

BATTERYDICT

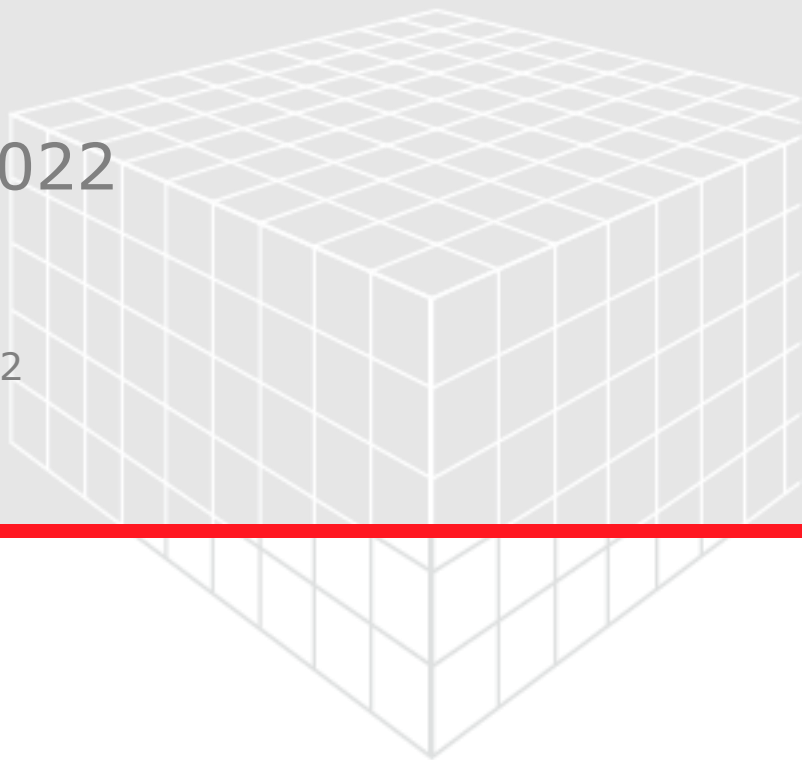
User Guide

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GEO DICT

BATTERYDICT - CHARGING & DISCHARGING SIMULATIONS FOR LI-ION BATTERIES

1

THEORETICAL BASIS	3
STATE OF CHARGE (SOC)	3
BATTERYDICT - SIMULATION OF CHARGING AND DISCHARGING PROCESS	5
BOUNDARY CONDITIONS AT THE CURRENT COLLECTORS	7
STOPPING CRITERIA FOR CHARGING SIMULATIONS	7
OVERPOTENTIALS IN BATTERY CHARGING SIMULATIONS	8
SIMULATION PARAMETERS	10
Tested parameter space	10
Overlapping OCV Curves for Several Active Materials	12
BATTERYDICT COMPUTATIONS	14
DESIGN BATTERY	15
Geometry	15
Anode and cathode	17
Setting up a Half-Cell simulation	18
More flexible geometries	19
ANALYZE BATTERY	20
CHARGE BATTERY	21
Constituent Materials	21
Parameter Options Dialogs	25
Experiment	30
Solver	34
Parallelization Benchmark Results	37
Output Options	39
Equations & References	40
CHARGE HALF CELL	41
Constituent Materials	41
Experiment	44
Solver, Output Options and Equations & References Tab	44
Parallelization Benchmark Results	45
CONTINUE INTERRUPTED SIMULATION	46
BATTERYDICT COMPUTATION RESULTS	47
RESULTS OF DESIGN BATTERY	47
RESULTS OF ANALYZE BATTERY	53
RESULTS OF CHARGE BATTERY	55
RESULT FOLDERS	70
DesignBattery folder	70
AnalyzeBattery folder	70
ChargeBatteryBESTmicro folder	71
LIR: the charge battery folder	71

BATTERYDICT - CHARGING & DISCHARGING SIMULATIONS FOR LI-ION BATTERIES

BatteryDict simulates the performance of secondary lithium-ion batteries during charging and discharging on the micro 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 in **BatteryDict** is composed of four different components: cathode, anode, separator, and the current collectors. The last two are represented as standardized layers, whereas the cathode and anode are individually modeled structures, consisting of multiple active materials, binder, and electrolyte. Since **GeoDict** 2020, it is possible to perform a half-cell simulation, by modelling cathode or anode as a lithium reservoir. Up to four different active materials can be handled for each electrode. Additionally, since **GeoDict** 2021, the LIR solver is available in **BatteryDict** as well, reducing considerably runtimes and memory consumption of battery simulations.

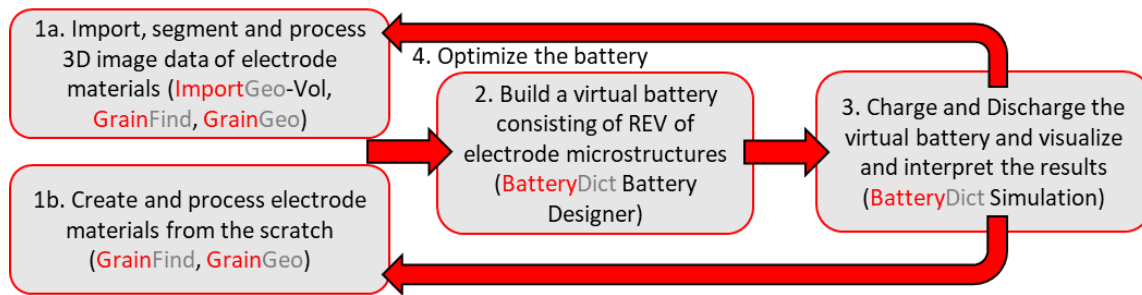
From **GeoDict** 2022 on, it is now possible to perform half-cell simulations for single electrode structures. Furthermore, it is now possible to define charging profiles with different stopping criteria. This functionality is especially useful to simulate consecutive charging and discharging processes in the battery.

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

The model used for simulation and the parameters to be defined are explained in more detail in the section *Theoretical Basis* (page [3](#)). In the section *BatteryDict Computations* (page [14](#)), 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* (page [47](#)).

The characteristic application for **BatteryDict** is to simulate and optimize the charging performance of a battery cell, based on realistic electrode microstructures. For analyzing or modeling electrode microstructures, also the use of other **GeoDict** modules is emphasized. Many properties of the microstructure, like porosity, pore size distribution, surface area, tortuosity, thermal conductivity, thermal flux, electric conductivity, electric flux, thermal expansion, permeability, diffusivity, etc. are vital for the performance of a battery. The **GeoDict** modules **FlowDict**, **GrainGeo**, **GrainFind**, **PoroDict**, **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 Li^+ ions initially stored in the active material of the cathode are transported to the anode side. During this process, the cathode active material is oxidized and Li^+ ions de-intercalate and diffuse through the electrolyte, towards the anode. This electrochemical process is induced by the applied charging potential, that drives the transport of free electrons through the cathode active material and through the binder with carbon black to the current collector. On the anode side, electrons flow from the current collector through the carbon black and active material. The active material of the anode is reduced by the Li^+ intercalation.

During discharging, Li^+ ions are transported in a corresponding process to the cathode side, while the electron flow powers the consumer device. The amount of lithium an electrode material can store per volume is defined as the volumetric energy density.

STATE OF CHARGE (SOC)

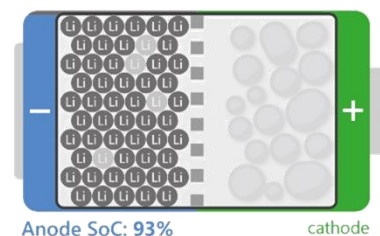
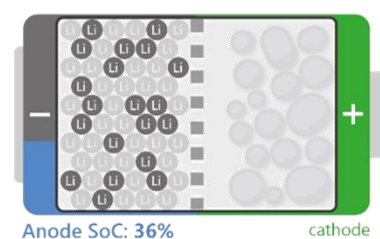
There are 3 different states of charge in a battery:

Anode state of charge: It measures the Li-ion content of the anode vs. 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 [10](#)).

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

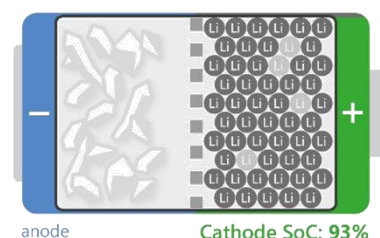
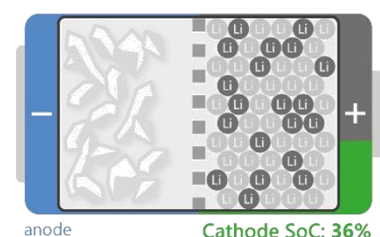
Anode State of Charge



Cathode State of Charge

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

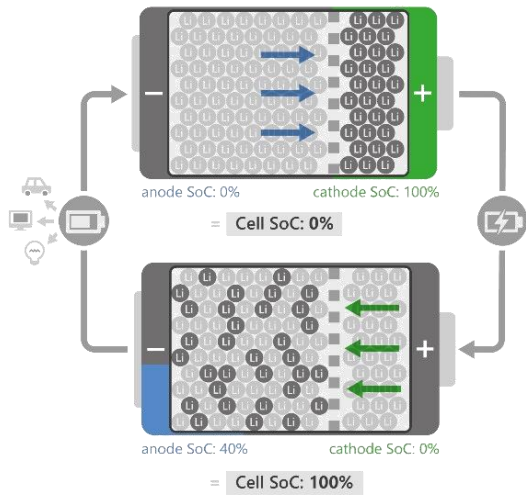
The cathode SOC is the mean value of the voxel SOC's of all active-material voxels in the cathode.



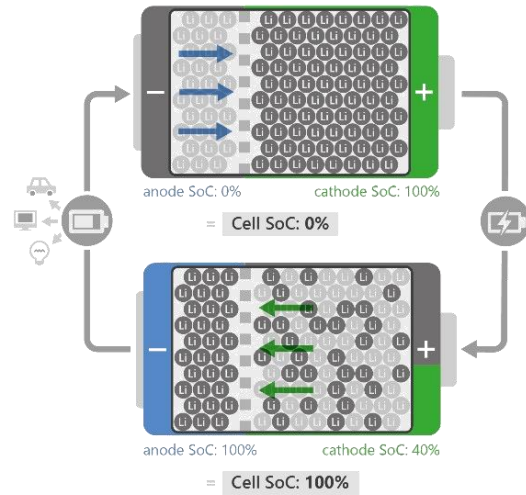
Charging and discharging simulations for Li-ion batteries

Cell state of charge: It describes the overall state of charge of the battery cell. It is 0% if the anode is empty *OR* the cathode is full. It is 100% if the anode is full *OR* the cathode is empty.

(Battery-)Cell State of Charge: **Anode has larger capacity**



(Battery-)Cell State of Charge: **Cathode has larger capacity**



For a half-cell simulation the lithium reservoir has always the same capacity as the other electrode.

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. The length scale considered in **BatteryDict** is above the scale where positive and negative charges can be resolved. Therefore, no free charges need to be considered. In the following, we shortly explain, how the principles of mass and charge conservation apply in the electrolyte and in the active material:

1. **In the electrolyte:** The movement of Li-ions is simulated in the whole electrolyte. Due to the mass conservation for Li-ions, the change of Li-ion concentration in time is equivalent to the divergence of the flux of the Li-ions. The movement of Li-ions, and therefore the flux, is driven by diffusion due to differences in Li-ion concentration and by migration, due to the applied current. In the case of constant Li transference number t_+ , the divergence of the migration is zero.

The current density of the electrolyte is given by gradients in the electric potential and in the Li-ion concentration. Due to the charge conservation, the sum of both is zero.

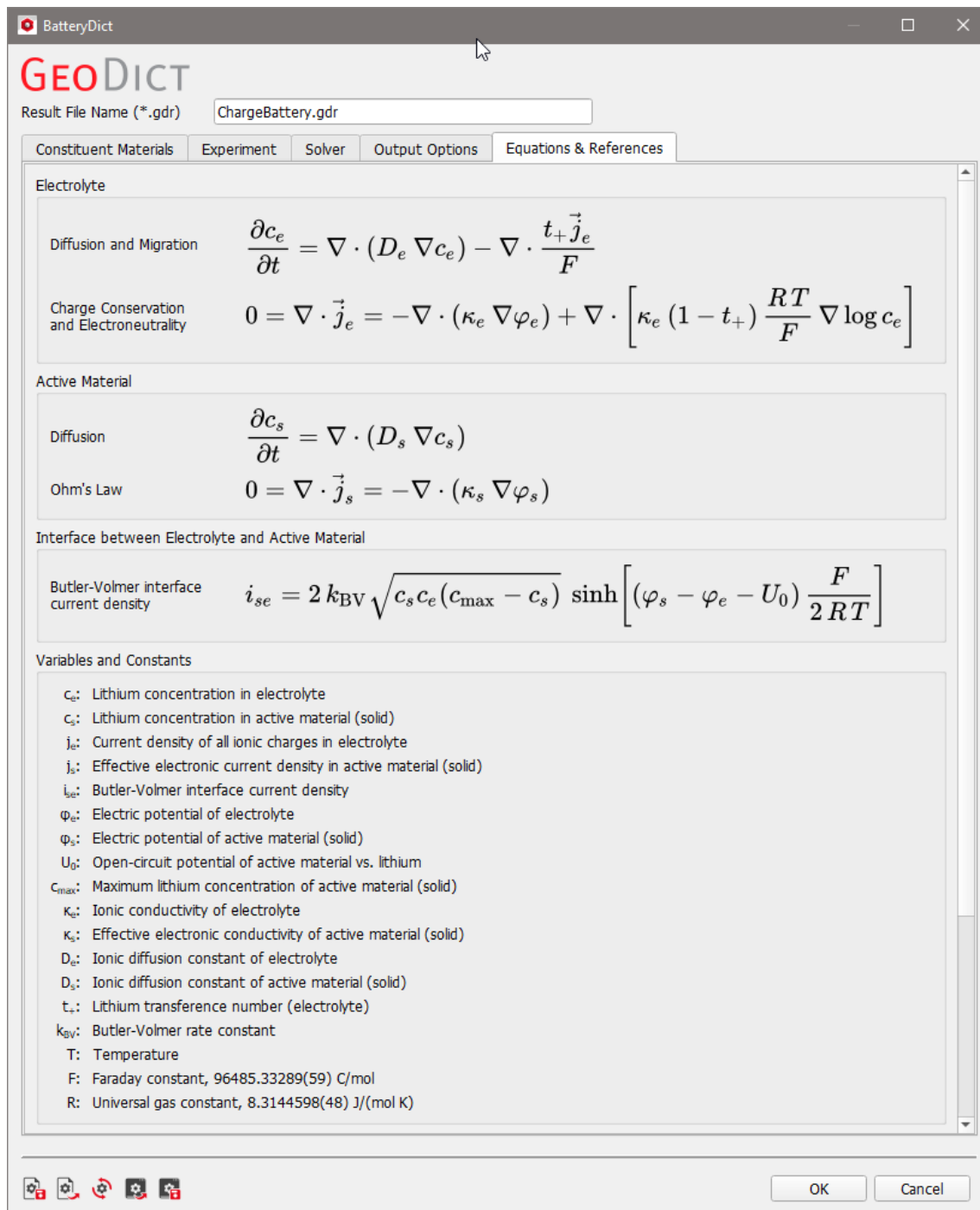
2. **In the active material:** The movement of Li atoms is not coupled to the electric field here. The reason is that Li-ions entering the active material, are combined directly with an electron. The resulting Li atoms do not contribute to the electric current. Mass and charge conservation equations are therefore simpler compared to the ones in the electrolyte. Again, changes in time of the Li concentration are equivalent to the divergence of the flux of the Li concentration. This flux consists here only of one term, the diffusion of Li atoms.

The current density is defined by gradients in the electric potential alone. This is Ohm's Law for the electrons.

3. **The interface of electrolyte and active material** is described by the Butler-Volmer interface current density. This is the flux of Lithium from the active material into the electrolyte and vice versa. This flux depends on the Li concentrations in both the electrolyte and the active material, and on the difference in chemical potentials. $i_{se} > 0$ means de-intercalation, i.e., movement of Lithium from the active material to the electrolyte, $i_{se} < 0$ intercalation.

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



BOUNDARY CONDITIONS AT THE CURRENT COLLECTORS

In **GeoDict** 2022, like in previous **GeoDict** versions, a constant current can be applied to the current collectors of the battery cell. This current can also be specified via a charge rate, which has the advantage of easily defining in which time the battery should charge. In the simulation result, it can easily be seen how far the cell potential will rise for this charge rate, and also if the charge rate diverges at some point, which means that the battery may have been charged too fast. Simulating at constant current has the advantage of seeing when the battery cannot be charged at a constant charge rate anymore due to the cell potential becoming too high.

Battery charging with constant potential can be simulated in **GeoDict** 2022. The time-dependent current, charge rate, etc. are like this not constant anymore and can be analyzed for the charging simulation in the **GeoDict** Result Viewer.

Additionally, in **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.

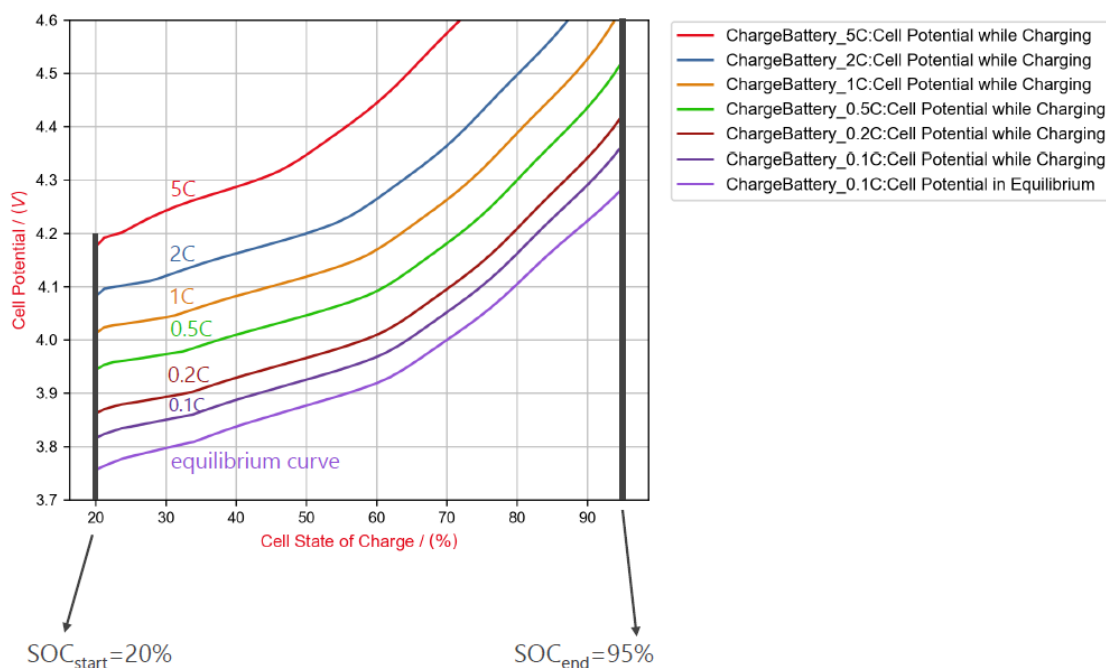
STOPPING CRITERIA FOR CHARGING SIMULATIONS

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 in previous **BatteryDict** releases.

In **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 criteria in the **GeoDict** GUI is explained on page [30](#) and [32](#).

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

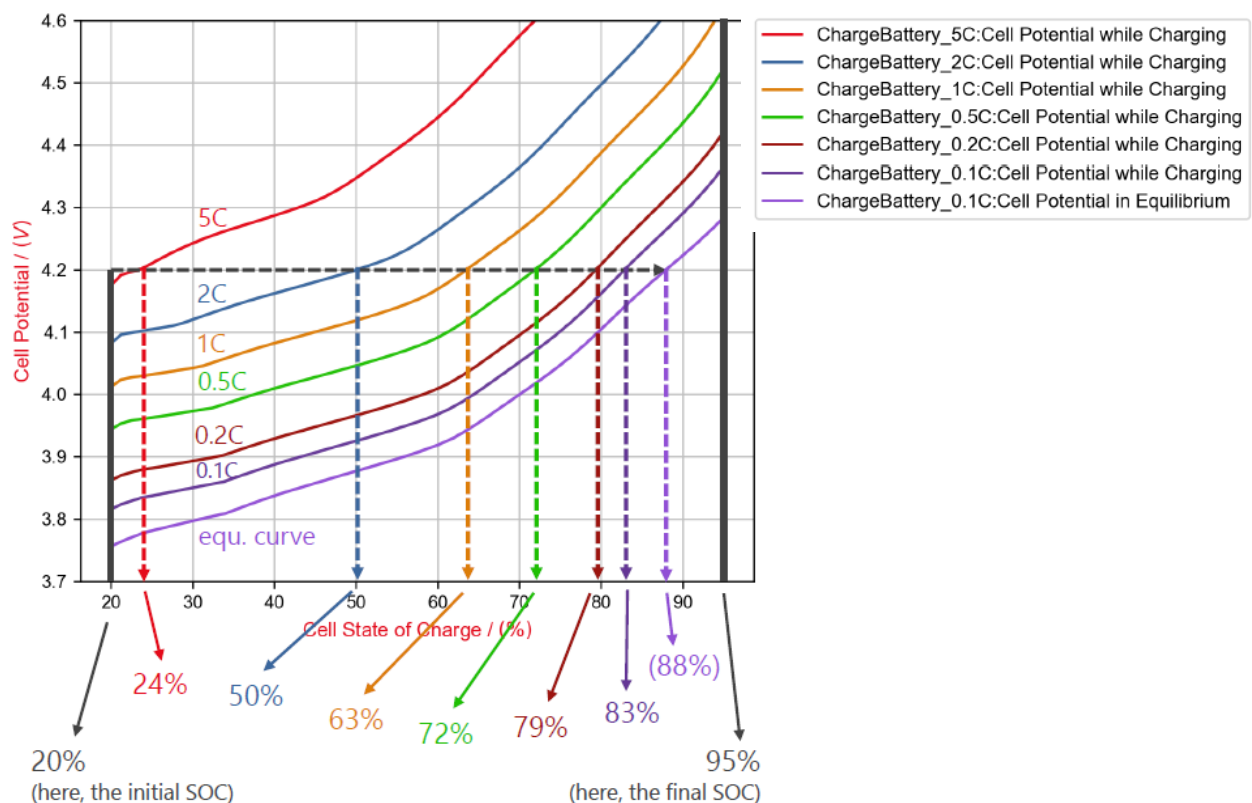
For simulations with constant charge rate, the time evolution of the cell potential depends on the charge rate selected. The higher the charge rate, the larger the deviation of the cell potential curve from the equilibrium charge curve. In the following figure, a charging simulation from state-of-charge 20% till 95% is shown for different charge rates for an example structure.



Charging and discharging simulations for Li-ion batteries

For the stopping criteria final state-of-charge, the computation runs always till the final state-of-charge, here 95%. Dependent on the charge rate, the cell potential reached for this final state-of-charge, is very different.

In contrast to this, if a final potential is defined as stopping criteria, here 4.2 V, the cell potential 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 the simulations with different charge rates.



OVERPOTENTIALS IN BATTERY CHARGING SIMULATIONS

From GeoDict 2022 on, overpotentials of the charging process, can be visualized for a finished simulation in the Result Viewer (see page [64](#)).

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

For charging the battery with a higher charge rate, an additional potential, i.e. additional energy, is necessary due to the inner electrical resistivities of the battery cell. In the same way, while discharging, these electrical resistivities are responsible for the potential difference compared to the equilibrium potential. Less energy can be taken out of the battery and produces heat instead, compared to the equilibrium situation. These differences are measured by the overpotentials. The larger the charge rate, the higher get the overpotentials. The overpotentials computed in GeoDict, distinguish three sources of overpotential:

- **Kinetic overpotentials** define the additional potential necessary for bringing the Lithium ions from the electrolyte into the active materials of cathode or anode. They depend on the Butler-Volmer current.
- **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 are therefore time-dependent and 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 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 part of the battery and which kind of current needs the largest amount of additional potential during charging and is responsible for the largest potential loss during discharging.

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 minimal and maximal reachable Lithium concentration. Usually, the minimal 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.
- **Electronic Conductivity:** Measures a materials ability to conduct electrons.
- **Ionic Conductivity:** Measures the electrolyte's ability to conduct ions (such as Li ions).
- **Ionic Diffusion Constant:** Measures a material's ability to equilibrate differences in concentration.
- **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.
- **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. It depends on the charging state of the electrode and is therefore a function of the state of charge (SOC) of the electrode $SOC=c/c_{max}$.
- **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.

TESTED PARAMETER SPACE

For any given set of material parameters (like conductivities), material structure parameters (morphological), and simulation parameters (like the applied current), the solver in **BatteryDict** strives to perform a physically accurate simulation. 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 58). 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.

One of the tests is a variation of the parameters for a realistic example structure, starting from the default values of the **BatteryDict** 2020 options dialog. From the default values, parameters were varied one at a time, and it was checked, whether the solver still produced meaningful results. Limits for this variation were defined by the regime, in which the parameter does not make sense physically anymore. Results of this variation lead to a n-dimensional box of minimum and maximum parameters in that the simulation with the varied parameters produced meaningful results. For a parameter combination in this box, it is very probable that the simulation will work, but it is not guaranteed since parameters are varied only one-by-one and the convergence behavior of the solver depends additionally on the geometry.

If the parameter combination chosen in the **BatteryDict** options dialog is outside the tested parameter range, a warning appears. This does not mean that the simulation will not work, but the user should check carefully if parameters are chosen in a physically meaningful range. If you have chosen physically meaningful parameters, but the solver does not produce meaningful results, please let us know by sending email to our support (support(at)math2market.de).

The tested parameter ranges of **BESTmicro** are listed in the following tables.

