR, BESTer:micro and BESTmicro with 32 threads are 10 h, 12 h, and 29 h.



## OUTPUT OPTIONS

---



In the **Output Options** tab, **Calculate Estimation Only** can be checked, and then, the full simulation is not performed, but only the cell potential is estimated. This estimation is much faster than the full simulation. It considers the cell potential in equilibrium as well as the charge rate and part of the structure information, like the solid volume percentages of the different materials of the battery. From this information, Ohm losses and overpotentials at the surfaces, but no overpotentials due to diffusion are considered in the estimation. In this case, no solver options need to be defined, and the **Solver** tab is inactive.

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.

## EQUATIONS & REFERENCES

The differential equations solved in the charging simulation are listed under the **Equations & References** tab and are described above in [Theoretical Basis](#).

The references for the methods used are listed on this tab. In this **BatteryDict** User Guide handbook they can be found on page [99](#).

**BatteryDict**

**GEO DICT**

Result File Name (\*.gdr)

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

**Electrolyte**

Diffusion and Migration 
$$\frac{\partial c_e}{\partial t} = \nabla \cdot (D_e \nabla c_e) - \nabla \cdot \frac{t_+ \vec{j}_e}{F}$$

Charge Conservation and Electroneutrality 
$$0 = \nabla \cdot \vec{j}_e = -\nabla \cdot (\kappa_e \nabla \varphi_e) + \nabla \cdot \left[ \kappa_e (1 - t_+) \frac{RT}{F} \nabla \log c_e \right]$$

**Active Material**

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

Ohm's Law 
$$0 = \nabla \cdot \vec{j}_s = -\nabla \cdot (\kappa_s \nabla \varphi_s)$$

**Interface between Electrolyte and Active Material**

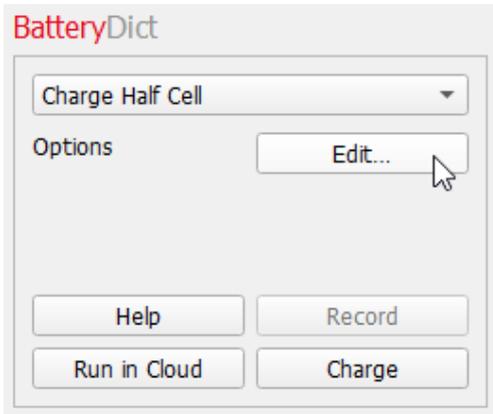
Butler-Volmer Interface Current Density 
$$i_{se} = 2 k_{BV} \sqrt{c_s c_e (c_{\max} - c_s)} \sinh \left[ (\varphi_s - \varphi_e - U_0) \frac{F}{2RT} \right]$$

**Variables and Constants**

- $c_e$ : Equilibrium Lithium Concentration in Electrolyte
- $c_s$ : Maximum Lithium Concentration in Active Material (Solid)
- $\vec{j}_e$ : Current Density of All Ionic Charges in Electrolyte
- $\vec{j}_s$ : Effective Electronic Current Density in Active Material (Solid)
- $i_{se}$ : Butler-Volmer Interface Current Density
- $\varphi_e$ : Electric Potential of Electrolyte
- $\varphi_s$ : Electric Potential of Active Material (Solid)
- $U_0$ : Open-Circuit Potential of Active Material vs. Lithium
- $c_{\max}$ : Maximum Lithium Concentration of active material (solid)
- $\kappa_e$ : Ionic Conductivity of Electrolyte
- $\kappa_s$ : Effective Electronic Conductivity of Active Material (Solid)
- $D_e$ : Ionic Diffusion Constant of Electrolyte
- $D_s$ : Ionic Diffusion Constant of Active Material (Solid)
- $t_+$ : Lithium Transference Number
- $k_{BV}$ : Butler-Volmer Rate Constant
- $T$ : Temperature
- $F$ : Faraday Constant, 96485.33289(59) C/mol
- $R$ : Universal Gas Constant, 8.3144598(48) J/(mol K)

OK Cancel

## CHARGE HALF CELL



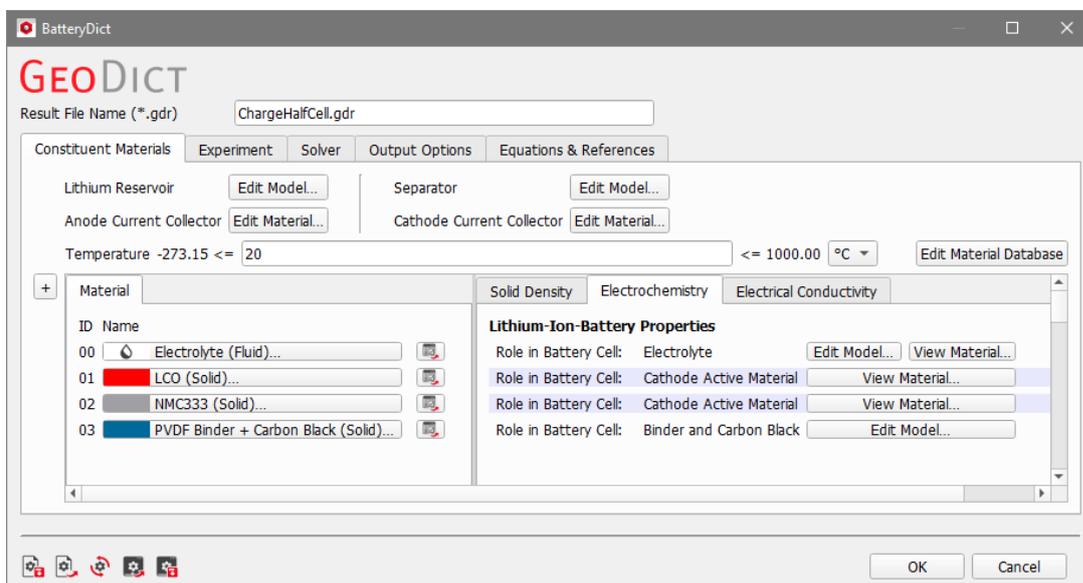
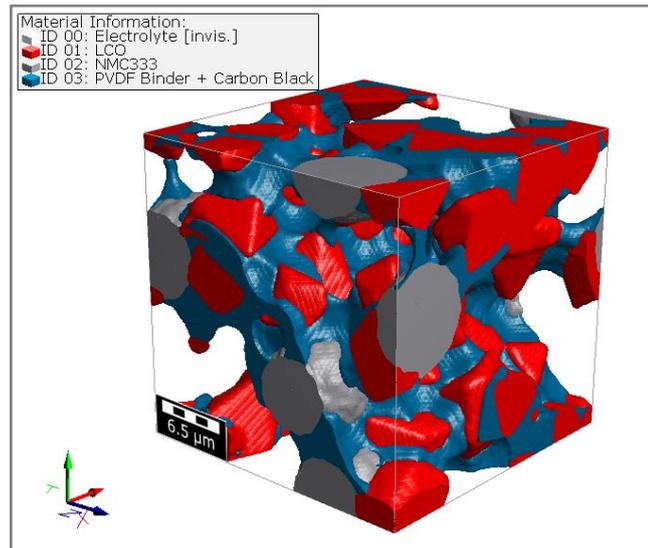
Since GeoDict 2022, the charging of a half-cell is available as separate functionality. It can be used for charging simulations of arbitrary structures loaded in GeoDict, consisting of a single electrode or an electrode together with a separator and/or a current collector without designing a battery first. Input parameters and results are adapted here, to fit for the simulation of a half-cell. The electrode can consist of cathode or anode active materials. Electrochemically, the lithium reservoir is always considered as the anode in the computation.

Click the options' **Edit** button to define the parameters for the simulation.

## CONSTITUENT MATERIALS

If a structure for a single electrode is loaded in GeoDict, this structure is considered as the cathode for a 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.

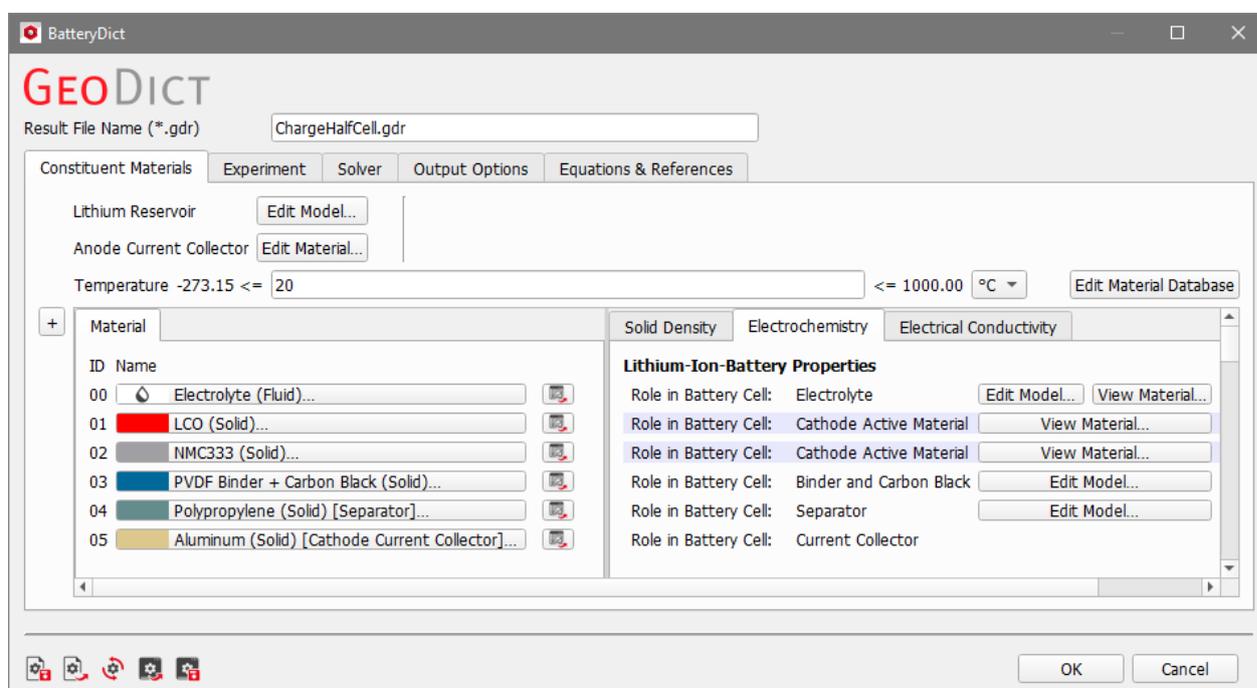
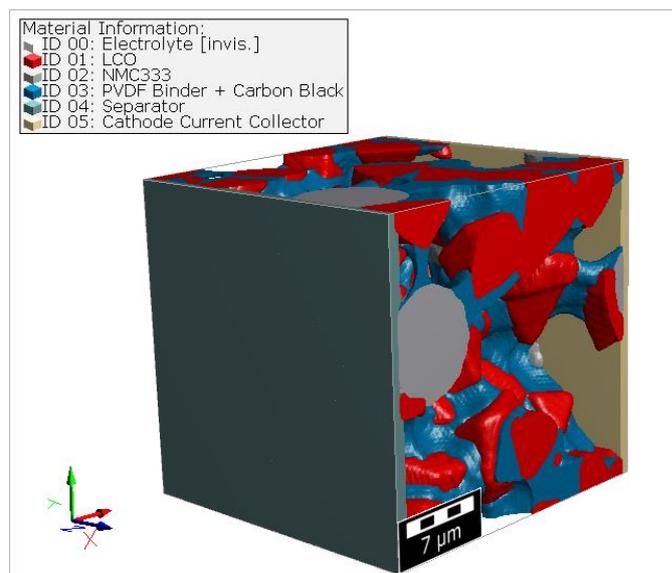
If a Material ID for the separator is available, it has to fit to the rule, that the half-cell is assembled in X-direction. In future GeoDict versions, the computation direction will be selectable in the GUI.



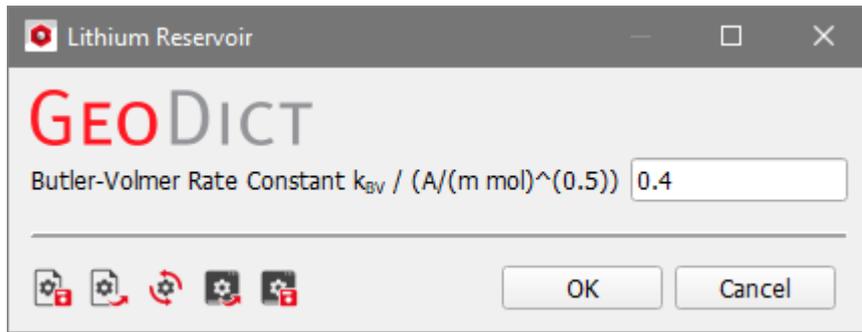
In the **BatteryDict** dialog, the materials available for the electrode are shown. In the same way as for battery charging, the parameters of the materials can be shown or modified. See page [31ff](#) for a more detailed description.

On top of the dialog, the parameters for anode current collector and lithium reservoir can be modified. If not defined by a separate Material ID in the structure, additionally the parameters for the separator and the cathode current collector can be defined.

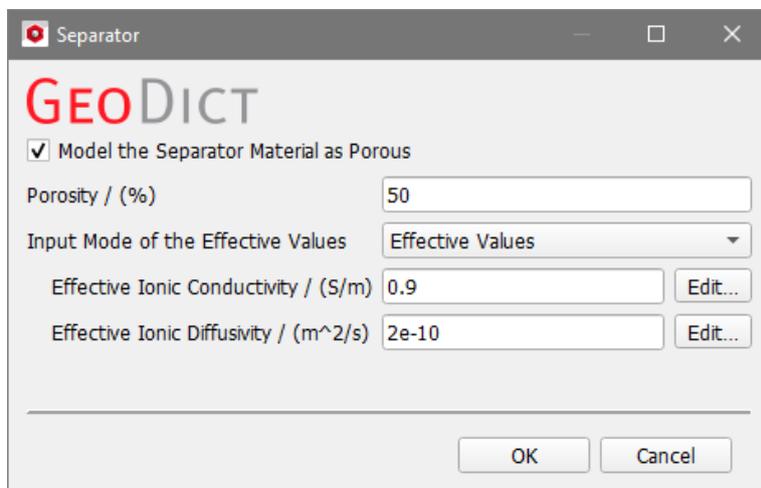
If the structure is created with separate Material IDs for cathode current collector and separator, these roles can be defined for the materials on the **Electrochemistry** subtab. In this case, the buttons for modifying the corresponding properties disappear from the top of the dialog.



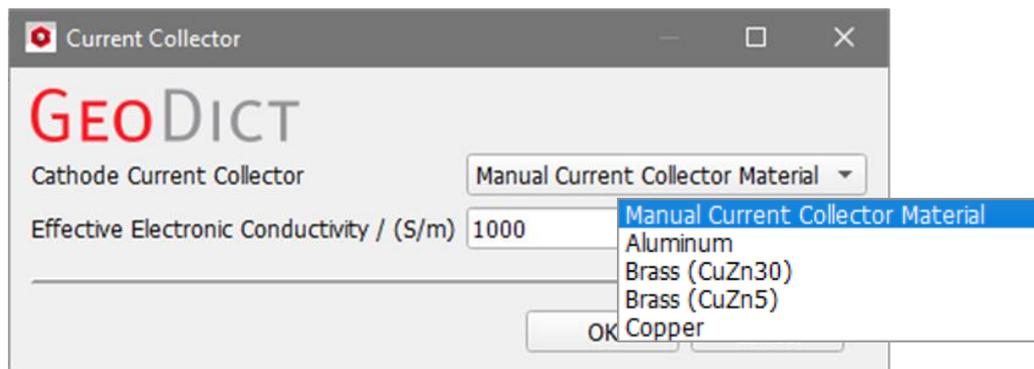
For the lithium reservoir, choose **Edit Model** to enter the Butler-Volmer Rate Constant for the simulation.



For the separator, with **Edit Model** the ionic conductivity and ionic diffusivity of the electrolyte can be selected (uncheck **Modify Effective Separator Properties**), or effective values can be defined. See page [39](#) for more details.



Material and electronic conductivity of the current collectors can be defined with the **Edit Material** buttons.



## EXPERIMENT

For the charging simulation of a half cell, the parameters that need to be selected on the **Experiment** tab, are nearly the same as for the simulation of a whole battery, see page [42](#).

Some differences occur because, for a half cell simulation, only the state of charge (SOC) of the investigated electrode needs to be considered. The other electrode is modelled as a never-ending lithium reservoir. Therefore, **Charge Electrode** simulates lithiation of the investigated electrode and **Discharge Electrode** delithiation of the investigated electrode vs the lithium reservoir. The **Start and End Condition** for the simulation are defined by selecting **Initial and Final Electrode SOC**.

To start the simulation from a lithium concentration in the half cell, 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 modelled as the lithium reservoir.

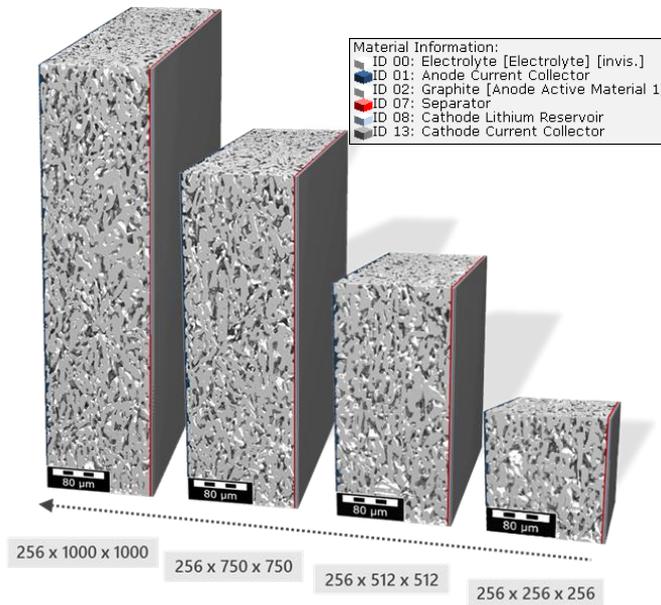
The **Computation Direction** is fixed in X direction in GeoDict 2023. In future GeoDict versions, it will be possible to decide about the coordinate direction in that the half-cell is assembled.

## SOLVER, OUTPUT OPTIONS, AND EQUATIONS & REFERENCES TAB

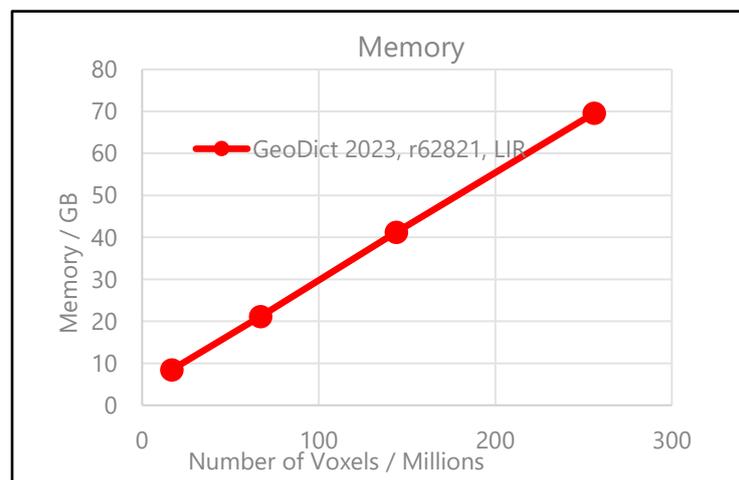
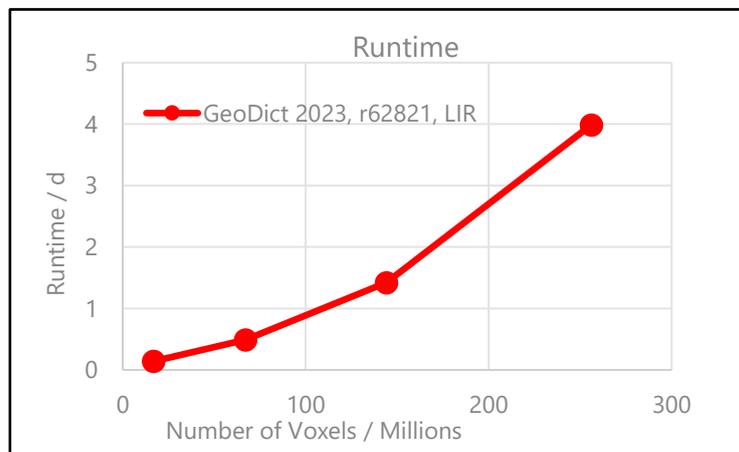
The options that can be selected on the **Solver** and the **Output Options** tab, as well as the equations on the **Equations & References** tab, are the same as for the charging of a whole battery. A description can be found on page [46ff](#).

