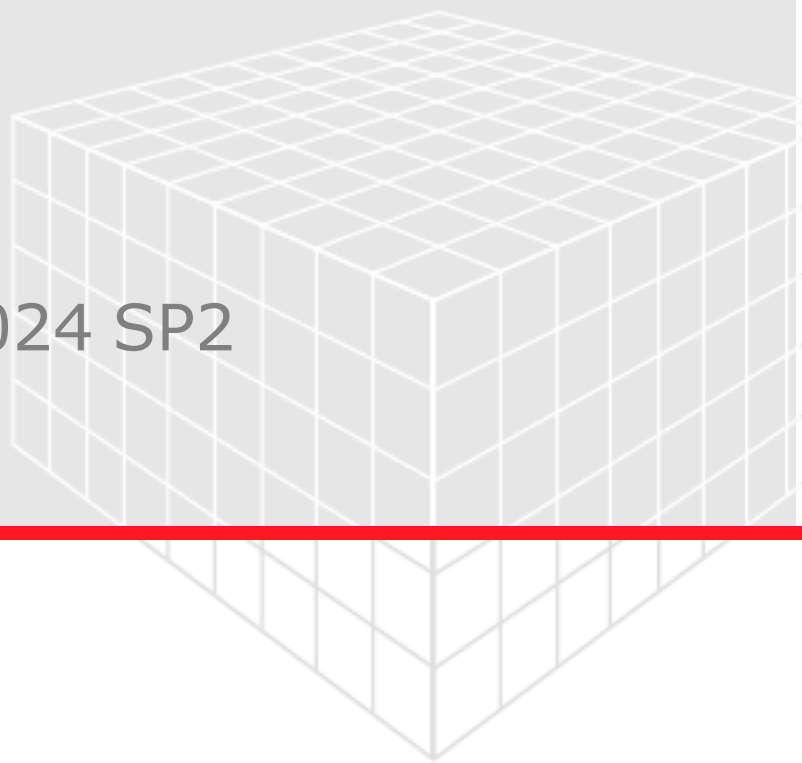


DIGITAL ANALYSIS OF BATTERY SEPARATOR STRUCTURES

Tutorial

GeoDict release 2024 SP2

Published: May 22, 2024



GEODICT

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Citation:

Janine Hilden, Anja Streit, Barbara Planas. Tutorials for GeoDict 2024.
Digital analysis of separator structures. Math2Market GmbH,
Germany.

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DIGITAL ANALYSIS OF BATTERY SEPARATOR STRUCTURES

INTRODUCTION

MOTIVATION

Even though battery separators are not an active part of the Li-ion battery assembly, the microstructure of the separator affects ion transport and has a considerable impact on the overall performance and lifetime of the battery. Understanding the influence of the separator microstructure on the battery performance opens a vast potential for improvement of battery design.

This tutorial illustrates the capabilities of the **GeoDict** software to digitally analyze and optimize the microstructure of battery separators. Following the tutorial, the user learns to import and crop the pre-processed microstructure of a segmented FIB-SEM scan of a Celgard® PP1615 Lithium-Ion Battery Separator in **GeoDict**. Then, the user calculates the geometric (morphological) and transport properties of the microstructure and identifies a representative elementary volume (REV). On this REV, the electrolyte-separator interaction is computed, and mechanical deformation is simulated. The geometric and transport properties are then discussed for the mechanically deformed structures as well.

BACKGROUND OF THE SAMPLE

The tutorial deals with the analysis of a sample of binarized focused ion beam scanning electron microscopic (FIB-SEM) tomography image stacks of a polymer-based separator microstructure. The scan of a Celgard® PP1615 Lithium-Ion Battery Separator was created by the MaDE group at ETH Zürich and can be accessed via <https://doi.org/10.3929/ethz-b-000265085> .

The scan was preprocessed at Math2Market to import the binarized data to the **GeoDict** structure format .gdt. The preprocessed structure is provided in the folder **Input-Data**, inside the provided tutorial folder.

Disclaimer:

The work for this tutorial was not endorsed nor funded by ETH Zurich

HOW TO USE THIS EXAMPLE TUTORIAL

The tutorial is organized into six parts that explain how to perform the computations step-by-step in the **GeoDict** GUI (Graphical User Interface). To proceed faster, the intermediate results can be loaded from the **Results-M2M** folder inside the **Digital-analysis-of-battery-separator-structures**.

The six steps are:

1. Importing and cropping the structure:

Load the FIB-SEM data and crop a segment for the computations.

2. Computing geometric and transport properties:

Compute geometric and transport properties of the cropped structure, like porosity, tortuosity, Euler characteristics, Gurley value and permeability.

3. Identifying a REV for geometric properties:

Identify a representative elementary volume (REV) of the structure for the computation of porosity and tortuosity.

4. Computing separator-electrolyte interaction:

Compute the thermal conductivity dependent on the wetting of the separator with electrolyte.

5. Computing the deformed structure for REV:

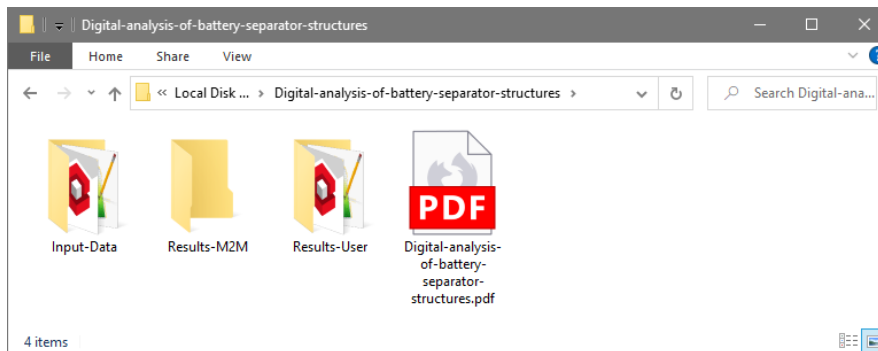
Compute the deformation for a mechanical load.

6. Computing properties of deformed structure:

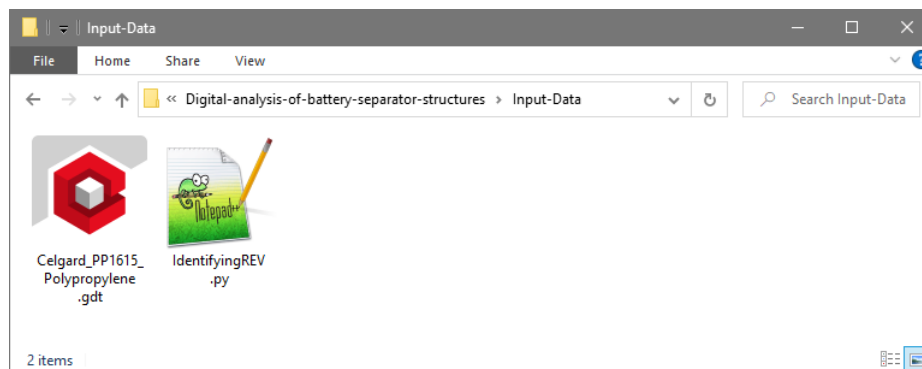
Compute geometric and transport properties again for the deformed geometries.

Modules needed to follow this tutorial:
GeoDict-Base, MatDict, DiffuDict, FlowDict, SatuDict,

Three folders and this PDF file are inside the **Digital-analysis-of-battery-separator-structures** folder.



- The **Input-Data** folder contains the segmented FIB-SEM data used as input structure for the computations in this tutorial and a GeoPy script (*.py) to identify an REV.

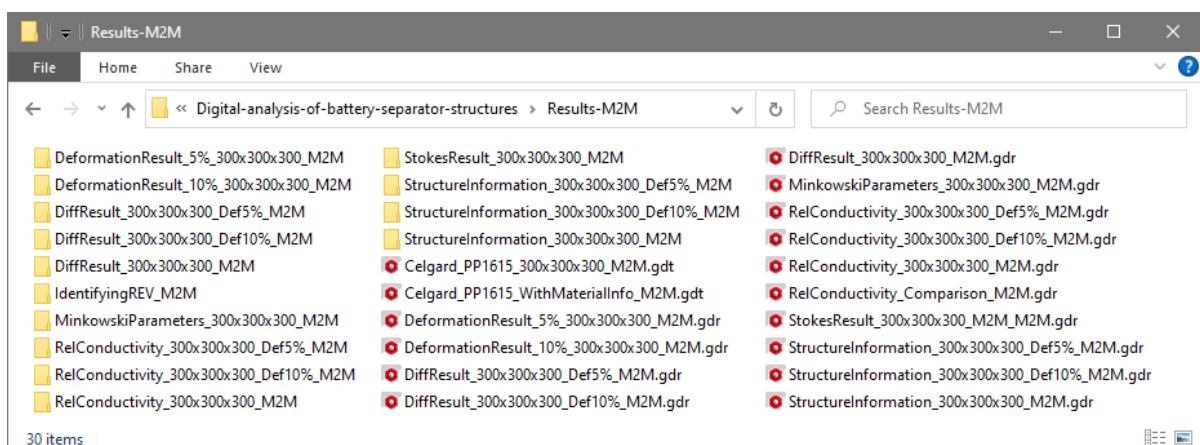


- The **Results-User** folder is empty. We recommend that, before starting to work through this tutorial, the user sets the **Results-User** folder as project folder in **GeoDict**.

For this, in the **GeoDict** GUI, select **File** → **Choose Project Folder** → **Select Project Folder** and navigate to the folder **Results-User**. In this way, the result files created when running the tutorial will not overwrite the files provided by **Math2Market**, even when using the same names.

- The **Results-M2M** folder contains the results that we at Math2Market obtained by following this tutorial.

Most of the results from each of the tutorial parts consist (as always in **GeoDict**) of a **GeoDict** result file (*.gdr) and a corresponding folder with the same name.