Electrolyte				
Parameter	Unit	Minimum	Default value	Maximum
Equilibrium Lithium Concentration	mol/m ³	12	1.2 e ⁰³	1.2 e ⁰⁷
Transference number	1	1 e ⁻⁰⁴	0.399	0.99
Ionic Diffusion Constant	m ² /s	3.0 e ⁻¹²	3.0 e ⁻¹⁰	3.0 e ⁻⁰⁶
Ionic Conductivity	S/m	1.0 e ⁻⁰⁴	1.0	1.0 e ⁰⁴

Anode				
Parameter	Unit	Minimum	Default value	Maximum
Maximum Lithium Concentration	mol/m ³	2.639	2.639 e ⁰⁴	2.639 e ⁰⁸
Butler-Volmer rate constant	A m ^{2.5} /mol ^{1.5}	8.8 e ⁻¹¹	8.8 e ⁻⁰⁷	8.8 e ⁻⁰⁵
Ionic Diffusion Constant	m ² /s	1.5 e ⁻¹⁵	5 e ⁻¹²	5 e ⁻⁰⁸
Electronic Conductivity	S/m	13	1.3 e ⁰⁵	1.3 e ⁰⁹

Cathode				
Parameter	Unit	Minimum	Default value	Maximum
Maximum Lithium Concentration	mol/m ³	2.3	2.3 e ⁰⁴	2.3 e ⁰⁸
Butler-Volmer rate constant	A m ^{2.5} /mol ^{1.5}	8.0 e ⁻¹⁰	8.0 e ⁻⁰⁶	8.0 e ⁻⁰⁵
Ionic Diffusion Constant	m ² /s	1.0 e ⁻¹⁴	1.0 e ⁻¹³	1.0 e ⁻⁰⁹
Electronic Conductivity	S/m	1.0 e ⁻⁰⁴	1.0 e ⁻⁰²	1.0 e ⁰⁶

OVERLAPPING OCV CURVES FOR SEVERAL ACTIVE MATERIALS

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.

The reason is that the 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 OCVs 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.

When performing simulations with **BatteryDict**, we will always start with an electrode in 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.

References

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References for comparisons of BESTmicro with experiments

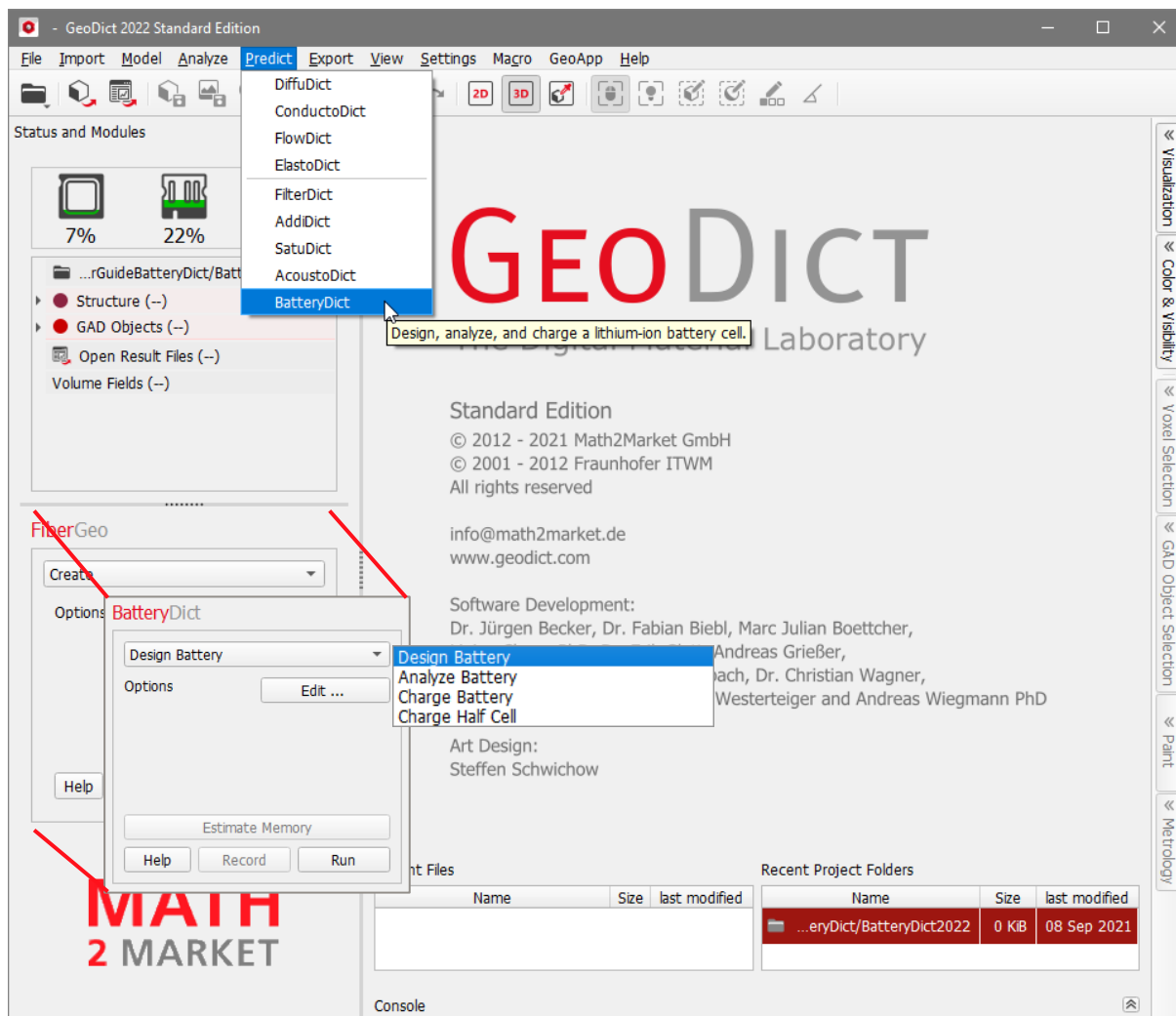
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BATTERYDICT COMPUTATIONS

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**, and to simulate the charging of a battery (**Charge Battery**) or a half-cell (**Charge Half Cell**).

In **GeoDict** 2021, the **BatteryDict** GUI 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.

DESIGN BATTERY

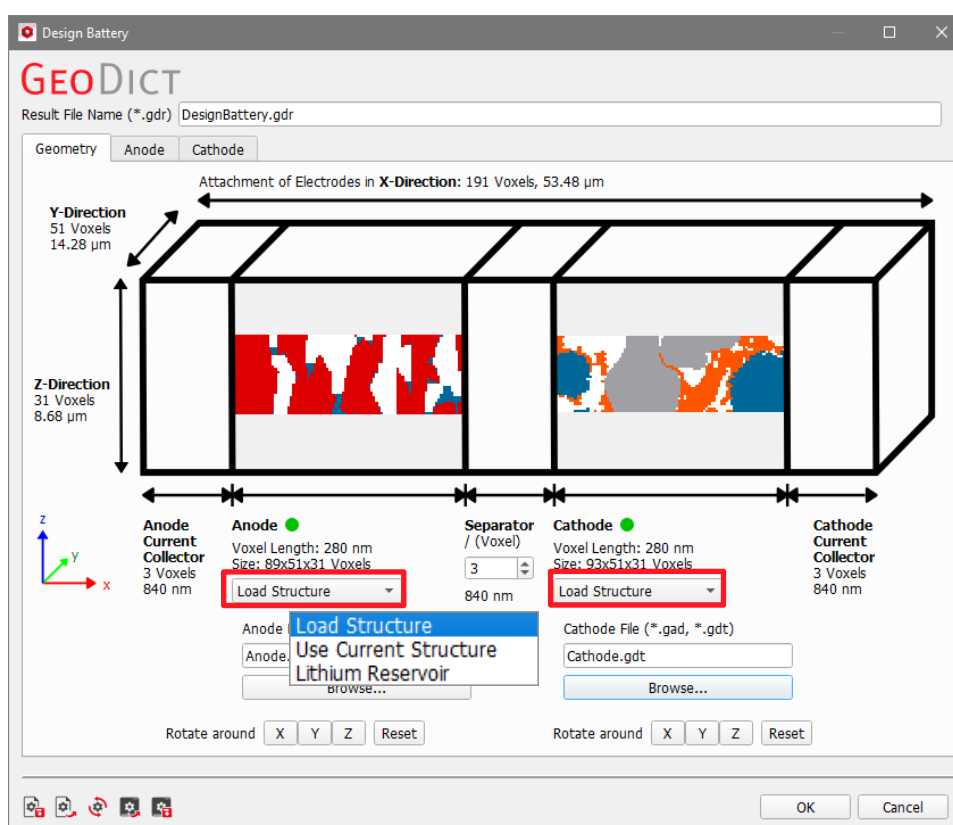
To design a battery, choose **Design Battery** from the pull-down menu and click **Edit...** to choose the options.

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 18, 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 in **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 41), a half cell simulation can be started from the microstructure of a single electrode alone.



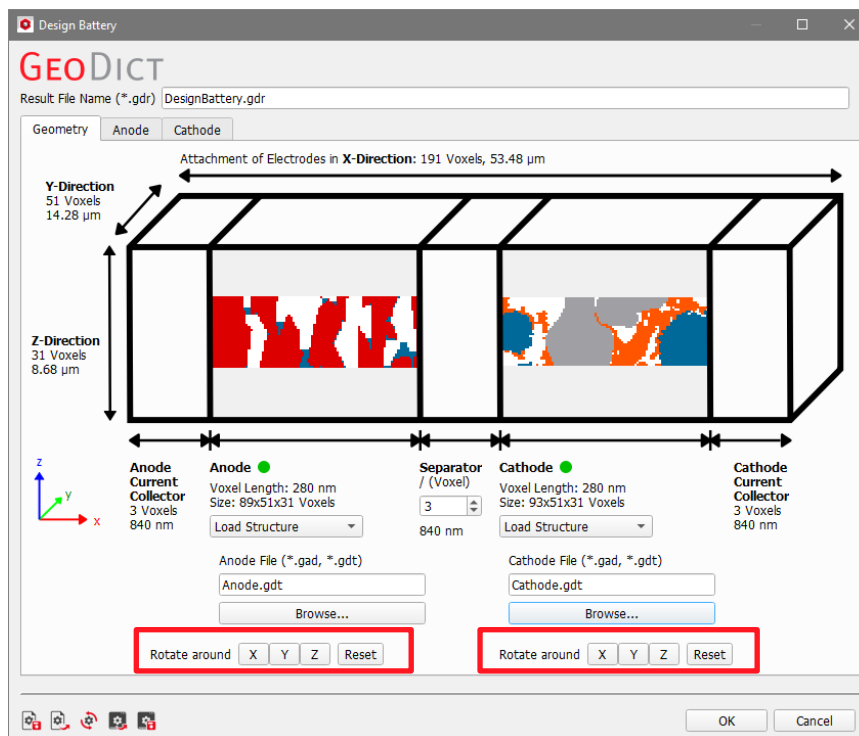
Choose **Load Structure** and use the **Browse...** buttons to select an input file for anode and cathode, in *.gad or *.gdt **GeoDict** formats. If the built-in default settings are used for the dialog, a default structure for anode and cathode from the BatteryDict/DesignBattery folder is loaded.

After selecting electrode files, a 2D representation of the anode and of the cathode appear in the dialog. For the example battery shown here, the anode material is a structure created in **GeoDict** using the **GrainGeo** module and the cathode material is part of a FIB/SEM image of a real cathode.

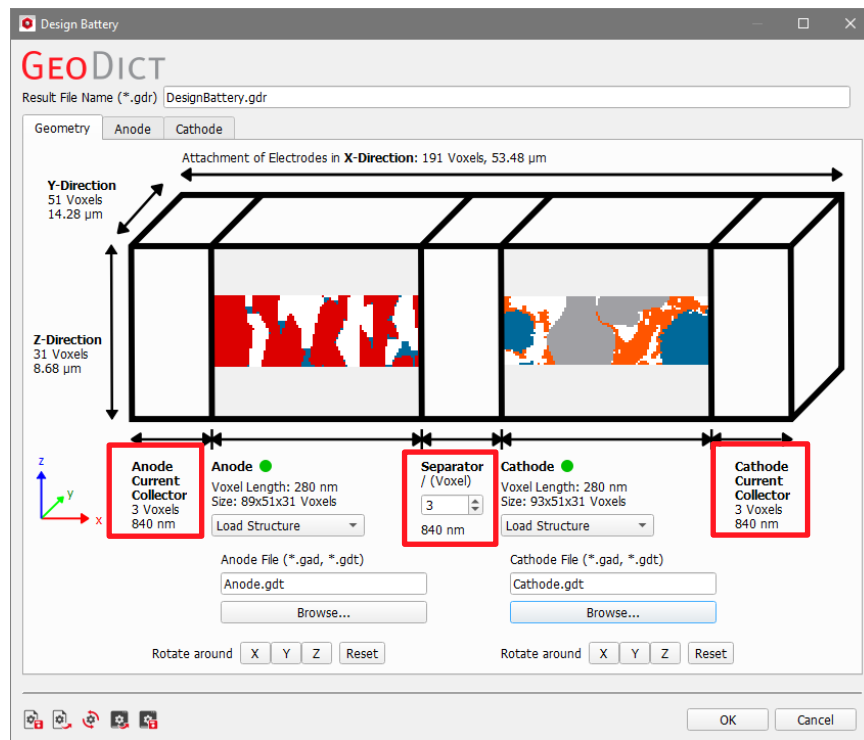
Charging and discharging simulations for Li-ion batteries

- 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.



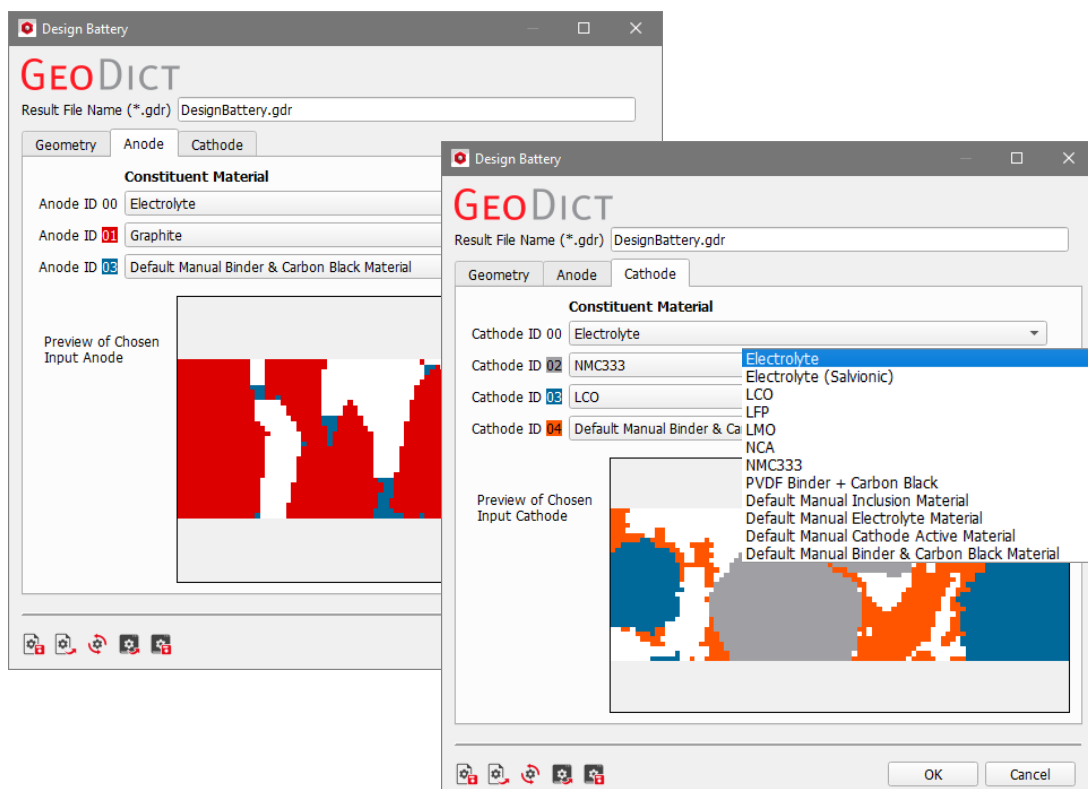
The **Rotate around X, Y and Z** buttons are used to rotate the structure 90° in X, Y or Z direction. Click **Reset** to go back to the original orientation of anode and cathode in the battery structure.



The number of voxels of the separator can be defined in the GUI. The default is 3 voxels. The length of anode and cathode 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.



Charging and discharging simulations for Li-ion batteries

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, the anode consists of one active material, whereas the cathode contains two active materials.

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.

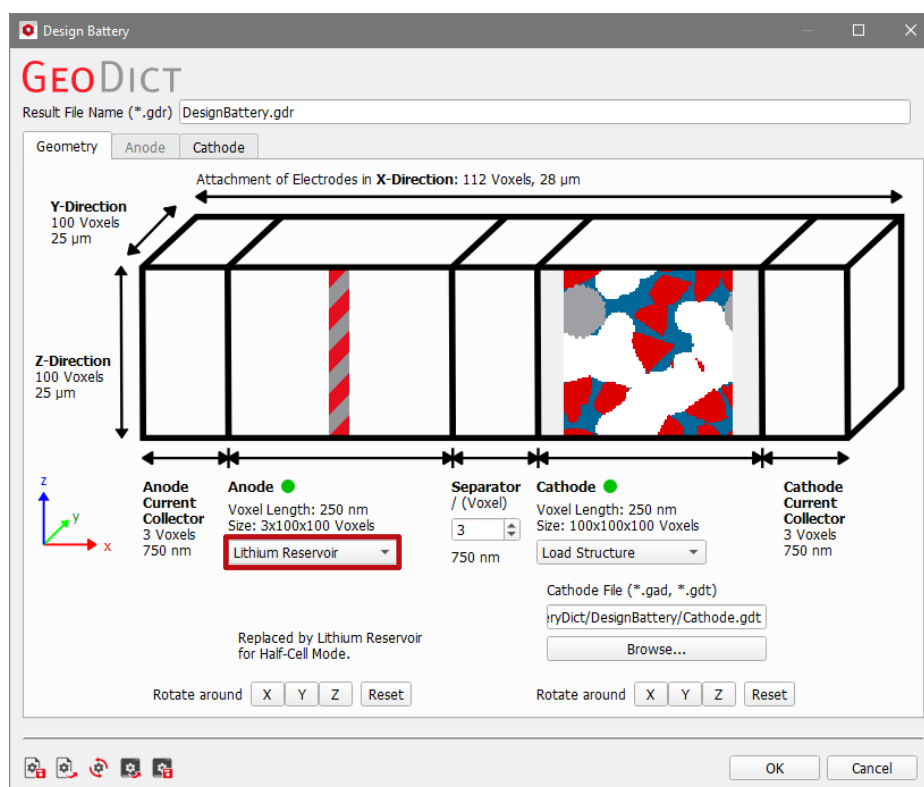
Click **Run** in the **BatteryDict** section of the GUI to create the battery.

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, in page [47](#)).

SETTING UP A HALF-CELL SIMULATION

To design a battery for a half-cell simulation, select **Lithium Reservoir** for either the anode or cathode structure, shown here for the anode. Choose the current structure or load one from a file for the other electrode.



A structure with 3 voxels in x-direction, and y- and z-dimension fitting to the other electrode, is created for the lithium reservoir. No materials need to be selected for an

electrode modelled as a lithium reservoir. In the charging simulation, it will be considered as a never-ending reservoir of lithium, not limiting the battery performance.

Notice that from GeoDict 2022 on, it is not necessary anymore to design a half-cell before performing a half cell simulation. A structure of a single electrode can be used to perform a half cell simulation directly, see page [41](#). For a half-cell created with the Battery Designer, it is recommended to use the functionality Charge Battery, see page [21](#).

MORE FLEXIBLE GEOMETRIES

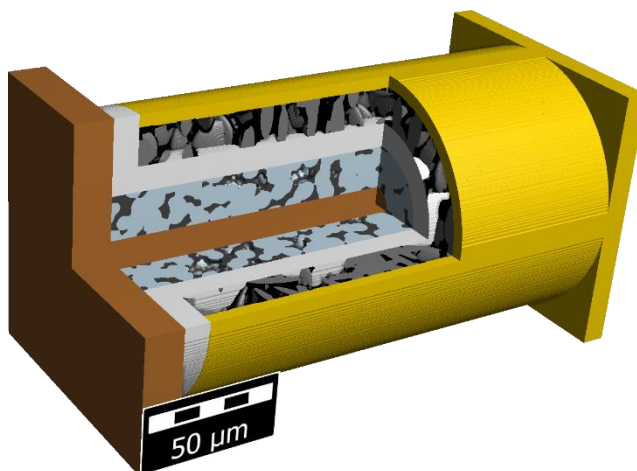
Since the GeoDict 2020 release, it is possible to use arbitrary battery geometries, not only cuboid ones, as shown in the **Geometry** on page [15](#).

In GeoDict 2022, arbitrary geometries can be chosen now without an additional expert setting for this.

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.

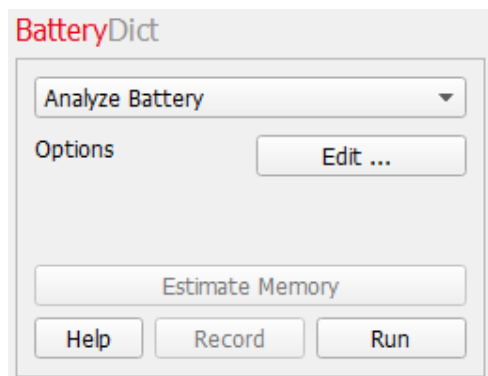
For geometries with circular cross sections, current collectors can be positioned like shown in the figure below.



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.

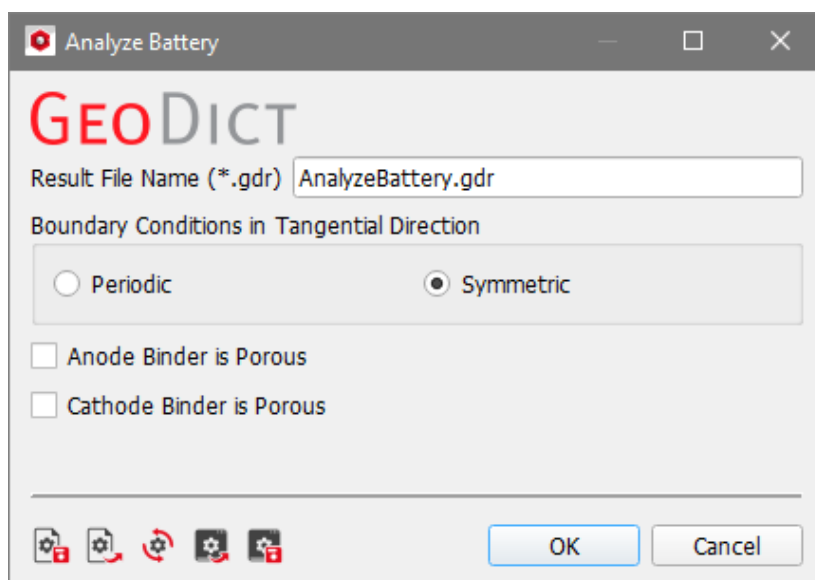
ANALYZE BATTERY

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 Li^+ ions and electrons are reflected at the boundary in y- and z-direction.

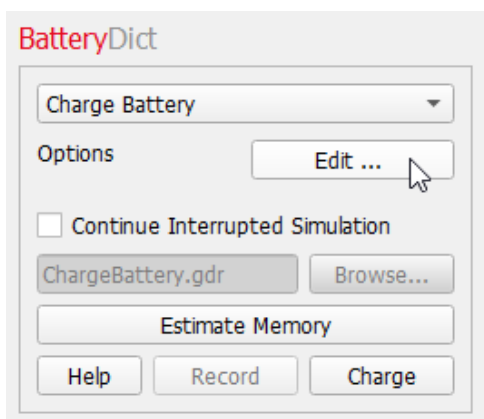
Boundary conditions are applied while identifying connected and unconnected material, since this depends on the continuation of the material in y- and z-direction. For a charging simulation, it can be chosen independent of the value selected here. Connected and unconnected material is identified again 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, filled with electrolyte and not resolved in the electrode structure.

Click **Run** in the **BatteryDict** section to start the analysis. If it is finished, a Result Viewer opens, see *Result of Analyze Battery* below, in page [53](#).

CHARGE BATTERY

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

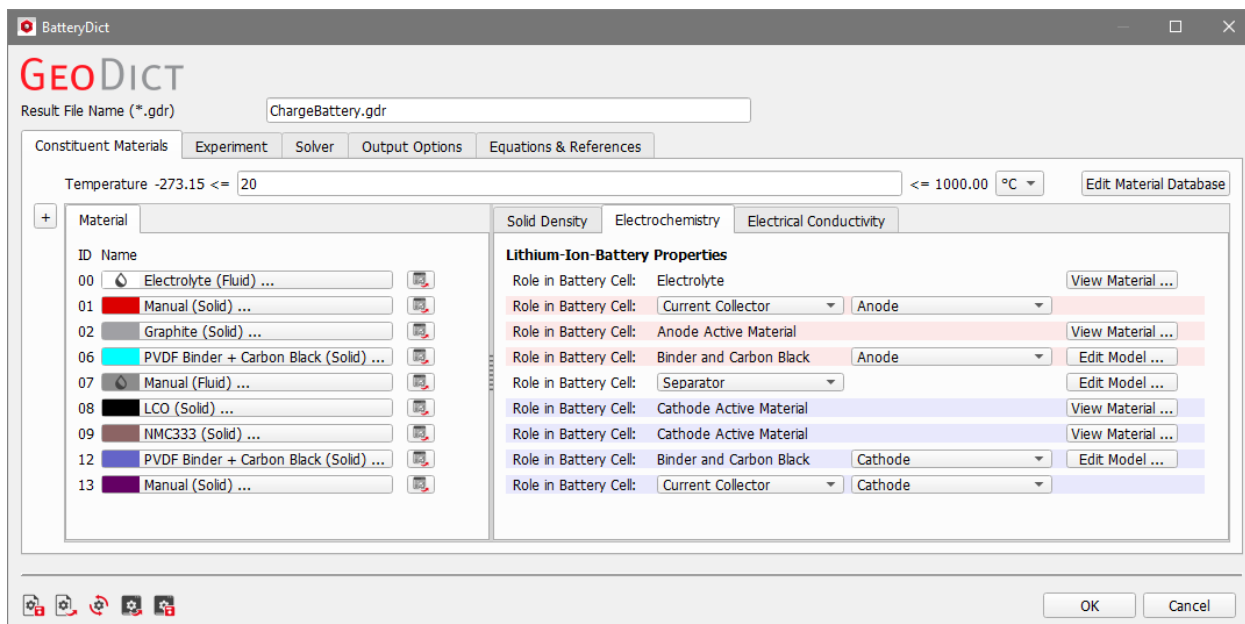


Then, click **Edit** to adjust the solver options.

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.