**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 ageing simulations.

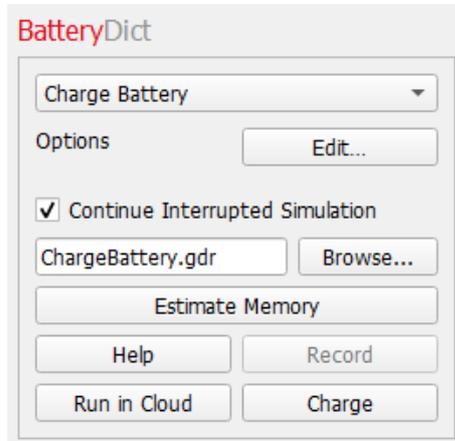


The simulation is run with LIR solver. The necessary memory for the computation is increasing linearly with the number of voxels simulated. Even a simulation with 250 million voxels can be run in 4 days, with only 70GB RAM required.



## CONTINUE INTERRUPTED SIMULATION

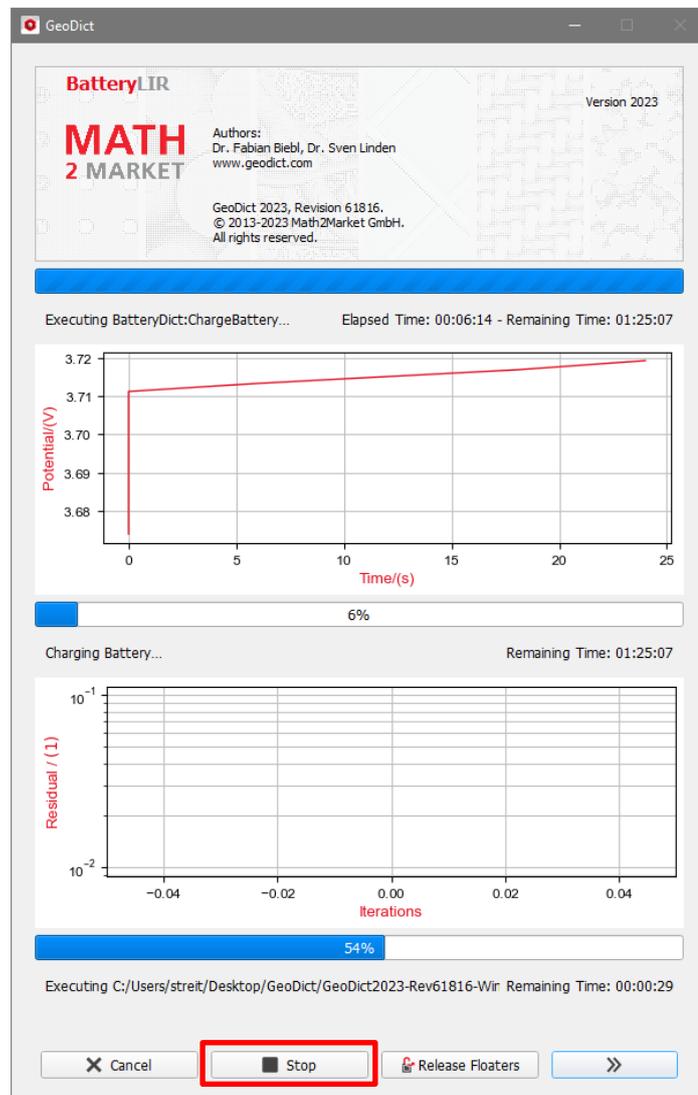
It is possible to continue a previously interrupted charging simulation.



If **Charge Battery** is selected from the **BatteryDict** pull-down menu, check **Continue Interrupted Simulation**.

Browse for the **GeoDict** result file, created earlier, and continue the unfinished simulation by selecting **Charge**.

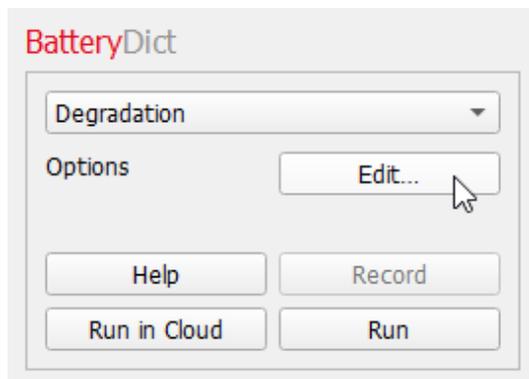
Continuing an interrupted simulation is possible, if a previously run charging simulation was stopped and **GeoDict** could create a result file.



If the simulation was canceled, it is not possible to continue the simulation later.

## DEGRADATION

In **GeoDict 2023**, the functionality to compute mechanical deformations of a battery cell due to Lithium intercalation is available as a command in **BatteryDict**.

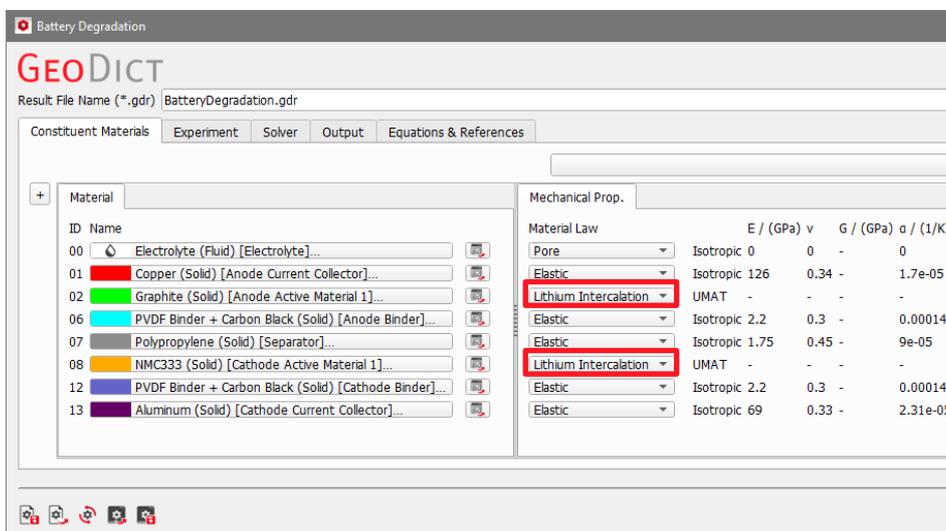


Select **Degradation** in the **BatteryDict** part of the main window and click **Edit ...** to open the options dialog for the simulation.

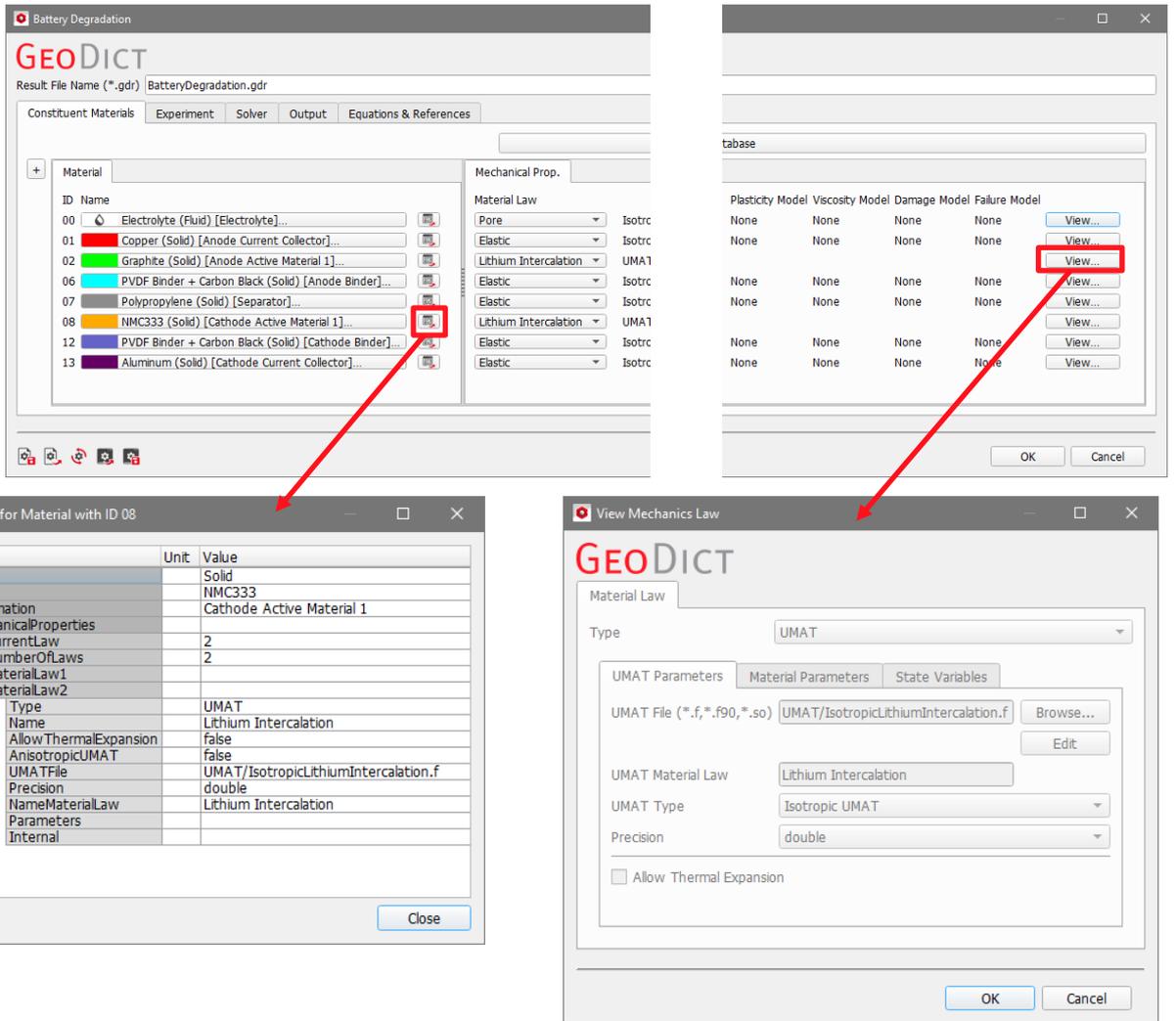
## CONSTITUENT MATERIALS

On the Constituent Materials tab, the mechanical properties of all materials are defined for the deformation simulation. Select the appropriate materials.

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 and Silicon with the Material Law Lithium Intercalation.

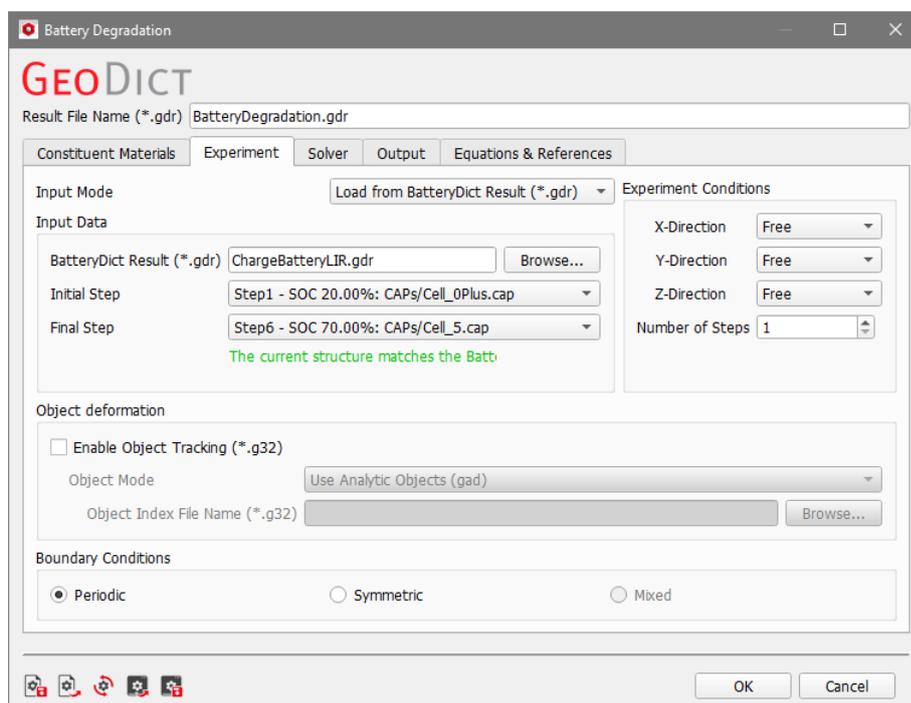


For all other solid materials, mechanical properties (Young's modulus and Poisson ratio) need to be defined for the simulation. Click **View** to see the parameters defined in the layout of the **GeoDict Material Database** or click the icon  to see the parameters as a report.



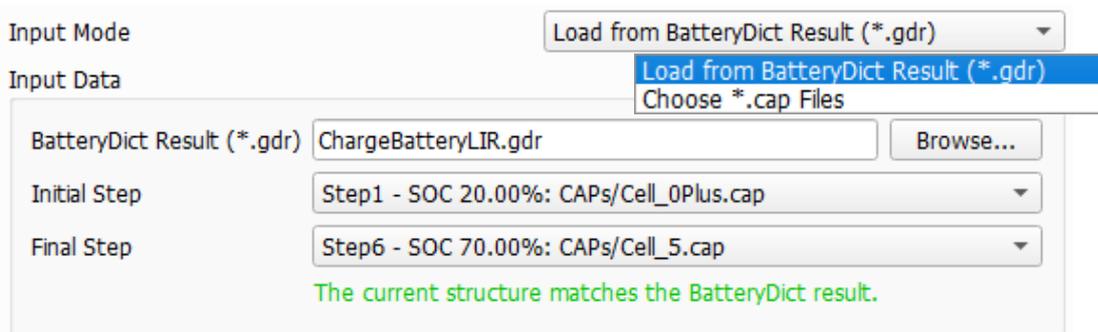
## EXPERIMENT

On the Experiment tab, define the parameters for the simulation itself.



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** (see page 31) or **Charge Half Cell** (see page 54) 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: Load from BatteryDict Result (\*.gdr) / Choose \*.cap Files

BatteryDict Result (\*.gdr): ChargeBatteryLIR.gdr [Browse...]

Initial Step: Step1 - SOC 20.00%: CAPs/Cell\_0Plus.cap

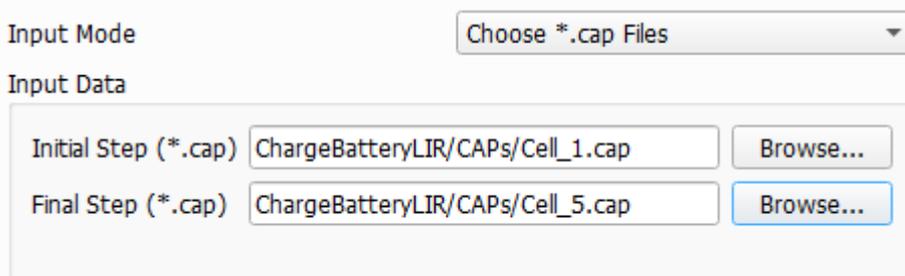
Final Step: Step6 - SOC 70.00%: CAPs/Cell\_5.cap

The current structure matches the BatteryDict result.

GeoDict checks if the battery currently in memory fits to the result file selected. If this is the case, this is displayed in green under the .cap files selected as initial and final step. If a different structure is currently loaded, a warning is displayed in red.

The current structure does not match the BatteryDict result.

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.



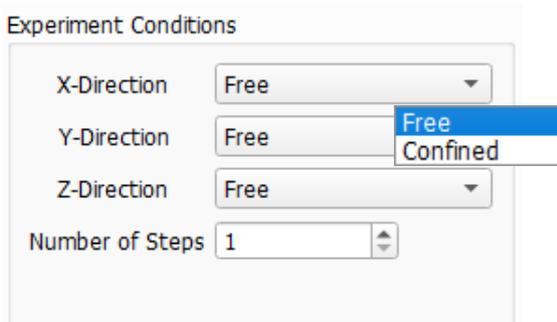
Input Mode: Choose \*.cap Files

Input Data: Initial Step (\*.cap): ChargeBatteryLIR/CAPs/Cell\_1.cap [Browse...]

Final Step (\*.cap): ChargeBatteryLIR/CAPs/Cell\_5.cap [Browse...]

In the upper right part of the dialog, choose the **Experiment Conditions**. In each coordinate direction, define if the cell can expand **Free** in this coordinate direction, or if it cannot expand at all (**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.



Experiment Conditions

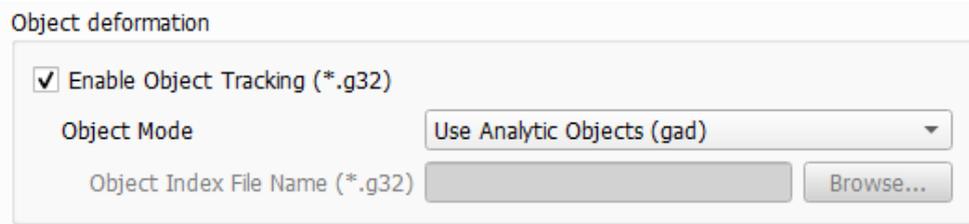
X-Direction: Free

Y-Direction: Free / Confined

Z-Direction: Free

Number of Steps: 1

**Enable Object Tracking** in the Object Deformation part of the dialog to keep object indices in the deformation simulation. Like this, it is possible to identify the deformation of every single 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,



or a previously created .g32 file can be selected.

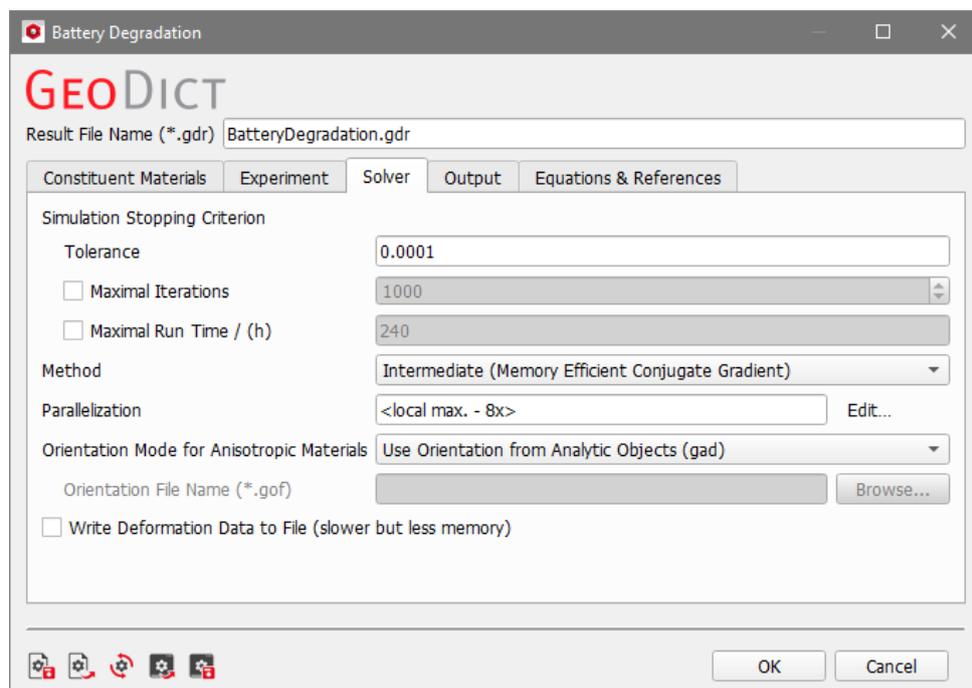


Finally, select the boundary conditions for the structure in the simulation. Use **periodic** if the structure is periodic in all coordinate directions, **symmetric** if it is not. Mixed boundary conditions are not available in BatteryDict-Degradation.



## SOLVER

On the Solver tab, specify the settings for the FeelMath solver. The settings are part of the FeelMath solver settings explained in more detail in the [ElastoDict](#) handbook of the [GeoDict](#) User Guide.



Under **Simulation Stopping Criterion** define the **Tolerance** and the **Maximal Iterations** and **Maximal Run Time** to control the iterative process of the solver. Only the tolerance must be set, the other two parameters are optional.

For each iteration step, the relative error of the current solution is computed. If this relative error is smaller than the given tolerance for ten subsequent steps, the computation is finished. When there is doubt about the quality of the solution, decrease the tolerance value by a factor of ten for that solver. In general, it is recommended to keep the default setting for tolerance.

Simulation Stopping Criterion

Tolerance	0.0001
<input type="checkbox"/> Maximal Iterations	1000
<input type="checkbox"/> Maximal Run Time / (h)	240

When the solver stops because the **Maximal Iterations** or the **Maximal Run Time(h)** are reached, the quality of solution might be doubtful since the requested accuracy is not achieved. Therefore, those two options are disabled by default and should only be selected if there are strong constraints on the allowed runtime.