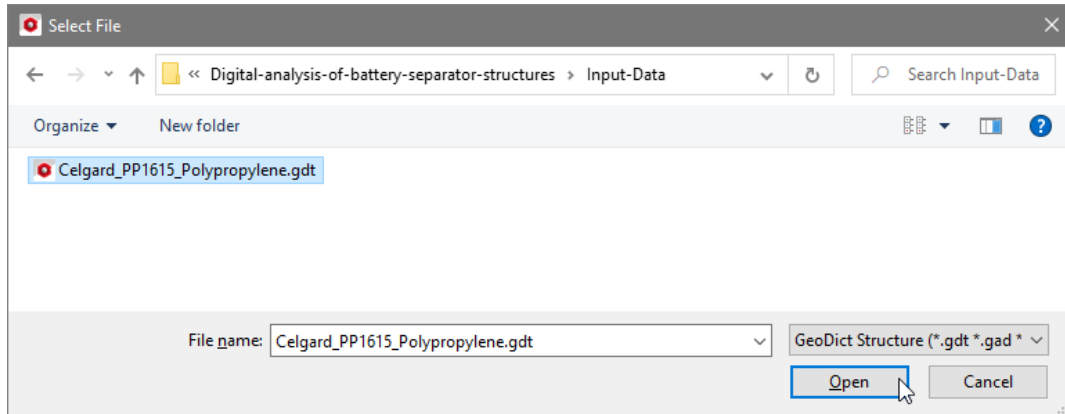
These files and folders are described in the following in the order shown above:

1. Cropped REV used in this tutorial to compute several properties for the separator:
Celgard_PP1615_300x300x300_M2M.gdt
2. Separator before cropping but already with materials info set-up:
Celgard_PP1615_WithMaterialInfo.gdt
3. **GeoDict** result files created by performing deformation simulations using the **ElastoDict** module once simulating 5% deformation and once 10%:. The results can be found in the accompanying folder:
DeformationResult_5%_300x300x300_M2M.gdr
DeformationResult_10%_300x300x300_M2M.gdr
4. **GeoDict** result files created by computing the tortuosity using the **DiffuDict** module once on the original cutout of the structure, once after 5% deformation, and once after 10%:
Diffusion_300x300x300_M2M.gdr
Diffusion_300x300x300_Def5%_M2M.gdr
Diffusion_300x300x300_Def10%_M2M.gdr
5. **GeoDict** result file created by computing the Euler characteristics using the **MatDict** module on the original cutout of the structure:
MinkowskiParameters_300x300x300_M2M.gdr
6. **GeoDict** result files created by computing the separator-electrolyte interaction using the **ConductoDict** module once on the original cutout of the structure, once after 5% deformation, and once after 10%:
RelConductivity_300x300x300_M2M.gdr
RelConductivity_300x300x300_Def5%_M2M.gdr
RelConductivity_300x300x300_Def10%_M2M.gdr
7. **GeoDict** result file created by computing the permeability using the **FlowDict** module on the original cutout of the structure:
StokesResult_300x300x300_M2M.gdr
8. **GeoDict** result files created by computing the porosity and other structure statistics using the **MatDict** module once on the original cutout of the structure, once after 5% deformation, and once after 10%:
StructureInformation_300x300x300_M2M.gdr
StructureInformation_300x300x300_Def5%_M2M.gdr
StructureInformation_300x300x300_Def10%_M2M.gdr
9. **IdentifyingREV_M2M** folder containing the results of the parameter study computing tortuosity and porosity for different cutout sizes. The results are combined in the plot **Plot_IdentifyingREV.png**

1. IMPORTING AND CROPPING THE STRUCTURES

Before starting the simulations, set-up the project folder as described on page 3.

1. Load the binarized example separator structure in **GeoDict**. For this, select **File** → **Open Structure (*.gdt, *.gad)...** from the menu bar and browse for the **Input-Data** folder inside the tutorial folder.
2. Select the file **Celgard_PP1615_Polypropylene.gdt** and click **Open**.

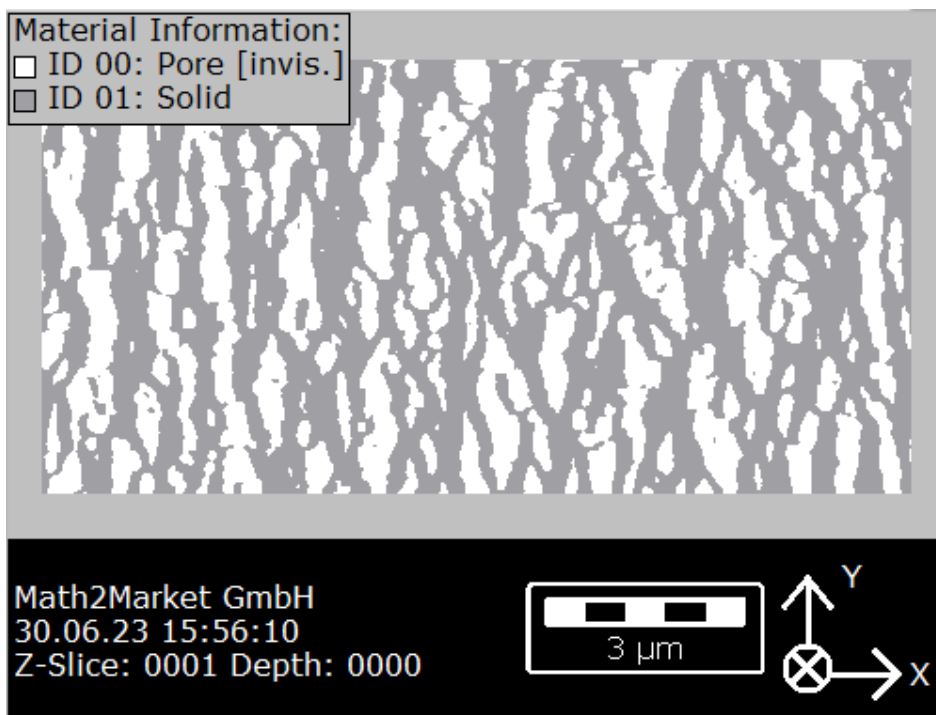


The structure is loaded in **GeoDict**.

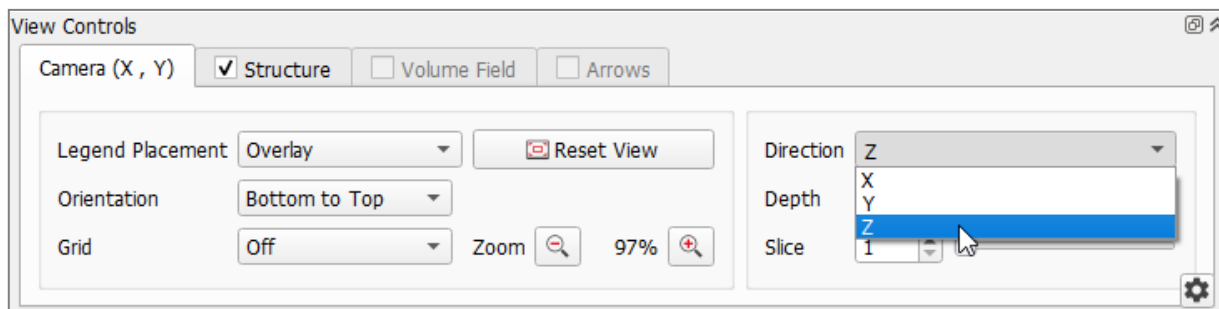
The structure appears in 2D in the Visualization area of the **GeoDict** GUI with the built-in visualization and view settings.

1.1 VISUALIZATION SETTINGS

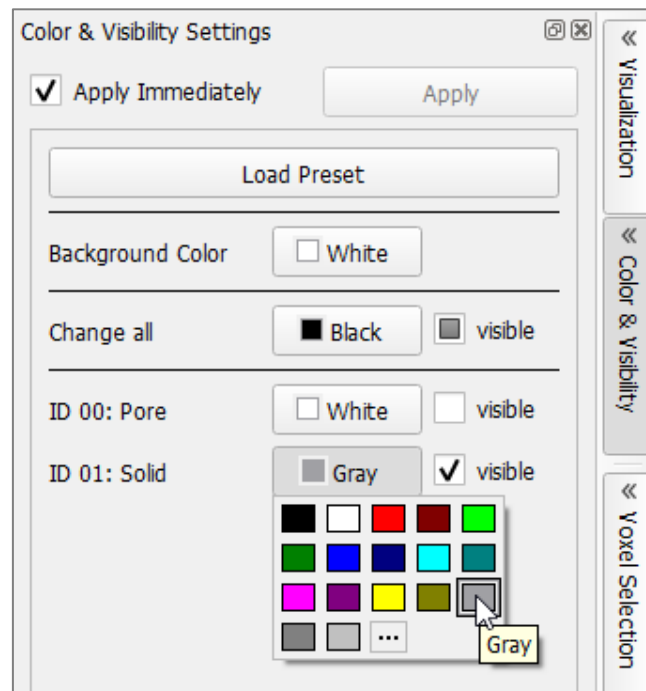
To obtain the display below, proceed as follows:




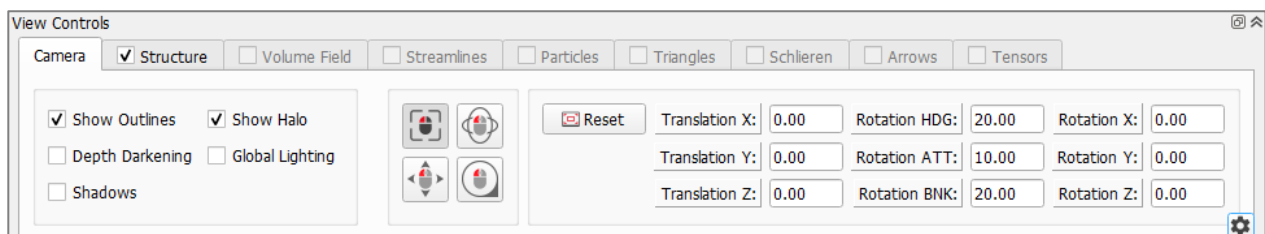
1. Above the visualization area, in the **View Controls** panel, go to the **Camera** tab and set the **Direction** to Z.



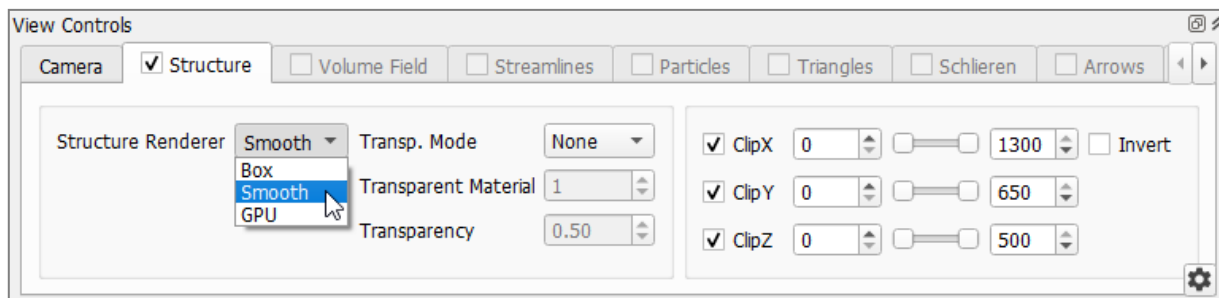
2. Change the color of the material with ID 01 from red to gray through the **Color & Visibility** tab from the side bar on the right of GeoDict.



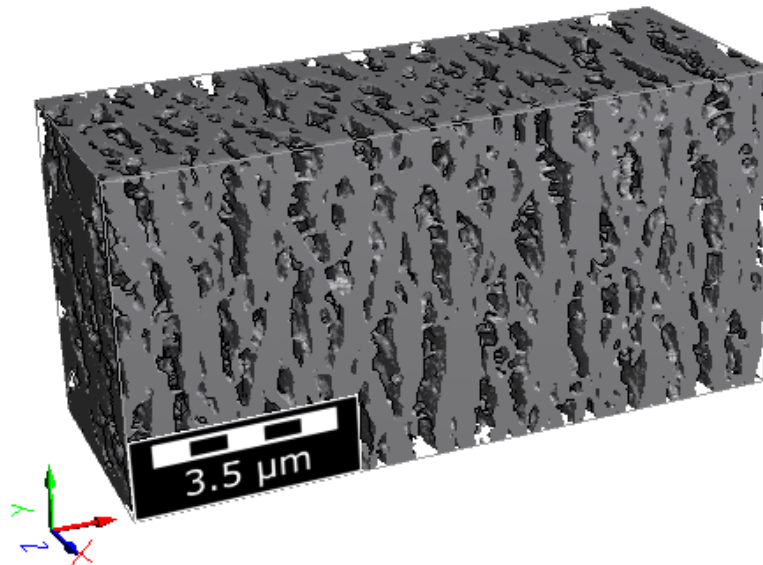
3. Click the 3D visualization icon  in the toolbar or select **View** → **3D Rendering** to display the structure in 3D view.
4. In the **Camera** tab check **Show Outlines** and **Show Halo**. For the camera angle we set the **Rotation** values as follows:
 - HDG 20
 - ATT 10
 - BNK 20



5. For a smooth representation of the structure, select **Structure Renderer** → **Smooth** under the **Structure** tab in the Visualization panel.