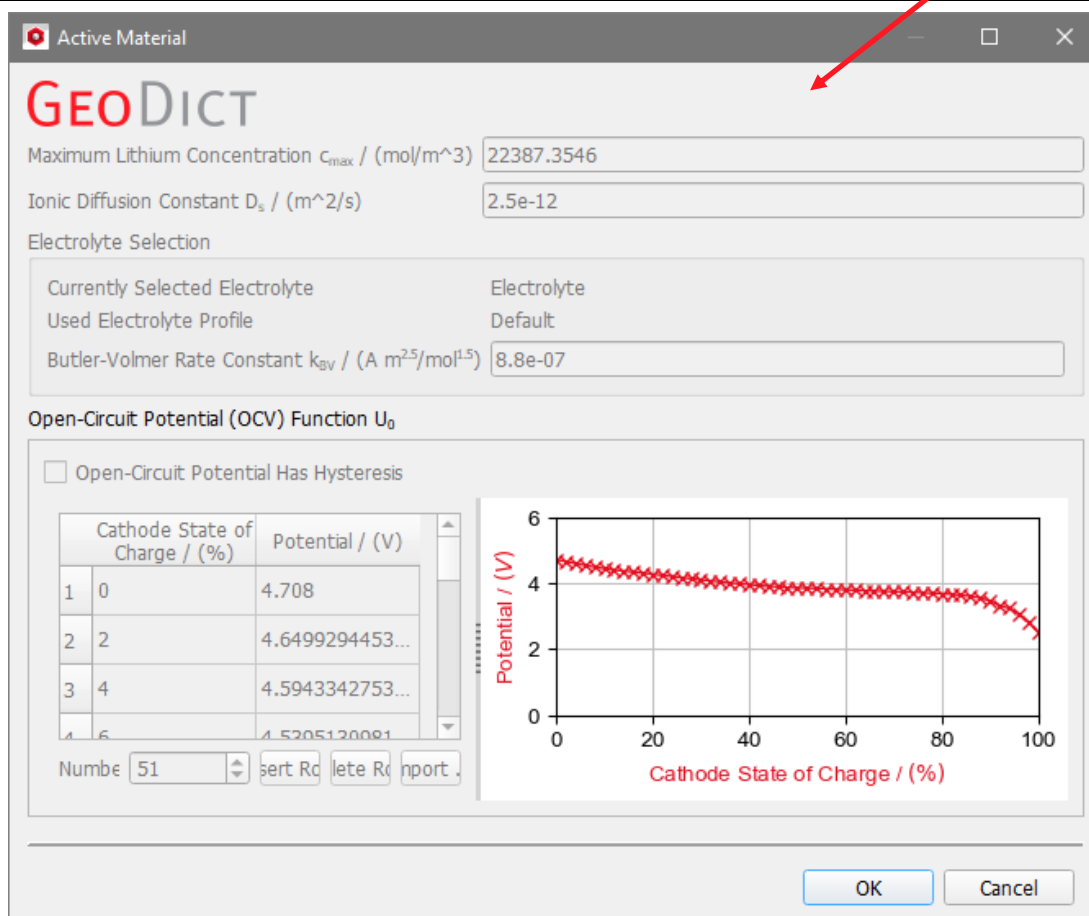
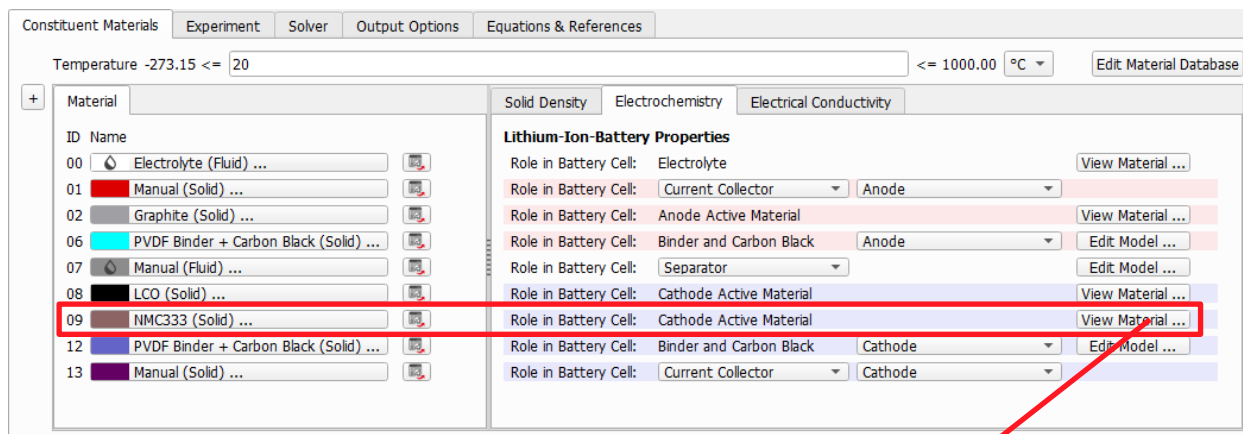
Material IDs of the structure and the assigned materials are listed on the left of the tab under **Material**.

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

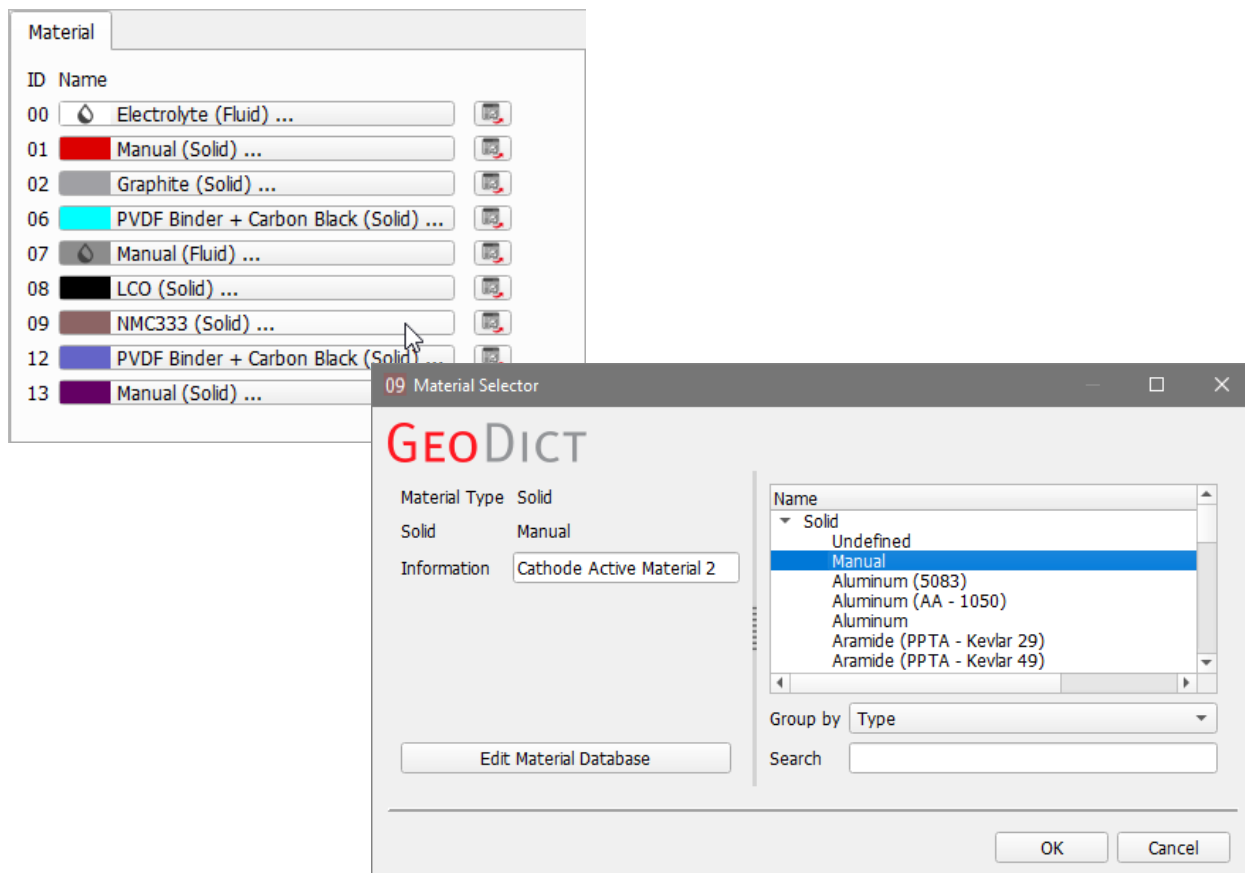
Charging and discharging simulations for Li-ion batteries

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.

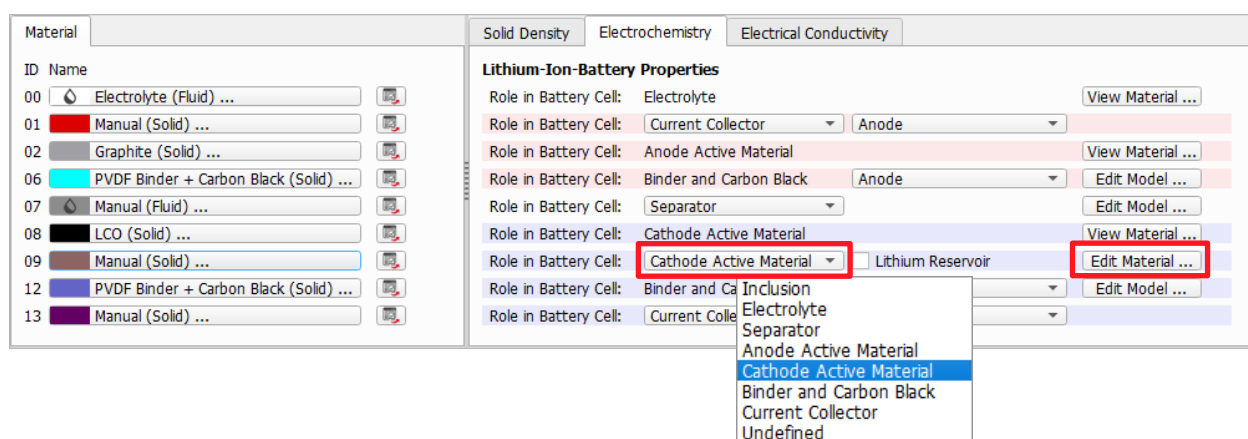
If a material from the GeoDict Material Database is selected for one Material ID (e.g. for ID 09 in the example shown), all parameters are set according to the database values. The electrochemical role of the material (here: Cathode Active Material) is shown and the parameters can be displayed by clicking the **View Material** button. Dependent on the electrochemical role of the material selected, the property dialog for **Active Material**, **Electrolyte**, **Binder & Carbon Black** or for **Separator** opens, showing the values of the database (see *Parameter Dialogs* below in page 25 for more details).



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 (as well as the other parameters under the **Solid Density** and **Electrical Conductivity** subtabs) can be modified.



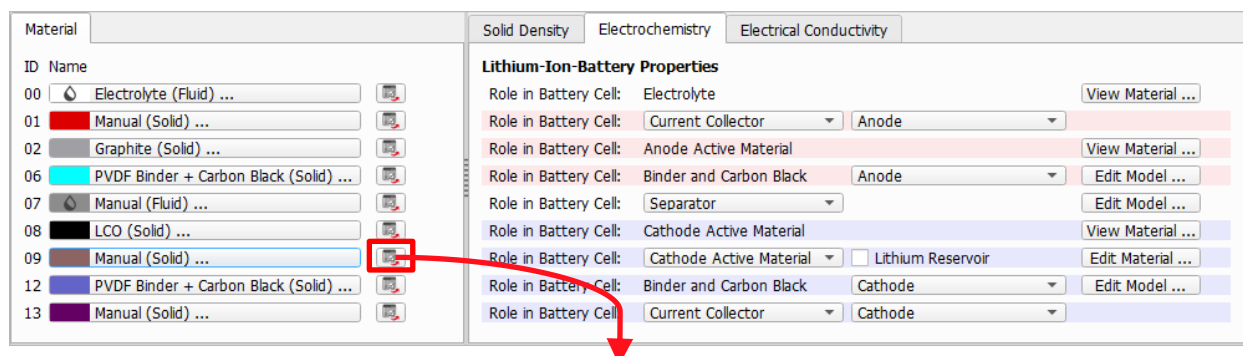
The electrochemical roles Separator, Binder and Carbon Black for each electrode and Current Collector for each electrode, can each be selected only for one material in the structure.

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.

Charging and discharging simulations for Li-ion batteries

Clicking **Edit Material** opens the property dialog for Active Material or Electrolyte for editing the values, **Edit Model** allows to change the Binder & Carbon Black or Separator model. See *Parameter Options Dialogs* below in page 25 for more details.

If the box **Lithium reservoir** is checked for a Cathode Active Material or an Anode Active Material, the **Edit Material** button is grayed out and no material parameters can be changed. This 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.



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

Report for Material with ID 09

Key	Unit	Value
Name		Manual
Type		Solid
Information		Cathode Active Material 2
▼ SolidProperties		
Density	kg/m ³	3750
▼ ElectricalConductivity		
CurrentLaw		1
NumberOfLaws		1
▼ MaterialLaw1		
Type		Isotropic
Name		Manual Law
Beta	S/m	0.9
▼ Electrochemistry		
▼ LilonBattery		
BatteryMaterialType		CathodeActiveMaterial
▼ CathodeActiveMaterial		
IsLithiumReservoir		false
MaxLiConcentration	mol/m ³	22387.35459
LiDiffusivity	m ² /s	2.5e-12
NumberOfElectrolytes		1
▼ Electrolyte1		
Name		Default
ButlerVolmerRate	A m ^{^(2.5)} /mol ^{^(1.5)}	8.8e-07
▼ OpenCircuitPotential		
HasHysteresis		false
StateOfCharge	%	0, 2, 4, 6, 8, 10, 12, 14, 16, ...
Potential	V	4.708, 4.649929445344823, ...

Close

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).

PARAMETER OPTIONS DIALOGS

Parameter dialogs for Active Materials, Binder & Carbon Black, Separator and Electrolyte are explained in the following. For an explanation of the meaning of the parameters, see *Simulation Parameters* above in page [10](#).

ACTIVE MATERIAL PARAMETER DIALOG

For all active materials, the simulation parameters **Maximum Lithium Concentration**, **Ionic Diffusion Constant**, **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.

Active Material

GeoDict

Maximum Lithium Concentration c_{max} / (mol/m³) 22387.3546

Ionic Diffusion Constant D_s / (m²/s) 2.5e-12

Butler-Volmer Rate Constant k_{BV} / (A m^{2.5}/mol^{1.5}) 8.8e-07

Open-Circuit Potential (OCV) Function U_0

☐ Open-Circuit Potential Has Hysteresis

	Cathode State of Charge / (%)	Potential / (V)
1	0	4.708
2	2	4.6499294453...
3	4	4.5943342753...
4	6	4.5395130981...
5	8	4.4856777104...
6	10	4.4373809168...
7	12	4.3987988782...
8	14	4.3659228500...

Number of f 51 Insert Row Delete Row Import ...

Potential / (V)

Cathode State of Charge / (%)

OK Cancel

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

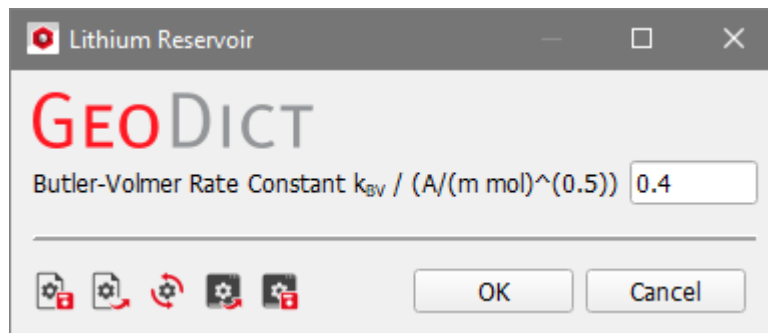
Values defining the **Open-Circuit Potential Function** can be modified directly in the table. Additionally, the number of value points can be changed by deleting or inserting new rows. Another possibility is to import the **Open-Circuit Potential Function** from a text file with two columns. The first 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.

Charging and discharging simulations for Li-ion batteries

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



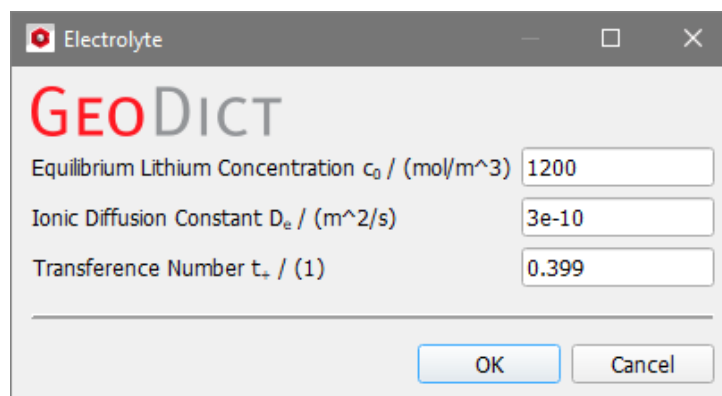
No other parameters need to be set for a lithium reservoir, since it will be considered as a never-ending reservoir of lithium, not limiting the battery performance.

ELECTROLYTE PARAMETER DIALOG

For the electrolyte, the **Equilibrium Lithium Concentration**, **Ionic Diffusion Constant**, and **Transference Number** need to be defined (see *Simulation Parameters* above, in page 10).

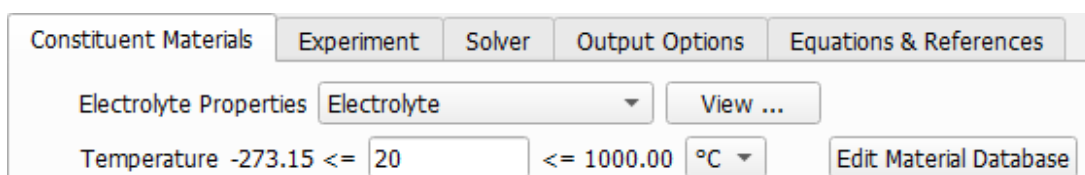
If a material from the GeoDict Material Database is selected for the electrolyte, values are shown in the **Electrolyte** dialog, but cannot be changed.

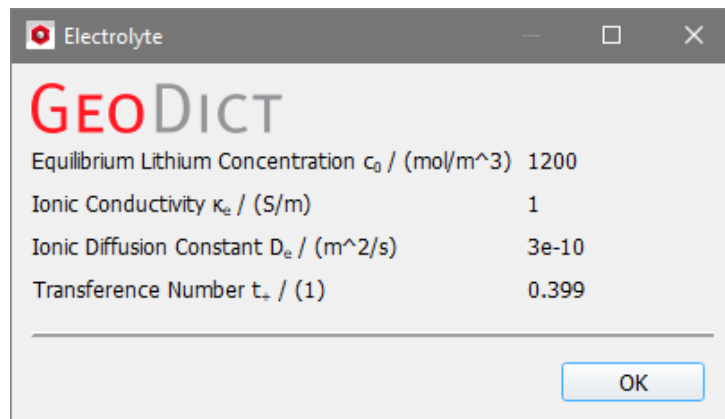
Set the electrolyte to **Manual (Fluid)** or **Manual (Solid)**, to modify the parameters.



The ionic conductivity of the electrolyte is the value for the electrical conductivity defined on the **Electrical Conductivity** tab. For electrolyte materials, ionic and electrical conductivity are the same since they have no electronic conductivity.

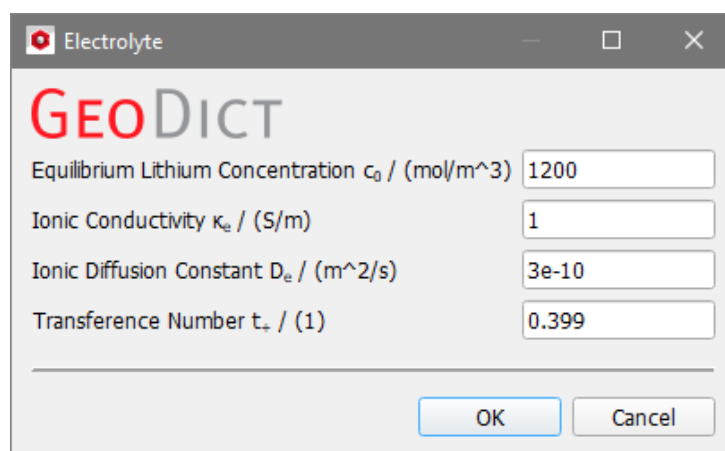
If no material ID with material defined as electrolyte exists, the electrolyte can be defined in the upper part of the Constituent Materials tab. In this case, no electrolyte exists in both electrodes, but only in the separator.





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.

Electrolyte Properties Manual Electrolyte Material Edit ...



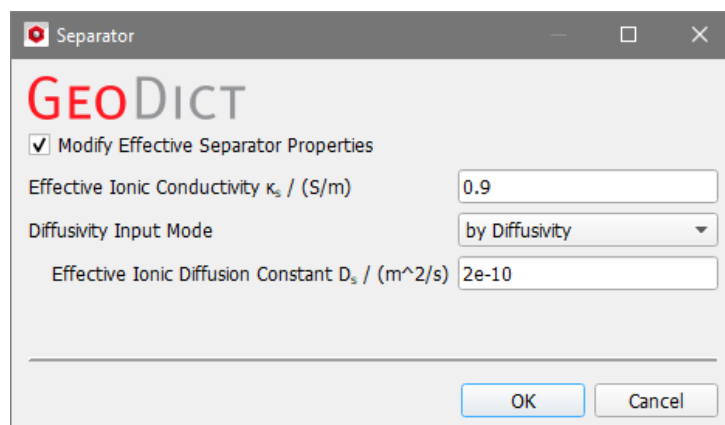
SEPARATOR PARAMETER DIALOG

If the box **Modify Effective Separator Properties** 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 **Modify Effective Separator Properties**. An **Effective Ionic Conductivity** and an **Effective Ionic Diffusion Constant** to account for the influence of the separator microstructure can be defined.

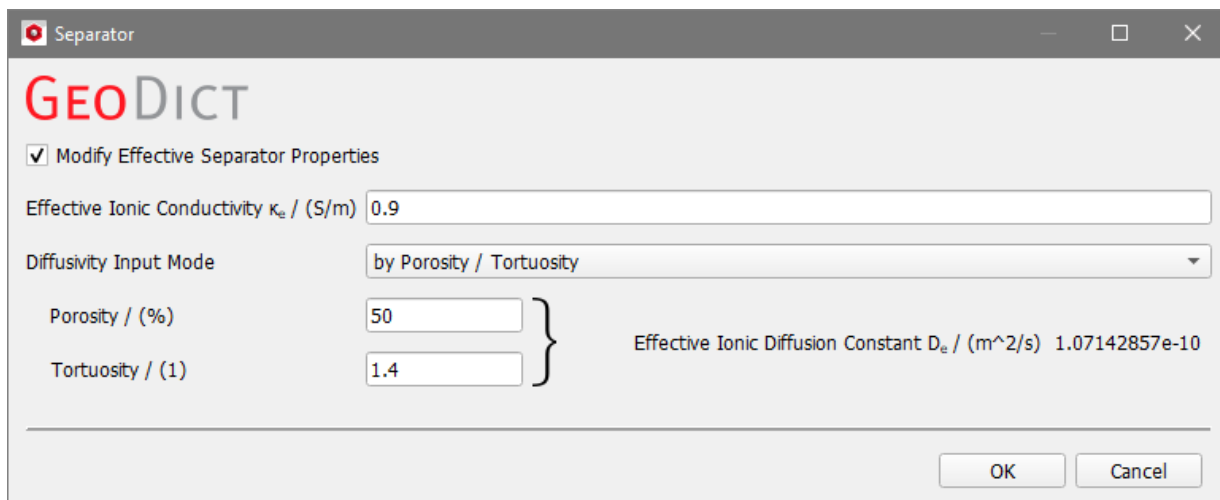
The **Effective Ionic Diffusion Constant** can be defined in two different ways:

- Set the value by choosing Diffusivity Input Mode **by Diffusivity** directly,



- Or select **by Porosity / Tortuosity** as Diffusivity Input Mode and define porosity and tortuosity of the separator.

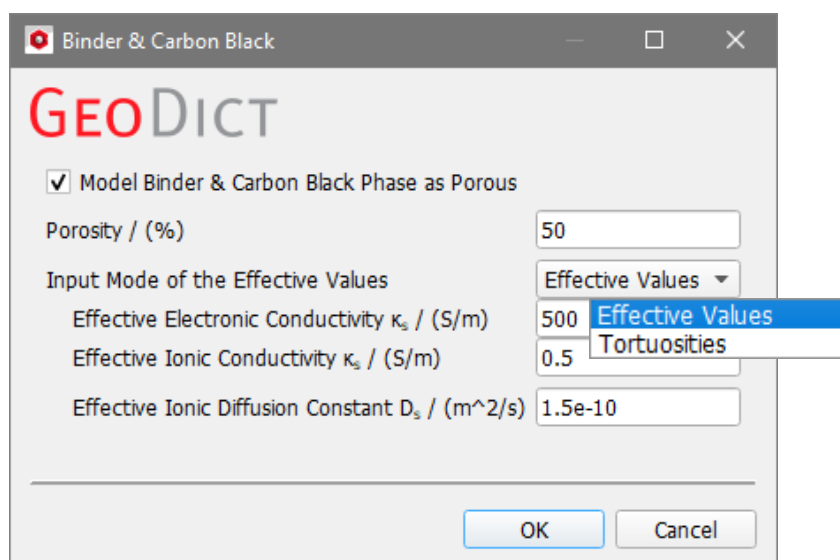
The effective ionic diffusion constant is computed from these values and the ionic diffusion constant of the electrolyte and shown in the dialog.



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 necessary 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 Diffusion Constant** 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** to set tortuosity values for both Solid and Fluid. Effective values are computed and shown on the right of the dialog. They cannot be changed there.