Method: Intermediate (Memory Efficient Conjugate Gradient)

- Fast (Conjugate Gradient)
- Intermediate (Memory Efficient Conjugate Gradient)
- Memory Efficient (Neumann Series)

For the **FeelMath-LD** 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 enough for the other methods.

The degradation simulation, like the charging simulation, can be accelerated by running the computation on multiple CPU cores, as explained on page [48](#). The maximum number of processes licensed for the degradation simulation is the number of licensed **ElastoDict** processes.

For information on how to set up and use **BatteryDict-Degradation** in a **Cluster** configuration, contact Math2Market.

Orientation Mode for Anisotropic Materials: Use Orientation from Analytic Objects (gad)

Orientation File Name (\*.gof): [Empty]

- Use Orientation from Analytic Objects (gad)
- Load Orientation Information from File (\*.gof)
- Use the Global XYZ-Coordinate System

**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.

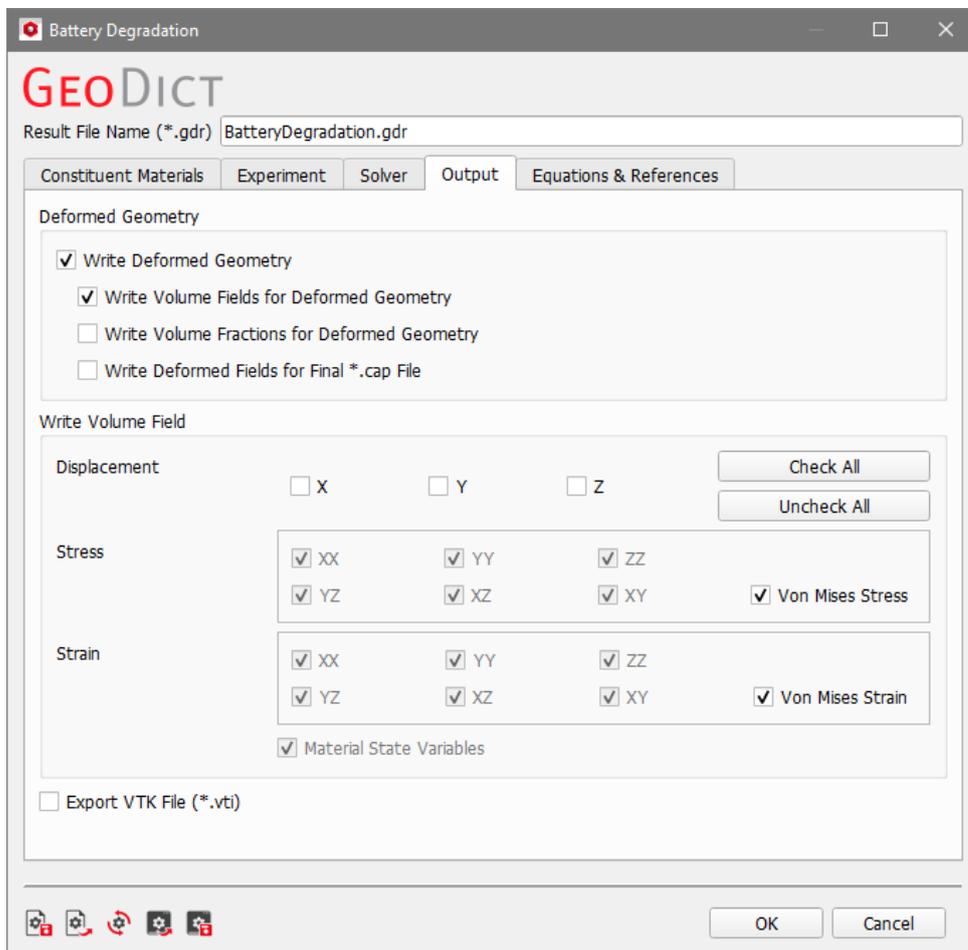
Write Deformation Data to File (slower but less memory)

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. Nevertheless, there is an issue with this approach: 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 the simulation down.

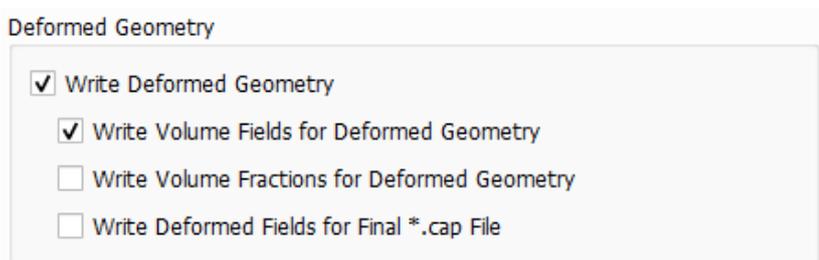
Therefore, the default is to keep the deformation data in memory. In most cases, the data fits into the main memory, and this option is many times faster (See benchmark results on page 41 in the [ElastoDict](#) handbook of the User Guide). We recommend keeping this setting, and to select **Write Deformation Data to File** only if the simulation fails because the data doesn't fit in the RAM.

## OUTPUT

The options available in the Output tab define which information is written to the hard disk during the computation.



In the **Deformed Geometry** section of the tab, select which information is exported for the deformed geometry.



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.

Under **Write Volume Field**, checking or un-checking the boxes for **Displacement**, **Stress**, and **Strain** determines whether these results outputs are available for visualization and post-processing after the run of the FeelMath solver.

Write Volume Field

Displacement	<input type="checkbox"/> X	<input type="checkbox"/> Y	<input type="checkbox"/> Z	<input type="button" value="Check All"/>
	<input type="button" value="Uncheck All"/>			
Stress	<input checked="" type="checkbox"/> XX	<input checked="" type="checkbox"/> YY	<input checked="" type="checkbox"/> ZZ	
	<input checked="" type="checkbox"/> YZ	<input checked="" type="checkbox"/> XZ	<input checked="" type="checkbox"/> XY	<input checked="" type="checkbox"/> Von Mises Stress
Strain	<input checked="" type="checkbox"/> XX	<input checked="" type="checkbox"/> YY	<input checked="" type="checkbox"/> ZZ	
	<input checked="" type="checkbox"/> YZ	<input checked="" type="checkbox"/> XZ	<input checked="" type="checkbox"/> XY	<input checked="" type="checkbox"/> Von Mises Strain
	<input checked="" type="checkbox"/> Material State Variables			

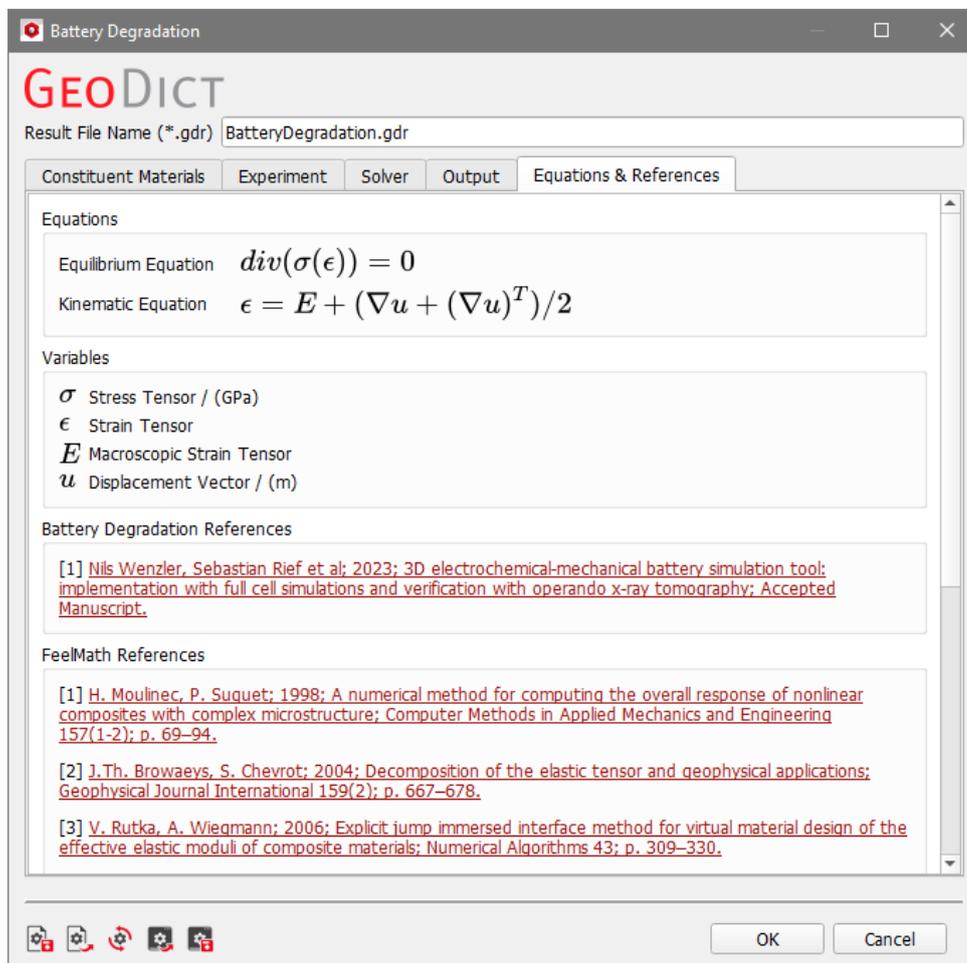
Different from **ElastoDict**, the stress and strain tensor itself (XX, YY, ...) is currently always exported in **BatteryDict-Degradation**, but Von Mises Stress and Strain can be checked or unchecked.

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)

## EQUATIONS & REFERENCES

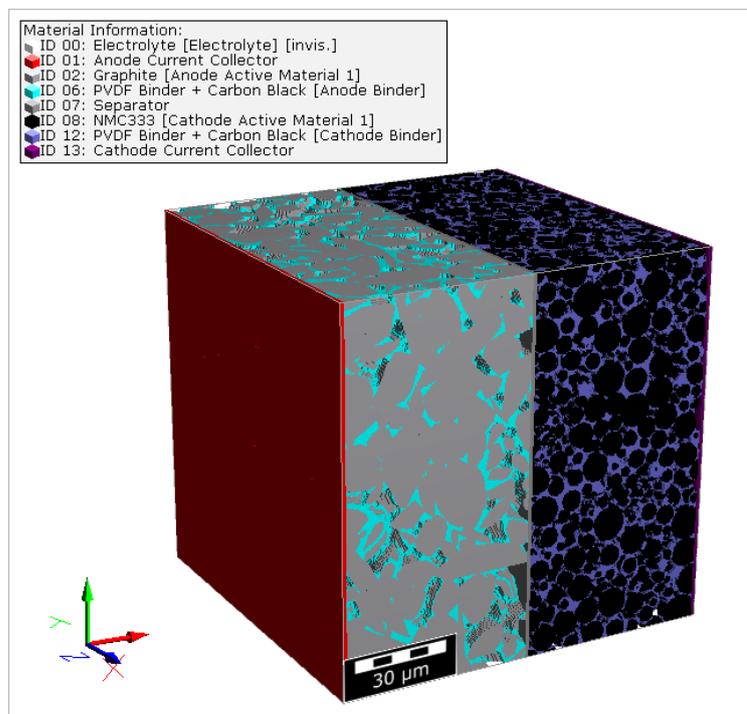
The differential equations solved in the simulation are listed under the **Equations & References** tab. Additionally, the references for the degradation simulation and the FeelMath solver are shown on this tab. In this **BatteryDict** User Guide handbook, the degradation references can be found on page [99](#).



## BATTERYDICT COMPUTATION RESULTS

### RESULTS OF DESIGN BATTERY

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

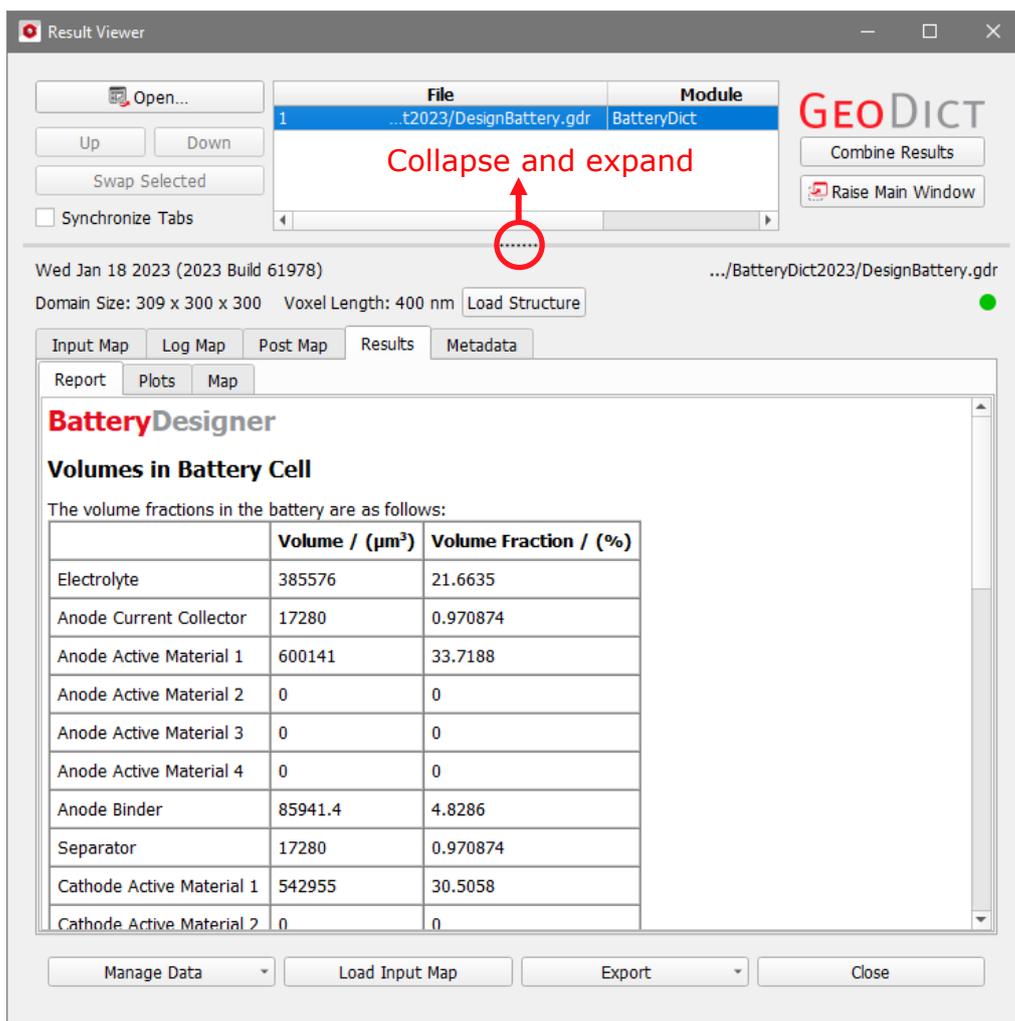


The .gdr file can be reopened at any time by choosing **File** → **Open Results (\*.gdr)...** in the menu bar. The **Result Viewer** opens at the **Results** tab.

In the **Result Viewer**, the list of all open result files is shown in a box in the upper part. The name of the result file currently displayed is highlighted in blue. This box in the upper part of the **Result Viewer** can be collapsed (and expanded) by pulling up (or down) the dotted line under the box.

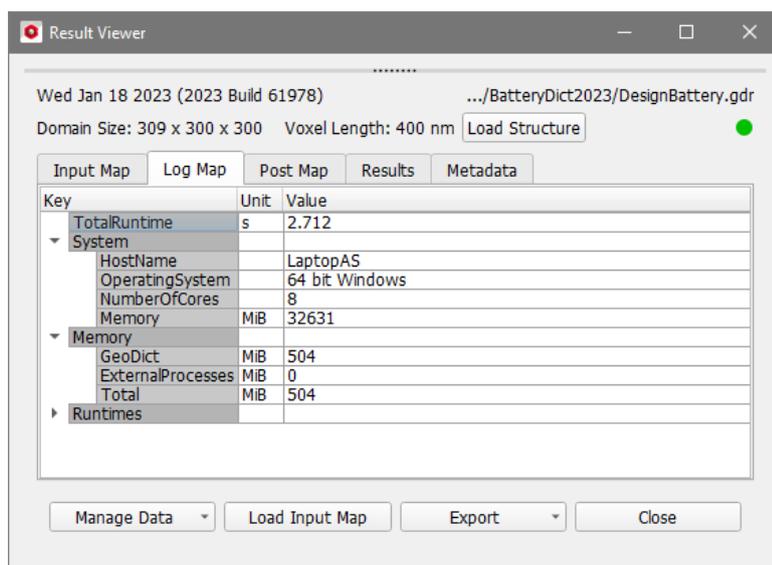
The green dot in the upper right part of the result viewer, indicates that the structure from that these results were obtained is loaded in the visualization area. This is always the case directly after creating the battery structure. If a result file (\*.gdr) is reloaded later through **File** → **Open Results (\*.gdr)...** or through clicking the **Open** button in the upper left part of the Result Viewer, the dot is red. The structure can be loaded into **GeoDict** memory and the visualization area by clicking the **Load Structure** button in the result viewer.

With the **Combine Results** button in the upper right part of the Result Viewer, the results of several selected .gdr files can be combined and shown in one plot in the **Result Viewer**. More details can be found in the [Result Viewer](#) handbook of this User Guide.



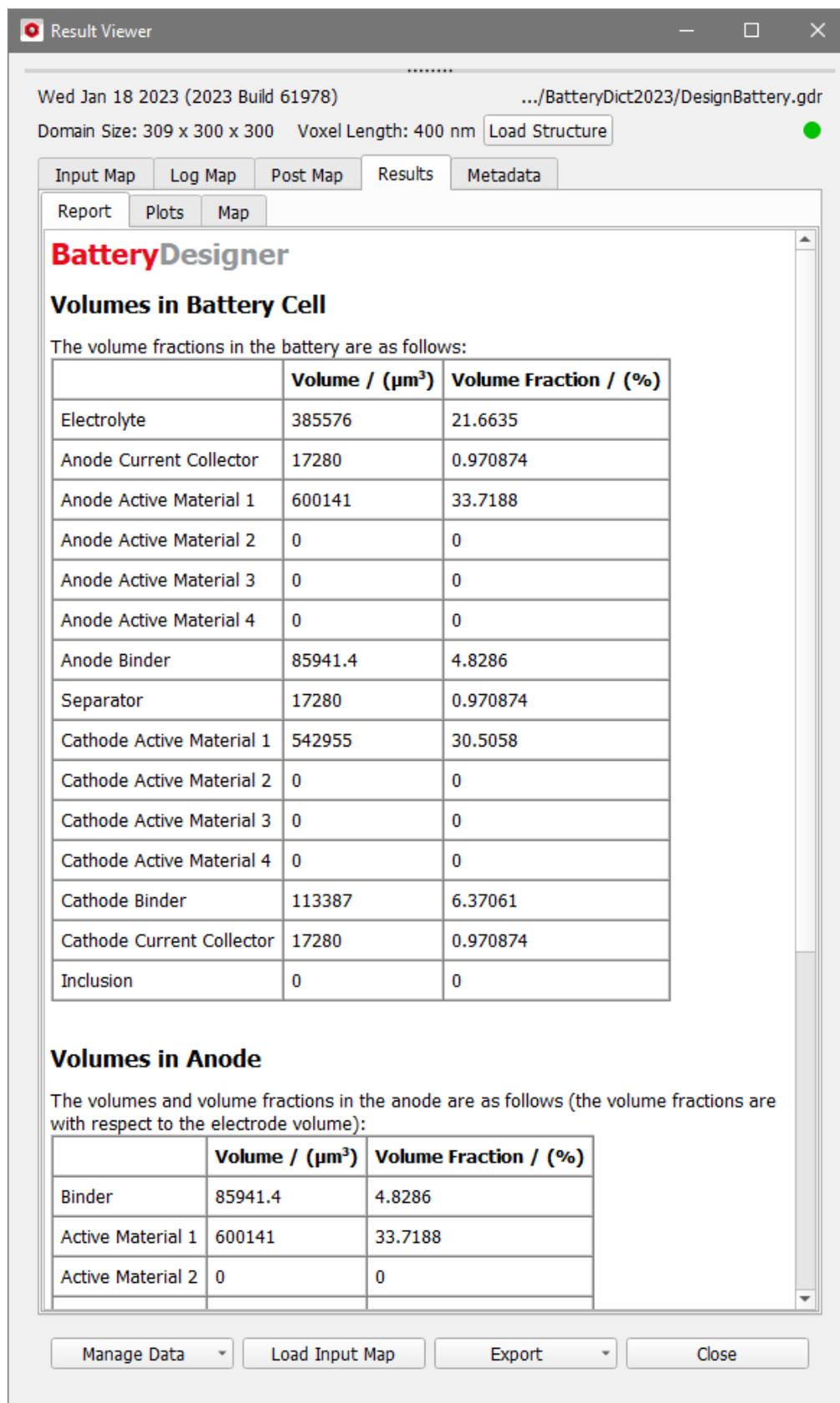
The **Input Map** tab contains all the input parameters of the battery creation.