Material Information:
 ID 00: Pore [invis.]
 ID 01: Solid



For this loaded segment of a polypropylene separator, the X-axis and Z-axis correspond to the in-plane directions of the separator, and the Y-axis indicates the through-plane direction.

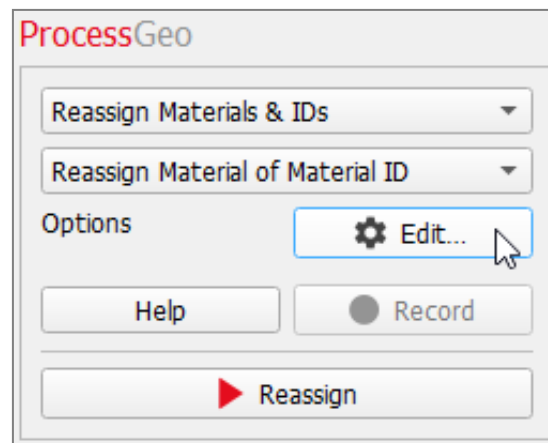
1.2 ASSIGN MATERIAL PROPERTIES

Now, assign materials to the pore and solid part of the structure.

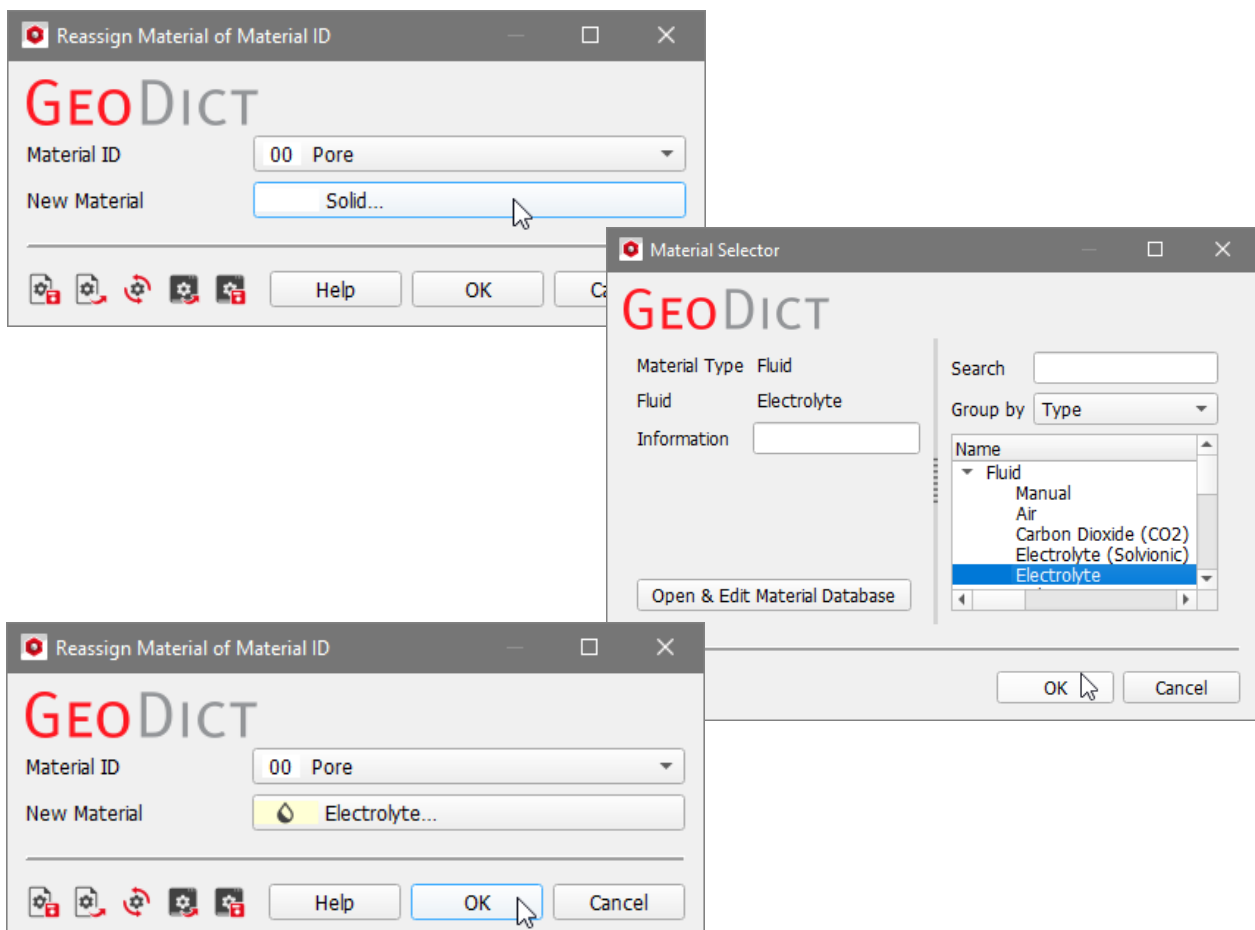
1. Select **Model** → **ProcessGeo** in the menu bar.

In the **ProcessGeo** module section, now appearing on the left of the **GeoDict** GUI, choose **Reassign Materials & IDs** from the first pull-down menu, and **Reassign Material of Material ID** from the second.

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

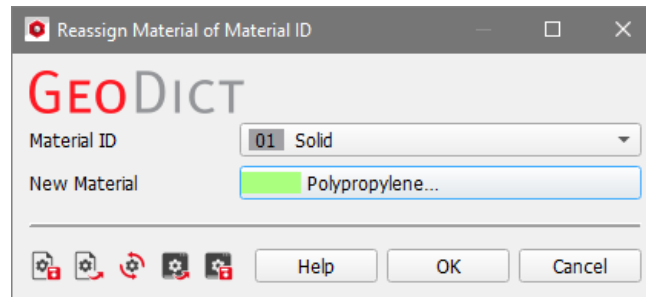


2. For the pore voxels with Material ID 00, set the **New Material** to **Electrolyte (Fluid)** by clicking on the box and selecting the material from the **Material Selector** and click **OK**.



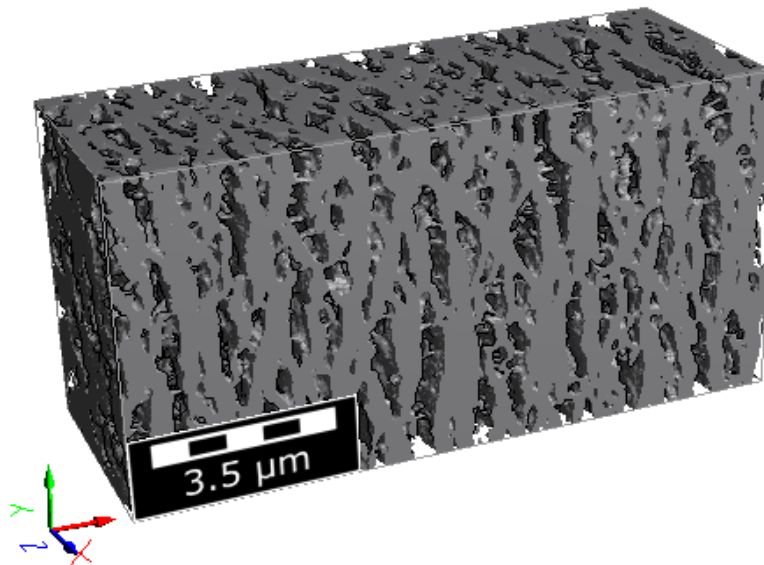
Click again **OK** in the **Reassign Material of Material ID** dialog and then **Reassign** in the **ProcessGeo** module section.

3. Repeat the same procedure to assign the material **Polypropylene (Solid)** to the solid part of the structure with Material ID 01.



The new material information is now shown above the structure in the **GeoDict Visualization** area. Properties of the constituent materials (Electrolyte, Polypropylene) are taken from the **GeoDict** Material Database and can now be used for the computations, where not only the geometric properties of the structure are relevant. Note that the material properties are not the specific ones of the Celgard® Separator structure used here.

Material Information:
 ID 00: Electrolyte [invis.]
 ID 01: Polypropylene



4. Select **File** → **Save Structure as...** in the menu bar to save the structure together with the material information in the project folder. Choose the filename **Celgard_PP1615_WithMaterialInfo.gdt**.

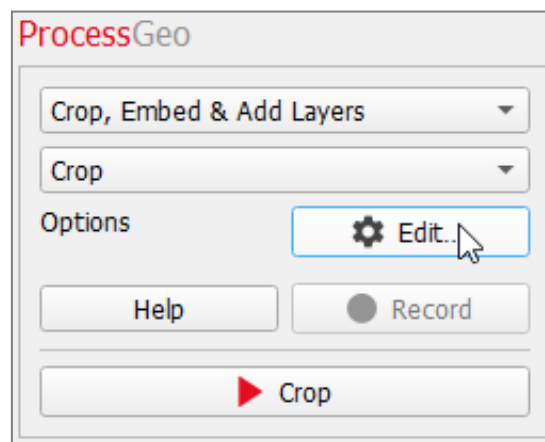
1.3 CROP STRUCTURE

Lagadec et al. [1] have reported that a segment of $3\mu\text{m}$ length in each coordinate direction is a representative elementary volume (REV) for this polypropylene separator regarding porosity, tortuosity, connectivity, and the effective transport coefficient.

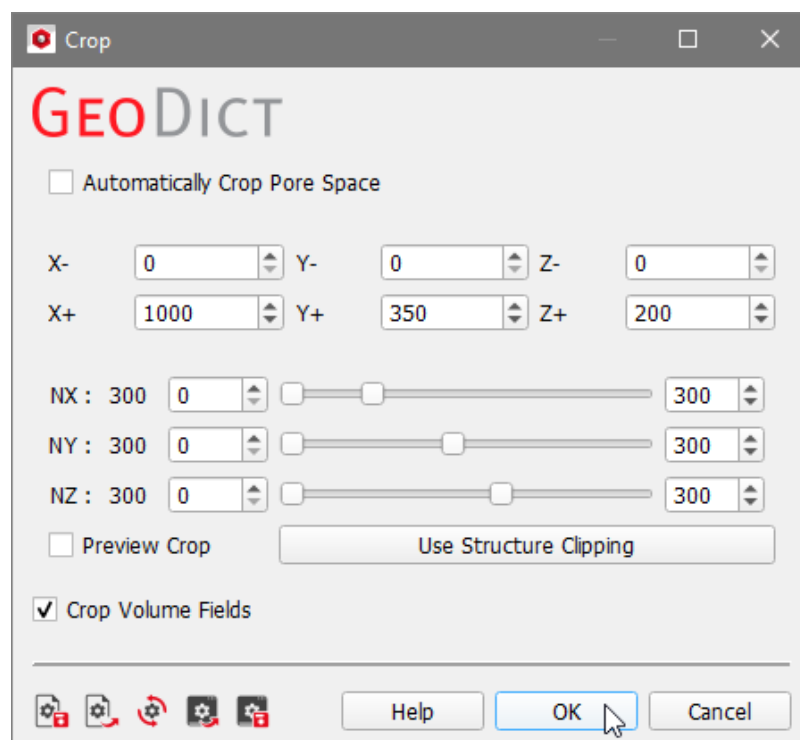
To pick a segment of $3\mu\text{m}$ side length, the structure is cropped using the **ProcessGeo** module as follows:

1. Select **Model** → **ProcessGeo** in the menu bar.
2. In the **ProcessGeo** module section, select **Crop, Embed & Add Layers** from the first pull-down menu and **Crop** from the second one.