Binder & Carbon Black

GEODict

☒ Model Binder & Carbon Black Phase as Porous

Porosity / (%)

Input Mode of the Effective Values

Tortuosity in Solid / (1)

Tortuosity in Fluid / (1)

Effective Values

Effective Electronic Conductivity / (S/m)

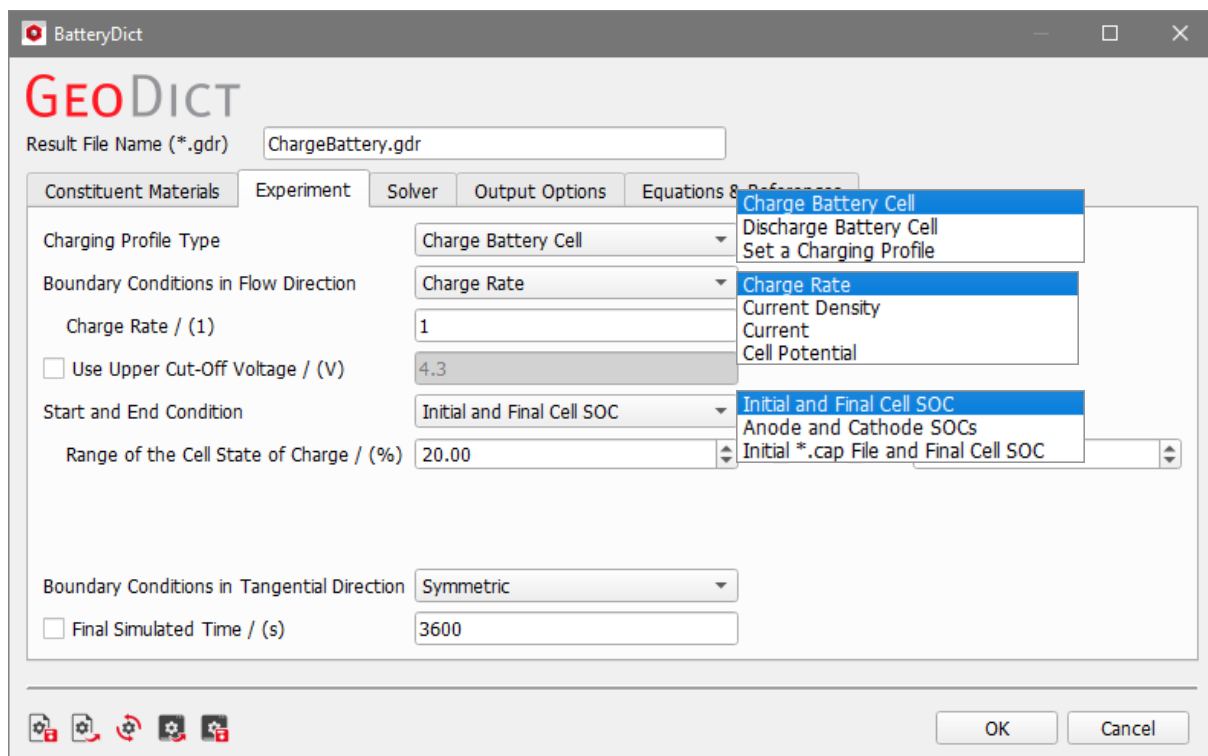
Effective Ionic Conductivity / (S/m)

Effective Ionic Diffusivity / (m²/s)

OK Cancel

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, in page [32](#).

The Applied Current can be specified by a **Charge Rate**, a **Charge Density**, by defining the **Current** itself in Ampère (A) or by defining the **Cell Potential**.

With an entered **Charge Rate**, 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 Ampère (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 Ampère takes ½ hour.

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

If the **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.

In **BatteryDict 2022**, 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, in page [3](#)) of the whole cell

Start and End Condition	Initial and Final Cell SOC	
Range of the Cell State of Charge / (%)	20.00	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	70.00
Range of the Cathode State of Charge / (%)	30.00	75.00

- by selecting an initial .cap file and defining a final SOC.

Start and End Condition	Initial *.cap File and Final Cell SOC	
Initial *.cap File (*.cap)	ChargeBattery/CAPs/Cell_1.cap	Browse...
Final Cell SOC / (%)	70	

This option is especially useful for simulating a charging or discharging process, starting from a non-equilibrium condition after a previous discharging or charging simulation.

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^+ 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
<input type="checkbox"/> 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

The screenshot shows the 'Experiment' tab in the BatteryDict GEODict software. The 'Result File Name (*.gdr)' is set to 'ChargeBattery.gdr'. The 'Charging Profile Type' is set to 'Set a Charging Profile'. The 'Initial Cell SOC' is set to 'Equilibrium' and the 'Initial Cell SOC / (%)' is set to '20'. Below these settings is a table with 4 rows defining simulation steps.

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

Below the table, 'Number of Rows' is set to 4, 'Boundary Conditions in Tangential Direction' is set to 'Symmetric', and 'Final Simulated Time / (s)' is set to 3600. At the bottom right are 'OK' and 'Cancel' buttons.

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,

This close-up shows the 'Set a Charging Profile' settings. The 'Charging Profile Type' is 'Set a Charging Profile', the 'Initial Cell SOC' is 'Equilibrium', and the 'Initial Cell SOC / (%)' is '20'.

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

This close-up shows the 'CAP File' selection settings. The 'Charging Profile Type' is 'Set a Charging Profile', the 'Initial Cell SOC' is 'CAP File', and the 'Initial *.cap File (*.cap)' is 'InitialCAP.cap'. A 'Browse...' button is also present.

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 boundary condition in flow direction and the corresponding value for the boundary condition, in the same way as for simple charging simulations, see page [30](#). 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

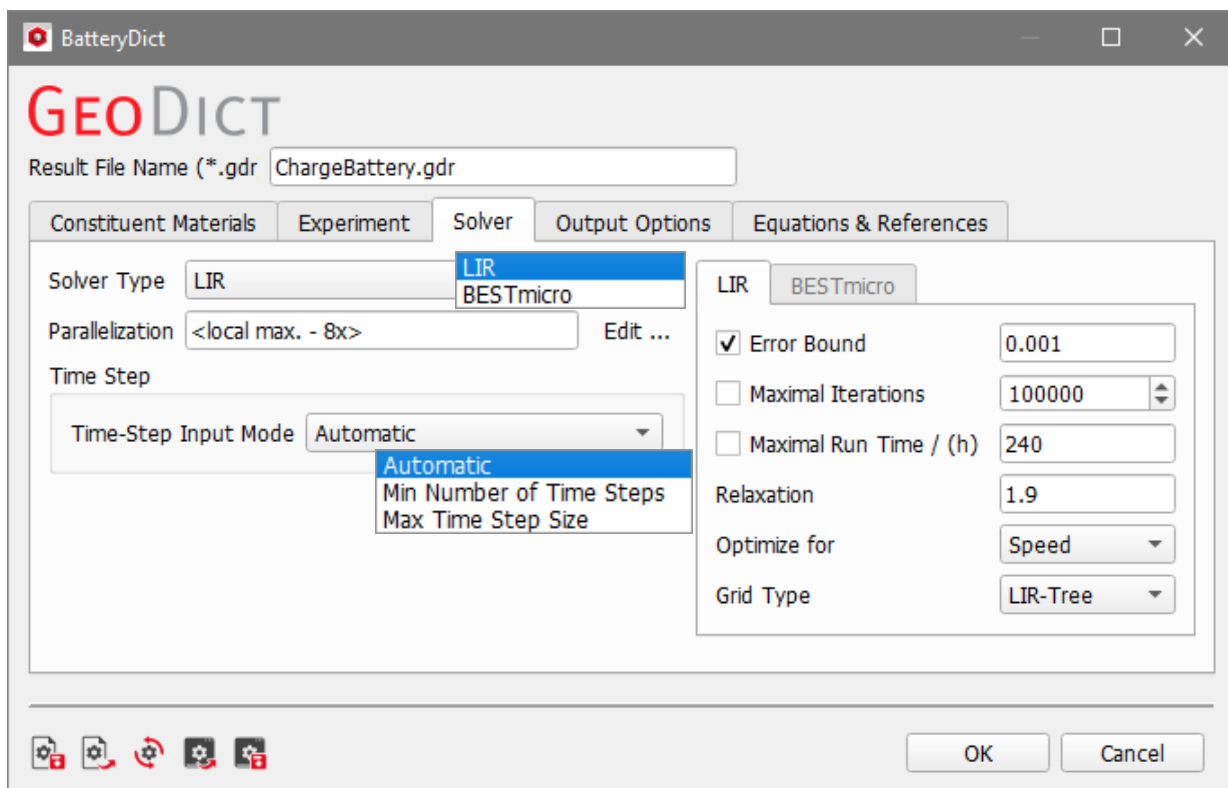
Boundary Conditions in Tangential Direction

☐ 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

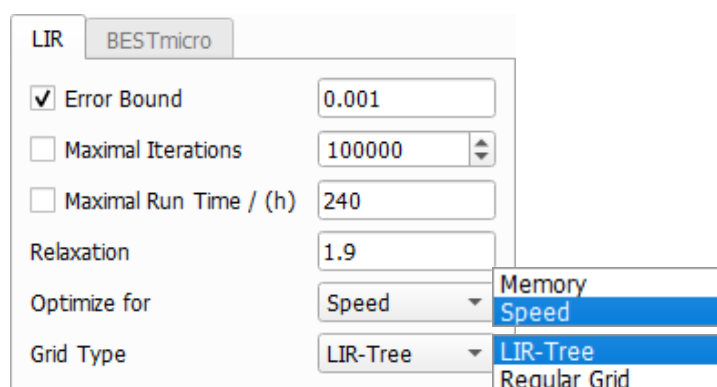
Under the **Solver** tab, the type of solver to apply when solving the system of partial differential equations is selected, as well as the solver options.



Select the **Solver Type** LIR or BESTmicro.

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.

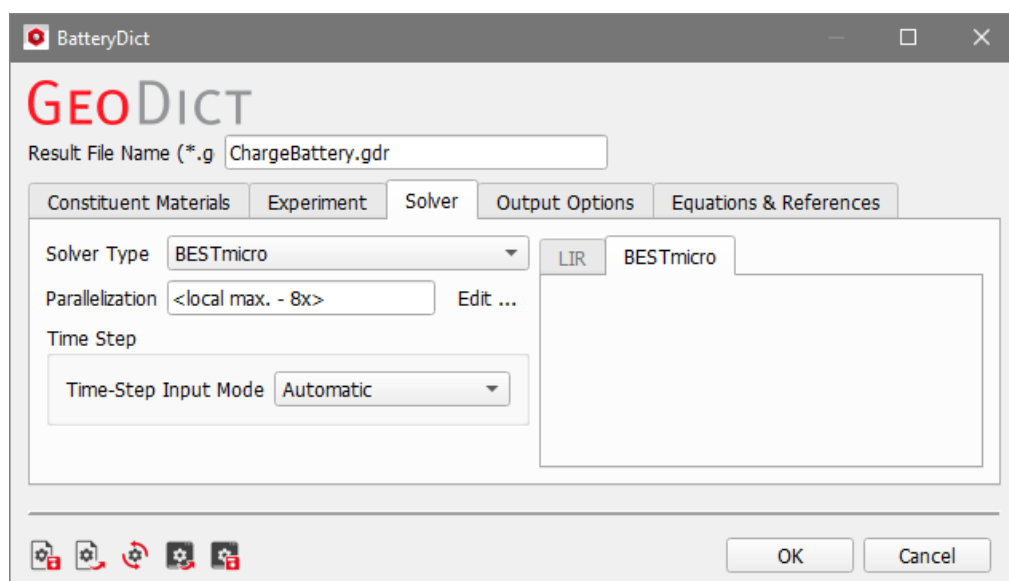
The **Grid Type** decides what kind of tree structure is used for the simulation.

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.

BESTMICRO SOLVER

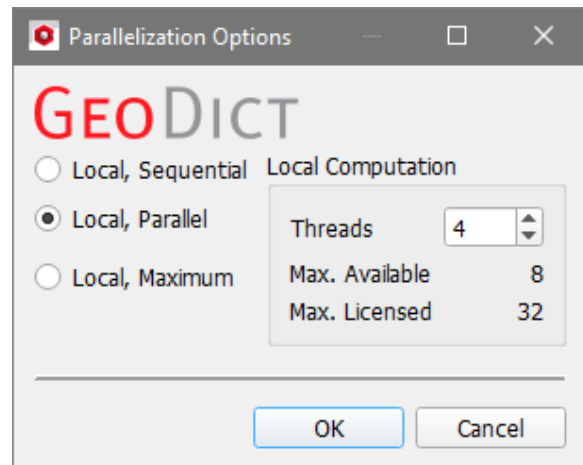
The BESTmicro solver uses algebraic multigrid methods to solve the system of partial differential equations of the battery charging process. Apart from the parallelization and the Time-Step Input Mode, no additional solver options need to be defined on the panel on the right for this solver.



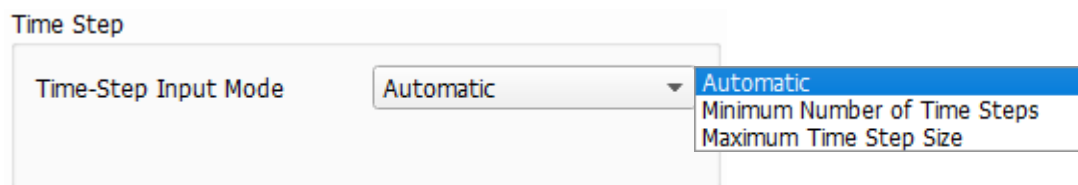
PARALLELIZATION AND TIME-STEP

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.



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 55). 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.

If a new battery state is found, the solver computes the Cell-SOC of the just found battery state via: $\text{Cell-SOC step} = \text{time step} * \text{charge rate} / (1 \text{ hour})$. So, it is not clear from the start which the next computed Cell-SOC in a simulation is, 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 [57](#)).

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

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

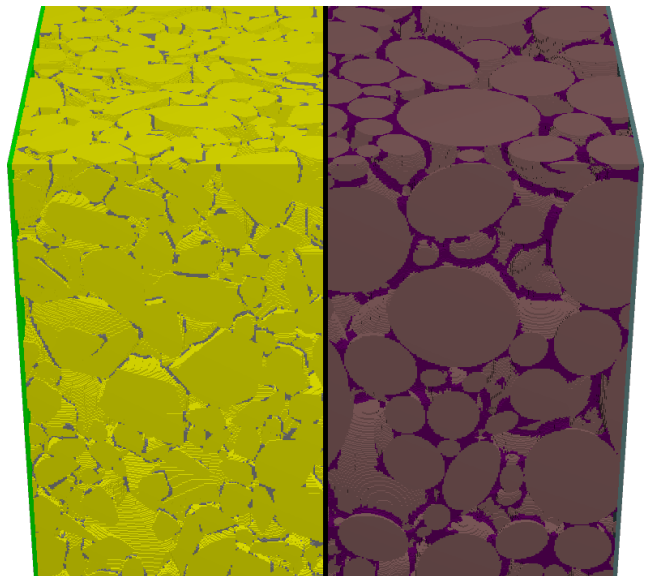
PARALLELIZATION BENCHMARK RESULTS

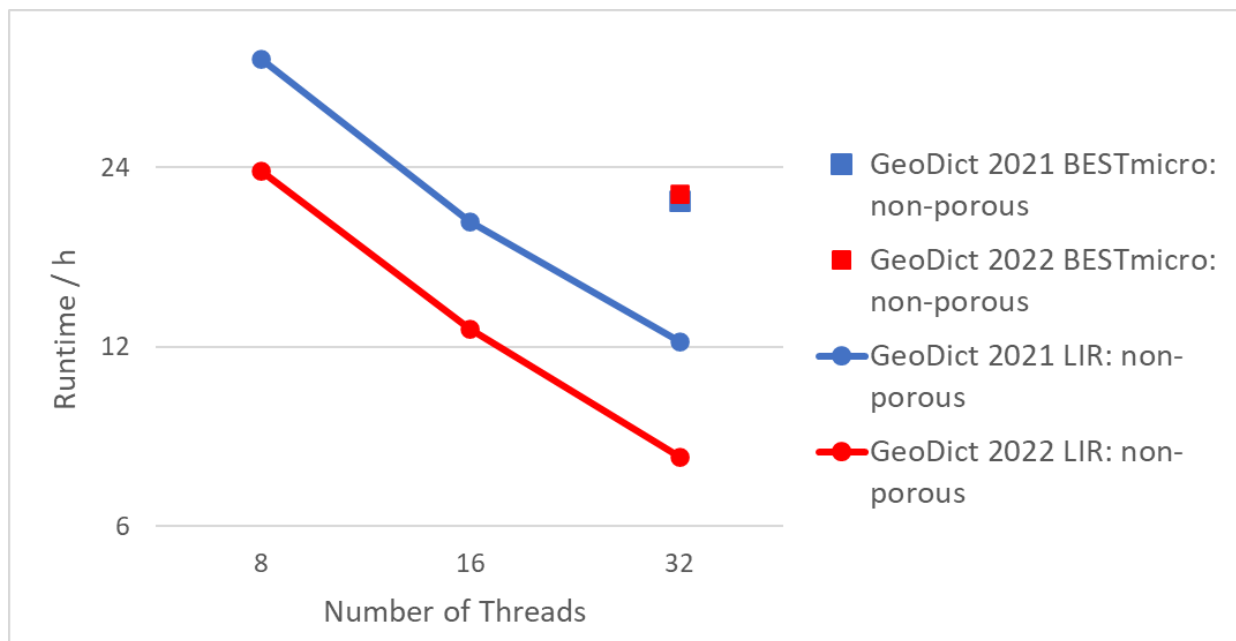
As an example for the parallelization, a full battery structure of size $409 \times 400 \times 400$ voxels with 200 nm voxel length is used to simulate the charging from the cell state of charge 20% till 70%. The computation is run on a server with 2 x Intel E5-2697A v4 processors with 16 cores each,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

The simulations are computed with **GeoDict** 2022, Service Pack 2.

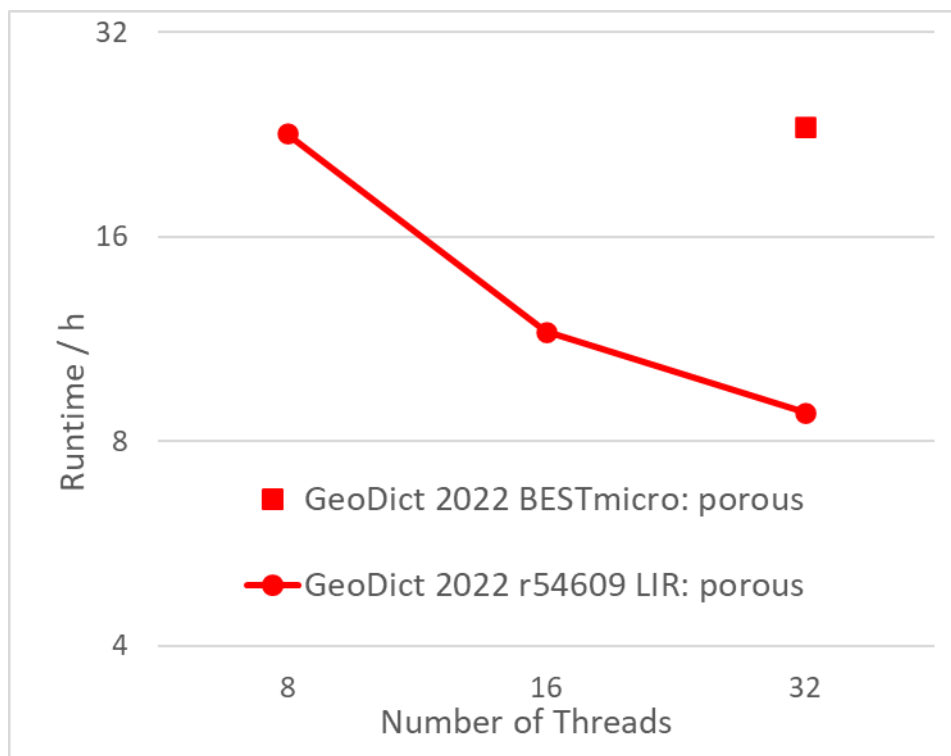
When the binder is considered as solid, the LIR solver needs only 1/3 of the runtime compared to BESTmicro with **GeoDict** 2022. In **GeoDict** 2022, with the LIR solver, the runtime is reduced by up to 35% compared to LIR in **GeoDict** 2021.

The LIR solver needs only 9.2 GB of RAM which is 3% of the memory required by BESTmicro. The speedup for LIR solver is nearly optimal.



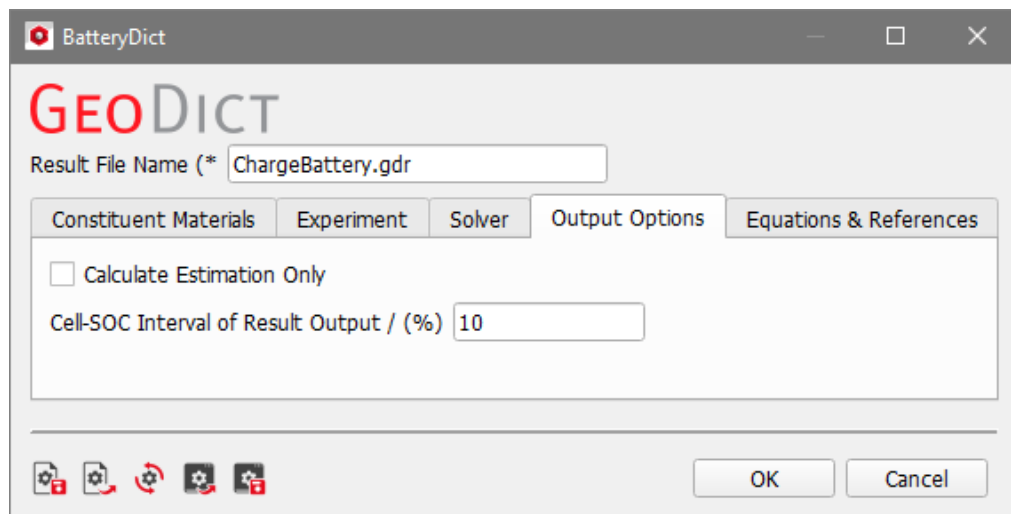


When the binder is considered as porous, since **GeoDict 2022**, LIR can also solve the porous case and the runtime and memory are both greatly reduced. The LIR solver needs 12 GB of RAM, only 3.5% of the memory required by BESTmicro, 345 GB. The runtimes of LIR and BESTmicro with 32 threads are 9 h resp. 23 h.



However, the runtimes of both solvers are not only dependent on the structure size, but also on the structure itself and the parameters set for the simulation.

OUTPUT OPTIONS



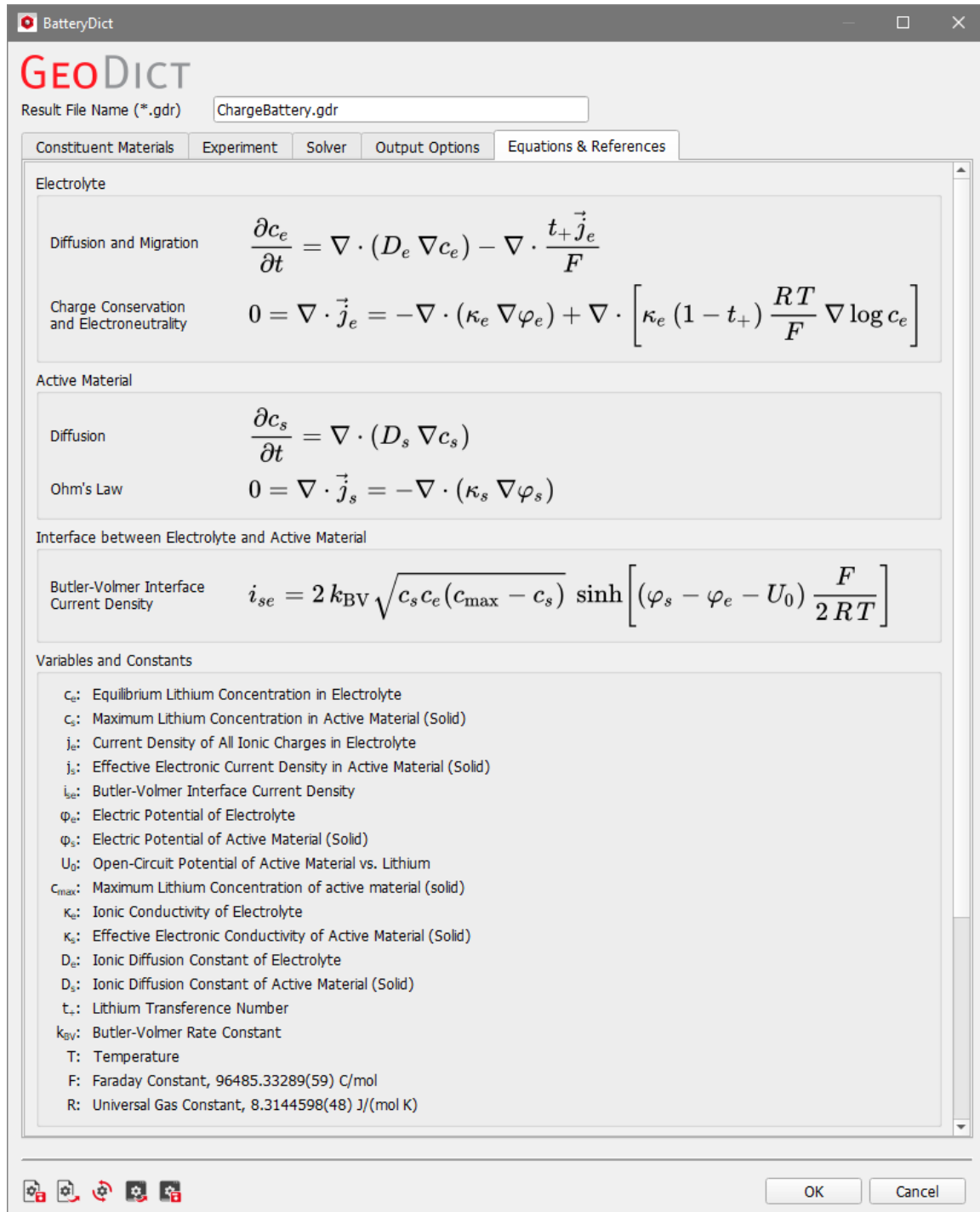
In the **Output Options** tab, **Calculate Estimation Only** can be checked, and then, the full simulation is not performed, but only the cell potential is estimated. This estimation is much faster than the full simulation. It considers the cell potential in equilibrium as well as the charge rate and 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.

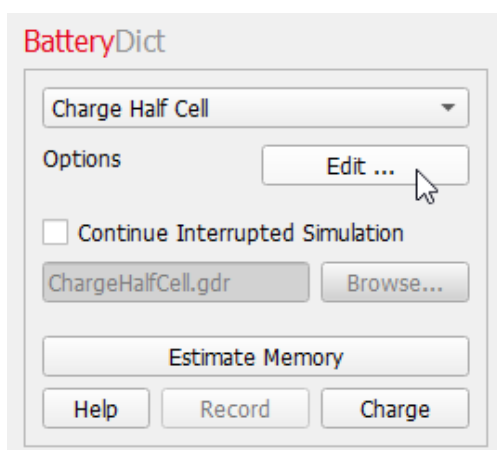
EQUATIONS & REFERENCES

The differential equations solved in the charging simulation are listed under the **Equations & References** tab and are described above in *Theoretical Basis* (page [3](#))

The references for the methods used are listed on this tab. In this **BatteryDict** documentation they can be found on page [13](#).