The **Log Map** tab shows the runtime and memory used as well as the information about the system on which the battery structure was created.



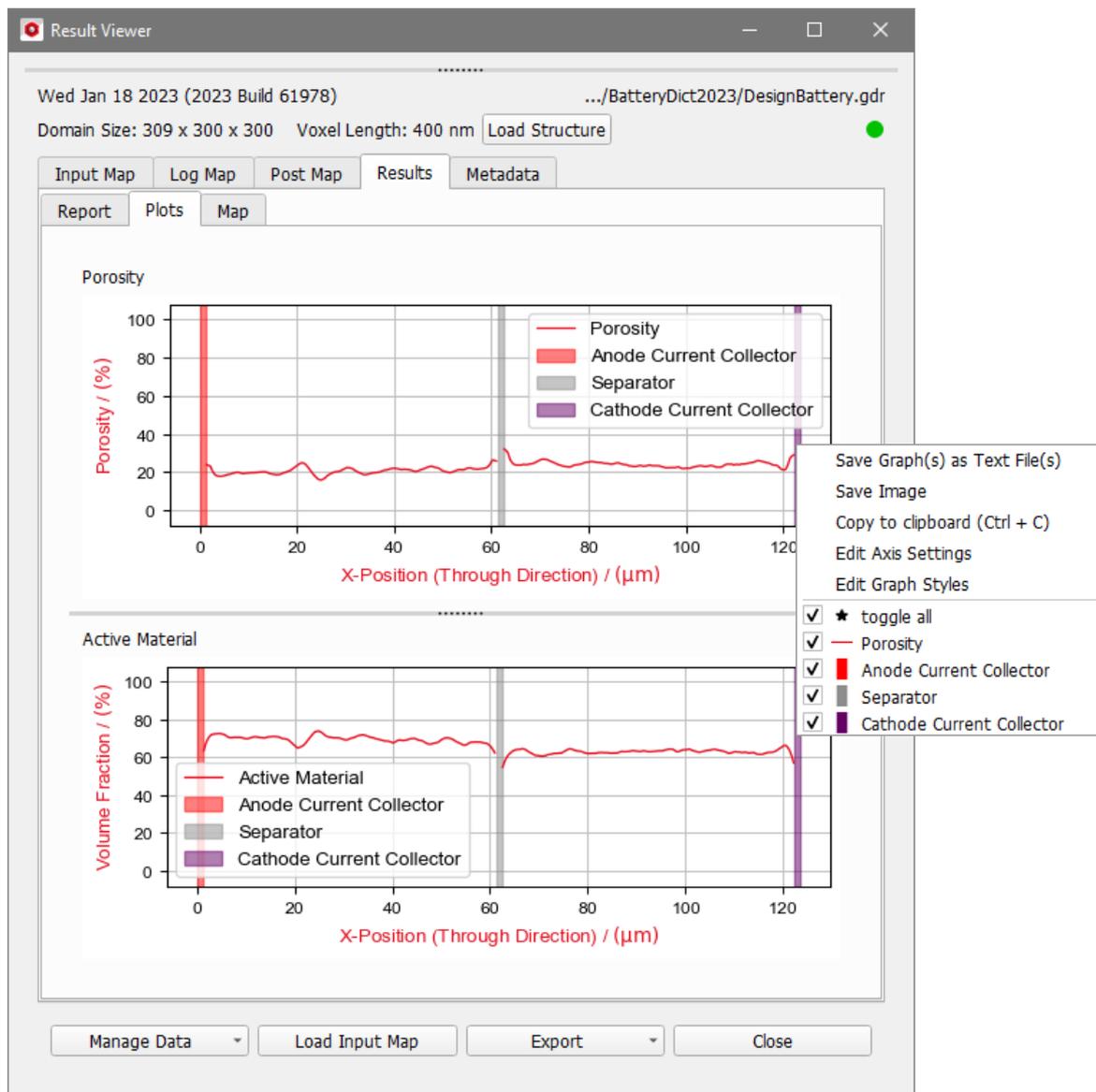
The **Post Map** tab shows parameter and graph data used for the plots on the **Results** tab.

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.



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.

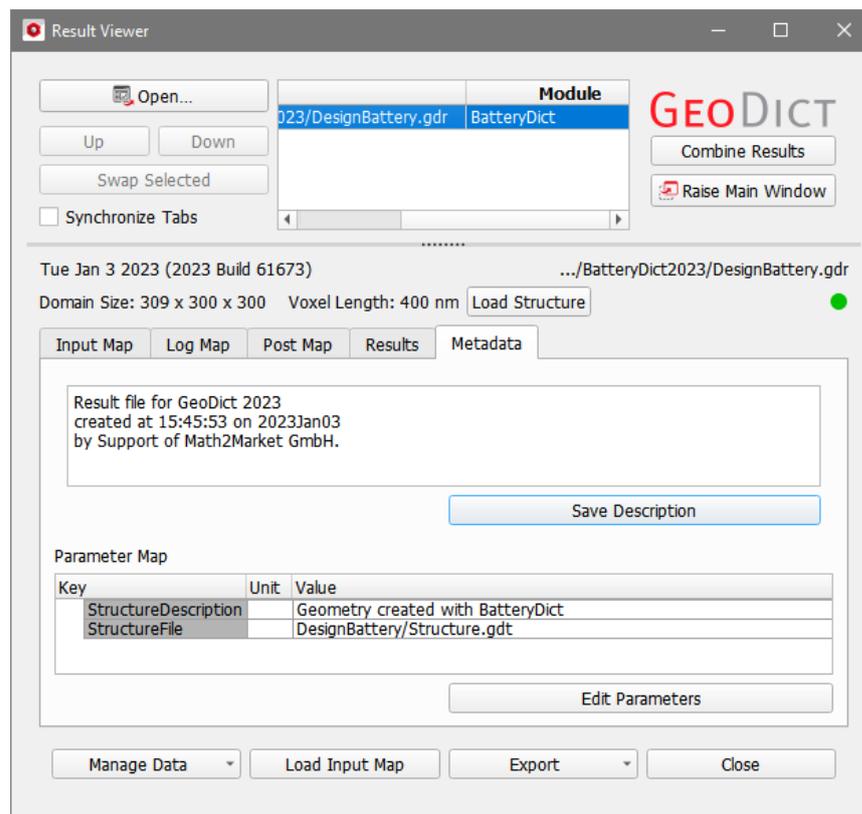
At the separator and both current collectors, no values are shown for porosity and active material since these structures do not contain active material and are not resolved into a microstructure in the Battery Designer. Also, the binder is considered as solid material in the computation of the porosity. Later, in the analysis of the battery or a charging simulation, binder can be considered as porous 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, text file or be copied to the clipboard.

The **Results - Map** subtab displays information on the volumes and volume fractions of the different materials of the whole battery, as well as for anode and cathode alone. This are the values also shown under the **Results - Report** subtab.

The **Metadata** tab displays a description of the .gdr file. The text can be modified here, and the modification can be saved to the .gdr file.



As usual for all **GeoDict** result files, several buttons for further processing are available at the bottom of the **Result Viewer**.



#### ■ **Manage Data:**

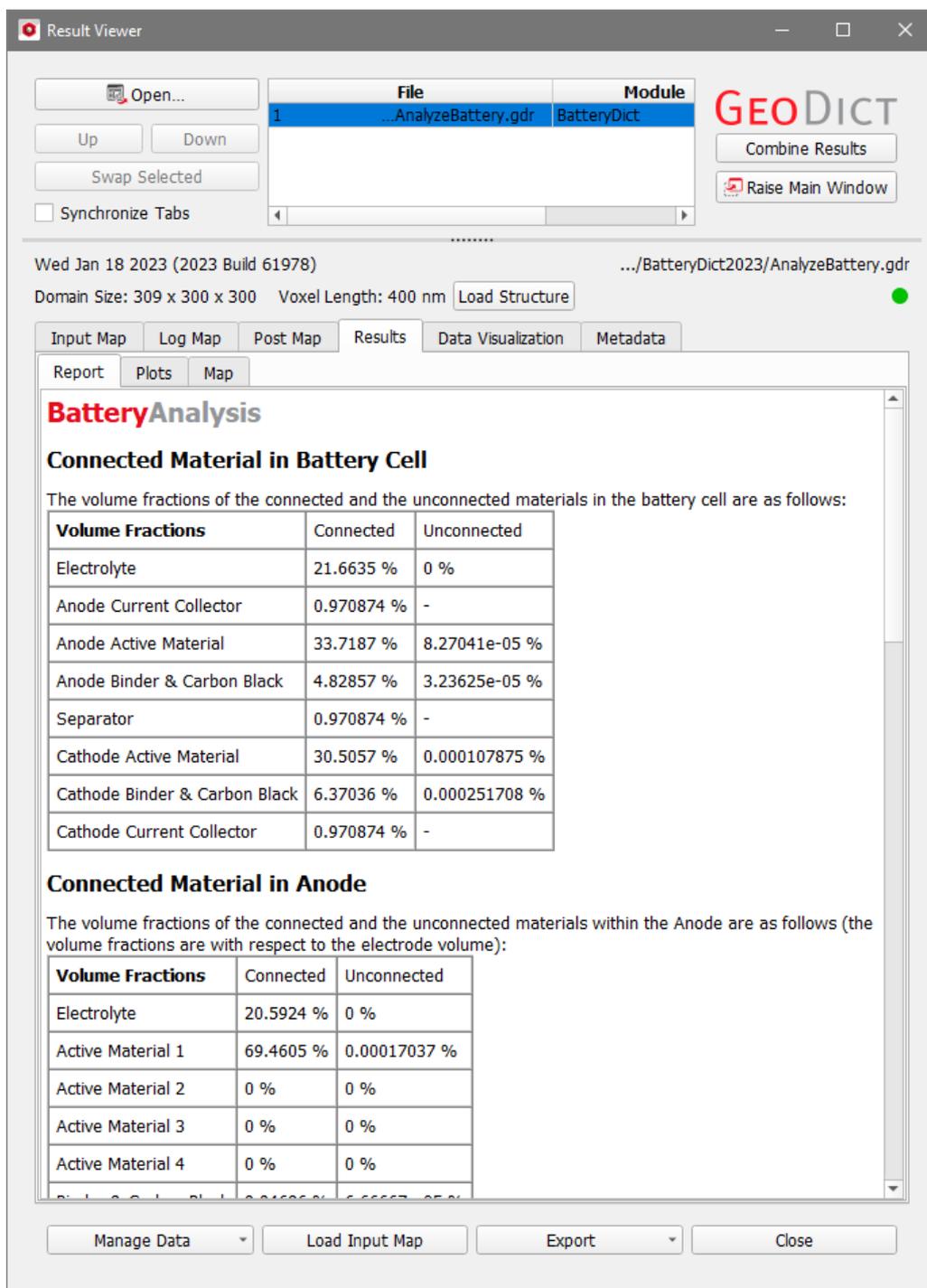
- **Clean-Up/Pack:** Zip the information contained in the result folder or clean-up the result folder.
- **Rename:** Change the name of result file and result folder.
- **Load Input Map:** Reload solver options and material parameters used for the computation of the results. After loading, these parameters are available in the **BatteryDict** dialogs.
- **Export:** Export the results for postprocessing with another tool
- **Excel (generic):** Export the information of the section Result Map of the **GeoDict** result file to Microsoft Excel®. You can analyze computation results in Microsoft Excel® using **GeoDexcel** provided with **GeoDict**. See the [GeoDexcel handbook](#) of the **GeoDict** User Guide for more information.
- **Excel (generic) – Python:** Export the information to an .xlsx Excel file in the same way as with **Excel (generic)** but using a Python script. This export does not need an Excel installation and can therefore also be used on Linux systems.

- **Matlab:** Open Matlab® if an installation and license is available, change to the project folder, and load the result file with **GeoLab**. See the [GeoLab](#) handbook the **GeoDict** User Guide for more information.
- **Store As Html:** Export the information shown in the **Results** tab to a html file.
- **Save Plots:** Export all plots to the **GeoDict** result folder.
- **Input Map as Python:** Export the solver options and material parameters used for the computation, together with the computation command to a Python file. This file can be executed as a **GeoDict** macro to rerun the computation, see the [Automation](#) handbook of the **GeoDict** User Guide for more detailed information.

## RESULTS OF ANALYZE BATTERY

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

The **Results – Report** subtab lists the information on the volume fractions of the connected and unconnected part for the different battery components. First, this volume fractions are shown for the whole battery cell, then for anode and cathode separately. The unconnected parts do not contribute to the performance of the battery, a small fraction of unconnected material is therefore desired.



The screenshot shows the 'Result Viewer' window with the 'Results' tab selected. The 'Report' sub-tab is active, displaying the 'BatteryAnalysis' report. The report is titled 'Connected Material in Battery Cell' and provides a table of volume fractions for various components. Below this, it also shows 'Connected Material in Anode' with another table of volume fractions.

**BatteryAnalysis**

**Connected Material in Battery Cell**

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

Volume Fractions	Connected	Unconnected
Electrolyte	21.6635 %	0 %
Anode Current Collector	0.970874 %	-
Anode Active Material	33.7187 %	8.27041e-05 %
Anode Binder & Carbon Black	4.82857 %	3.23625e-05 %
Separator	0.970874 %	-
Cathode Active Material	30.5057 %	0.000107875 %
Cathode Binder & Carbon Black	6.37036 %	0.000251708 %
Cathode Current Collector	0.970874 %	-

**Connected Material in Anode**

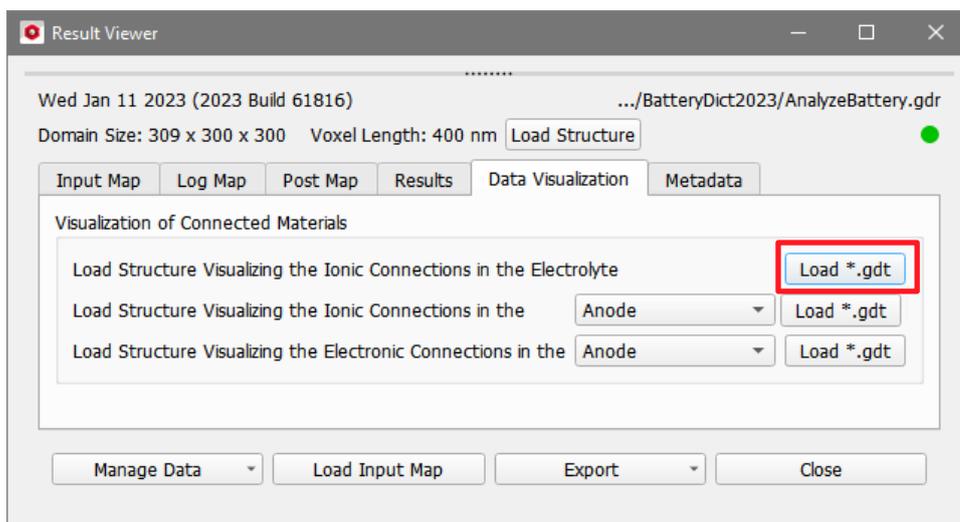
The volume fractions of the connected and the unconnected materials within the Anode are as follows (the volume fractions are with respect to the electrode volume):

Volume Fractions	Connected	Unconnected
Electrolyte	20.5924 %	0 %
Active Material 1	69.4605 %	0.00017037 %
Active Material 2	0 %	0 %
Active Material 3	0 %	0 %
Active Material 4	0 %	0 %

After the information about connected and unconnected parts of the battery, in the **Results - Report** tab follows a list of the volume and volume fractions of each component for the whole battery cell as well as for anode and cathode separately. This is the same information also shown in the result file of the Battery Designer, see page [71](#).

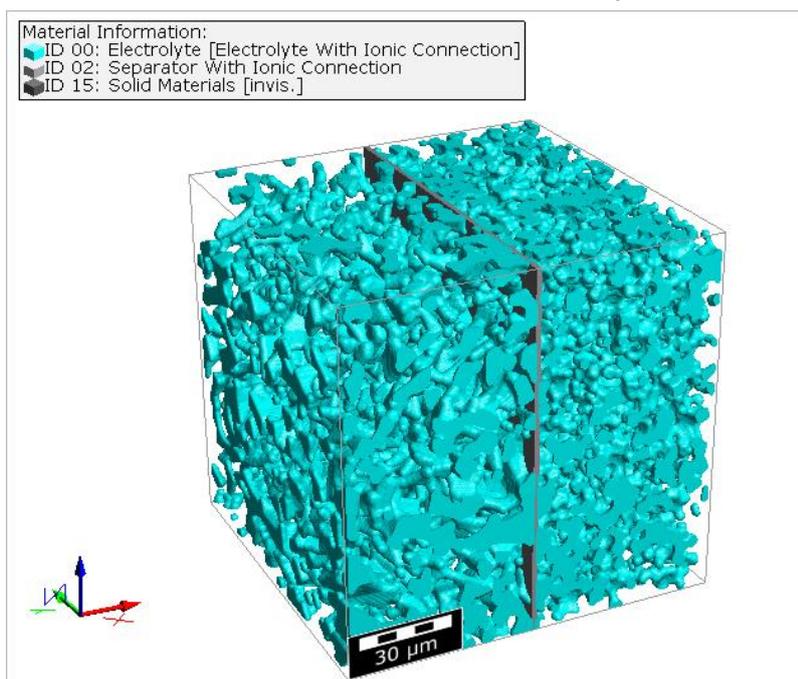
Under the **Results - Plots** subtab, the porosity, and the distribution of active material over the whole battery are shown as averaged values over each slice in y- and z-direction. This is the same plot as shown for a result file of the battery designer, see page [72](#).

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 containing the electronic as well as the ionic connections are available for anode and cathode and for the electrolyte connections, see page [96](#).

As an example, here the structure for the ionic connection in the Electrolyte is shown. No unconnected electrolyte exists in the example battery shown here.



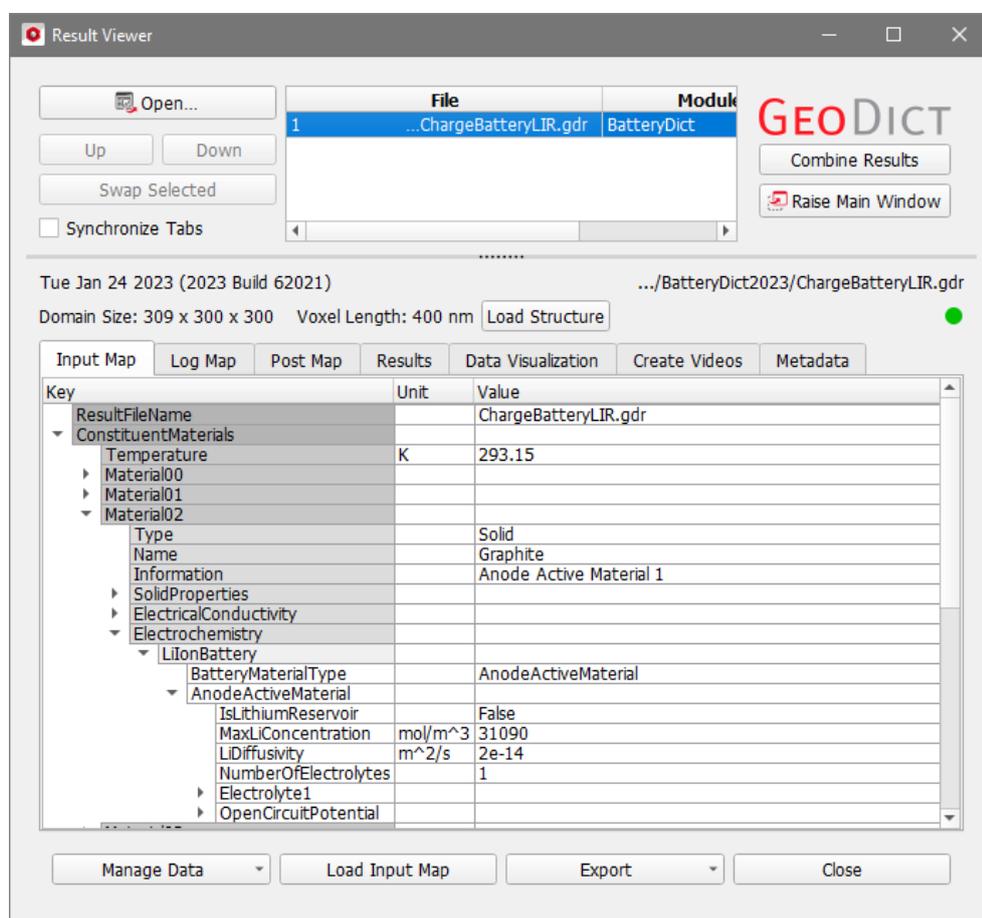
## RESULTS OF CHARGE BATTERY

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

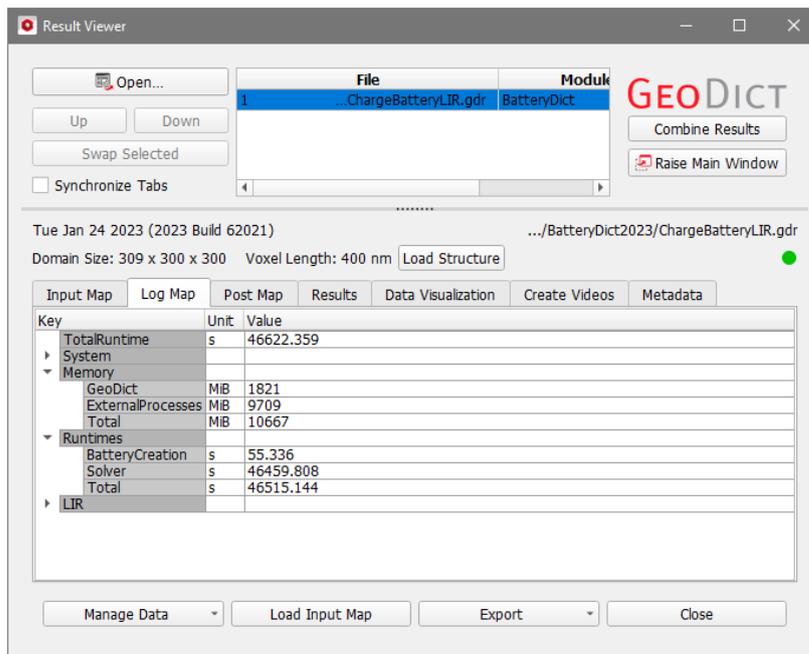
These results are accessible at any time by loading the .gdr file from the menu bar (**File** → **Open Results (\*.gdr) ...**). The **Load Structure** button and the buttons available at the bottom of the **Result Viewer** are the same as for other result files and are explained on page [69](#).