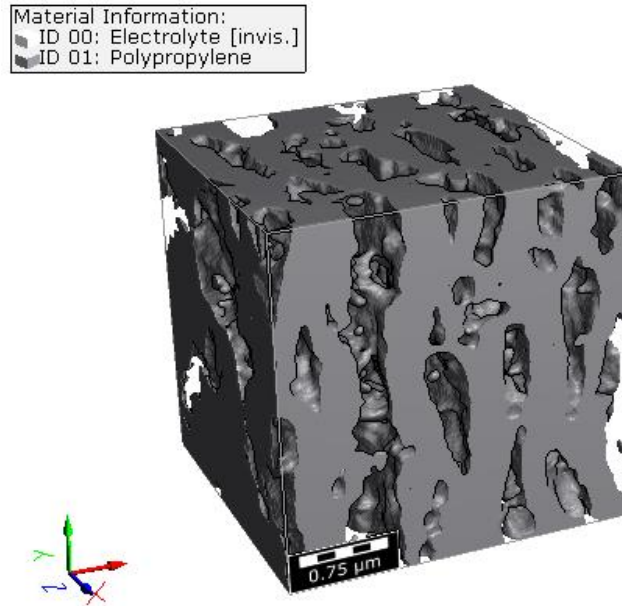
Then, click **Edit** to open the options dialog.




3. Crop the sample in each direction to 300 voxels. For this, enter the values 0 – 300 for **NX**, **NY** and **NZ**. Click **OK** to close the dialog, then click **Crop** in the **ProcessGeo** section to start the cropping process.



The smaller structure is now displayed in the Visualization area.



4. Select **File** → **Save Structure as...** or the corresponding icon in the toolbar  to save the cropped segment of the structure with the filename **Celgard_PP1615_300x300x300.gdt** in the project folder.

2. COMPUTING GEOMETRIC AND TRANSPORT PROPERTIES

In the second step, different geometric and transport properties are computed on the cropped segment.

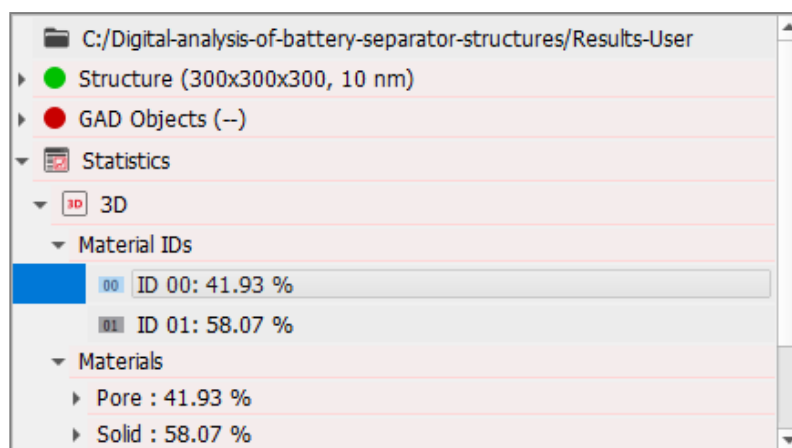
1. Select the **Results-User** folder as project folder, as described on page 3.
2. Load the cropped segment of size 300x300x300 (unless it is still in memory) as follows: **File** → **Open Structure (*.gdt, *.gad)...** and select the **Celgard_PP1615_300x300x300.gdt** file from the project folder or from the **Results-M2M** folder.



2.1 POROSITY

Now, let's obtain the porosity of the structure as follows:

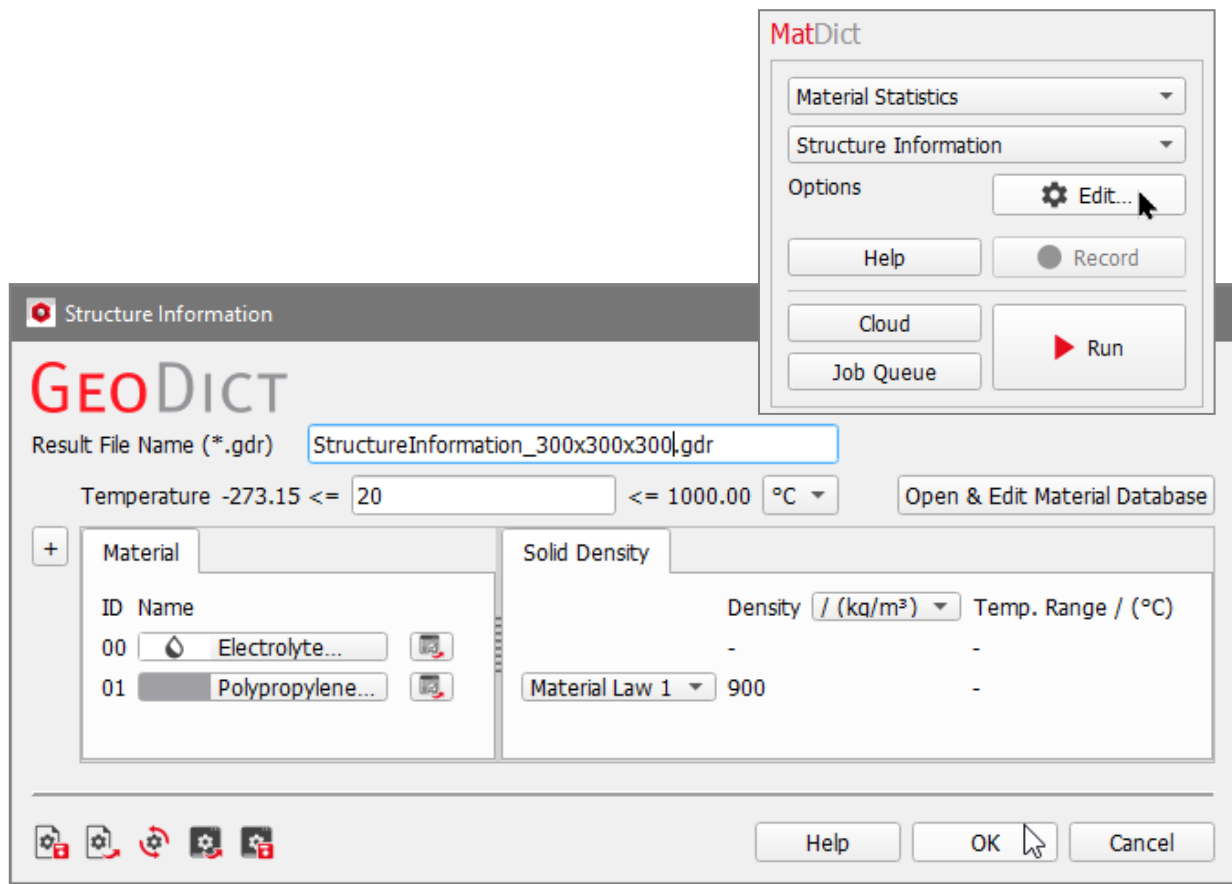
1. Find the Project Status panel on the left side of the **GeoDict** GUI. Here, unfold the **Statistics** section. Expand the **3D** section and the list of **Material IDs**, to observe the volume percentage for each material ID. The original pore space (now filled with Electrolyte) occupies 41.93% of the segment, i.e., the porosity is 41.93%.



2. To get a **GeoDict** result file containing the porosity value, select **Analyze** → **MatDict** from the menu bar.

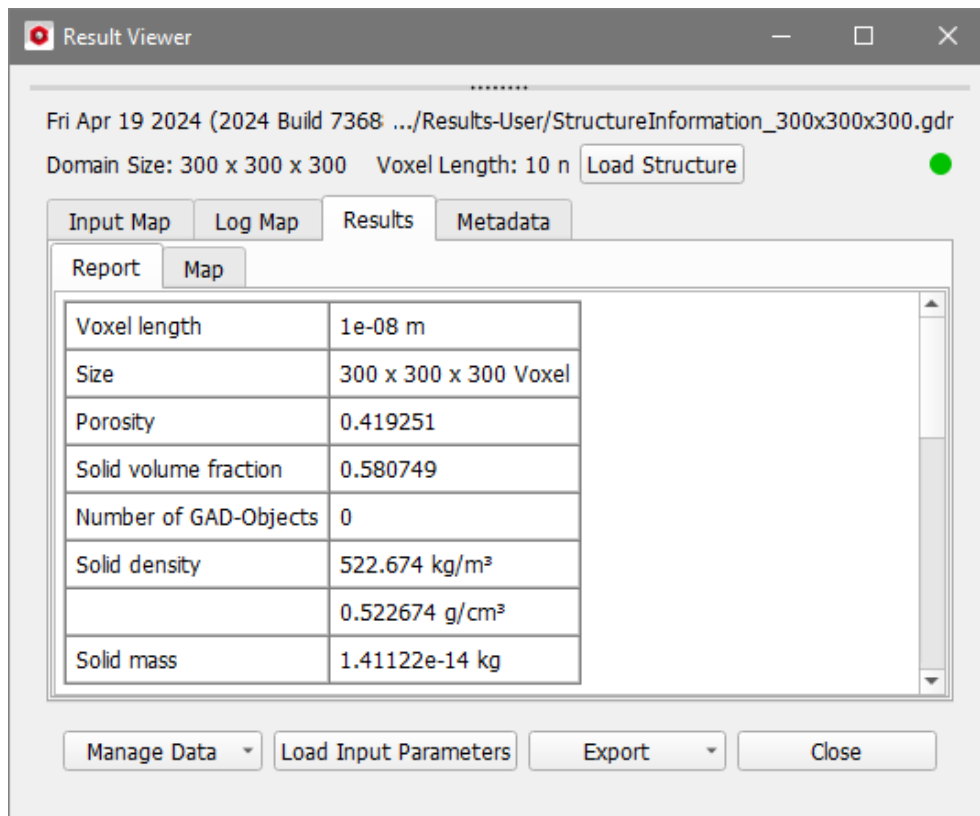
In the **MatDict** module section, on the left of the **GeoDict** GUI, select **Material Statistics** from the first pull-down menu and **Structure Information** from the second one. Then click **Edit...** to open the options dialog.

3. In the **Structure Information** dialog that opens, define the Result File Name as **StructureInformation_300x300x300.gdr** and close the dialog by clicking **OK**.



Start the computation by clicking **Run** in the **MatDict** module section.

4. The **Result Viewer** of the result file opens automatically, showing size, voxel length, porosity, and other geometric properties.