CHARGE HALF CELL



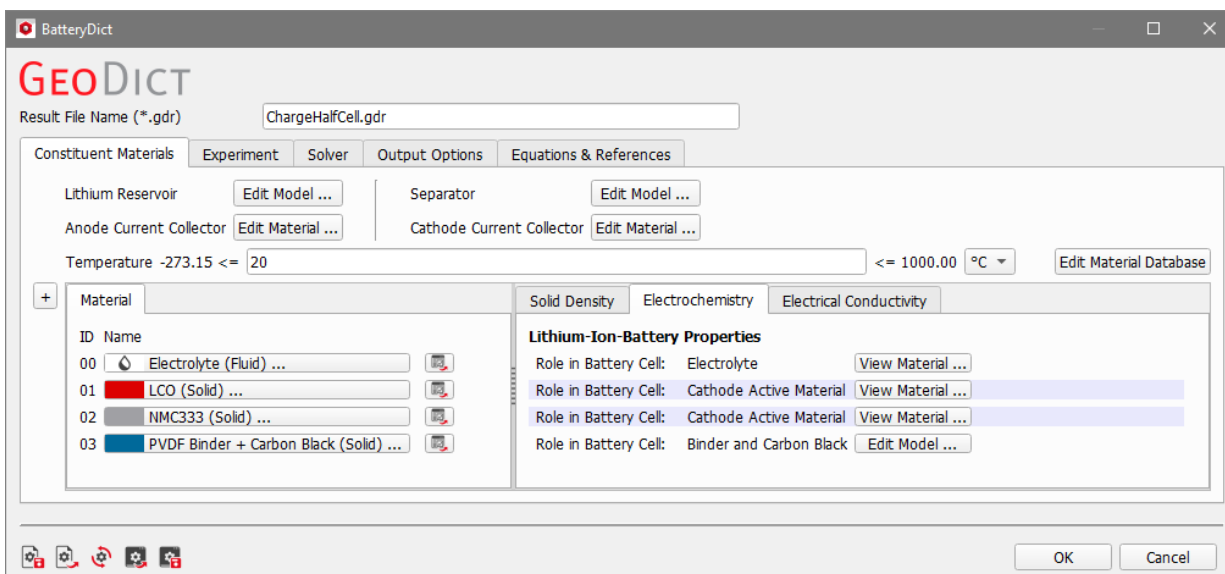
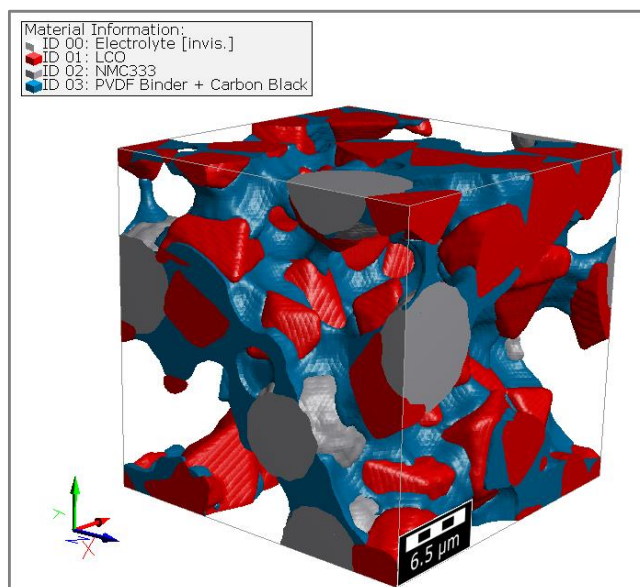
In **GeoDict** 2022, the charging of a half-cell is available as separate functionality. It can be used for charging simulations of arbitrary structures loaded in **GeoDict**, consisting of a single electrode or an electrode together with a separator and/or a current collector without designing a battery first. Input parameter 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.



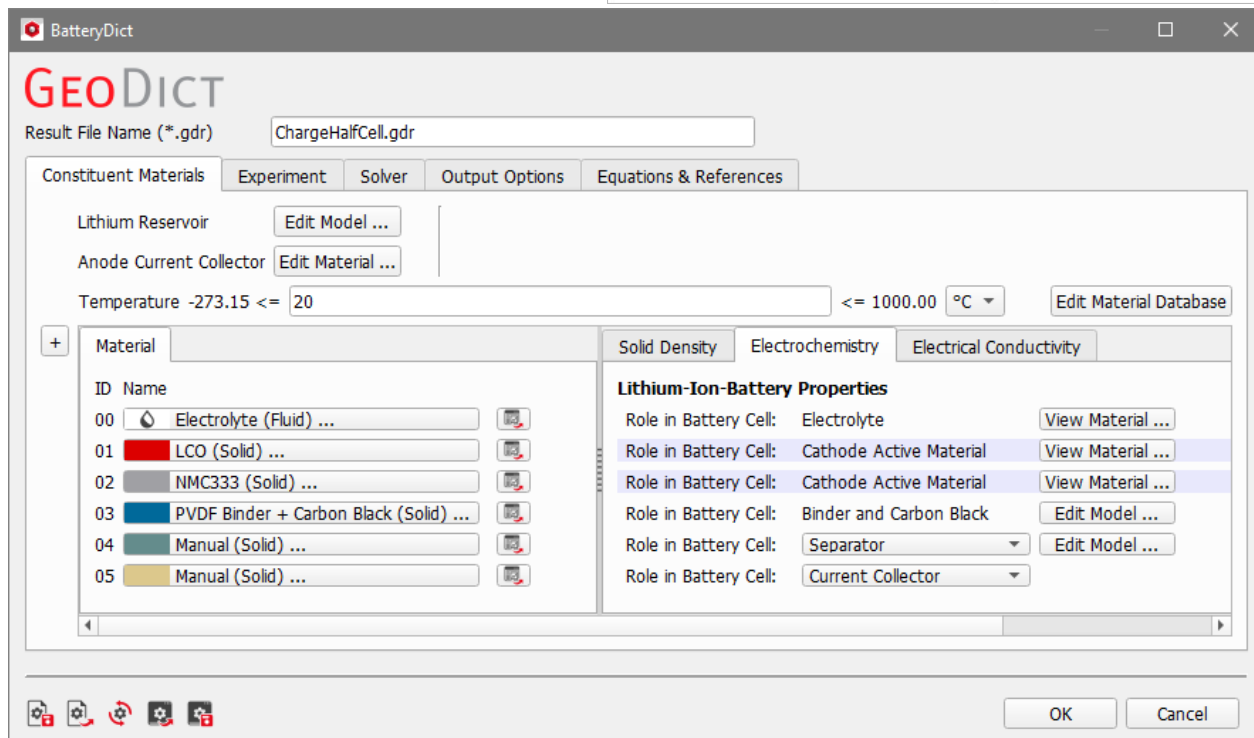
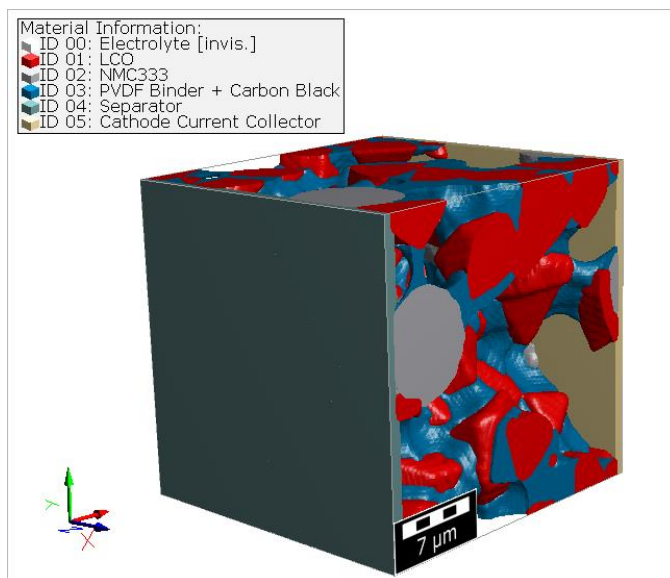
Charging and discharging simulations for Li-ion batteries

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 [21ff](#) for a more detailed description.

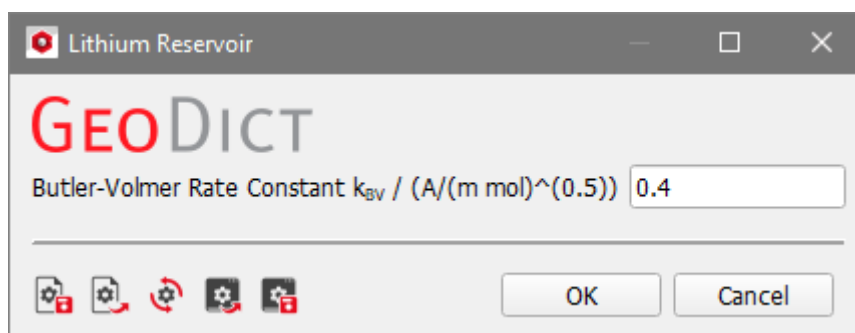
On top of the dialog, the parameters for anode current collector and lithium reservoir can be modified. If not defined by a separate Material ID in the structure, additionally the parameters for the separator and the cathode current collector can be defined.

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.

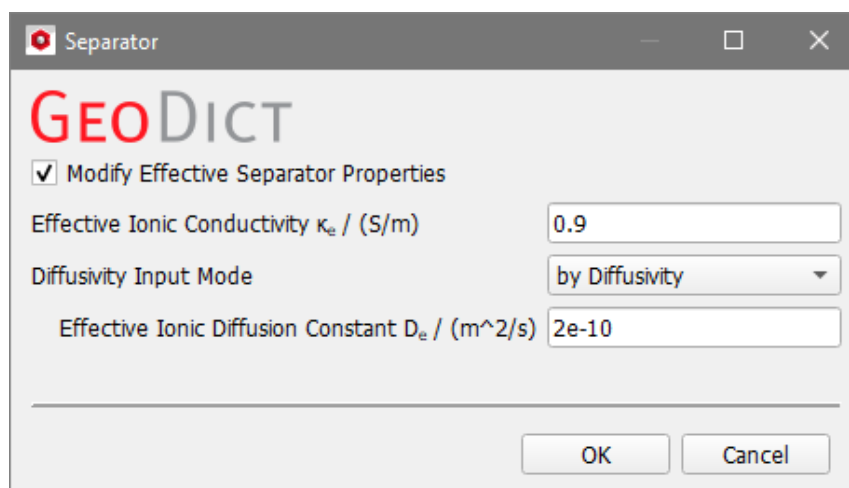
In this case, the buttons for modifying the corresponding properties disappear from the top of the dialog and the modification is possible only on the Electrochemistry tab.



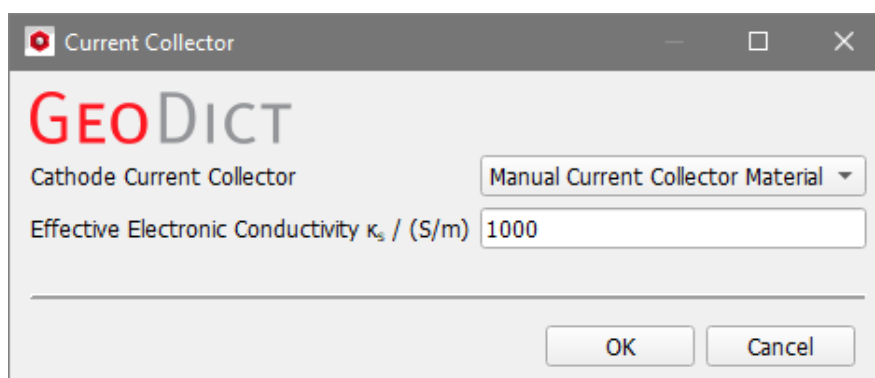
For the lithium reservoir, choose **Edit Model** to enter the Butler-Volmer Rate Constant for the simulation.



For the separator, with **Edit Model** the ionic conductivity and ionic diffusion constant of the electrolyte can be selected (uncheck **Modify Effective Separator Properties**), or effective values can be defined. See page [27](#) for more details.



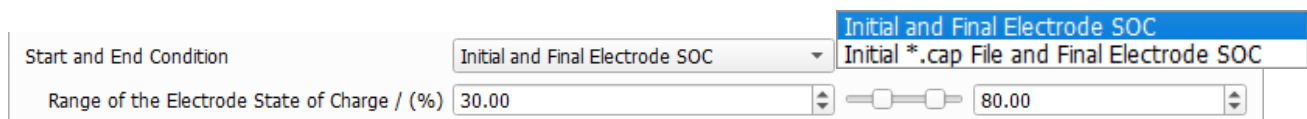
Material and electronic conductivity of the current collectors can be defined with the **Edit Material** buttons.



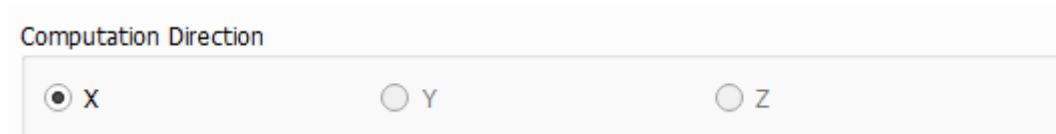
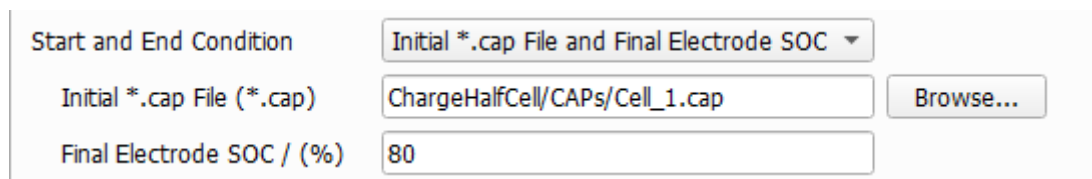
EXPERIMENT

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 [30](#).

A difference is in the selection of **Start and End Condition** for the simulation. Since for a half cell simulation one of the electrodes is modelled as a never-ending reservoir of lithium, only the state of charge (SOC) of the other electrode needs to be 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.



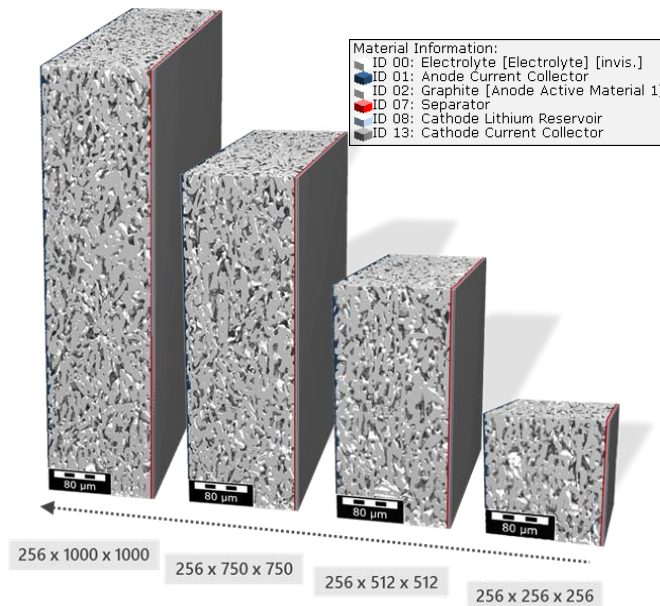
The **Computation Direction** is fixed in X direction in GeoDict 2022. In future GeoDict versions, it will be possible to decide about the coordinate direction in that the half-cell is assembled.

SOLVER, OUTPUT OPTIONS AND EQUATIONS & REFERENCES TAB

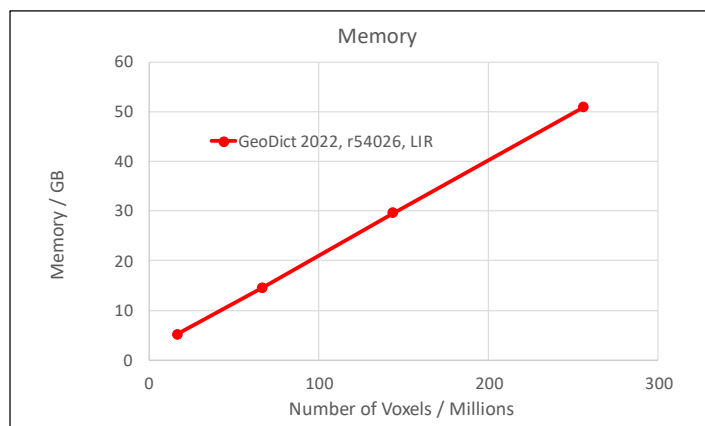
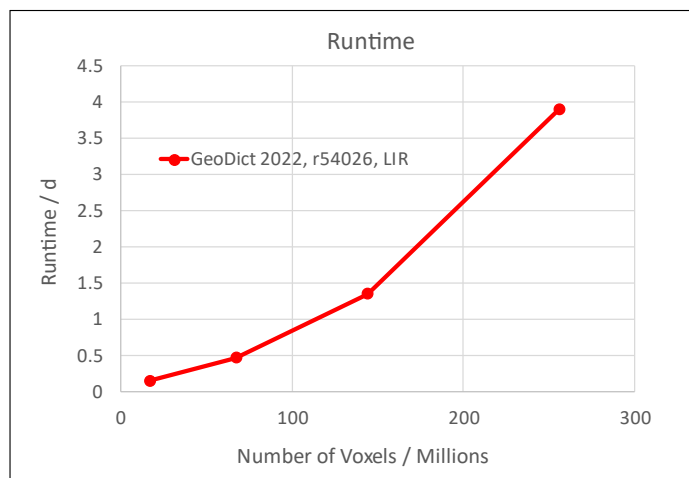
The options that can be selected on the **Solver** and the **Output Options** tab, as well as the equations on the **Equations & References** tab, are the same as for the charging of a whole battery. A description can be found on page [34ff](#).

PARALLELIZATION BENCHMARK RESULTS

A half cell consisting of a graphite anode and a lithium reservoir is simulated. It is charged from 5% to 91%. The simulation is run for increasing structure size to account for inhomogeneities or for battery ageing simulations.

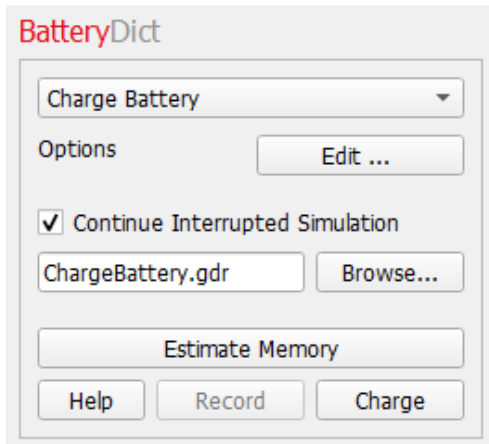


The simulation is run with LIR solver. The necessary memory for the computation is increasing linearly with the number of voxels simulated. Even a simulation with 250 million voxels can be run in 4 days, with only 50GB RAM required.



CONTINUE INTERRUPTED SIMULATION

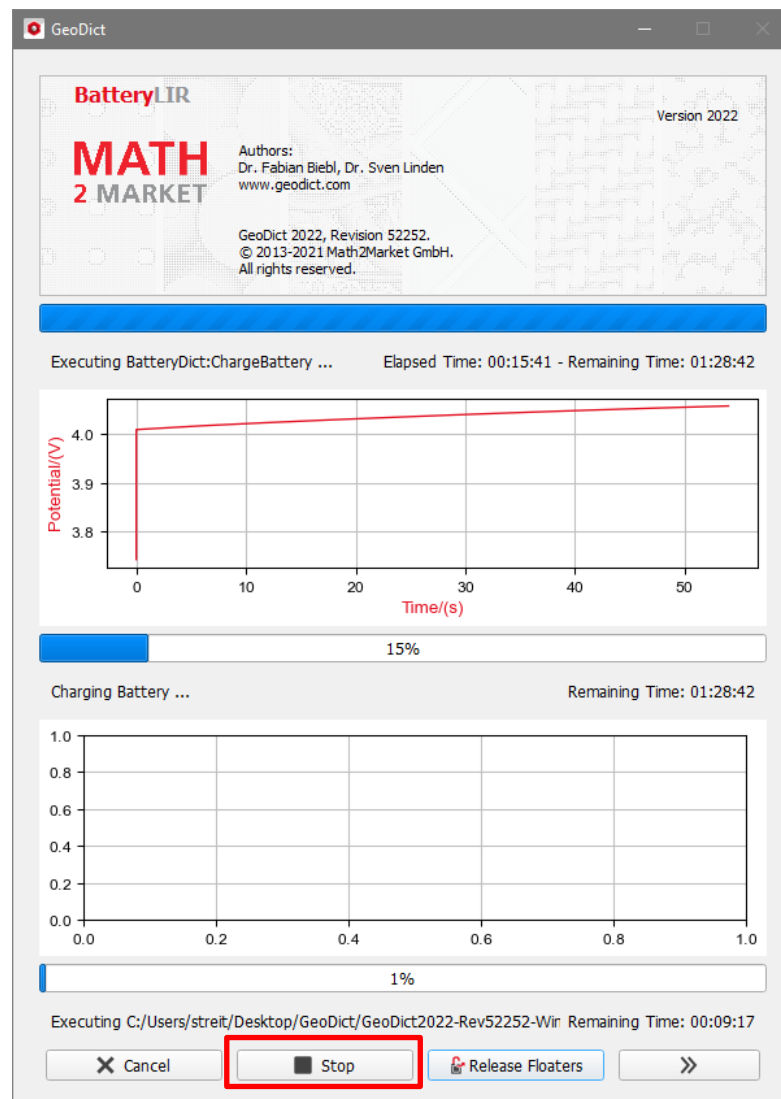
Since **GeoDict 2021**, it is possible to continue a previously interrupted simulation.



If **Charge Battery** or **Charge Half Cell** 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.

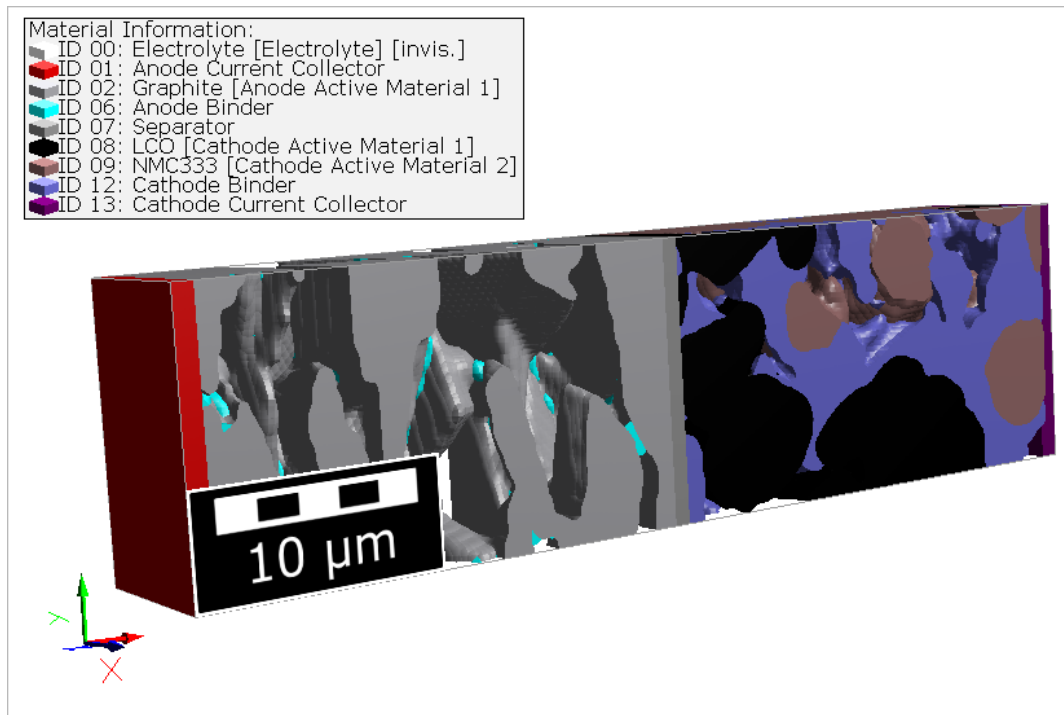


If the simulation was canceled, it is not possible to continue the simulation later.

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.



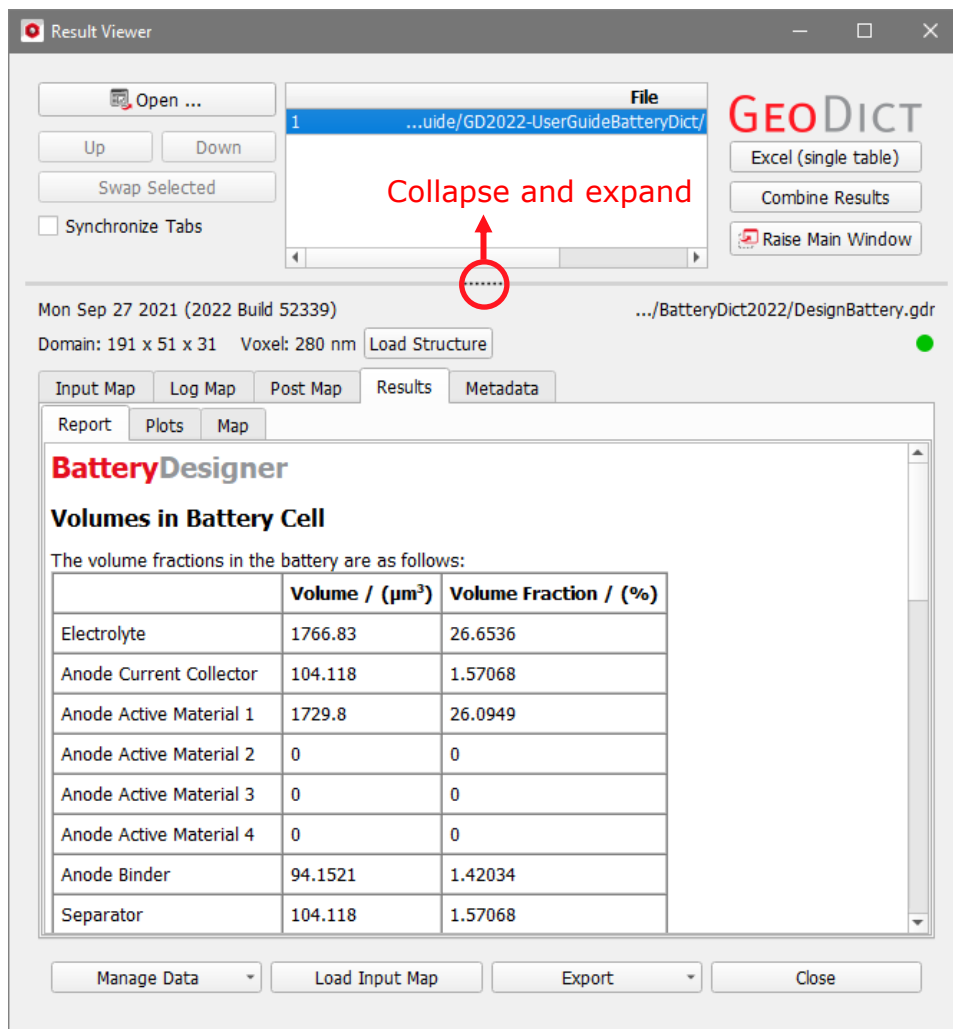
The .gdr file can be reopened at any time by choosing **File → Open Results (*.gdr)...** in the menu bar. The **Result Viewer** opens at the **Results** tab.