In the following, results of a simulation with the battery designed above are shown.

The **Input Map** tab displays the input data for the simulation. All parameters can be displayed here, e.g., the material parameters defined for the (first) active material of the anode.

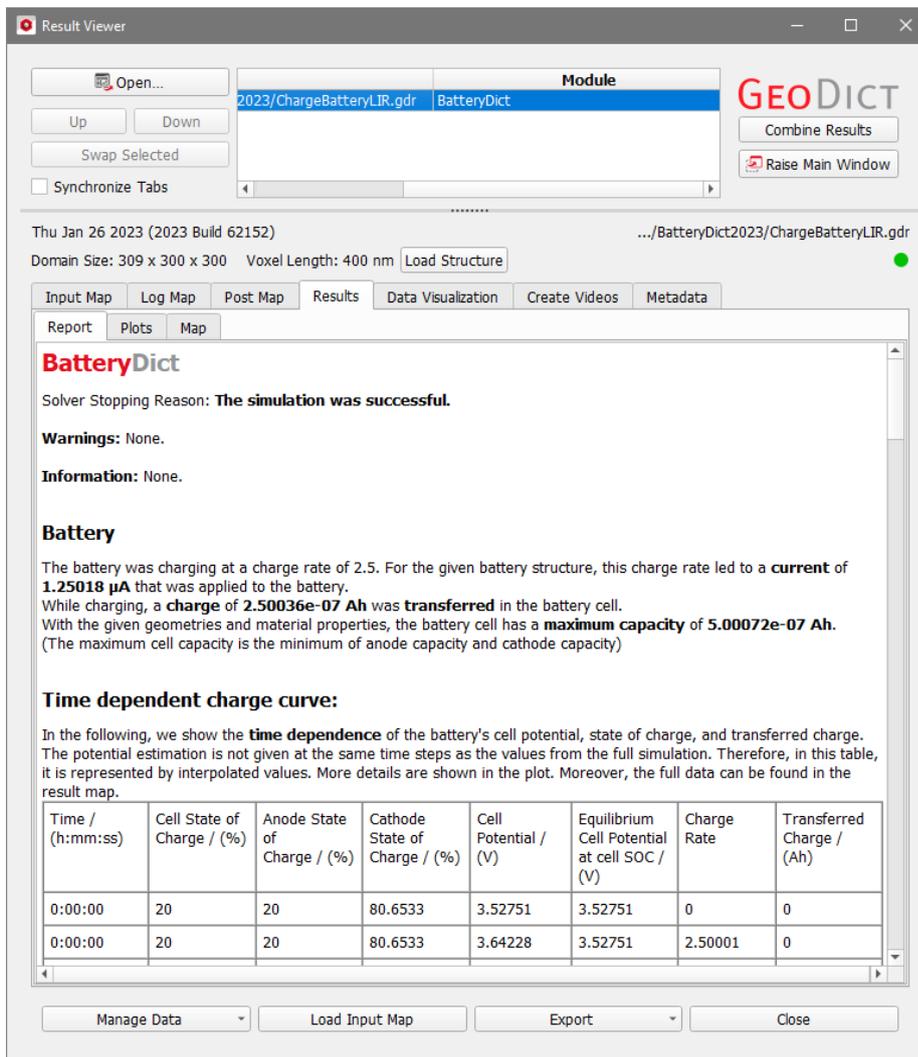


On the tab **Log Map**, the runtime and memory used for the simulation, as well as information about the machine, are shown.

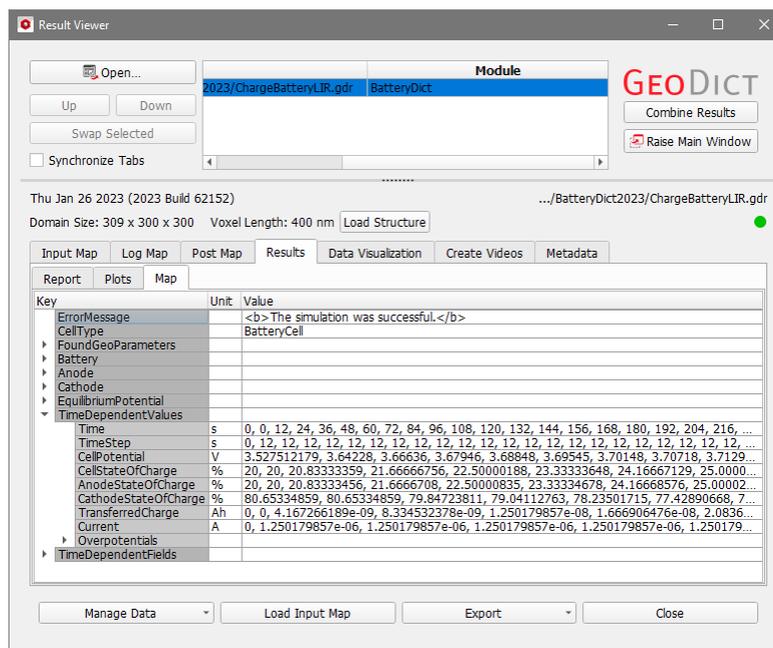


The **Post Map** tab lists information about plots shown in the **Results** tab. Parameters chosen for the plots as well as data for the graphs are shown here.

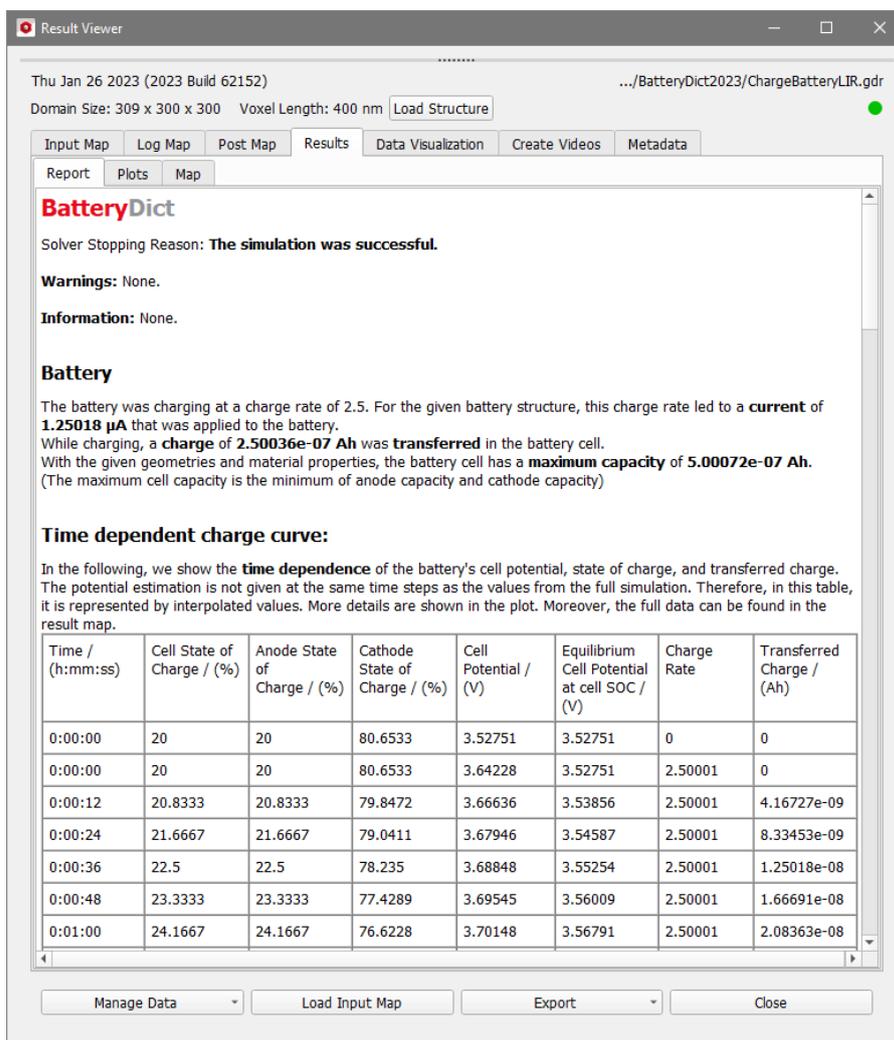
The **Results** tab shows the results of the computation in several forms.



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



In the **Results - Report** subtab, part of this information is shown, with explanations about the computation results. The table **Time dependent charge curve** shows part of the time dependent values in a clearly arranged way.



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 is shown there.

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

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

$$C_{B,max} = \min(C_{A,max}, C_{C,max}),$$

with

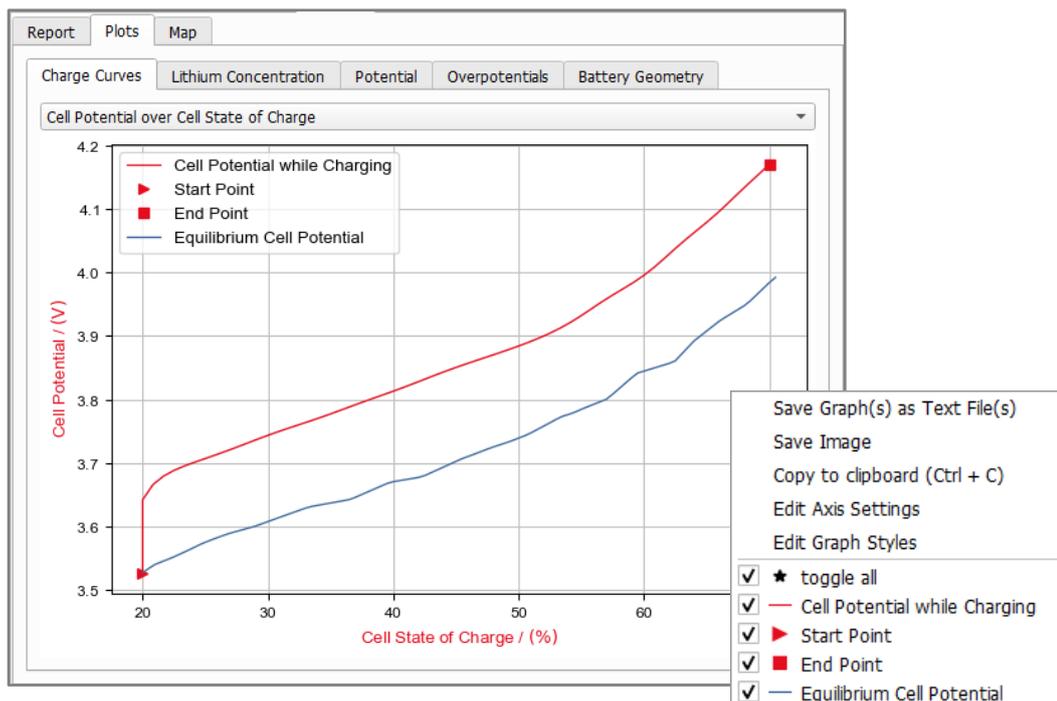
$$C_{A,max} = l_V^3 * F * \sum_{V \in \{Anode \ Active \ Material \ Voxels\}} c_{max}(V)$$

and

$$C_{C,max} = l_V^3 * F * \sum_{V \in \{Cathode \ Active \ Material \ Voxels\}} c_{max}(V)$$

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

Under the **Results - Plots** subtab, several standard plots for the visualization of the **BatteryDict** simulation results are available: On the tab **Charge Curves**, **Cell Potential**, **Cell State of Charge**, **Cell Capacity Density**, **Charge Rate**, **Current Density**, **Current** and **Transferred Charge** are plotted over **Time**. Additionally, the **Cell Potential** and the **Electrode State of Charge** can be plotted over the **Cell State of Charge** and the **Cell Potential** over the **Cell Capacity Density**.



Clicking the right mouse button, allows to change properties of each plot shown, to save the image or to copy the values to the clipboard. Graphs shown can be switched on and off there as well.

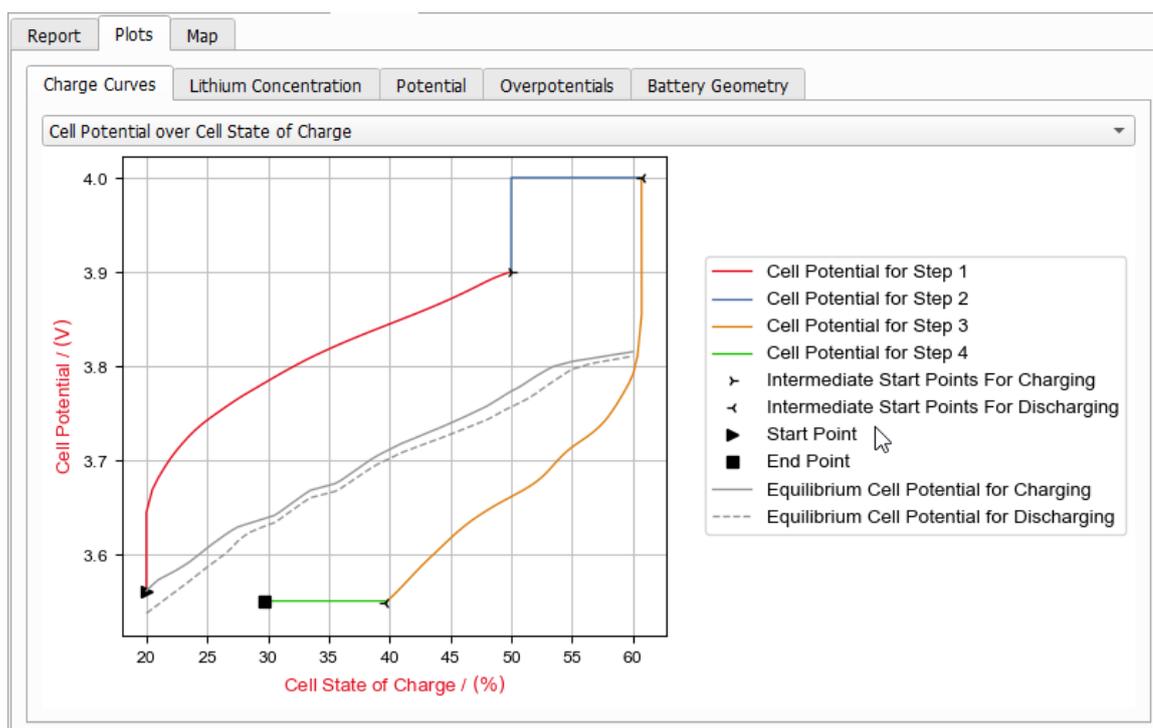
In the **Cell Potential over Cell State of Charge** plot (above), the cell potential while charging or discharging is compared to the cell potential in equilibrium, i.e., while loading in infinite time. While charging or discharging the battery infinitely slow, the battery is always in equilibrium state.

In contrast to this, charging or discharging the battery in finite time, the battery is not in equilibrium state anymore. Charging curves have therefore always higher values than the equilibrium curve, i.e., charging the battery requires a higher potential than the optimum one. Discharging curves are always below the equilibrium curve.

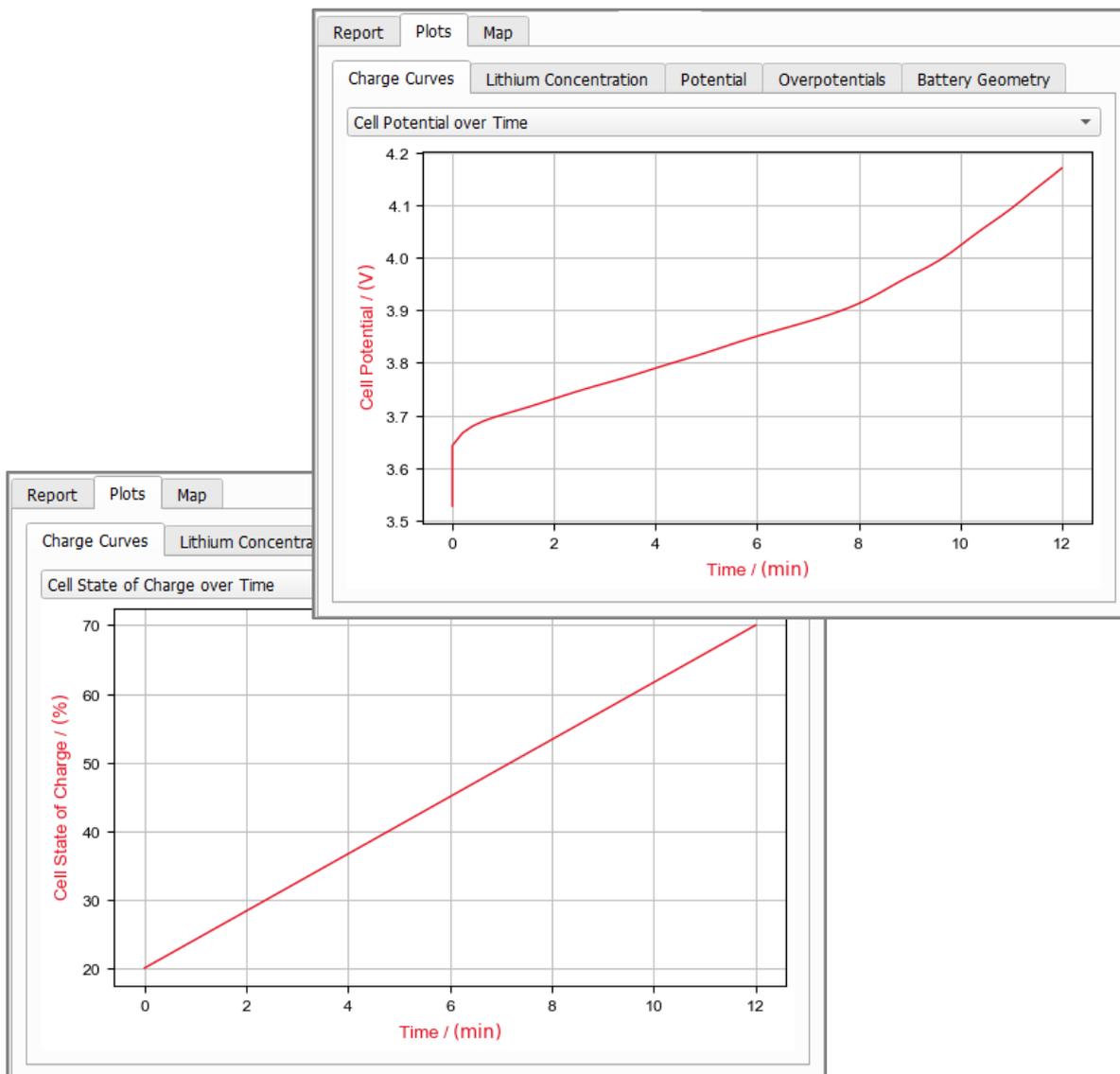
If [Calculate Estimation Only](#) was chosen as option, the estimation of the cell potential is shown instead of the computed time evolution of the potential.