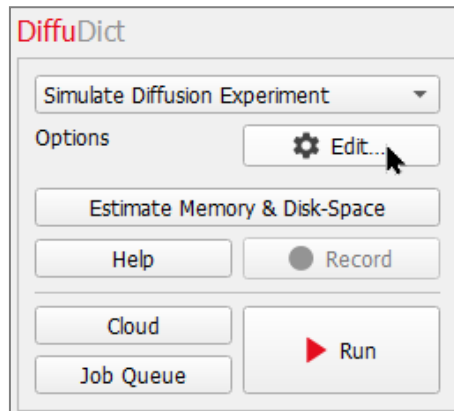


2.2 DIFFUSIVITY AND TORTUOSITY

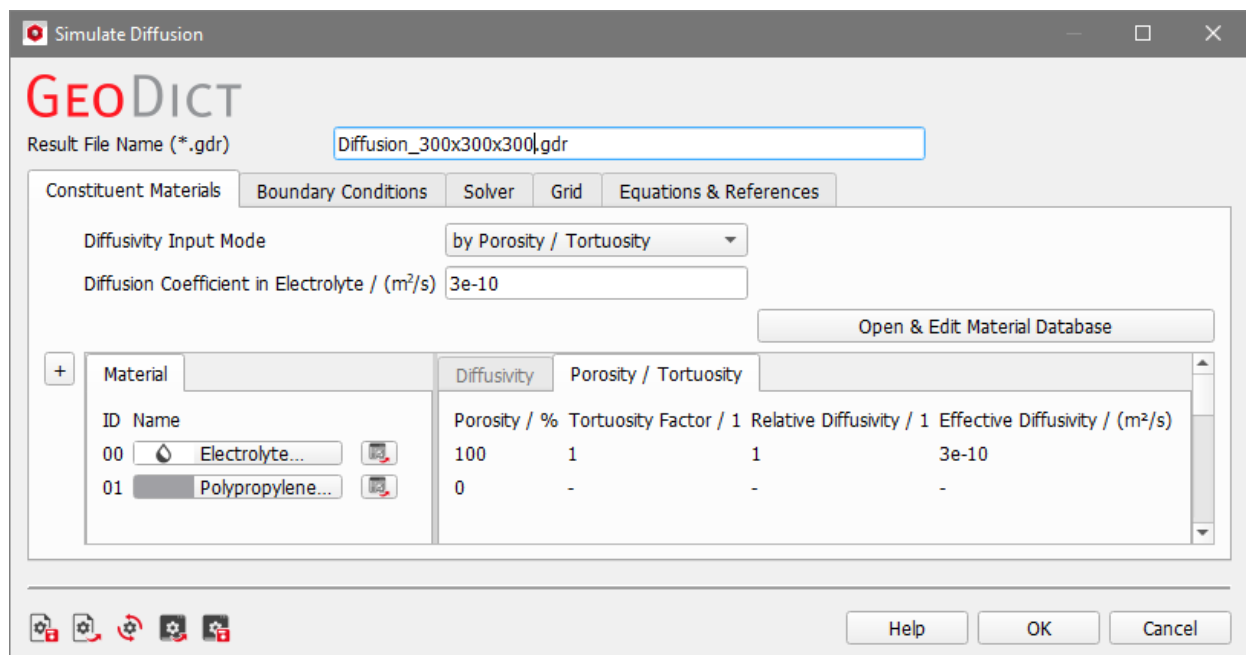
Now, let's compute diffusivity and tortuosity using the **DiffuDict** module.

1. Select **Predict** → **DiffuDict** from the menu bar.
2. From the pull-down menu in the **DiffuDict** module section, choose **Simulate Diffusion Experiment**, to compute the effective diffusivity of the structure.

Click **Edit...** to open the **Simulate Diffusion** dialog.



3. Enter **Diffusion_300x300x300.gdr** as result file name. Nothing must be changed under the **Constituent Materials** tab.



4. Under the **Boundary Conditions** tab, select to compute the diffusion in Y-direction.

Choose **Symmetric (Dirichlet)** Boundary Conditions in diffusion direction and **Periodic** boundary conditions in tangential directions.

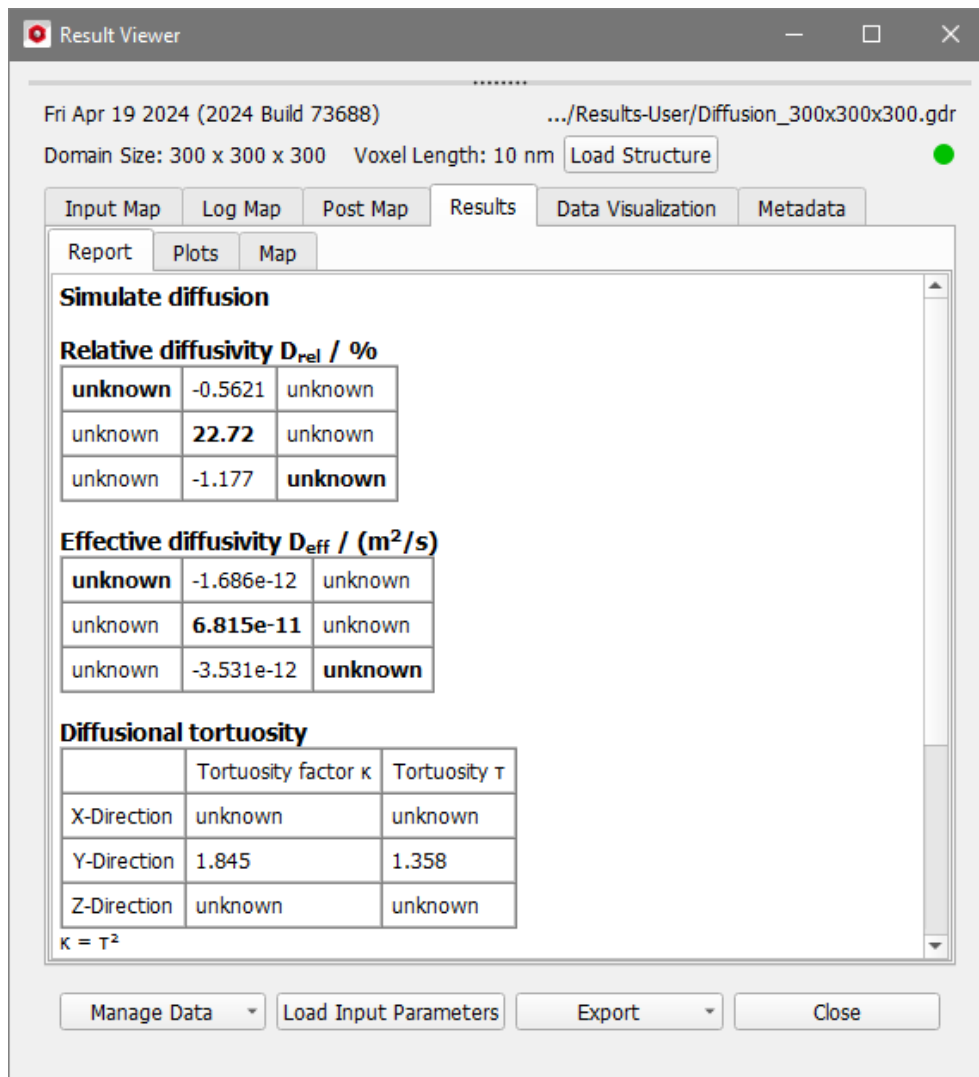
The screenshot shows the 'Boundary Conditions' tab of a software interface. It contains several sections: 'Computation Directions' with checkboxes for X, Y (checked), and Z; 'Boundary Conditions in Diffusion Direction' with radio buttons for Periodic and Symmetric (Dirichlet) (selected); 'Experiment Input' with text boxes for 'Concentration at Inlet' (1) and 'Concentration at Outlet' (0), both with units of mol/m³; and 'Boundary Conditions in Tangential Directions' with radio buttons for Periodic (selected), Symmetric, Encase, and Expert.

- Under the **Solver** tab, select the LIR solver and leave all its default settings.

The screenshot shows the 'Solver' tab of the software interface. A dropdown menu is open, showing 'LIR' selected. Below the menu, the 'Simulation Stopping Criterion' section has 'Error Bound' checked with a value of 0.01, and 'Maximal Iterations' set to 100000. 'Maximal Run Time / (h)' is set to 240. 'Restart Save Interval / (h)' is set to 6. 'Parallelization' is set to '<local max. - 8x>'. There are checkboxes for 'Restart from .gdr File' and 'Discard PDE Solver Files'. 'Orientation Mode' is set to 'Use Orientation from Analytic Objects (gad)'. There is a checkbox for 'Write Diffusion Flux into Solution File' and a collapsed 'Advanced Options' section.

- Click **OK** to close the dialog box and click **Run** in the **DiffuDict** module section to start the computations.
- When the computation finishes, the Result Viewer of the result file opens automatically. The **Results - Report** subtab shows the **Relative diffusivity** in Y-direction and the **Effective diffusivity** as well as the **Tortuosity factor** and the geometric **Tortuosity**.

Since we ran the computations only in Y-direction, the values in X-direction and Z-direction appear listed as unknown in the tables.



2.3 EULER CHARACTERISTIC

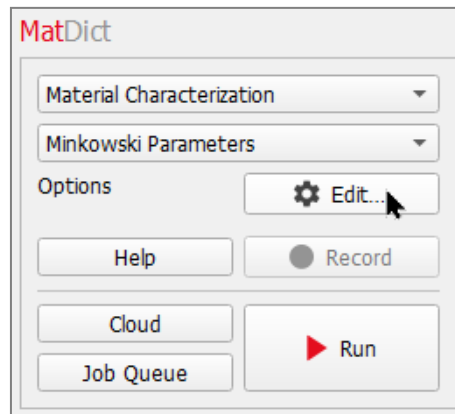
Now, let's compute the Euler Characteristic using the **MatDict** module.

The Euler characteristic (or Euler number) is a topological invariant, a number describing a topological space's shape or structure regardless of the way it is bent (see e.g. https://en.wikipedia.org/wiki/Euler_characteristic).

In the context of the 3D microstructure of a separator, it can be used as a measure for the connectivity of the pore space. The more negative the Euler characteristic is, the better the pore network is interconnected. Besides porosity and tortuosity, the connectivity was identified as one of the most relevant parameters to determine the ion concentration distribution and the performance of the separator [1]. In this step, the Euler number is calculated using **MatDict**.