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 which 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.

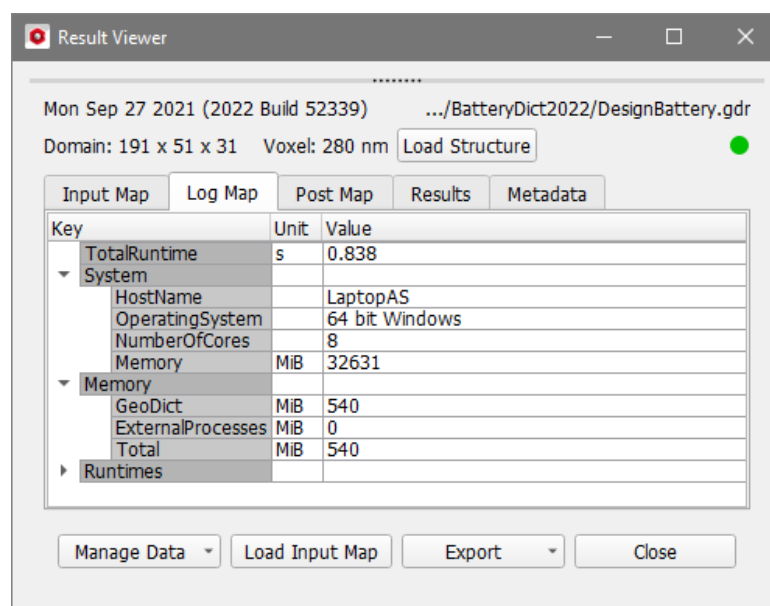
At the top of the result viewer, clicking the button **Excel (single table)** exports the information of this result file to Microsoft Excel®. A single worksheet is created that contains the information of the Results tab from the result file.

With the **Combine Results** button, 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.

Result Viewer

Mon Sep 27 2021 (2022 Build 52339)

.../BatteryDict2022/DesignBattery.gdr

Domain: 191 x 51 x 31

Voxel: 280 nm

Load Structure

Input Map

Log Map

Post Map

Results

Metadata

Report

Plots

Map

BatteryDesigner

Volumes in Battery Cell

The volume fractions in the battery are as follows:

	Volume / (μm^3)	Volume Fraction / (%)
Electrolyte	1766.83	26.6536
Anode Current Collector	104.118	1.57068
Anode Active Material 1	1729.8	26.0949
Anode Active Material 2	0	0
Anode Active Material 3	0	0
Anode Active Material 4	0	0
Anode Binder	94.1521	1.42034
Separator	104.118	1.57068
Cathode Active Material 1	745.292	11.2431
Cathode Active Material 2	1367.19	20.6248
Cathode Active Material 3	0	0
Cathode Active Material 4	0	0
Cathode Binder	613.251	9.25122
Cathode Current Collector	104.118	1.57068
Inclusion	0	0

Volumes in Anode

The volumes and volume fractions in the anode are as follows (the volume fractions are with respect to the electrode volume):

	Volume / (μm^3)	Volume Fraction / (%)
Binder	94.1521	1.42034
Active Material 1	1729.8	26.0949
Active Material 2	0	0
Active Material 3	0	0
Active Material 4	0	0

Manage Data

Load Input Map

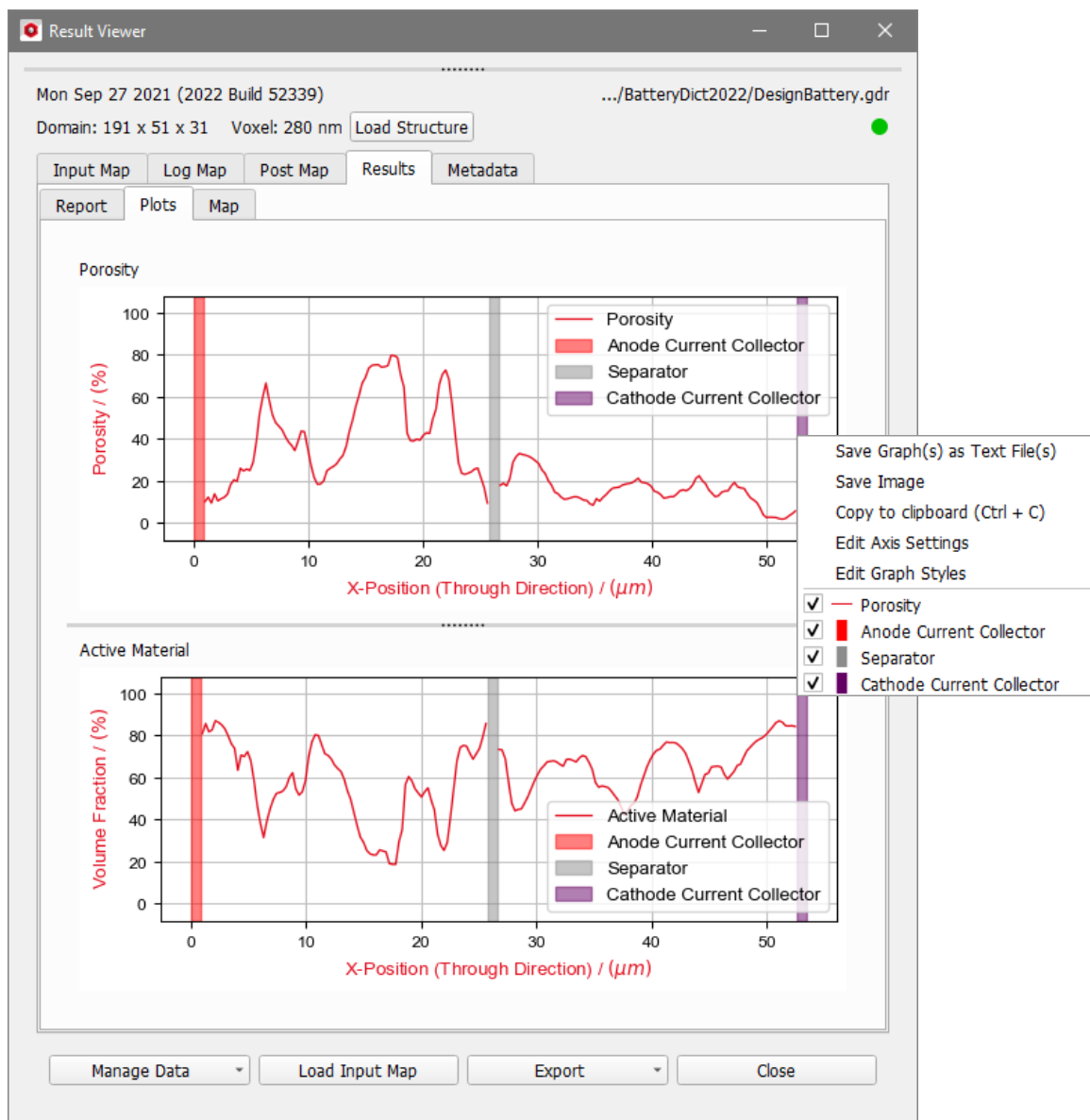
Export

Close

Charging and discharging simulations for Li-ion batteries

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.

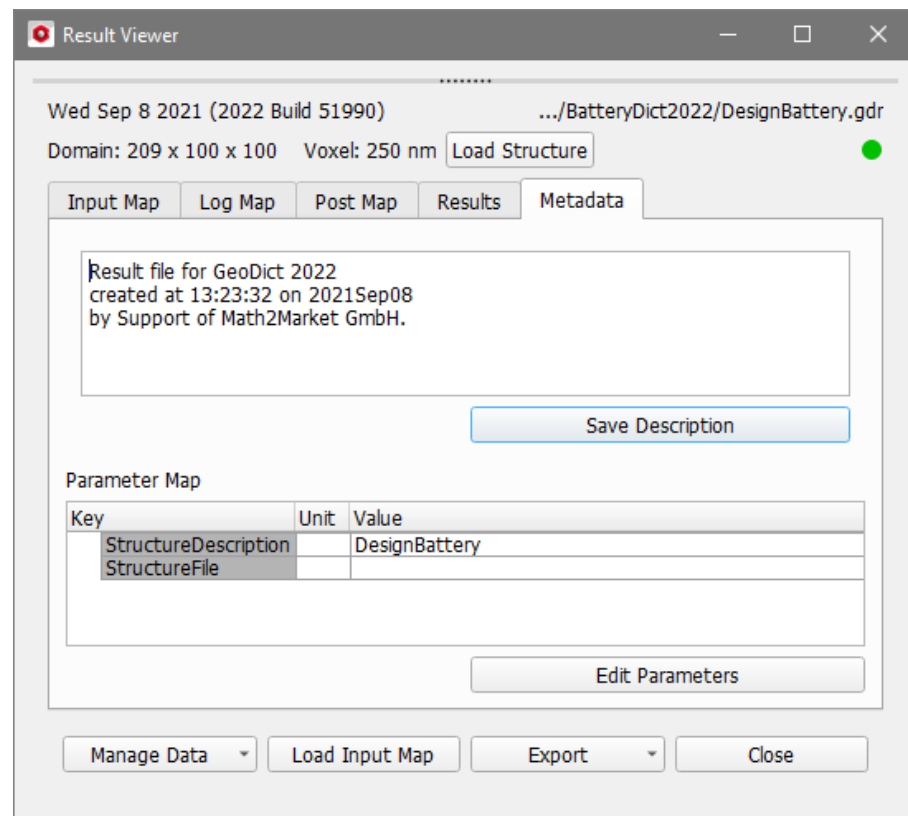
At the separator and both current collectors, no values are shown for porosity and active material since these structures do not contain active material and are not resolved into a microstructure in the Battery Designer. Also, the binder is considered as solid material in the computation of the porosity. 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 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:**

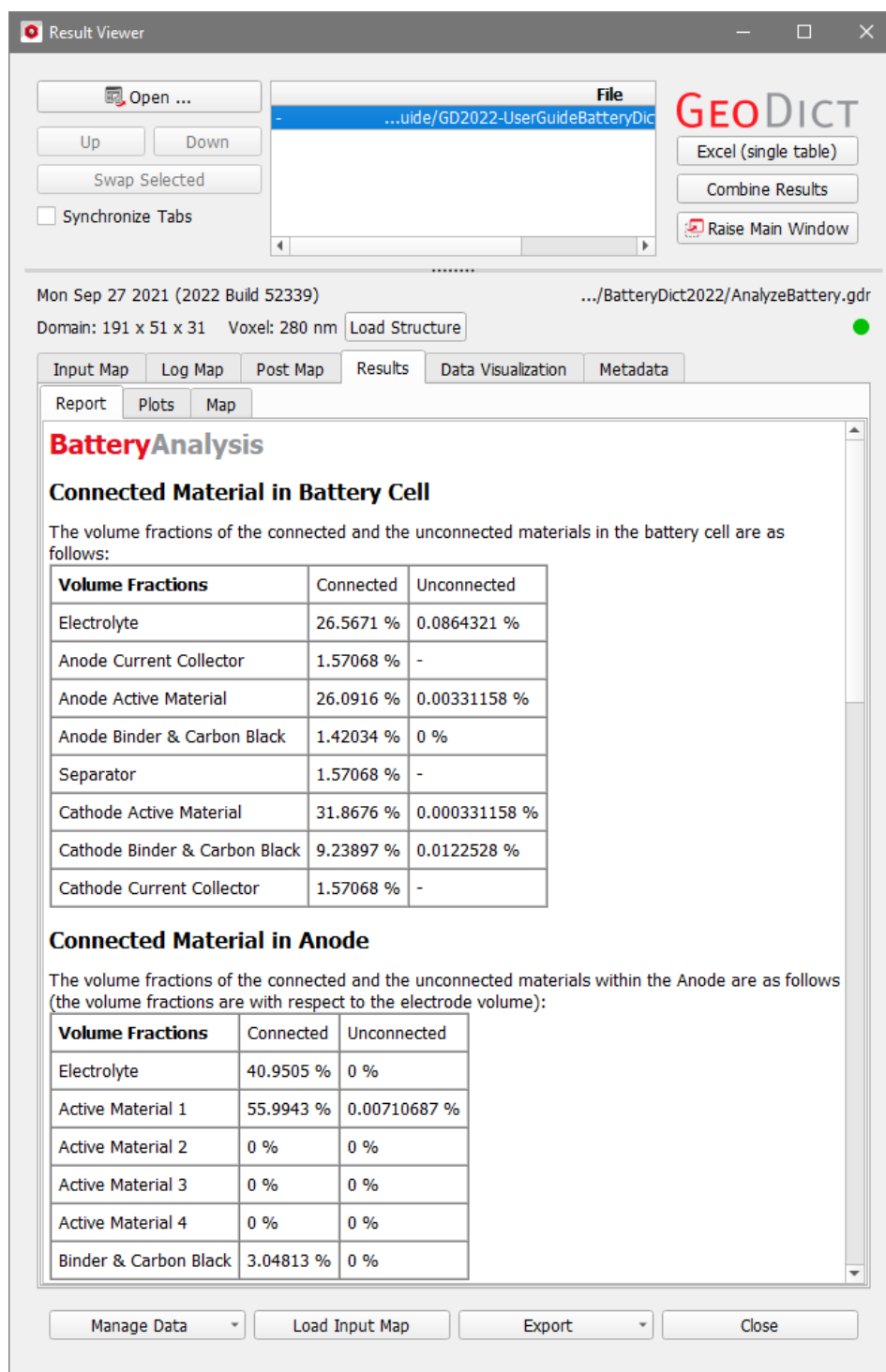
- **Clean-Up/Pack:** Zip the information contained in the result folder or clean-up the result folder.
- **Rename:** Change the name of result file and result folder.
- **Load Input Map:** Reload solver options and material parameters used for the computation of the results. After loading, these parameters 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](#) 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](#) 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](#) 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 part of unconnected material is therefore desired.



The screenshot shows the GeoDict Result Viewer window. The 'Results' tab is selected, and the 'Report' subtab is active. The report is titled 'BatteryAnalysis' and 'Connected Material in Battery Cell'. It displays the volume fractions of connected and unconnected materials for various battery components.

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	26.5671 %	0.0864321 %
Anode Current Collector	1.57068 %	-
Anode Active Material	26.0916 %	0.00331158 %
Anode Binder & Carbon Black	1.42034 %	0 %
Separator	1.57068 %	-
Cathode Active Material	31.8676 %	0.000331158 %
Cathode Binder & Carbon Black	9.23897 %	0.0122528 %
Cathode Current Collector	1.57068 %	-

Connected Material in Anode

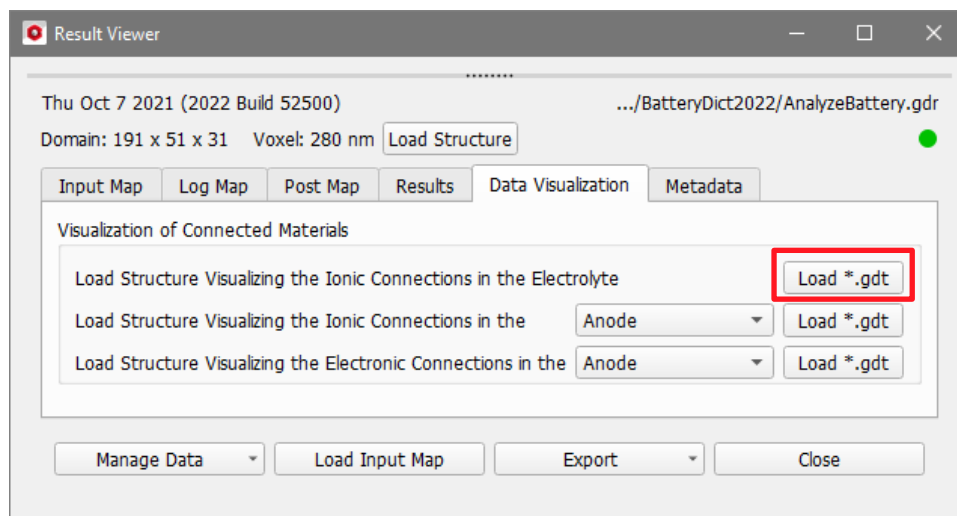
The volume fractions of the connected and the unconnected materials within the Anode are as follows (the volume fractions are with respect to the electrode volume):

Volume Fractions	Connected	Unconnected
Electrolyte	40.9505 %	0 %
Active Material 1	55.9943 %	0.00710687 %
Active Material 2	0 %	0 %
Active Material 3	0 %	0 %
Active Material 4	0 %	0 %
Binder & Carbon Black	3.04813 %	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 [49](#).

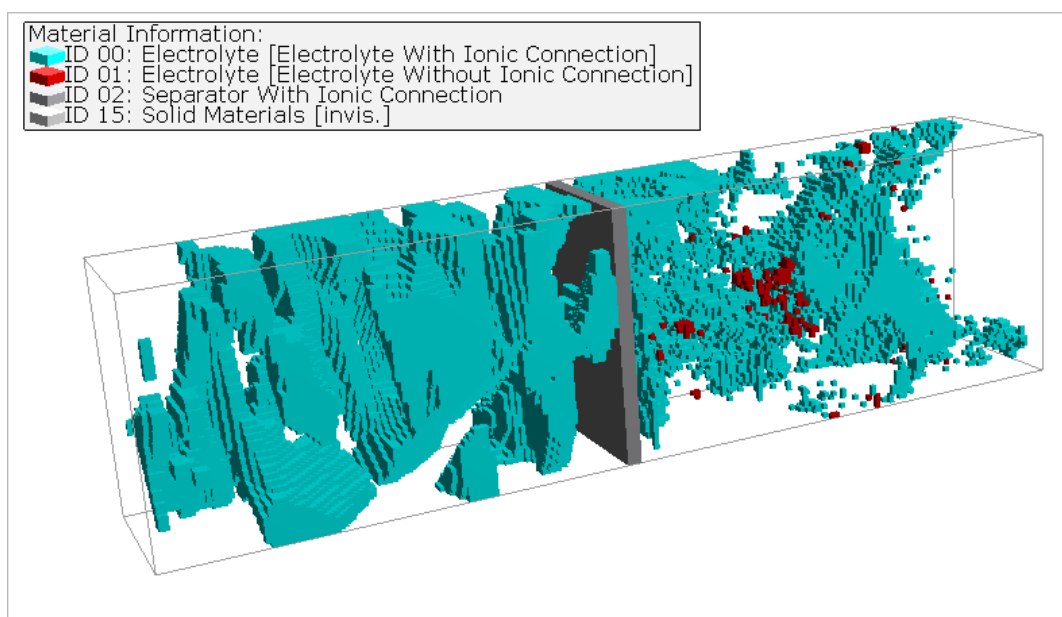
Under the **Results - Plots** subtab, the porosity, and the distribution of active material over the whole battery are shown as averaged values over each slice in y- and z-direction. This is also the same plot as shown for a result file of the battery designer, see page [50](#).

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 [70](#).

As an example, here the structure for the ionic connection in the Electrolyte is shown.



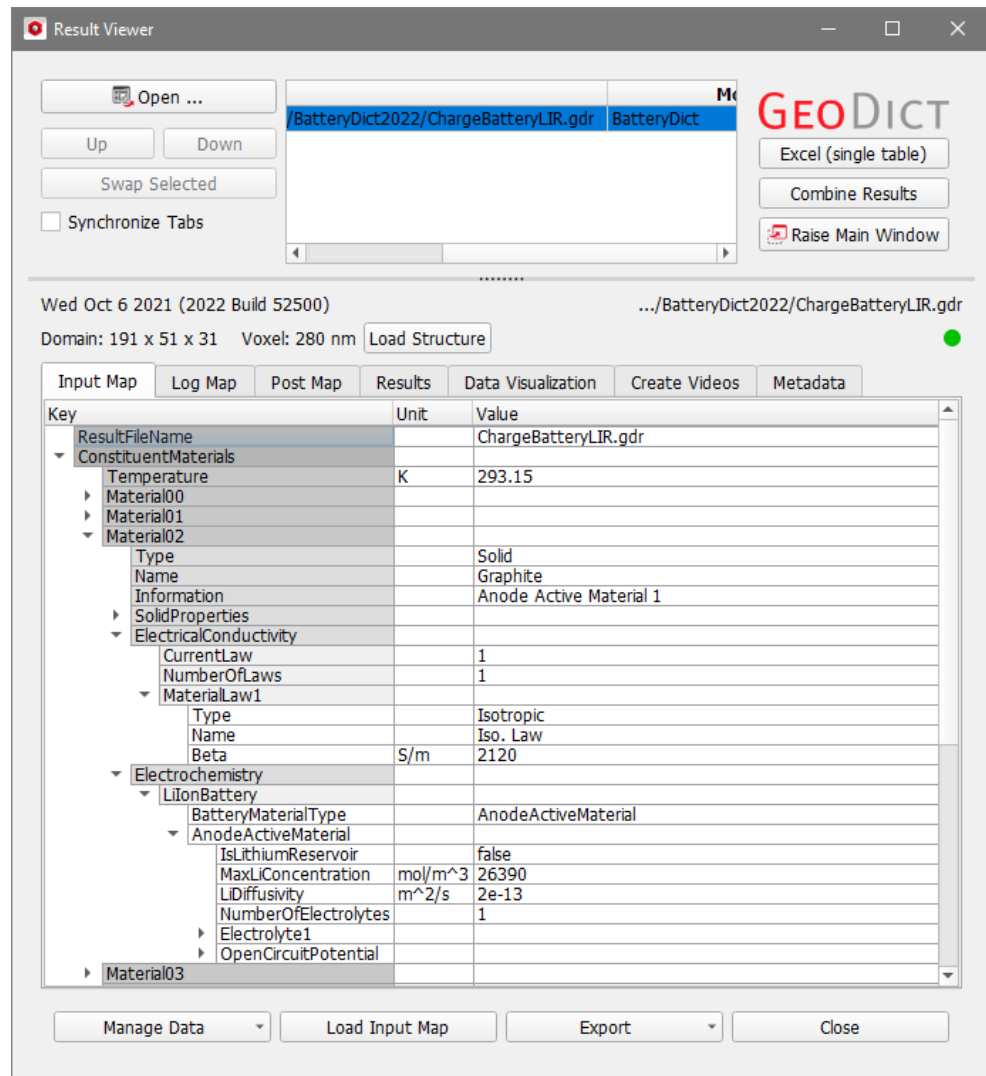
RESULTS OF CHARGE BATTERY

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.

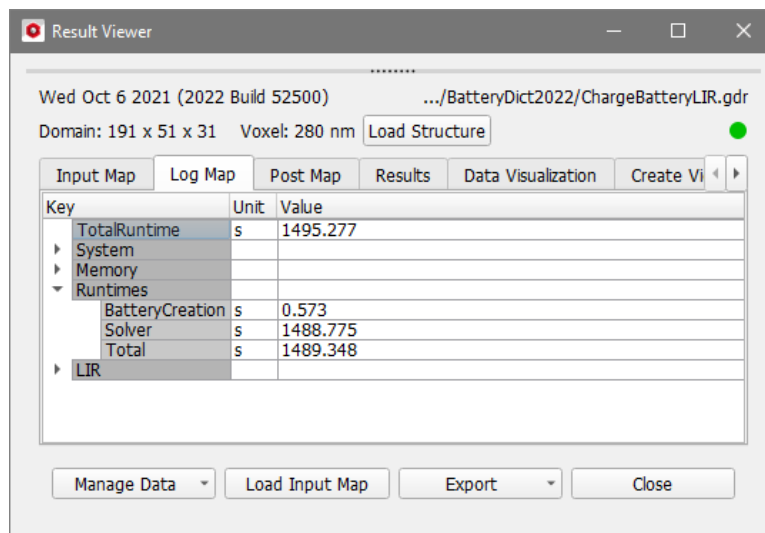
These results are accessible at any time by loading the .gdr file from the menu bar (**File** → **Open Results (*.gdr) ...**). The **Load Structure** button and the buttons available at the bottom of the **Result Viewer** are the same as for other result files and are explained on page 47.

In the following, the 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.

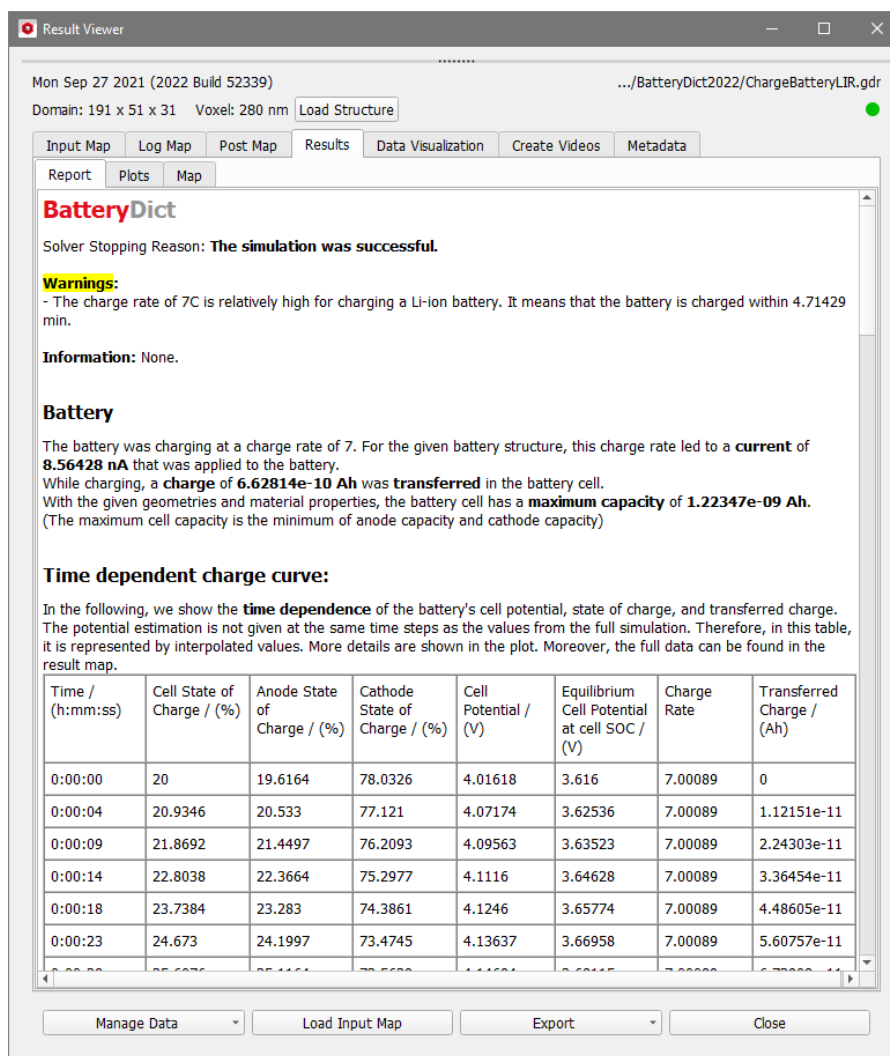


On the tab **Log Map**, the runtime and memory used for the simulation, as well as information about the machine, are shown.