In case a charging profile was selected for the simulation (see page 44), the cell potential is shown for each simulation step 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.



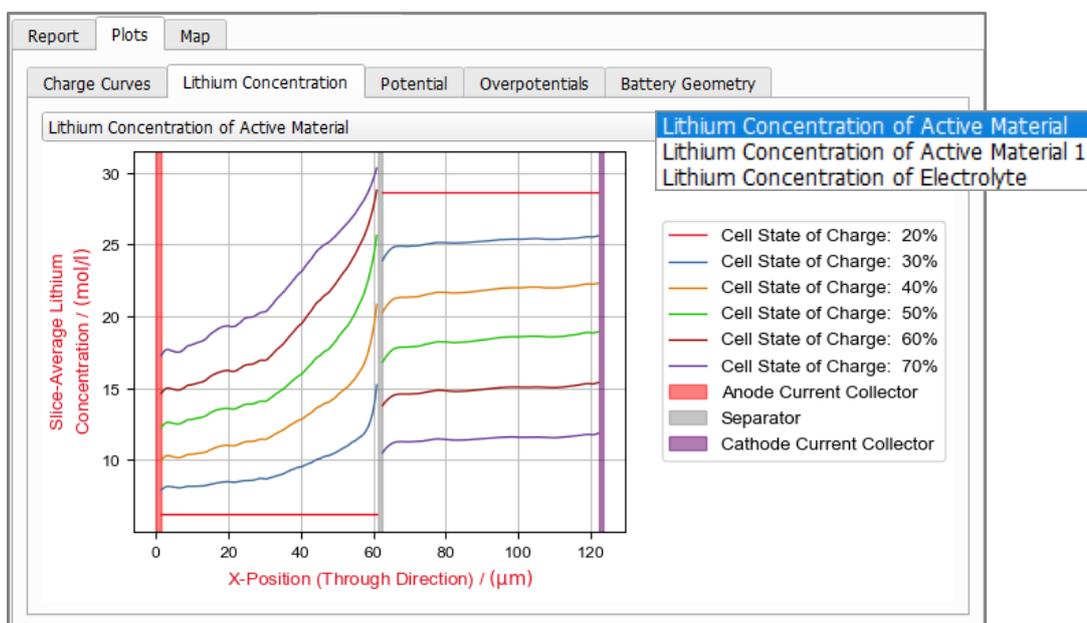
Due to the simulation with a constant charge rate and without the selection of an upper cut-off voltage in the example shown, the state of charge increases linearly with the simulated time. The trend of the cell potential over time is therefore the same as for the **Cell Potential over Cell State of 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 **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.).

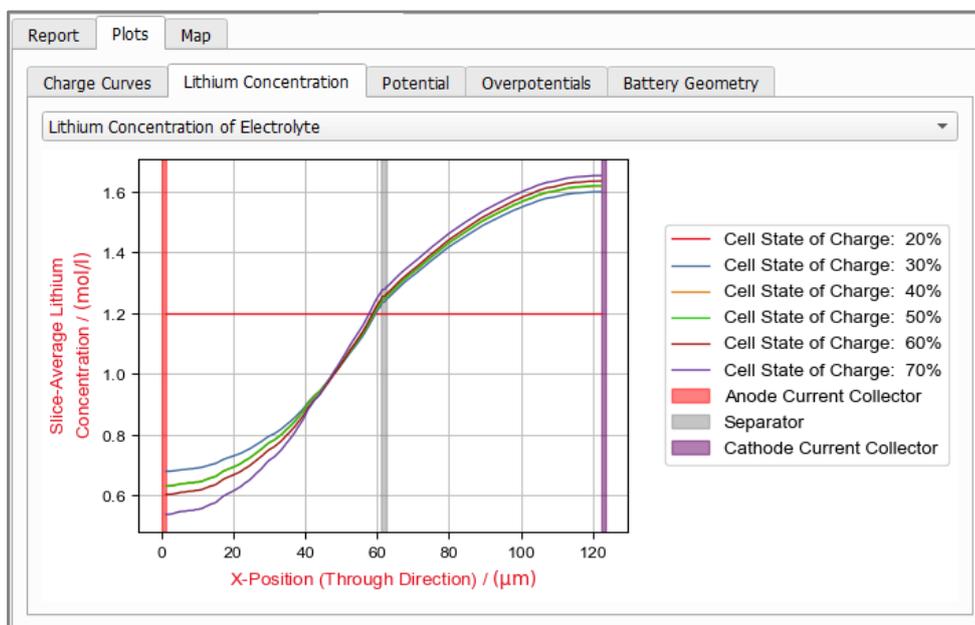
A separate curve is shown in these plots for each state of charge with an intermediate result available. As can be seen in the following plot, the concentration of lithium ions in the cathode (right-part of the plot) is decreasing during charging of the battery, while the concentration in the anode is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



In 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.

During charging, the cathode releases Li-ions into the electrolyte. Therefore, the Li-ion concentration grows in the electrolyte on the cathode side. At the same time, the Li-ions intercalate into the anode.

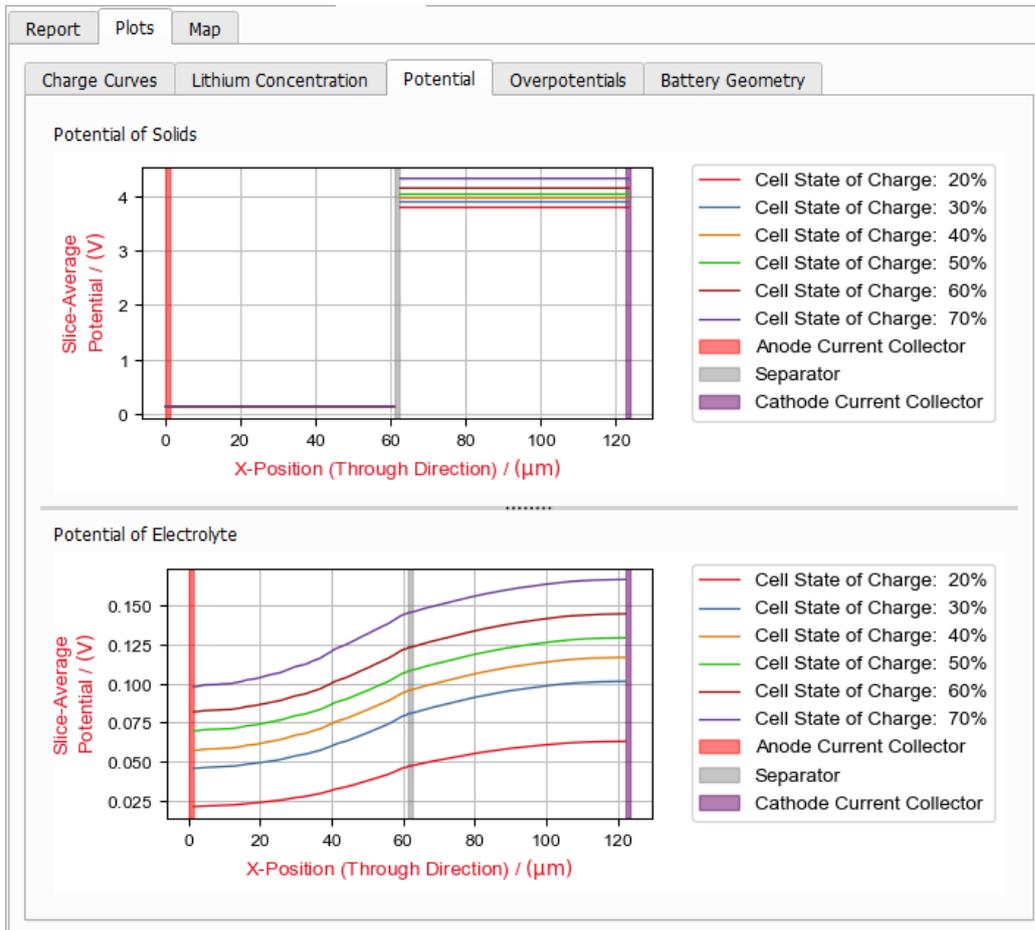
Since, the diffusion of the Li-ions takes some time, the gradient of the Li-ion concentration in the electrolyte is visible in the example.



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. Again, for each state of charge with an intermediate result available, a separate curve is shown in the plot. Click the right mouse button in the plot to change view settings.

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

In the example shown, 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.

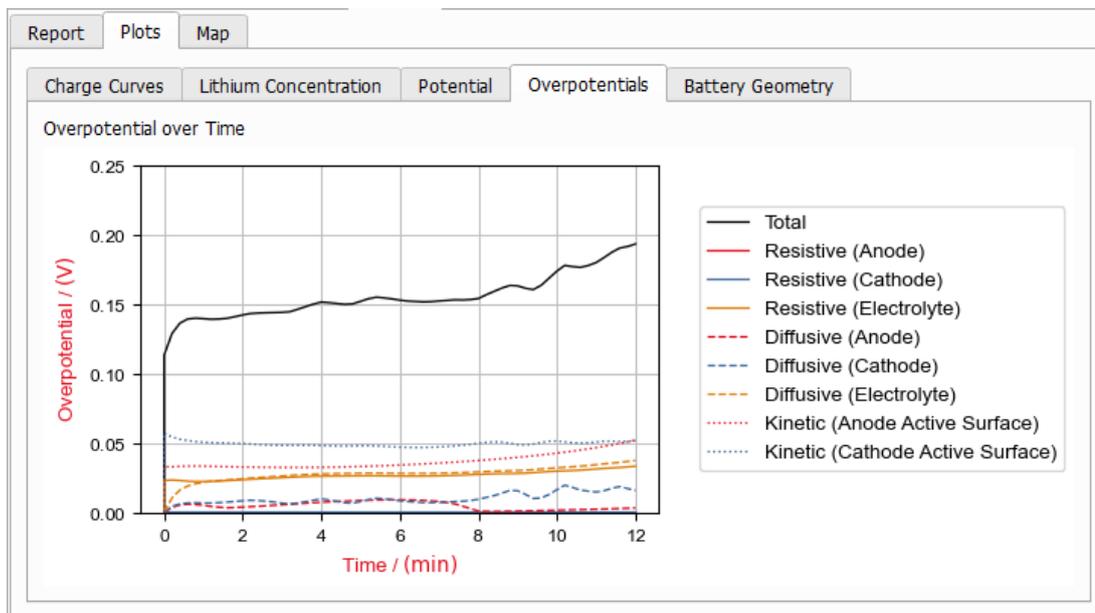


The current is only dependent on the potential difference and not on the total potential offset. The latter can be chosen freely.

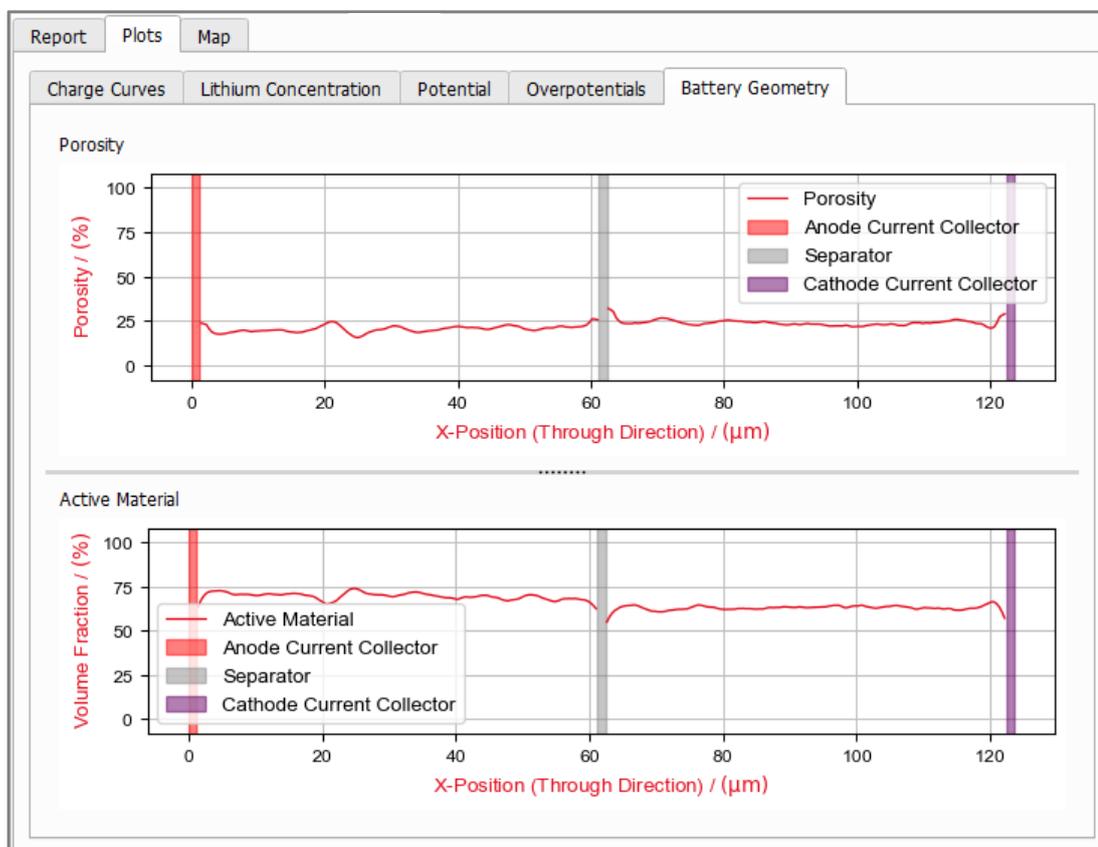
For the potential of the electrolyte, a gradient is visible between the anode current collector and the cathode current collector. This gradient is increasing for higher charge rates and the potential grows from left to right. This is caused by the charge current that is driven by the ions resolved in 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.

Note that the **Lithium Concentration** and the **Potential** subtabs of the **Plots** tab do not exist for simulation results computed with BESTmeso. For the meso scale simulation, the voxel and slice based information shown on this two tabs is not available.

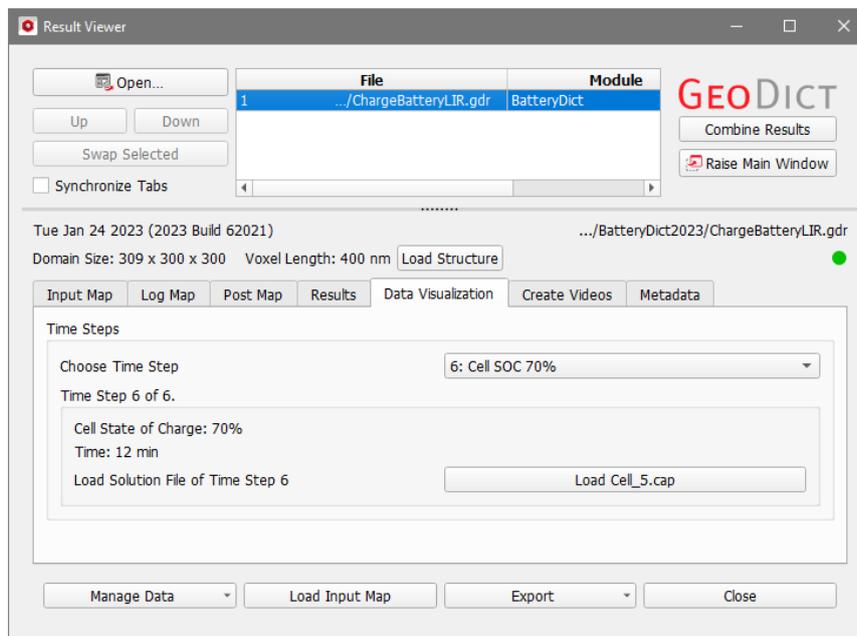
On the **Overpotentials** tab, the evolution of the different overpotentials over time is visualized. For an explanation of the overpotentials see page [12](#).



The **Battery Geometry** tab shows the mean of porosity and the volume fraction of active material for each slice in y- and z-direction.



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](#) (see above).

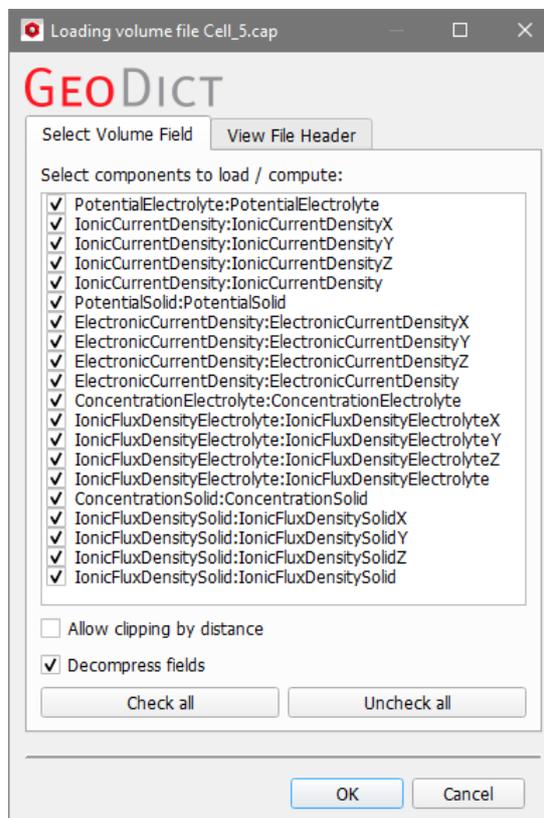


For instance, let us select the solution file at a state of charge of 70%. For the example shown here, we just need to select step 6. By clicking **Load Cell\_5.cap**, the available volume fields (tab Select Volume Fields) of the file can be selected. Additionally, the user may have a look at the file header of the result file (View File Header).

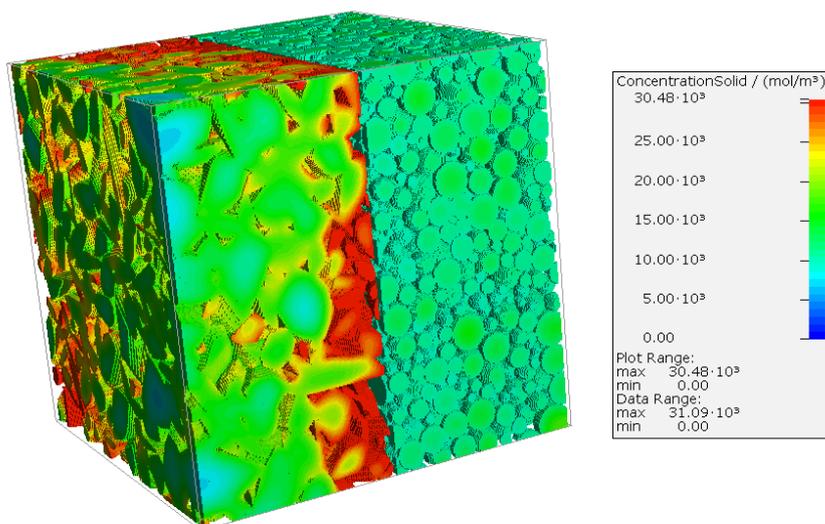
Volume Fields available depend on the solver used for the computation (LIR or BESTmicro) and on the fact whether porous binder is used or not.

Load, for example, only the concentration in the solid part of the battery.

In this case, first click **Uncheck all**. Select **ConcentrationSolid:ConcentrationSolid**. After clicking **OK**, the selected field is loaded into the **GeoDict** GUI.



The concentration field of lithium ions for the active materials is visualized here. More information on visualization of results is available in the [Visualization](#) handbook of this User Guide.



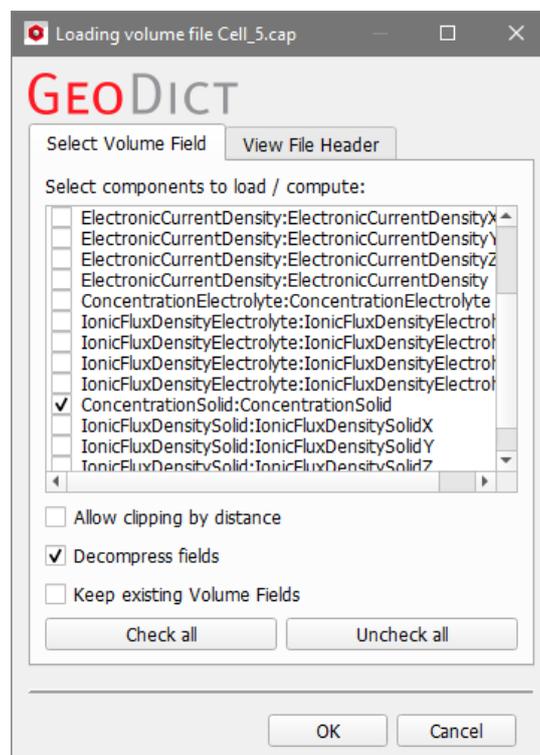
The concentration gradient in the anode (left part of the battery) is in the example shown higher as in the cathode (right part of the battery).