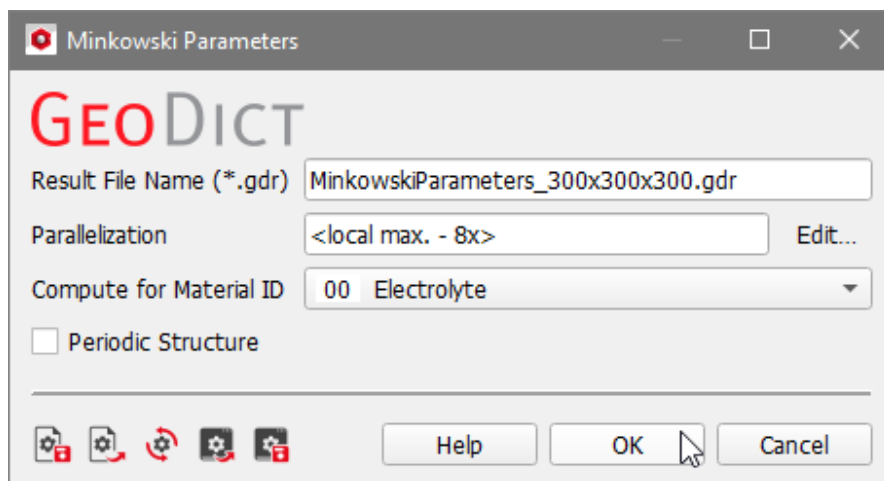
1. Select **Analyze** → **MatDict** from the menu bar.
2. Then, from the first pull-down menu in the **MatDict** module section, select **Material Characterization** and from the second one **Minkowski Parameters** to compute the Euler characteristic and other Minkowski parameters.

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



3. Then, select **MinkowskiParameters_300x300x300.gdr** as Result File Name and compute the parameters for the pore space filled with electrolyte.

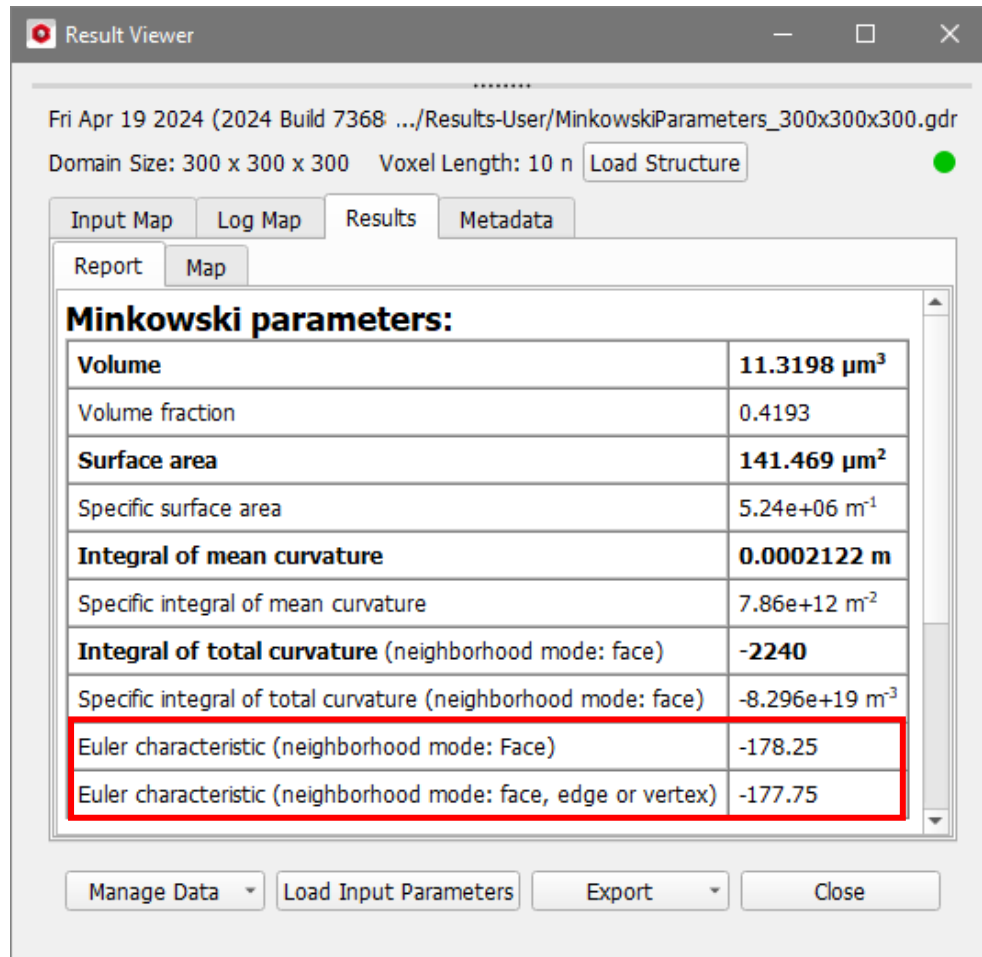
Since our structure is not periodic, uncheck **Periodic Structure**.



4. Click **OK** to close the dialog box and click **Run** in the **MatDict** section to start the computation.

5. The **Result Viewer** of the result file opens automatically for the computed Minkowski parameters.

The Euler characteristics are given by the last two values in the table. For the structure studied here both values are similar, i.e., the neighborhood mode selected has only a small influence on the connectivity.

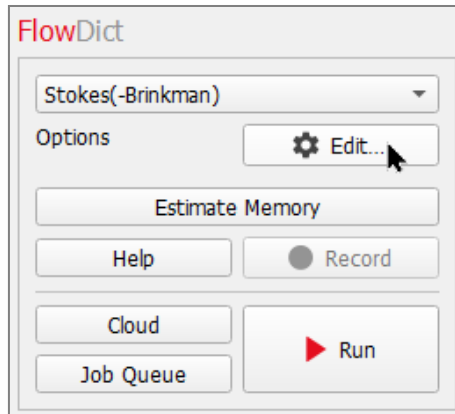


2.4 PERMEABILITY AND GURLEY VALUE

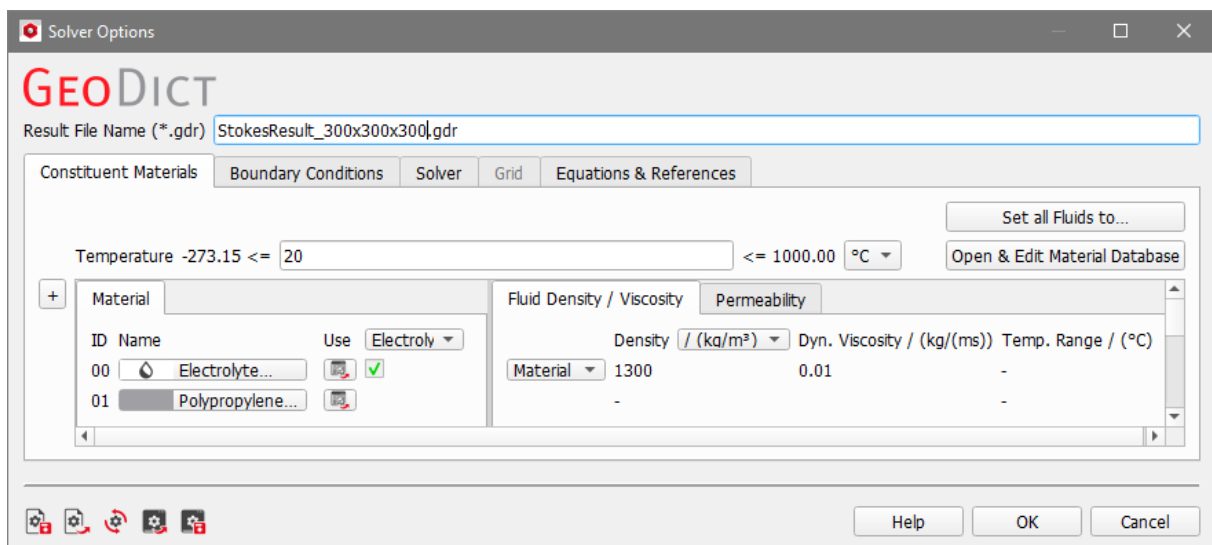
Now, let's compute permeability and Gurley value with **FlowDict**:

1. Select **Predict** → **FlowDict** from the menu bar.
2. Then, from the pull-down menu in the **FlowDict** module section, select **Stokes(-Brinkman)**, to compute the flow through the structure by solving Stokes equations.

Click the **Edit...** button to open the dialog and set the solver options.



3. Enter **StokesResult_300x300x300.gdr** as Result File Name. Nothing needs to be changed under the **Constituent Materials** tab.



4. In the **Boundary Conditions** tab, select to compute the flow in Y-direction and to use symmetric boundary conditions in flow direction.

All other options are kept at the default values.

The screenshot shows the 'Boundary Conditions' tab in the FlowDict software. The 'Computation Directions' section has three checkboxes: 'X' (unchecked), 'Y' (checked), and 'Z' (unchecked). The 'Boundary Conditions in Flow Direction' section has four radio buttons: 'Periodic' (unchecked), 'Symmetric (Dirichlet)' (checked), 'Velocity inlet, Pressure outlet' (unchecked), and 'Add implicit region / (Voxel):' (unchecked). Below this are two input fields for 'inflow' and 'outflow', both set to 10. The 'Experiment Input / Output' section has three radio buttons: 'Pressure Drop' (checked), 'Mean Velocity' (unchecked), and 'Flow Rate' (unchecked). The 'Pressure Drop' section has a value of 0.02 and a unit of Pa. The 'Mean Velocity' section has a value of 0.1 and a unit of m/s. The 'Flow Rate' section has a value of 60 and a unit of l/min. The 'on Flow Area' section has a value of 100 and a unit of cm². The 'Boundary Conditions in Tangential Direction' section has four radio buttons: 'Periodic' (checked), 'Symmetric' (unchecked), 'No-Slip' (unchecked), and 'Expert' (unchecked). The 'Pore-Solid Boundary Conditions' section has a label 'Slip Length / (m)' and a value of 0.

5. Click **OK** to close the dialog box and click **Run** in the **FlowDict** module section to start the computation.

We run the simulation on eight cores. Running the simulation on a different number of cores can lead to slightly different results.

6. The **Result Viewer** of the result file opens automatically, showing the **permeability** vector computed for the Y-direction.

Again, the entries for the X-direction and Z-direction are marked as unknown in the table since the computation was not run for these directions.

The **Gurley value** can be found under the results for the **Y-direction** below.

Result Viewer

Fri Apr 19 2024 (2024 Build 73688) .../Results-User/StokesResult_300x300x300.gdr

Domain Size: 300 x 300 x 300 Voxel Length: 10 nm Load Structure

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

Media Thickness Y / (m) 3e-06

Permeability Unit m²

Flow Rate Unit l/s

Characteristic Length Numerical Length

Apply

☒ Back-up result file

Plot Options

Report Plots Map

Permeability tensor / (m²)

unknown	-1.37974e-18	unknown
unknown	4.59273e-16	unknown
unknown	-1.80222e-17	unknown

Error bound tensor

unknown	0.616284%	unknown
unknown	0.674392%	unknown
unknown	2.23271%	unknown

Maximum error bound is 2.23271%
 (green): error <= 2 %; (yellow): 2 % < error <= 5 %; (red): error > 5 %.