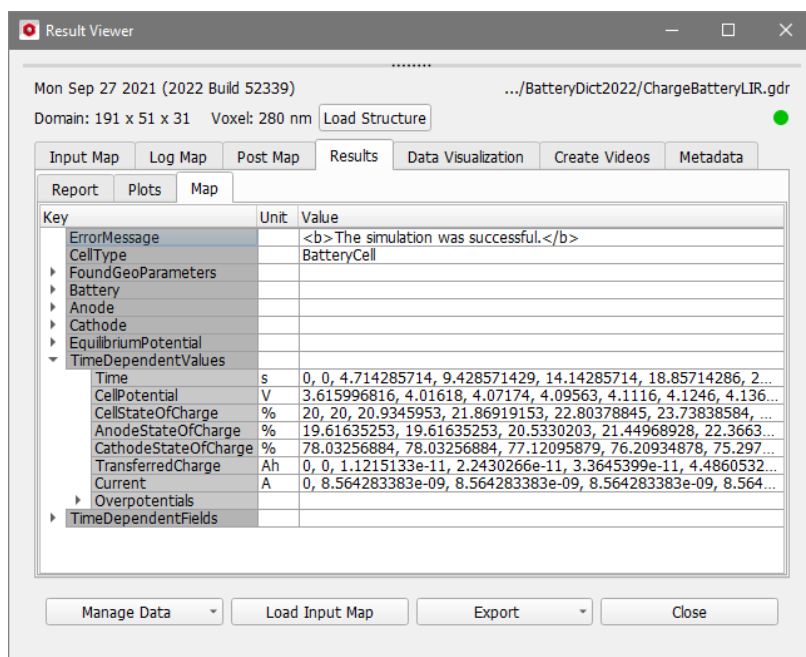


The **Post Map** tab lists information about plots shown in the **Results** tab. Parameters chosen for the plots as well as data for the graphs are shown here.

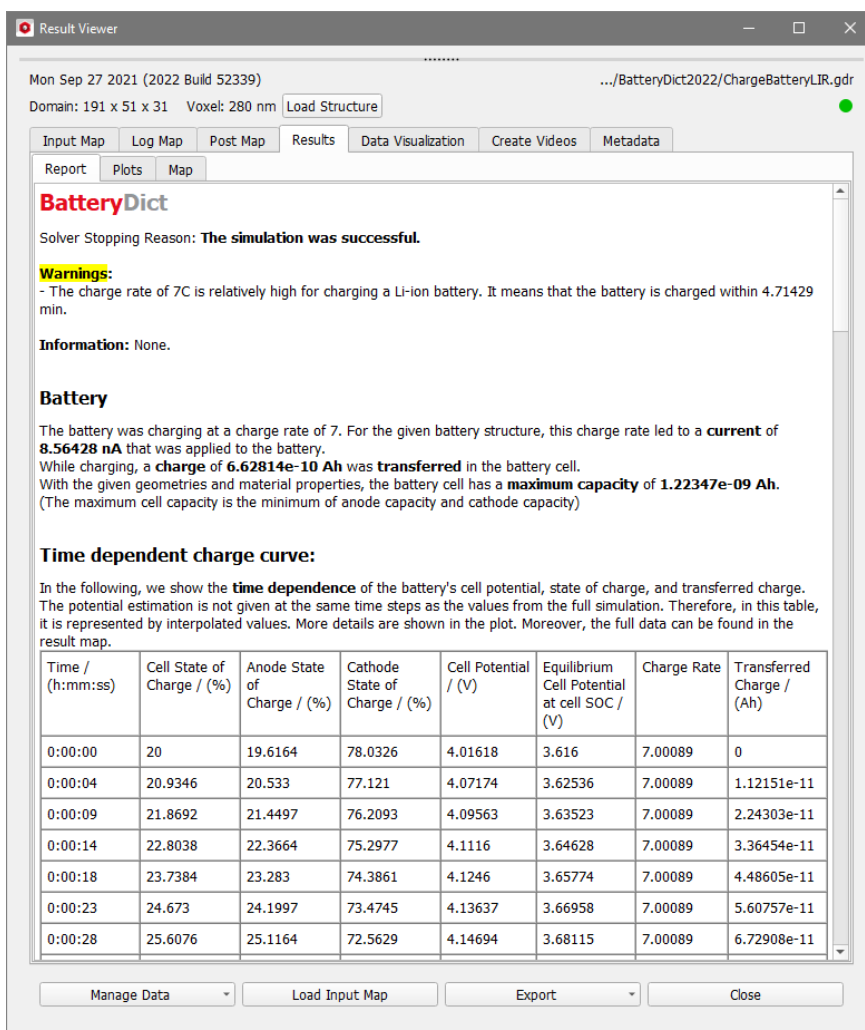
The **Results** tab shows the results of the computation in several forms.



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, see *Tested Parameter Space* above in page 10) and information about the simulation steps for a charging profile is shown there. In the example shown here, a warning appears due to the high charge rate applied.

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

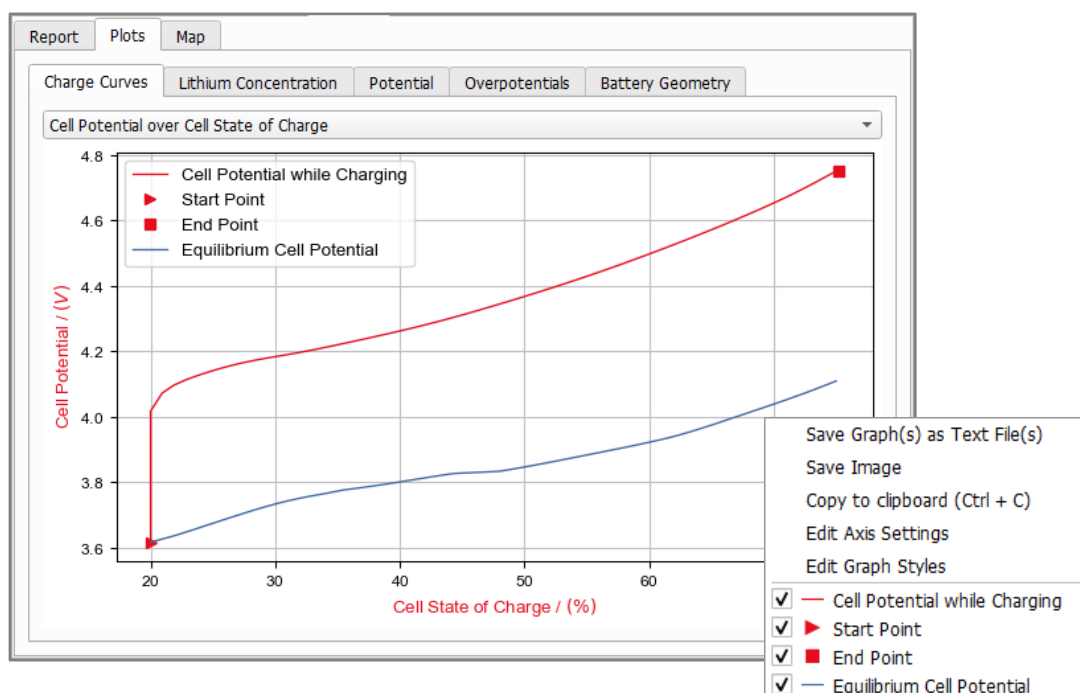
$$C_{A,max} = l_V^3 * F * \sum_{V \in \{Anode \text{ Active Material Voxels}\}} c_{max}(V)$$

and

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

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.

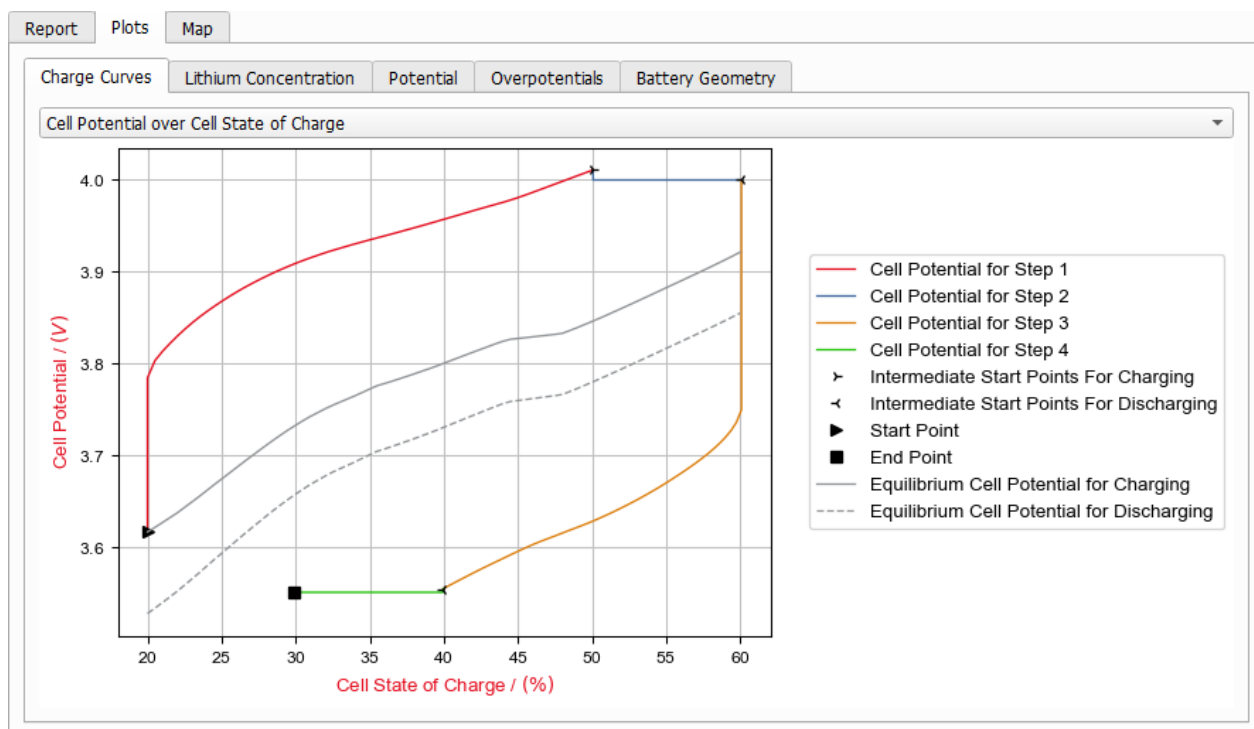
In the **Cell Potential over Cell State of Charge** plot (above), the cell potential while charging or discharging is compared to the cell potential in equilibrium, i.e., while loading in infinite time. While charging or discharging the battery infinitely slow, the battery is always in equilibrium state,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

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.

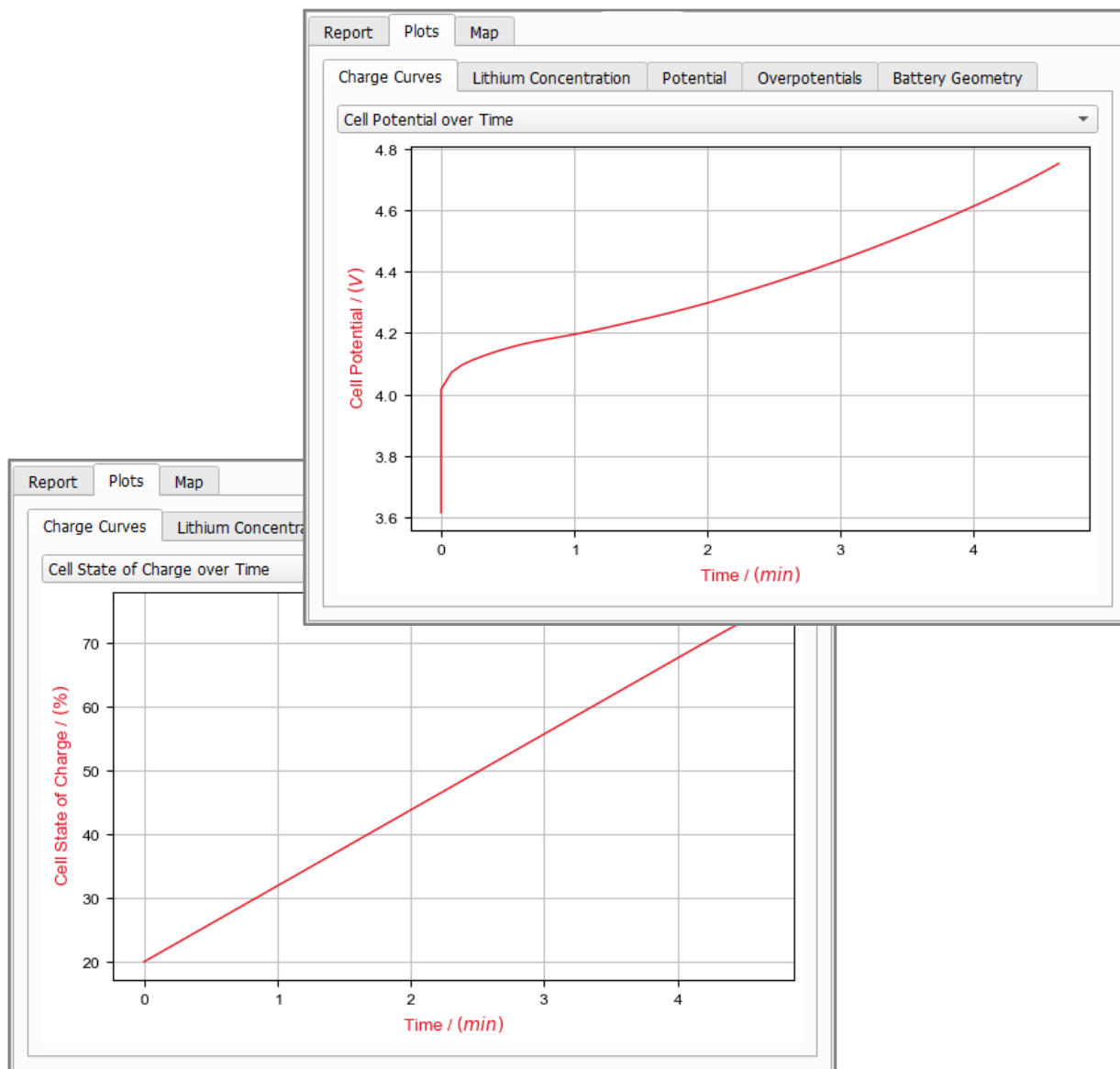
If **Calculate Estimation Only** (page [39](#)) was chosen as option, the estimation of the cell potential is shown instead of the computed time evolution of the potential.

In case a charging profile was selected for the simulation (see page [32](#)), the cell potential is shown for each simulation step in the profile in a different color. If the charging profile consists of charging and discharging steps, the equilibrium cell potential is shown both for charging and discharging.

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



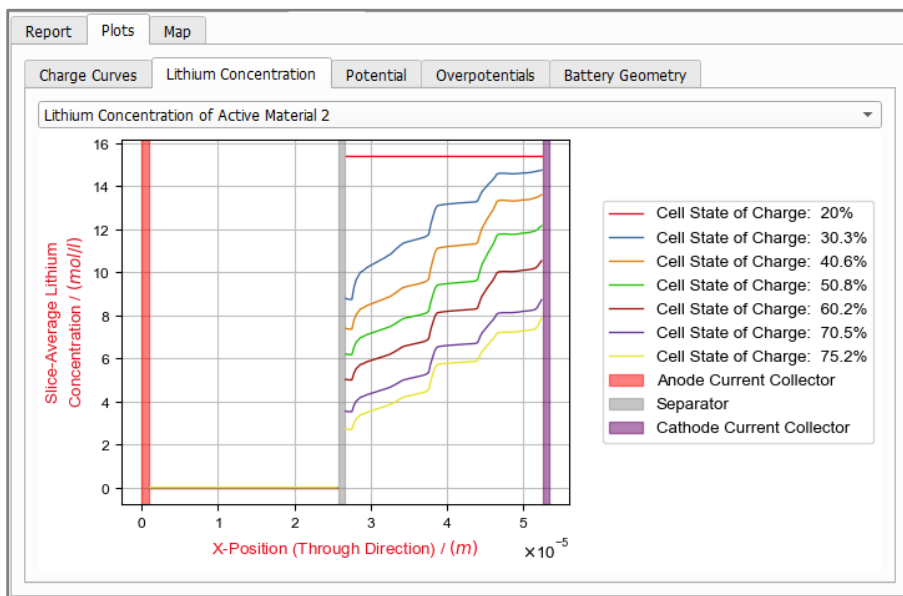
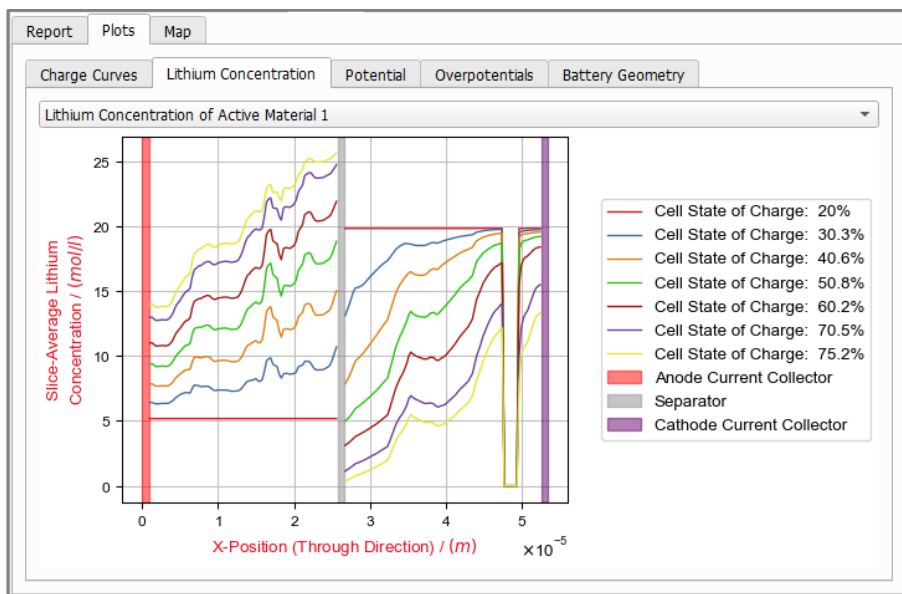
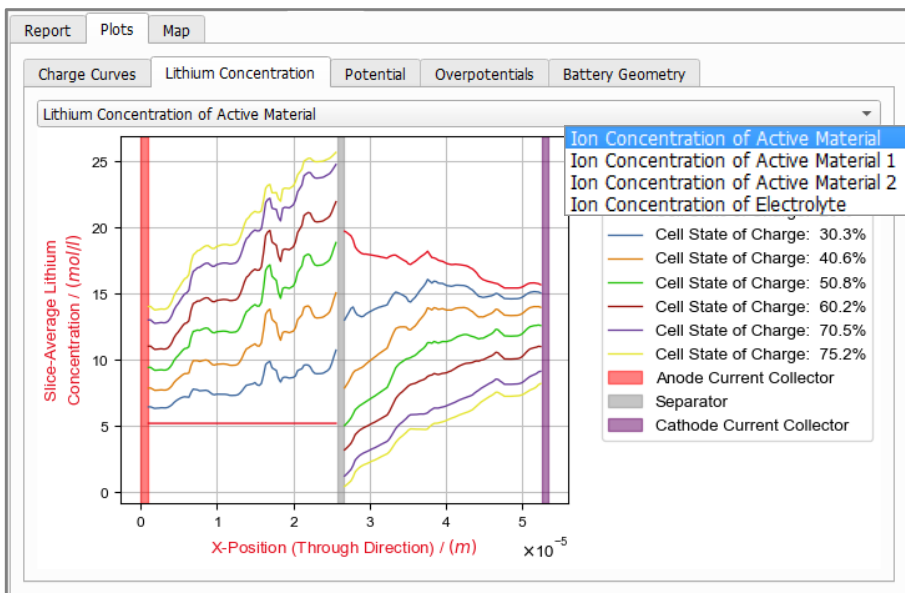
Due to the simulation with a constant charge rate and without the selection of an upper cut-off voltage in the example shown, the state of charge increases linearly with the simulated time. The trend of the cell potential over time is therefore the same as for the **Cell Potential over Cell State of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



Charging and discharging simulations for Li-ion batteries

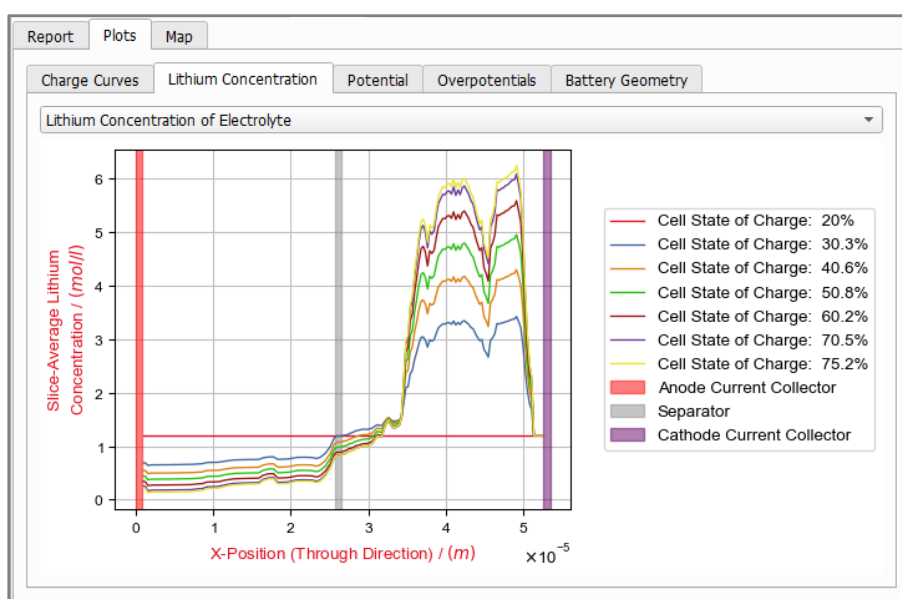
The lithium concentration of the cathode changes more uniformly if only the concentration of one of the active materials is selected to be displayed.

Note, that for the **X-Position** between 48 and 50 μm no Active Material 1 is contained in the cathode. Therefore, a jump is visible there. For the anode, only one active material was used in the battery cell. Therefore, the ion concentration shown for Active Material 2 is zero.

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.

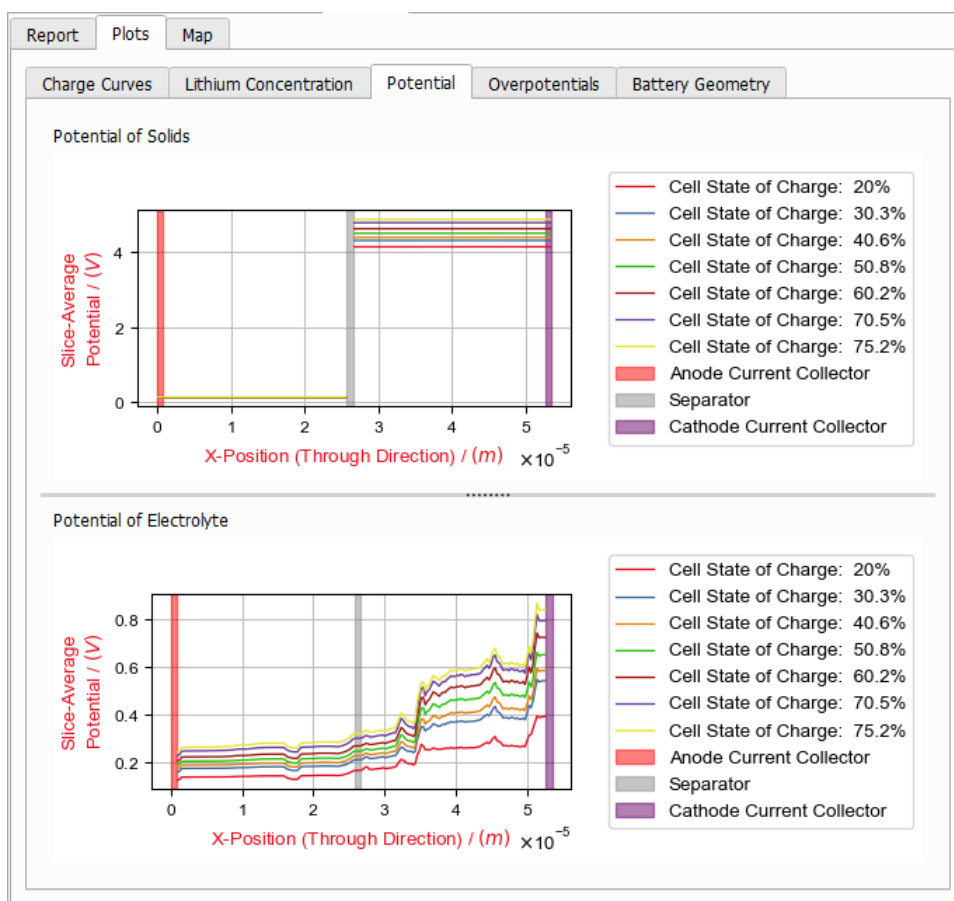
Since, the diffusion of the Li-ions takes some time, the gradient of the Li-ion concentration in the electrolyte is visible in the example.



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 one 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.

The solvers calculate 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. The solvers choose the potential to be zero at the anode current collector. Therefore, the potential in the anode always starts at zero for all times. As explained before, the potential is as good as constant in the anode. Hence, in this example, the potential in the anode solid is very close to zero everywhere for all time steps.

Over the time, the intercalation of Li-ions into the anode becomes more costly. At the same time, the potential gain from the deintercalation of Li-ions out of the cathode decreases. Therefore, the potential difference between anode and cathode grows, which can be seen in the example.