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.

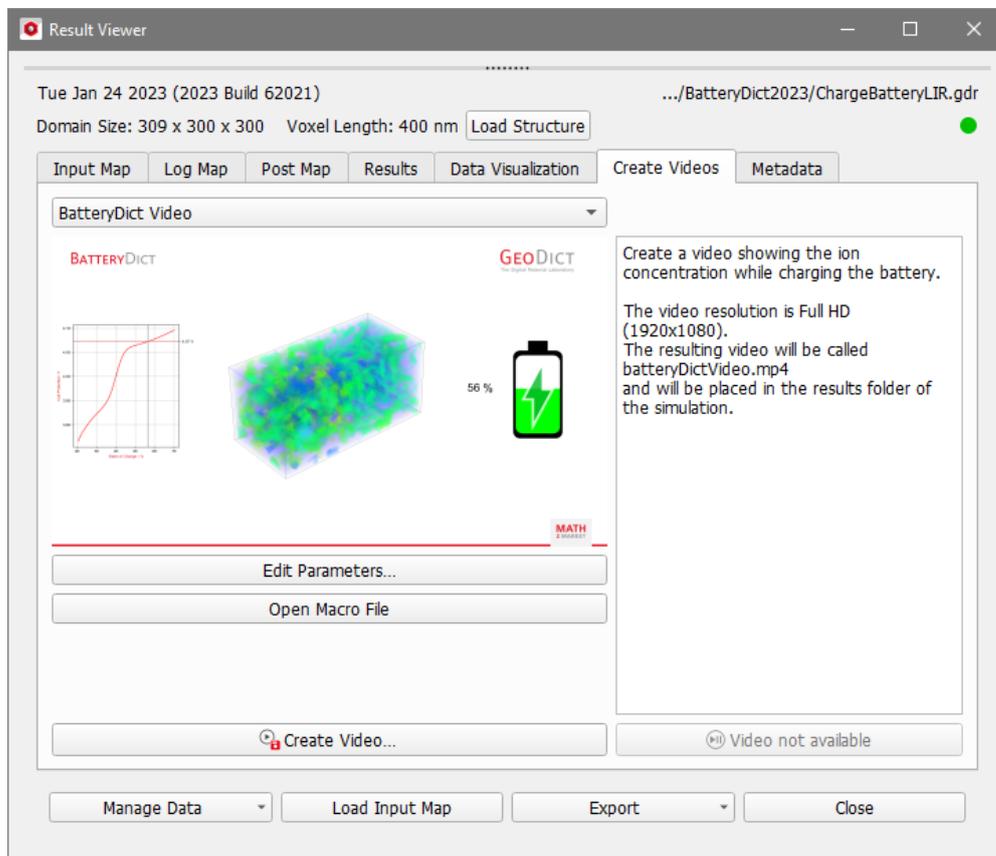
Check **Keep existing Volume Fields** if you repeat loading result fields for another time step or have other previously loaded volume fields in memory that you want to keep. If this box is not checked, previously loaded volume fields are discarded.

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.

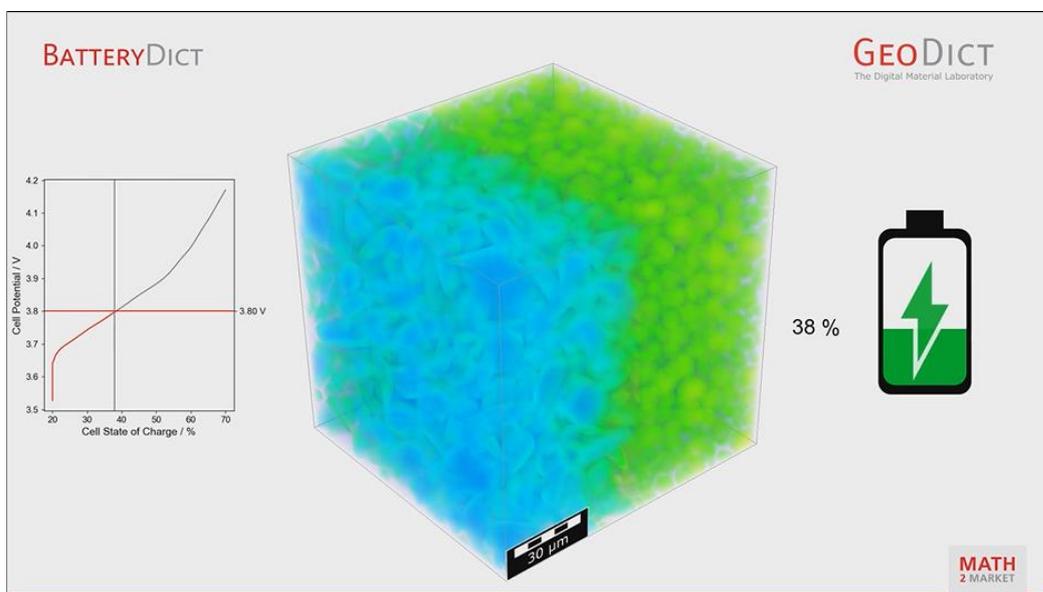


Through the **Create Videos** tab, a video showing the ion concentration while charging or discharging of the battery can be created. The first part of the video shows the cropping of the battery structure together with the ion concentration at the start of the simulation.



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

A screen shot of such a video is shown here. The left side of the video shows a graph of the cell potential over state of charge. The actual state of charge value is displayed there. In the middle, the ion concentration in the battery structure is shown. On the right, the actual state of charge of the battery is shown schematically.



Click **Open Macro File**, under the **Create Videos** tab, to open the GeoDict Python macro used to create the video, if you are interested in modifying it with a text editor.

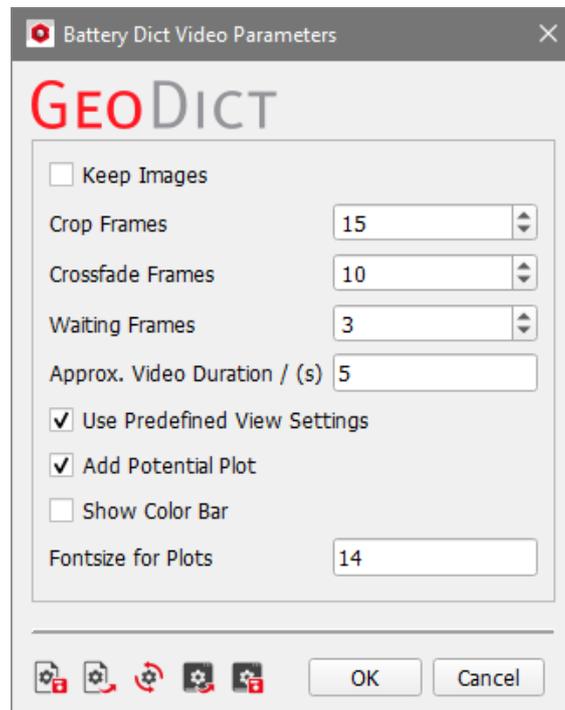
Click **Edit Parameters...** to modify the default settings of the video creation.

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 field. The shorter the time defined here, the faster the charging is shown in the video.

**Waiting Frames:** A higher number here means 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 GUI.

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**.

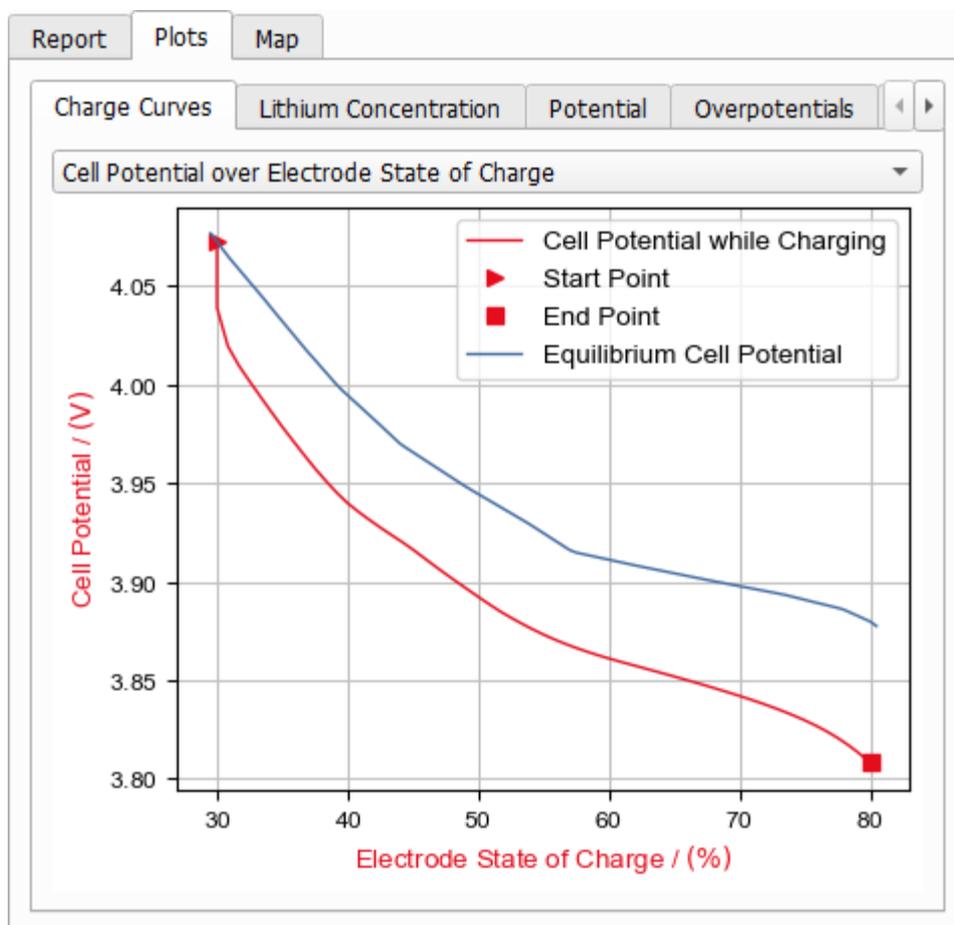
If the video is created, the **Play Video** button is activated on the **Create Videos** tab.

## RESULTS OF CHARGE HALF CELL

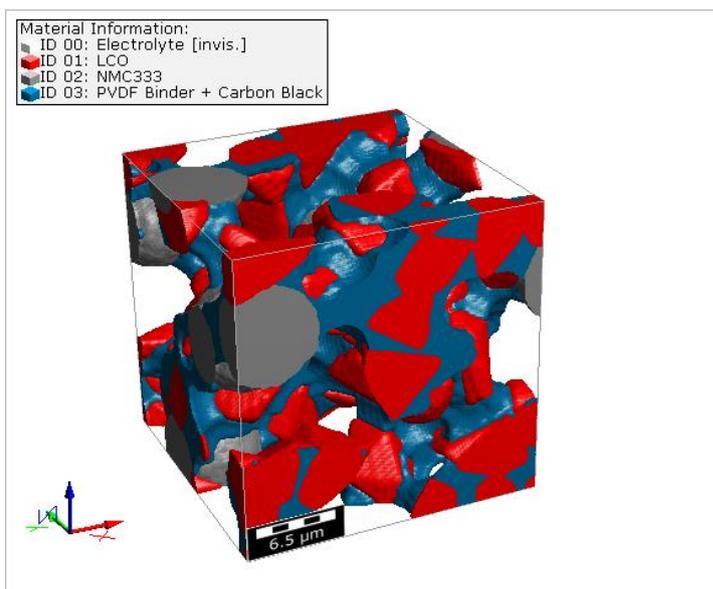
When the simulation of charging the half-cell has finished, a GeoDict result file (.gdr) is available in the project folder and the Result Viewer of this result file automatically opens.

For the charging simulation of a half cell, the same information as for charging a whole battery is available in this result file. It is shown and can be visualized or further processed in the same way, see page 77ff.

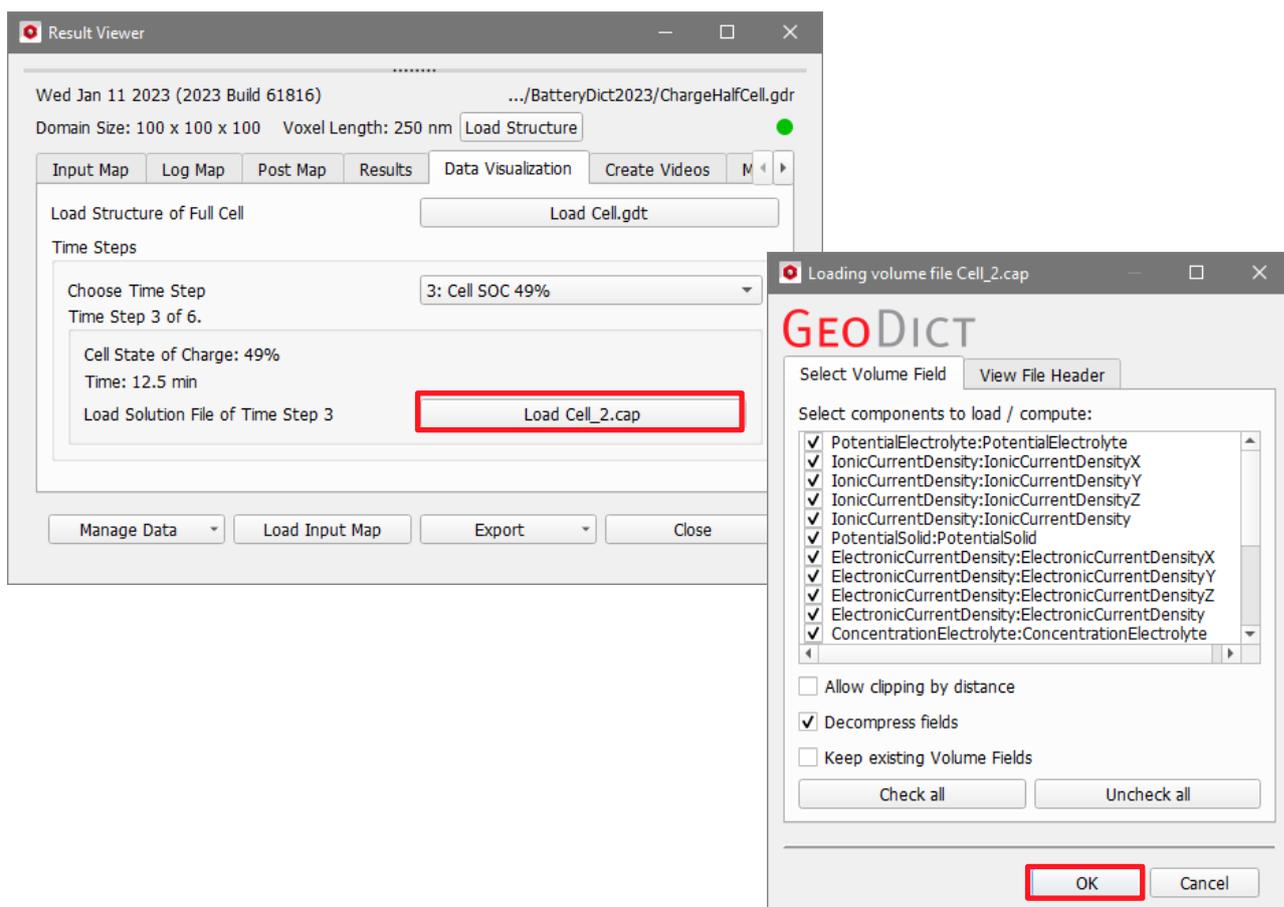
Note that for the charging simulation of a half cell, the modelled electrode is electrochemically always considered as the cathode (see page 54). Charging the cathode, i.e. increasing the electrode state of charge, means discharging the half-cell. On the **Results -Plots – Charge Curves** subtab the cell potential is shown over the electrode state of charge and is therefore decreasing during the charging simulation of the half-cell.

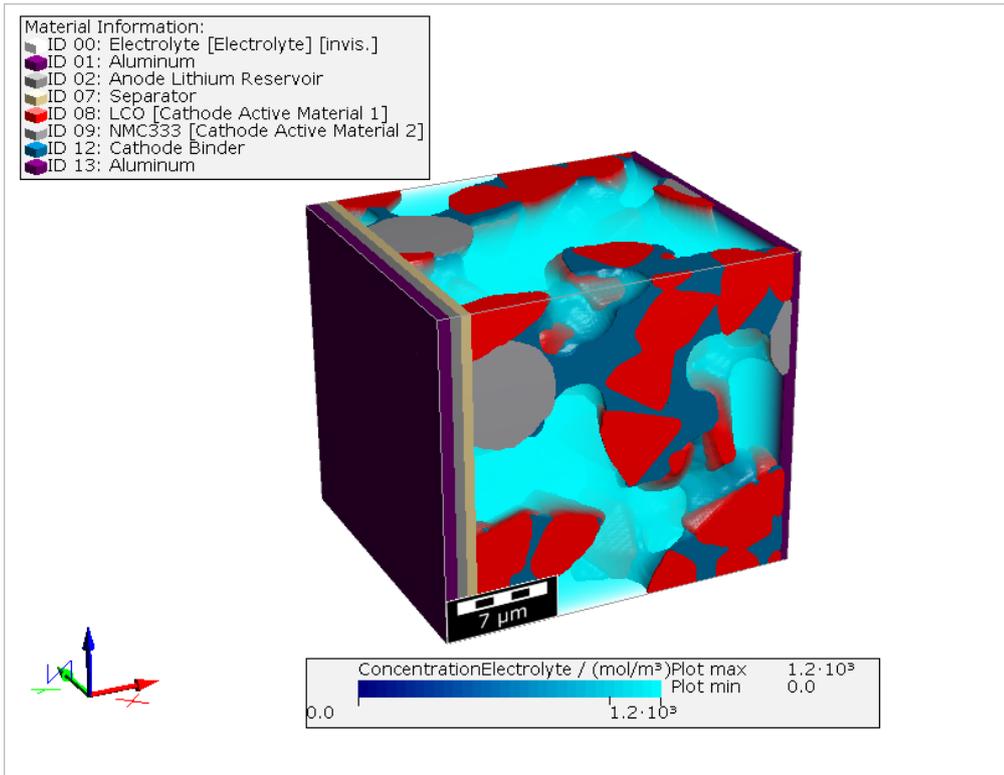


Note also, that in the volume files of the simulation (\*.cap files), the result fields are stored for the whole half-cell structure (electrode, both current collectors, separator and lithium reservoir), and not for the electrode alone. If the structure used as input for the simulation (and shown in 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.



If one or more volume field(s) are loaded on the **Data Visualization** tab, the structure shown in the Visualization area is therefore extended to contain the missing half-cell components as well.





## RESULTS OF A DEGRADATION SIMULATION

If the degradation simulation finished successfully, the GeoDict Result Viewer opens for the result file (\*.gdr file created).

The screenshot shows the 'Result Viewer' window for a simulation titled 'BatteryDegradation'. The window displays the following information:

- File: .../BatteryDict2023/BatteryDegradation.gdr
- Domain Size: 309 x 300 x 300, Voxel Length: 400 nm
- Simulation based on: BatteryDict:ChargeBattery result file ChargeBatteryLIR.gdr.