Y-direction

Average (superficial) flow velocity at 0.02 Pa: **3.06182e-10 m/s**.
 Volume flow rate: 3.06182e-07 l/(s m²)
 Reynolds number 8.53019e-13 for characteristic length 2.14307e-08 m.
 Flow resistivity: 2.17735e+13 kg/(m³s).
 Gurley value: 15.302 s.
 Asymptotic estimate of permeability: 4.58061e-16 m²
 --- Solver: LIR, Threads: 8, Iterations: 400, Runtime: 34.649 s, Number of cells: 3211719, Memory usage: 559.831 MiB, and stopped successfully for error bound ---

Manage Data Load Input Parameters Export Close

3. IDENTIFYING A REV FOR GEOMETRIC PROPERTIES

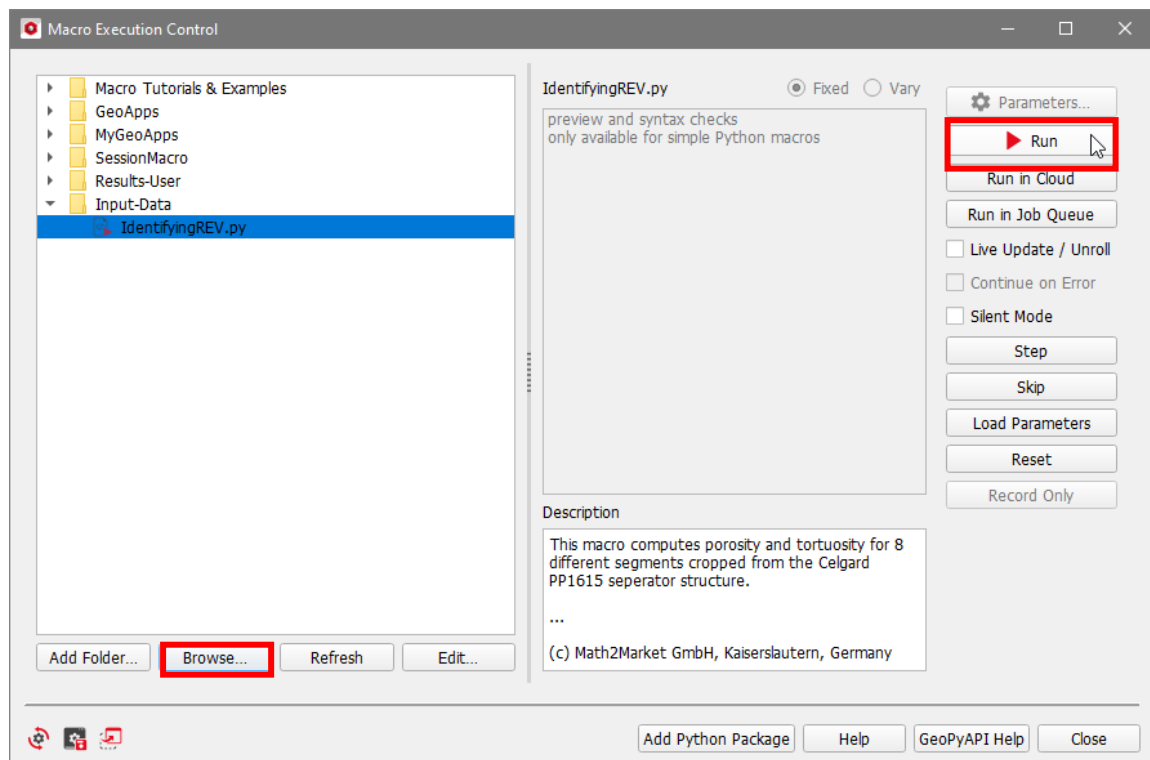
The cropped segment of size 300x300x300 voxels was cut following the recommendation published by Lagadec et al. [11]. We want to study properties of the deformed geometry as done for the original geometry in the previous unit starting on page 12. Since the computation of a deformed geometry is costly in time and memory, it is convenient to use a structure as small as possible for this computation.

In this step, we proceed to identify a REV for a structure regarding porosity and tortuosity. The basic idea is to compute the properties for the whole structure and for smaller cropped segments and compare the results. As long as the value computed on the small segment is the same as for the whole structure, it is enough to use the small segment for the computation.

We repeat the steps outlined in chapter 1.3 **Crop structure** on page 10 to cut parts of the structure of different sizes as well as the steps in 2.1 **Porosity** and 2.2 **Diffusivity and tortuosity** on pages 12 and 14, respectively, to compute geometric properties of the cut segments.

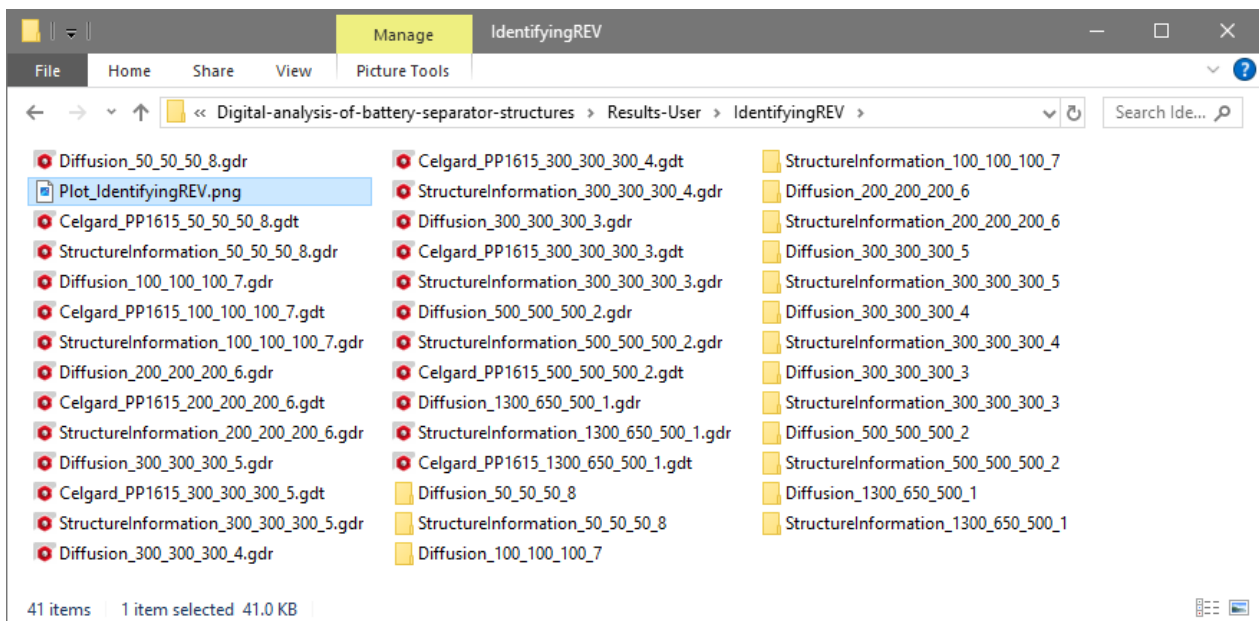
This task can be automated. To learn how to do that, have a look at the macro file **IdentifyingREV.py** provided in the **Input-Data** folder of this tutorial folder. The file can be opened in any text editor, e.g. Notepad++. How to run the macro is shown in the following. If you want to do the task manually, follow the steps done in 3.1 and 3.2 on the next page.

1. To execute the macro, open the macro execution control by selecting **Macro → Execute Macro /Script** from the menu bar. **Browse** for the **Input-Data** folder and select the Python file **IdentifyingREV.py**.



Clicking **Run** produces the folder **IdentifyingREV** inside the project folder **Results-User**. The macro loads the separator structure 8 times to crop it to the eight different segments and compute porosity and tortuosity on them. Finally,

the results are plotted into one graph inside the new folder as shown on page [25](#). On our machine with 8 cores, the macro needed 14 minutes.



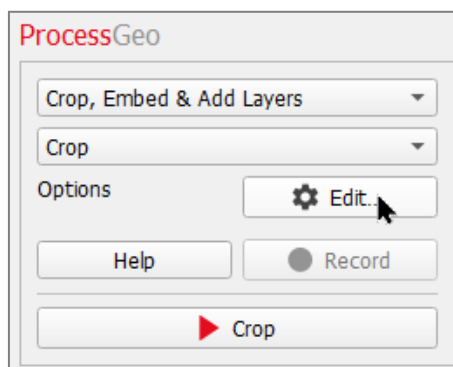
To learn more about automation in **GeoDict**, refer to the [GeoPy scripting](#) handbook of the User Guide.

3.1 CROP SEGMENTS

For each segment to cut, make sure to have the project folder set as described on page [3](#).

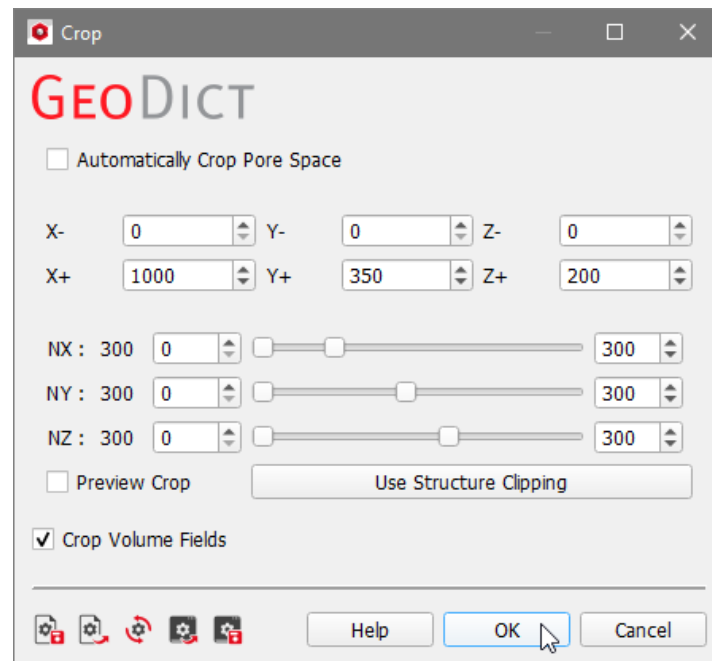
1. Start always with the large structure **Celgard_PP1615_WithMaterialInfo.gdt**. Select **File** → **Open Structure (*.gdt, *.gad)...** and choose the file from the **Results-User** folder.
2. Select **Model** → **ProcessGeo** in the menu bar.
3. In the **ProcessGeo** module section, select **Crop, Embed & Add Layers** from the first pull-down menu and **Crop** from the second one.

Then, click **Edit...** to open the options dialog.



4. Choose the size of the segment that should be cut out by choosing the start and end voxel in each direction.

For a segment of size 300x300x300, the values are shown in the screenshot below.



The resulting structure is the **Celgard_PP1615_300x300x300_3.gdt** and the third row in the table below.

For other structure sizes, choose the ranges shown in the following table for all three coordinate directions.

Size of segment	NX	NY	NZ	Filename extension
1300x650x500	0-1300	0-650	0-500	_1300x650x500_1
500x500x500	0-500	0-500	0-500	_500x500x500_2
300x300x300	0-300	0-300	0-300	_300x300x300_3
300x300x300	100-400	100-400	100-400	_300x300x300_4
300x300x300	200-500	200-500	200-500	_300x300x300_5
200x200x200	0-200	0-200	0-200	_200x200x200_6
100x100x100	0-100	0-100	0-100	_100x100x100_7
50x50x50	0-50	0-50	0-50	_50x50x50_8

The structures 4 and 5 are two other segments of size 300x300x300. The computed properties depend not only on the size of the segment chosen but also on the segment itself. Therefore, it is better to consider not only one segment of a specific size but several instead. As examples, we choose therefore 3 different segments of size 300x300x300.