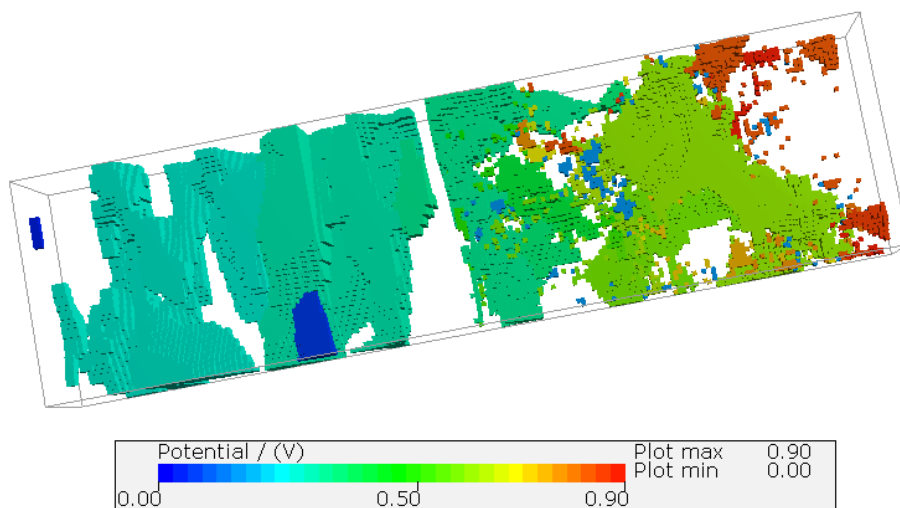
For the potential of the electrolyte, a gradient is visible between the anode current collector and the cathode current collector. This gradient is increasing for higher charge rates. Disregarding the noise, the potential grows from left to right. This comes from the charge current that is driven by 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. The potential gradient is larger on the right, because there, the electrolyte is not as good connected as on the left side.

The noise visible in the electrolyte potential stems from electrolyte voxels which are not connected to the separator via other electrolyte voxels. In these 'unconnected' electrolyte voxels, the potential is rather extreme (either quite high or quite low).

The potential of the electrolyte voxels is shown in the figure below. On the right side (cathode), unconnected voxels are red (high electrolyte potential) or blue (low electrolyte potential).

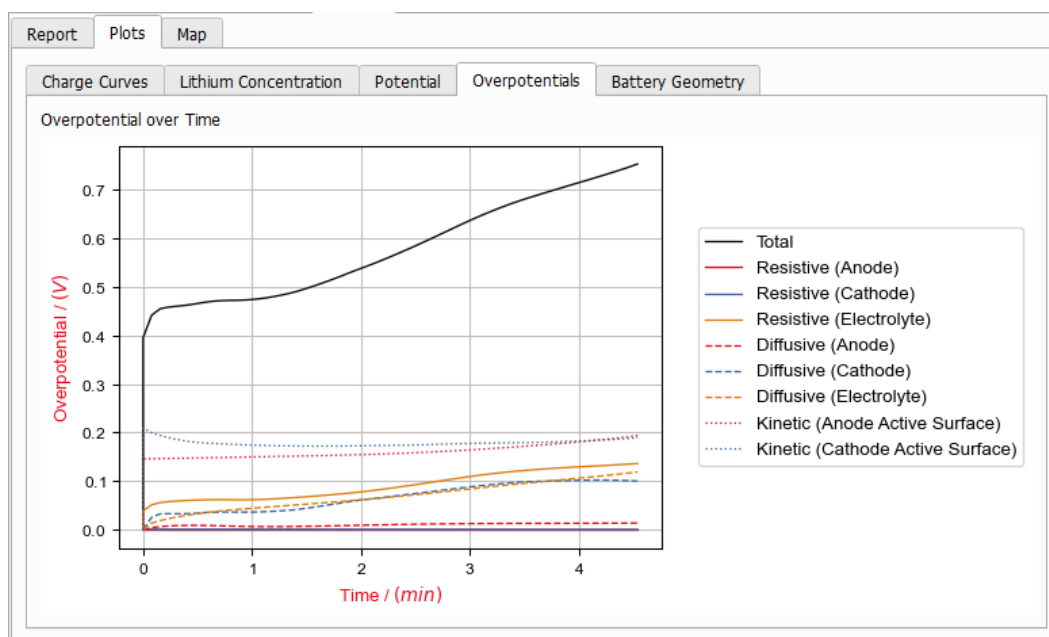
The blue voxels are not connected to active material. This connection would be the only way for electrolyte to change the potential (via the Butler-Volmer interface current).

The red voxels are connected to active material and roughly have the potential of the cathode solids minus the overpotential from the interface of active material and electrolyte. They have a higher potential than the electrolyte connected to the separator, because they do not have currents that would lead to a potential drop.

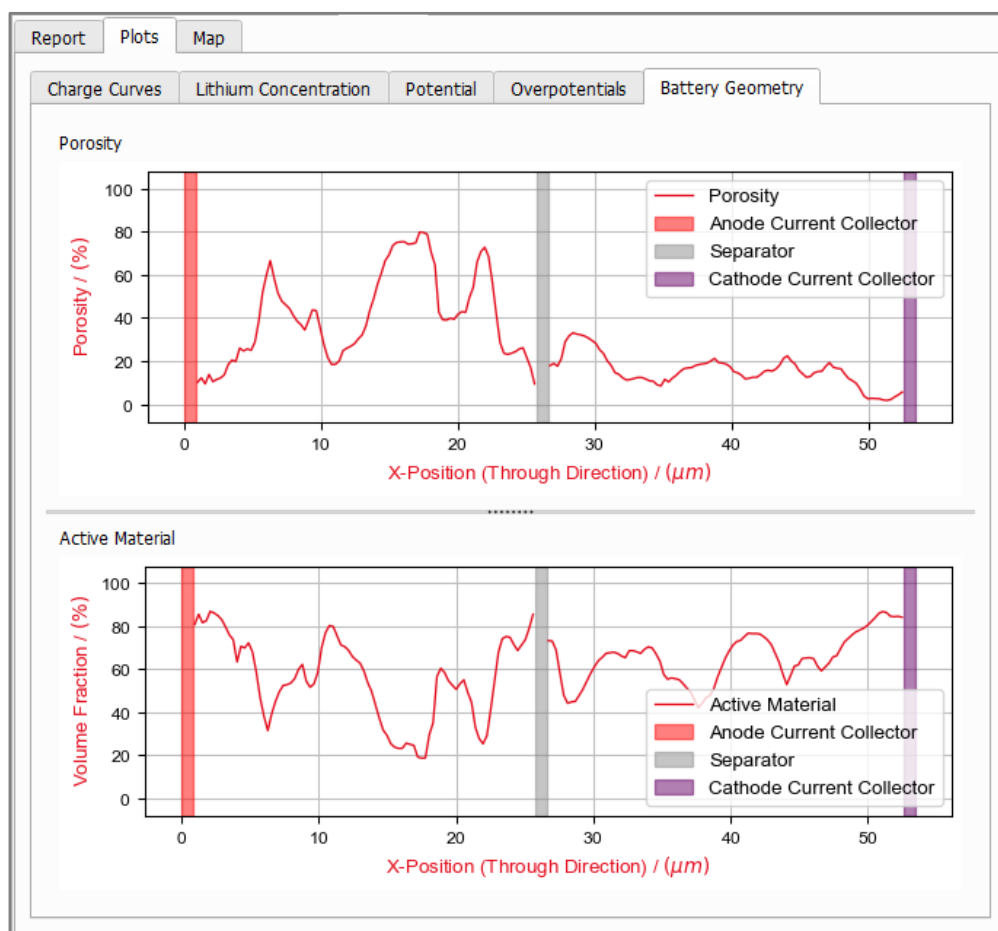


On the anode side, all voxels with electrolyte have a low potential even in the case of them being connected to active material only, because they either have kept their potential from the beginning (0 Volt) or have the potential of the anode solids plus the overpotential on the interface of active material and electrolyte. Unconnected electrolyte voxels have a lower potential than the electrolyte connected to the separator, because they do not have current that would cause a potential difference.

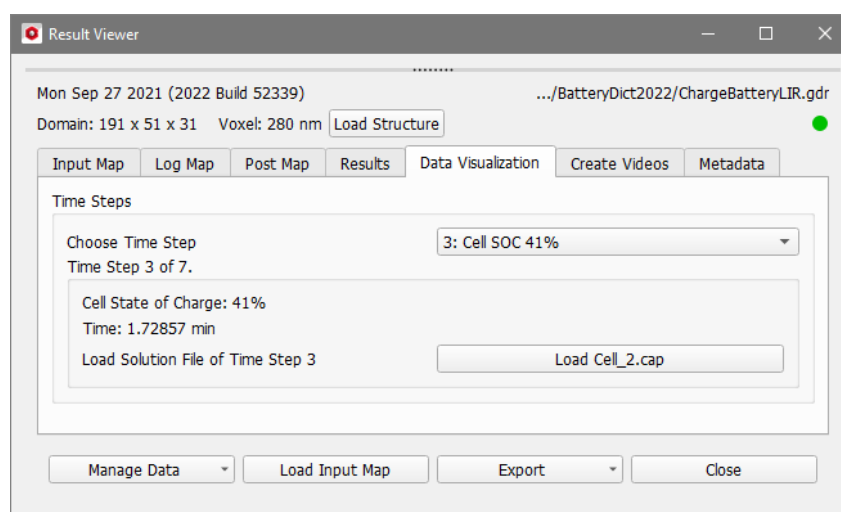
On the **Overpotentials** tab, the evolution of the different overpotentials over time is visualized. For an explanation of the overpotentials see page [8](#).



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 in page 39).

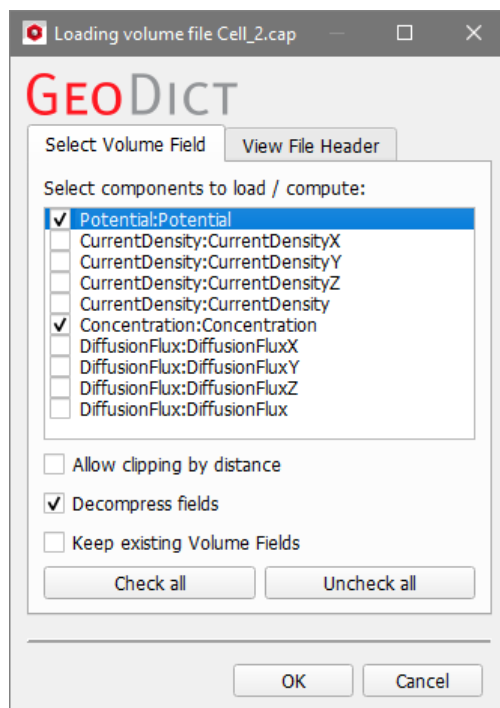


For instance, let us select the solution file at a state of charge of 40%. For the example shown here, we just need to select step 3. By clicking **Load Cell_2.cap**, the available volume fields (tab Select Volume Fields) of the file can be selected. Additionally, the user may have a look at the file header of the result file (View File Header).

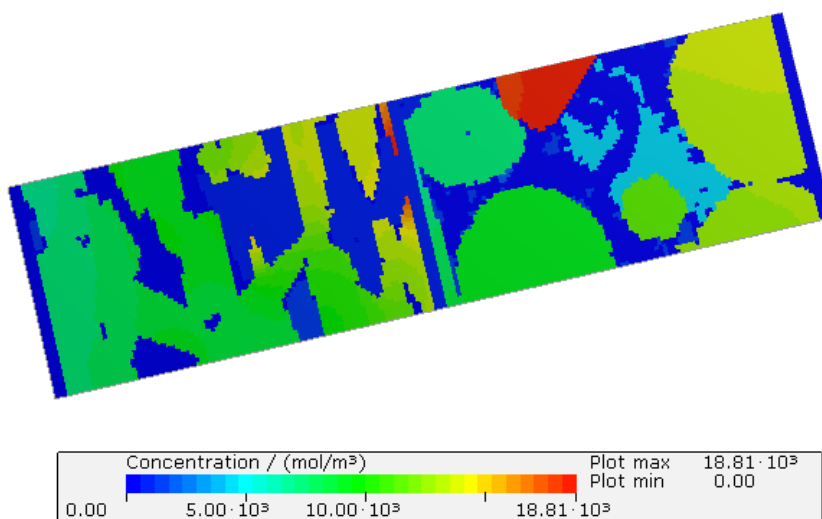
Volume Fields available depend on the solver used for the computation (LIR or BESTmicro) and on the fact whether porous binder is used or not.

Load, for example, only the **Concentration** and **Potential** fields.

In this case, first click **Uncheck all**. Then, select **Concentration:Concentration** and **Potential:Potential**. After clicking **OK**, both selected fields are loaded into the GeoDict GUI.



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



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.

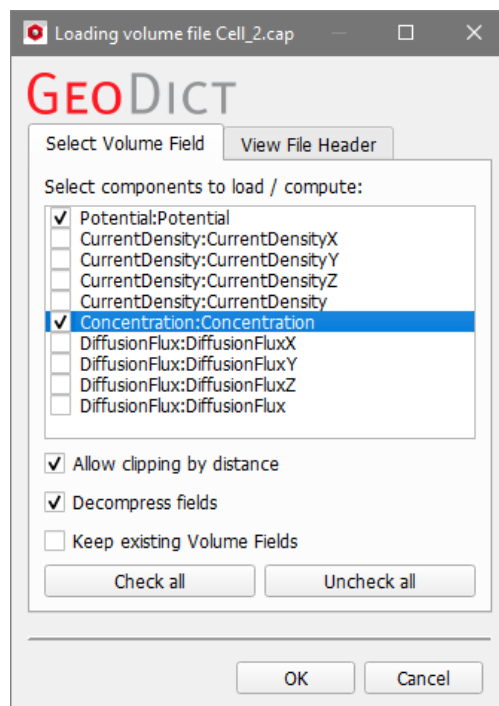
For example, if you are only interested in the Li-ion concentration inside of the electrolyte, check **Allow clipping by distance** when you load the volume field. In

this way, in the visualization, you can choose to clip the ionic concentration by positive values of the created distance map.

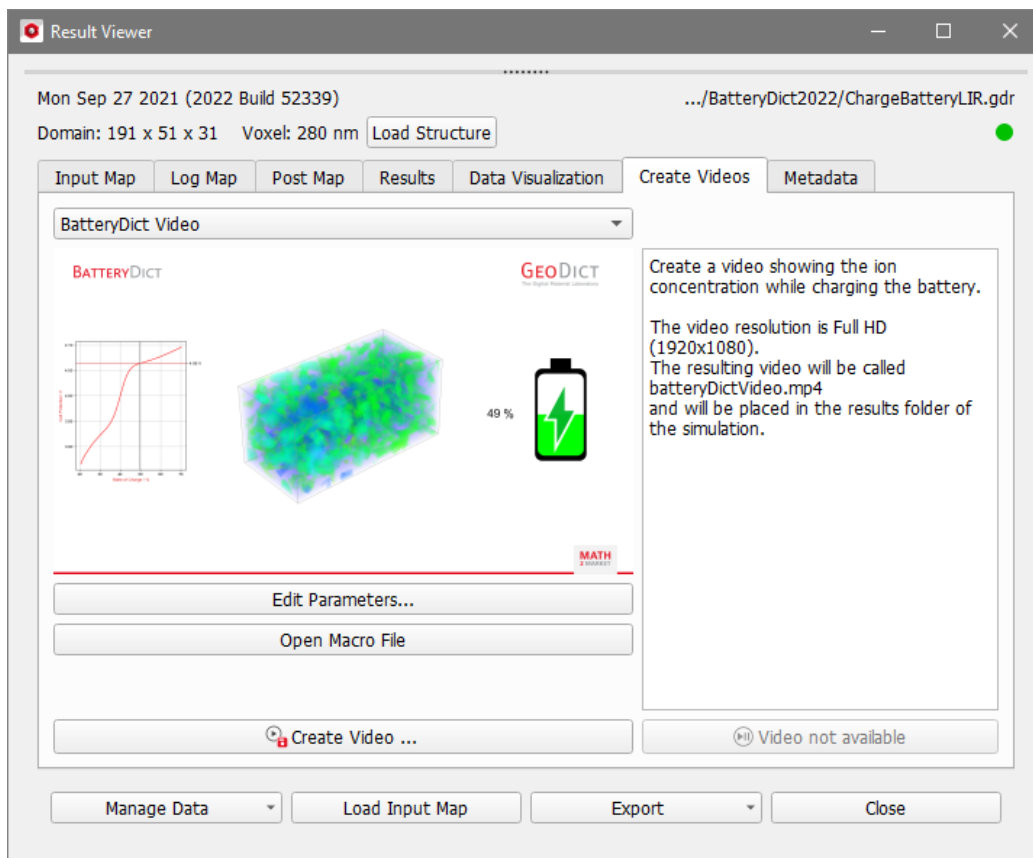
Check **Keep existing Volume Fields** if you repeat loading result fields for another time step or have other previously loaded volume fields in memory that you want to keep. If this box is not checked, previously loaded volume fields are discarded.

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.

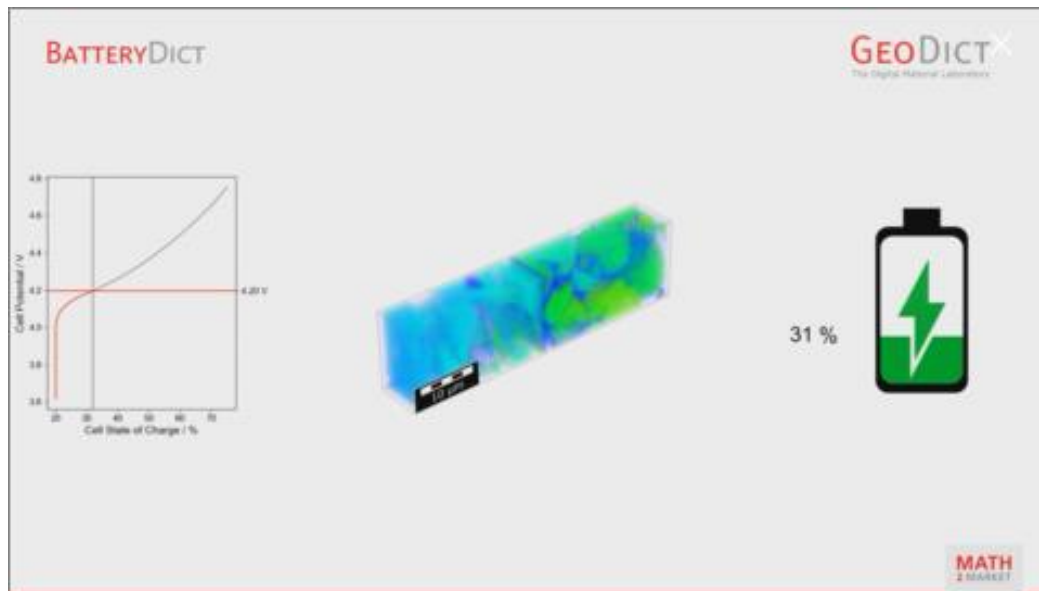


Through the **Create Videos** tab, a video showing the ion concentration while charging or discharging of the battery can be created. The first part of the video shows the cropping of the battery structure together with the ion concentration at the start of the simulation.



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.

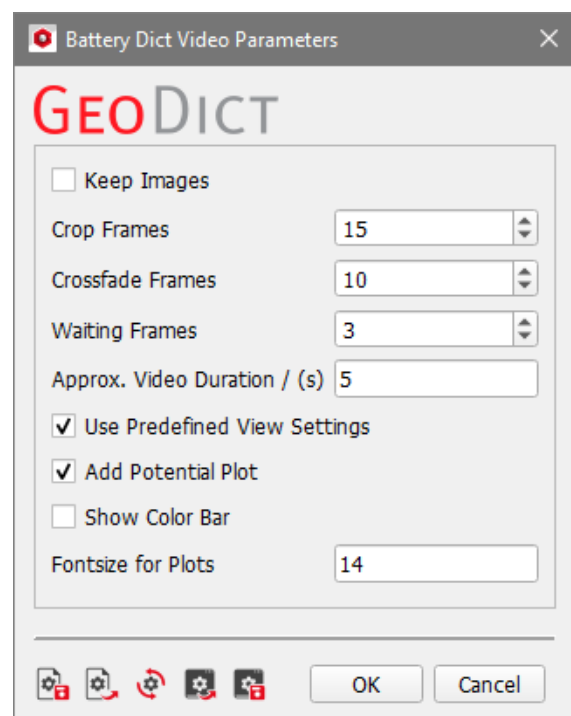
Click **Edit Parameters...** to modify the default settings of the video creation.

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.

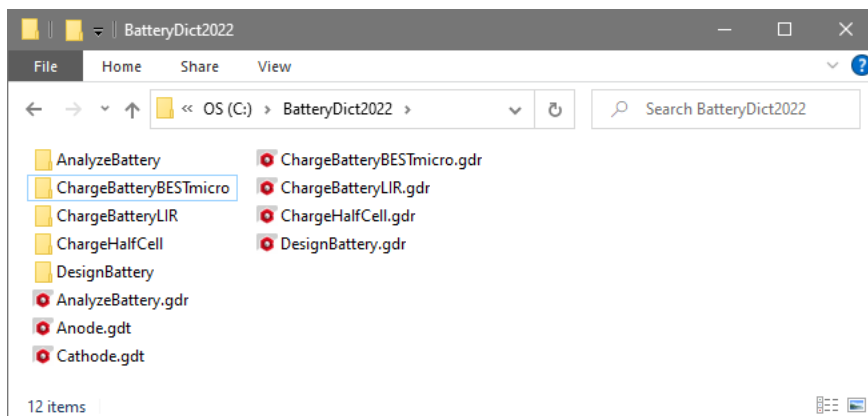
Check **Show Color Bar** to add an additional color bar for the ion concentration below the structure.

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.

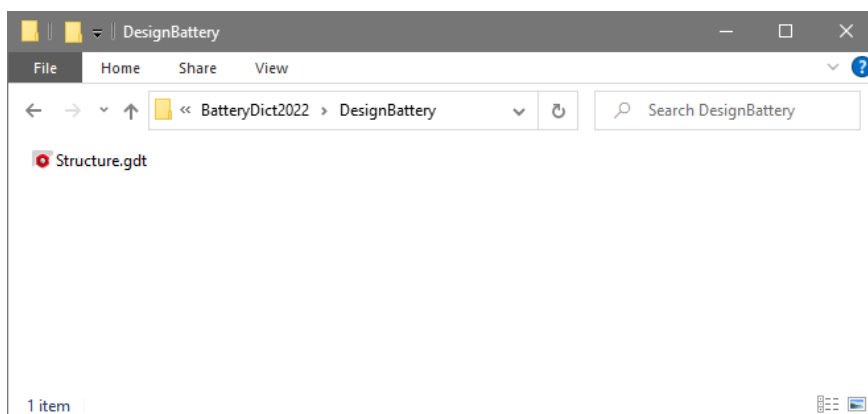
RESULT FOLDERS

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.



DESIGNBATTERY FOLDER

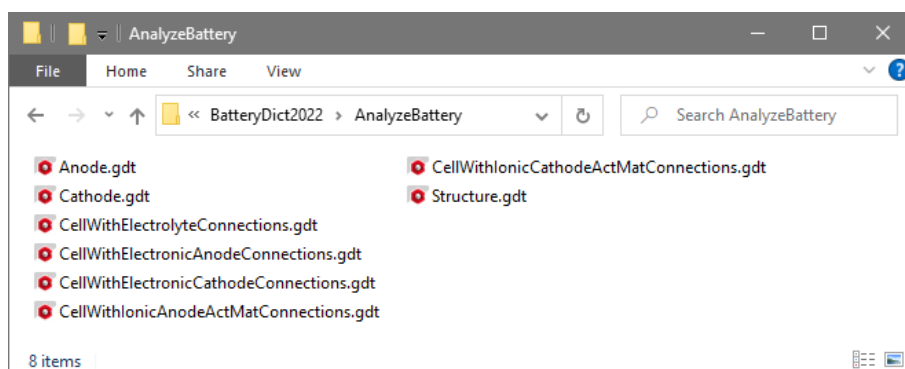
After the generation of a battery structure, a **GeoDict** result file (.gdr) is created in the selected project folder. A subfolder with the same name as the result file contains the generated battery structure.



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

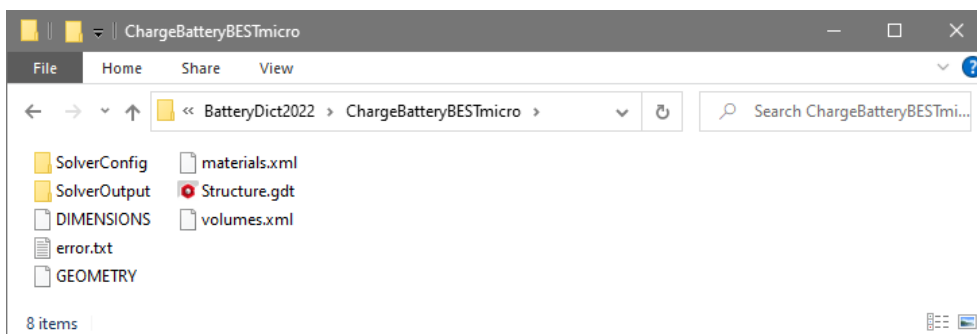
ANALYZEBATTERY FOLDER

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.



CHARGE BATTERY BEST MICRO FOLDER

After running a charging simulation, a **GeoDict** result file (.gdr) is created in the selected project folder. A subfolder with the same name as the result file contains two subfolders called **SolverConfig** and **SolverOutput**.



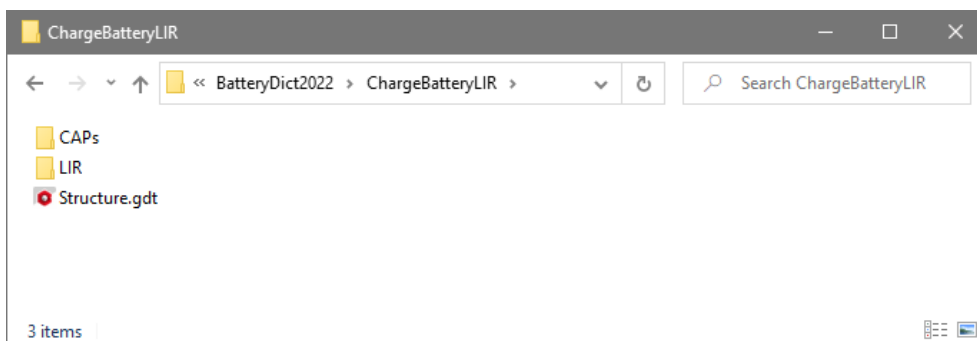
SolverConfig contains files with the input parameters for the charging simulation.

The **SolverOutput** folder contains some log-files from the solver, as well as a subfolder **output** with *.cap files containing volume fields. Such a *.cap file is written for the initial state, for the final state, and for each time step with intermediate output. These volume fields can be loaded from the **Load Results** button under the Result Visualization tab of the Result Viewer or directly from the **GeoDict** GUI by selecting **File → Load Volume Field ...** 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 fields for initial, final and each time step with intermediate output. The folder **LIR** contains files for each time step computed.



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