The 'Results' tab is active, showing a 'Report' section with two tables:

### Average Strain

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	0.0094639	0.00063168	0.00070602	-0.0001842	-0.00059112	8.2745e-05	0.0088616	0.0036005

### Average Stress

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	-4.2498e-07	-3.5564e-07	-3.4932e-07	0.00066331	-0.0047214	0.00013137	0.0082611	-3.7665e-07

**References:**

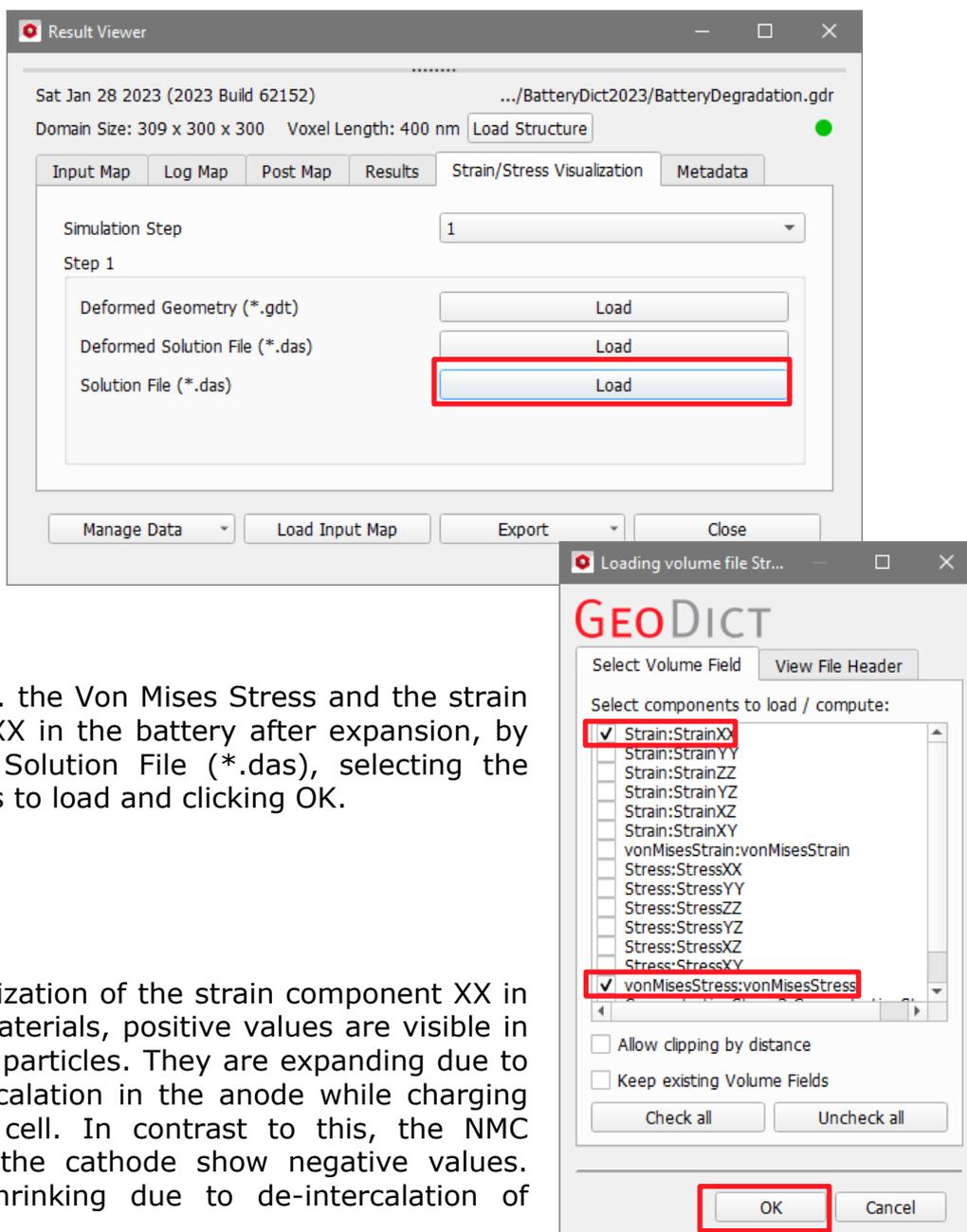
[1] Nils Wenzler, Sebastian Rief et al; 2023; 3D electrochemical-mechanical battery simulation tool: implementation with full cell simulations and verification with operando x-ray tomography; Accepted Manuscript.

--- Total runtime: 2.22592 h, Total memory usage: 17.019 GiB ---

At the bottom of the window, there are buttons for 'Manage Data', 'Load Input Map', 'Export', and 'Close'.

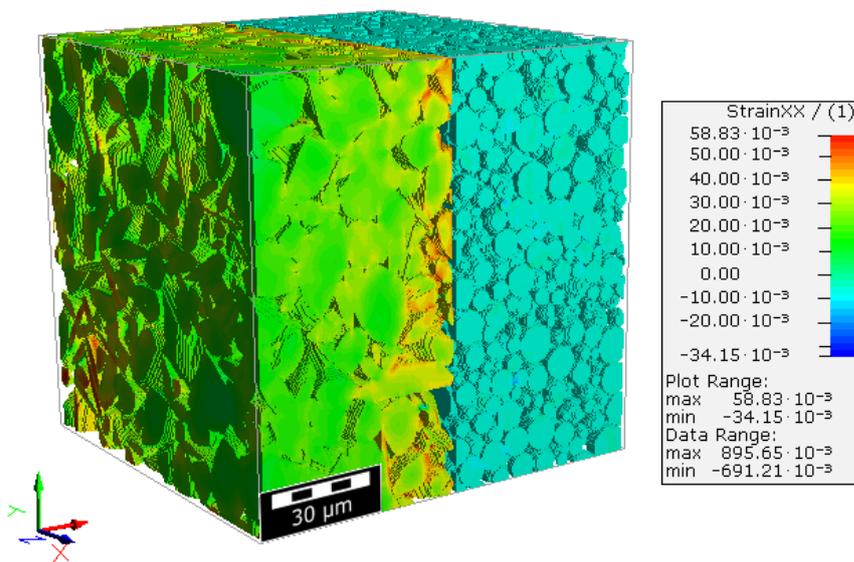
On the **Results** tab, the **Report** shows the average strain and stress tensor as well as the average Von Mises and hydrostatic strain and stress for each computation step.

On the **Strain/Stress Visualization** tab, the volume fields for each simulation step can be loaded by clicking on the **Load button** for Solution File (\*.das). If the deformed geometry and the volume fields for the deformed geometry are written to the hard disk (see page 66), they can be loaded for visualization here as well. For details on the (deformed) solution files, we refer to the [ElastoDict](#) handbook of the GeoDict User Guide.

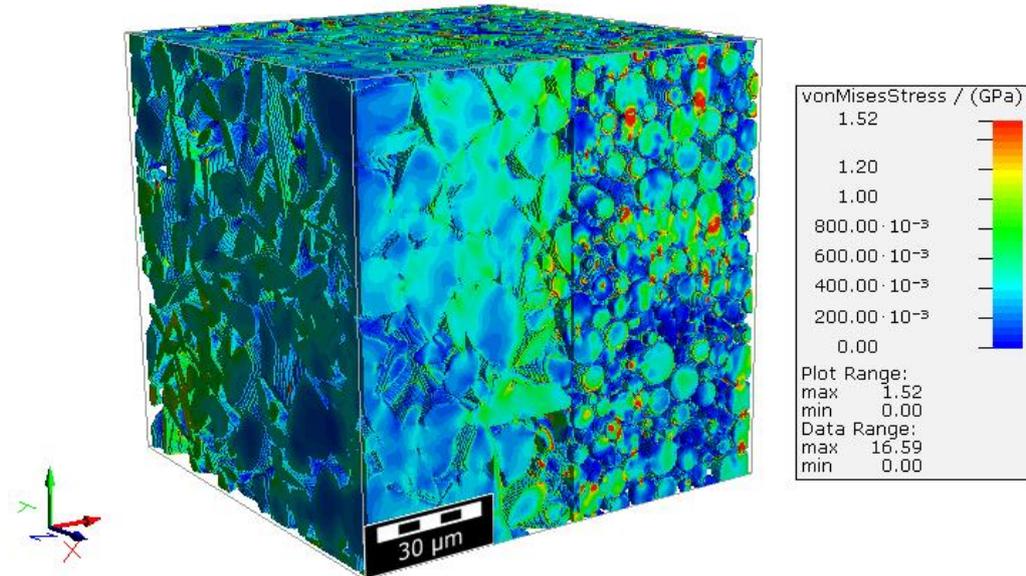


Visualize e.g. the Von Mises Stress and the strain component XX in the battery after expansion, by loading the Solution File (\*.das), selecting the volume fields to load and clicking OK.

In the visualization of the strain component XX in the active materials, positive values are visible in the graphite particles. They are expanding due to lithium intercalation in the anode while charging the battery cell. In contrast to this, the NMC particles in the cathode show negative values. They are shrinking due to de-intercalation of lithium.

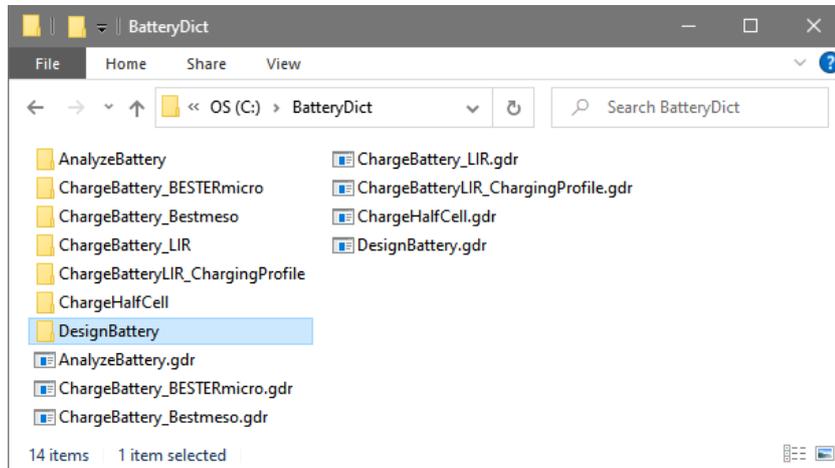


The Von Mises Stress in the cathode, shows its highest values at the boundary of the NMC grains where they are in contact to neighboring grains. This is reasonable since breaking contacts during shrinking of the active material is not yet possible in BatteryDict-Degradation.



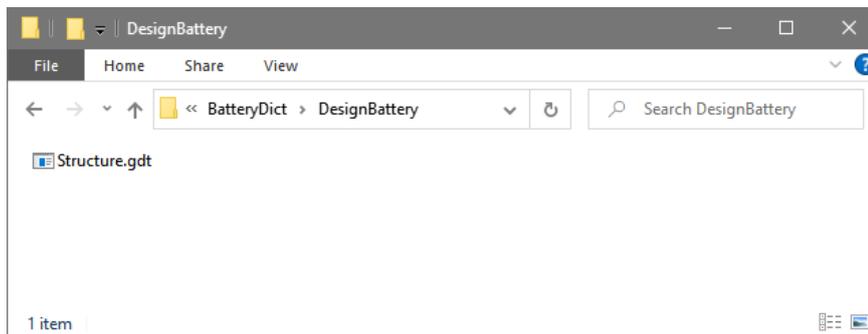
### RESULT FOLDERS

After designing a battery or running a charging simulation with BESTmicro or LIR, result files and the corresponding result folder are found in the project folder.



### DESIGN BATTERY FOLDER

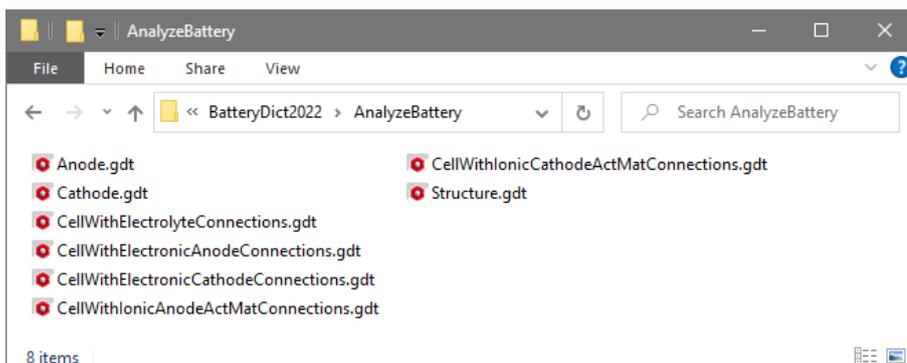
After the generation of a battery structure, a **GeoDict** result file (.gdr) is created in the selected project folder. A subfolder with the same name as the result file contains the generated battery structure.



The result file (.gdr) can be loaded at any time by selecting **File** → **Open Results (\*.gdr) ...** in the menu bar.

### ANALYZE BATTERY FOLDER

In the folder created for a battery analysis, the input structures used for both electrodes, as well as **GeoDict** structure files showing electronic and ionic connections in the active materials, the electrolyte and the binder and carbon black are available.



## BESTMICRO: THE CHARGE BATTERY FOLDER

After running a charging simulation with BESTmicro or BEST:er-micro, a GeoDict result file (.gdr) is created in the selected project folder. A subfolder with the same name as the result file contains three subfolders called **SolverConfig**, **SolverConfig0** and **SolverOutput**.



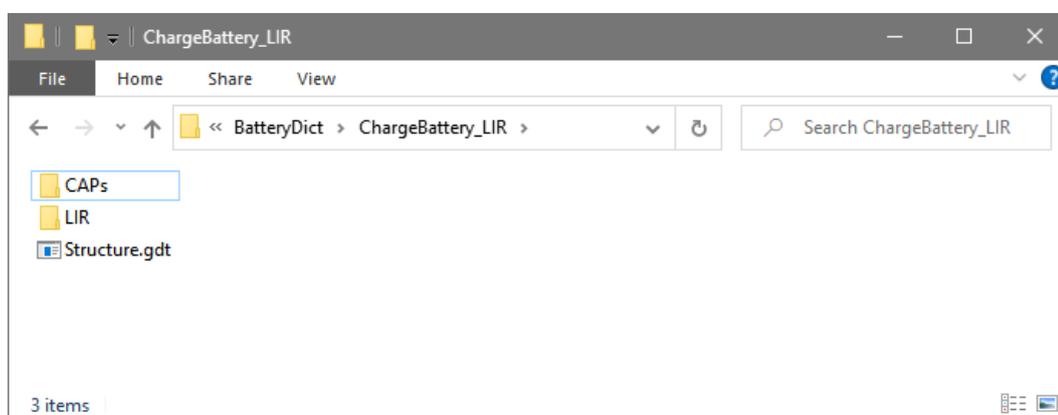
**SolverConfig** and **SolverConfig0** contain files with the input parameters for the charging simulation.

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

The additional files as well as the two additional folders **configuration** and **geometry** in **SolverOutput** contain some internal solver information and cannot be loaded in the GeoDict GUI.

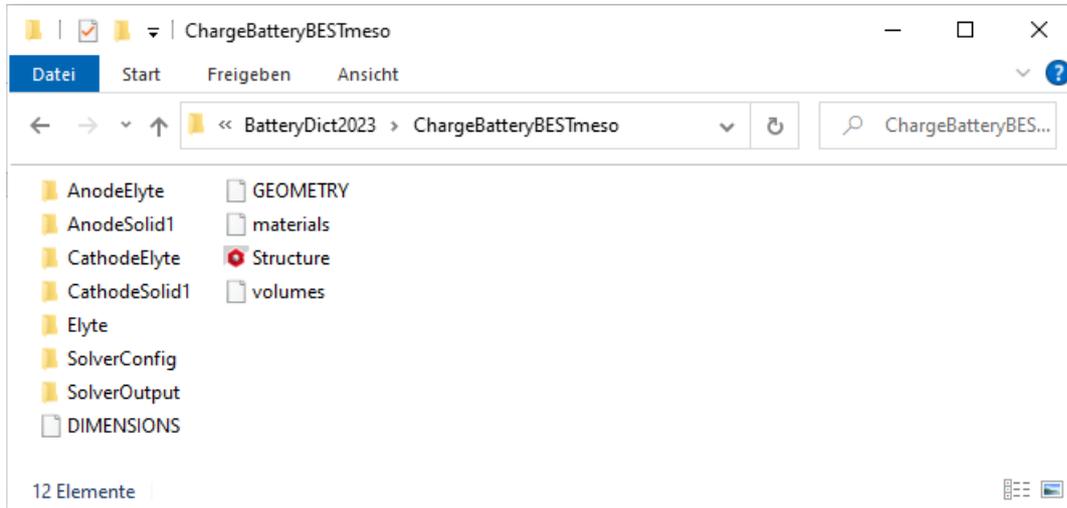
## LIR: THE CHARGE BATTERY FOLDER

If the charging simulation was run with LIR solver, the result folder contains two subfolders. The folder **CAPs** contain 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 CHARGE BATTERY FOLDER

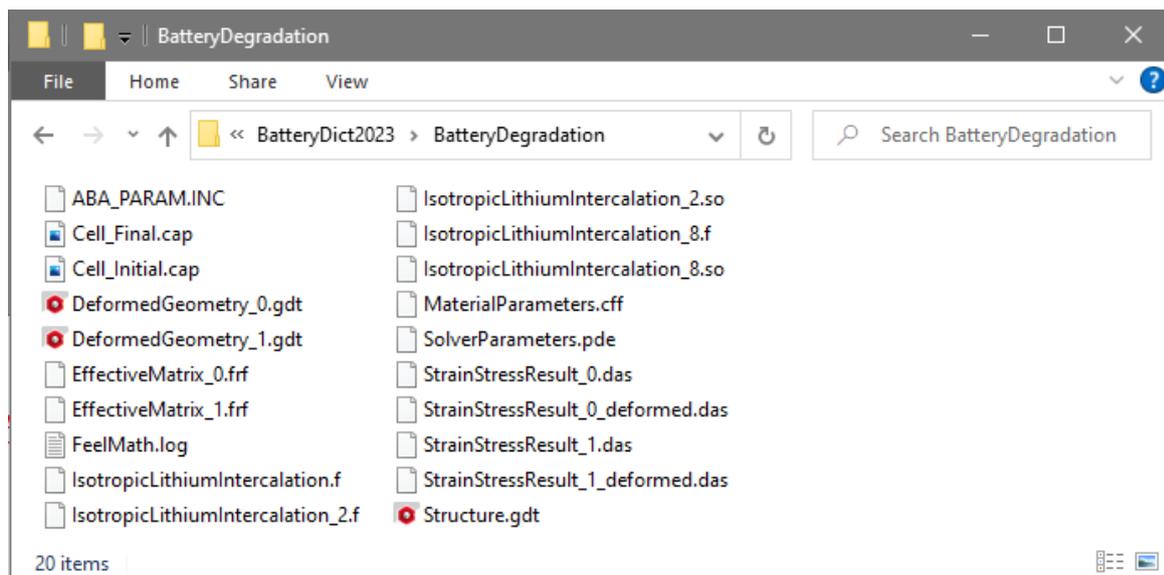
The result folder of a meso-scale simulation with BESTmeso contains subfolders with information about the solver configuration and output. Additionally, subfolders with the effective material parameters of electrolyte and active materials, derived from the microstructure, are available.



## DEGRADATION 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 tab, see page 66, 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.



## References

- [1] Latz, Arnulf, and Jochen Zausch. "Thermodynamic consistent transport theory of Li-ion batteries." *Journal of Power Sources* 196.6 (2011): 3296-3302.
- [2] J. Newman, K. Thomas-Alyea. *Electrochemical systems*, 2004, Wiley, ISBN 3175723993
- [3] A. Latz and J. Zausch. Thermodynamic derivation of a Butler–Volmer model for intercalation in Li - ion batteries. *Electrochim. Act.*, 110:358–362, 2013
- [4] Weppner, W. R. A. H., and Robert A. Huggins. "Determination of the kinetic parameters of mixed-conducting electrodes and application to the system Li<sub>3</sub>Sb." *Journal of The Electrochemical Society* 124.10 (1977): 1569.
- [5] Ecker, Madeleine, et al. "Parameterization of a physico-chemical model of a lithium-ion battery: I. Determination of parameters." *Journal of The Electrochemical Society* 162.9 (2015): A1836.
- [6] Schmalstieg, Johannes, et al. "Full cell parameterization of a high-power lithium-ion battery for a physico-chemical model: Part I. Physical and electrochemical parameters." *Journal of The Electrochemical Society* 165.16 (2018): A3799.
- [7] Schmalstieg, Johannes, and Dirk Uwe Sauer. "Full cell parameterization of a high-power lithium-ion battery for a physico-chemical model: Part II. Thermal parameters and validation." *Journal of The Electrochemical Society* 165.16 (2018): A3811.
- [8] Barai, Anup, et al. "A study of the open circuit voltage characterization technique and hysteresis assessment of lithium-ion cells." *Journal of Power Sources* 295 (2015): 99-107.
- [9] Nitta, Naoki, et al. "Li-ion battery materials: present and future." *Materials today* 18.5 (2015): 252-264.
- [10] Wenzler, Nils et al, 3D electrochemical-mechanical battery simulation tool: implementation with full cell simulations and verification with operando x-ray tomography, 2023, Accepted Manuscript, *Journal of the Electrochemical Society* 170 020511, <https://doi.org/10.1149/1945-7111/acb5c9>

## References for comparisons of BESTmicro with experiments

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- [12] T. Danner et al. Thick electrodes for Li-ion batteries: A model based analysis, *J. Power Sources* 334, 191-201 (2016).
- [13] M. A. Cabañero et al. Investigation on the temperature dependence of lithium plating in commercial Li-ion batteries, *Electrochimica Acta* 171, 1217-1228 (2017).

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