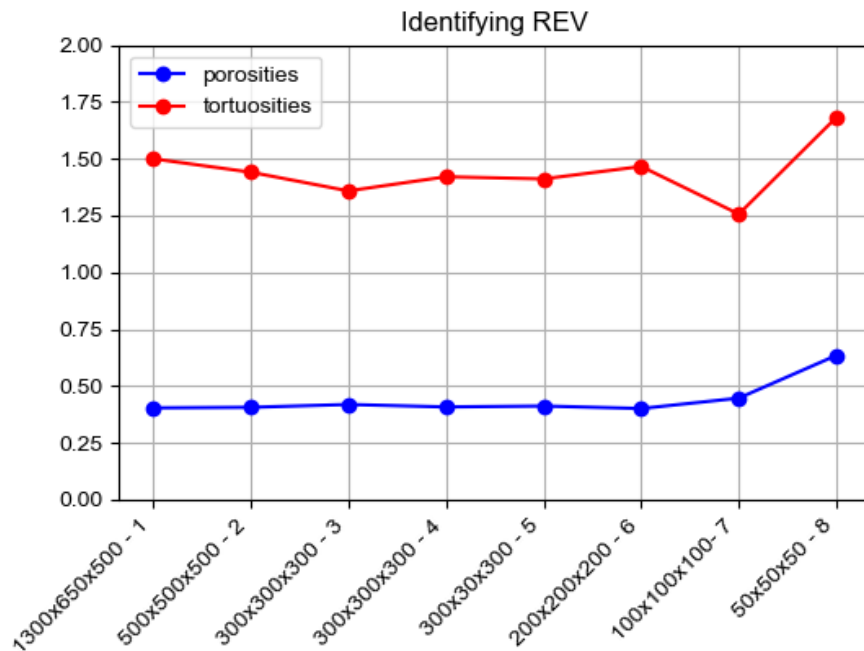
Save the cut segments with the name **Celgard_PP1615_extension.gdt**, with the filename **extension** selected according to the last column of the table above.

3.2 COMPUTE POROSITY AND TORTUOSITY FOR ALL SEGMENTS

For each segment, perform the steps outlined in **2.1 Porosity** and **2.2 Diffusivity and tortuosity** on pages [12](#) and [14](#), respectively to determine the porosity and the geometric tortuosity. Load the file **Celgard_PP1615_extension.gdt** for each of the segments and choose the result file names

StructureInformation_extension.gdr and **Diffusion_extension.gdr** accordingly.

Results for porosity and geometric tortuosity for all segments are shown in the following graph, which is generated by the **IdentifyingREV.py** using the Python package matplotlib. For structure sizes larger than 100x100x100 voxels, both the values for porosity and for geometric tortuosity do not deviate much from those of the whole structure. For structure size 100x100x100 a larger deviation for the tortuosity value and for structure size 50x50x50 also for the porosity can be observed.



Considering only the porosity and the geometric tortuosity, using the segment of size 200x200x200 would be enough. However, since we want also to examine other properties for the deformed structure, we proceed here with the larger structure of size 300x300x300.

4. COMPUTING SEPARATOR-ELECTROLYTE INTERACTION

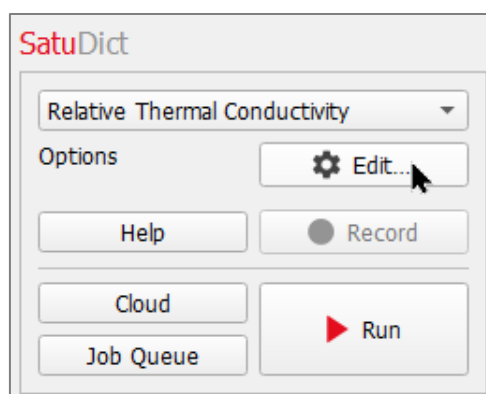
Besides the geometric and transport properties of a separator, the interaction with the electrolyte is very important for the separator performance. For example, the thermal conductivity changes depending on the wetting of the separator with electrolyte.

To show this effect, we compute the thermal conductivity for different saturations of the separator with electrolyte using **SatuDict**.

1. Select the **Results-User** folder as project folder as described on page 3.
2. Load the cropped segment of size 300x300x300 (unless it is still in memory) as follows: **File** → **Open Structure (*.gdt, *.gad)...** and select the **Celgard_PP1615_300x300x300.gdt** file from the project folder.

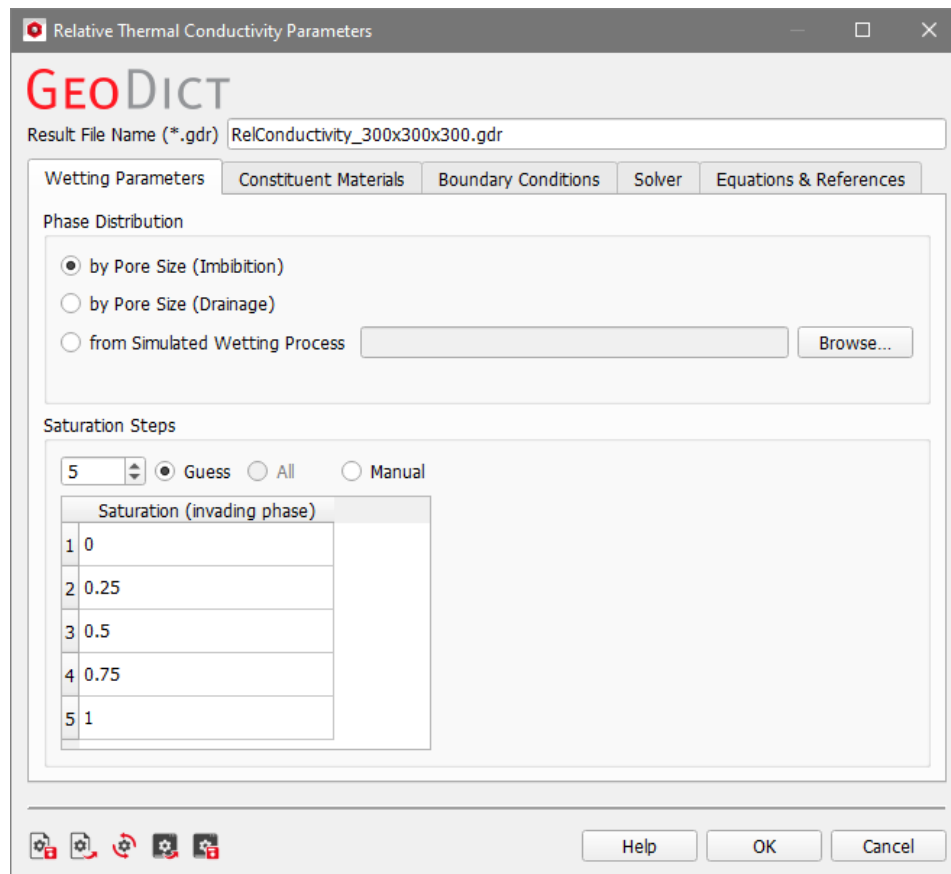


3. Select **Predict** → **SatuDict** from the menu bar.
4. Next, select **Relative Thermal Conductivity** in the **SatuDict** module section.
5. Open the parameters dialog by clicking the **Edit...** button.



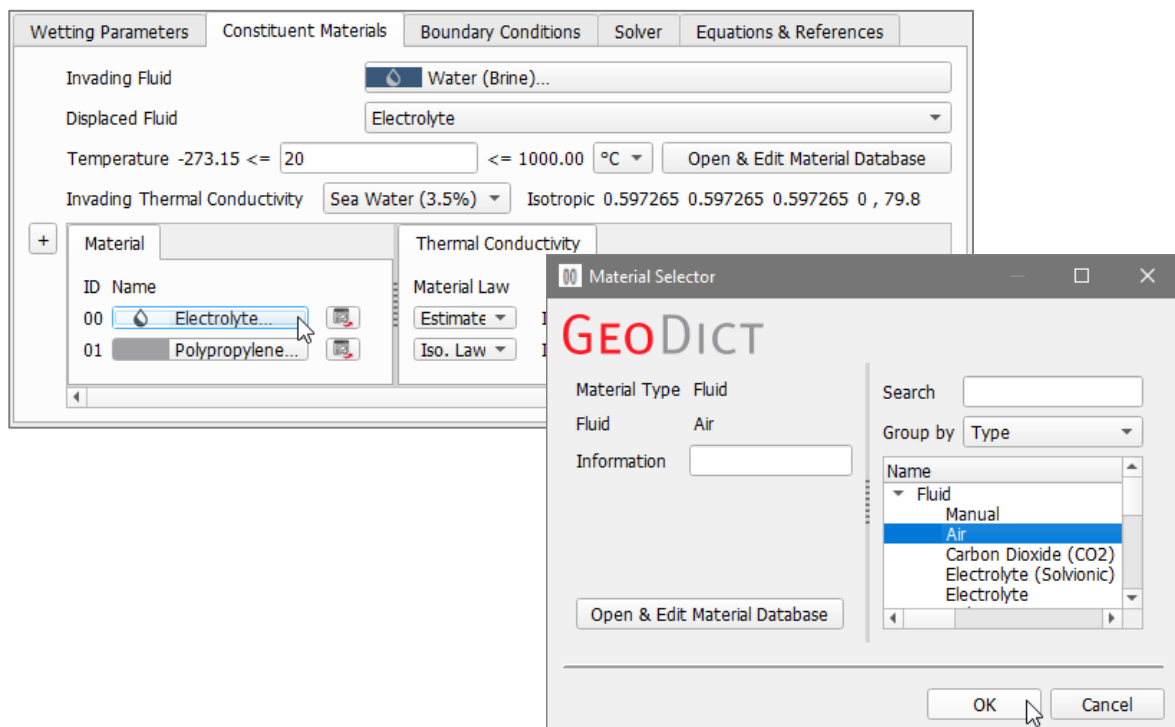
6. Enter **RelConductivity_300x300x300.gdr** as Result File Name.

Under the **Wetting Parameters** tab, keep the default settings of running the computation for five different saturation steps (0%, 25%, 50%, 75% and 100%).



7. On the next tab, **Constituent Materials**, the fluids involved in the simulation of the wetting process need to be defined.

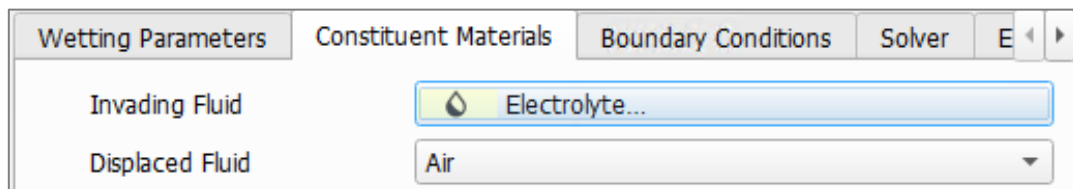
We want to simulate the wetting of the separator with electrolyte, starting with the pore space being full of air. Therefore, we set the material in the pore space to Air, by clicking on the material with Material ID 00 and selecting Air in the Material Selector.



The thermal conductivities of the materials Air and Polypropylene, available in the structure at the start of the simulation, are displayed on the right of this tab:

Material		Thermal Conductivity				
ID	Name	Material Law	Long. / (W/(mK))	Trans. 1 / (W/(mK))	Trans. 2 / (W/(mK))	Temp. Range / (°C)
00	Air...	Iso. Law	Isotropic 0.0257	0.0257	0.0257	-150 , 400
01	Polypropylene...	Iso. Law	Isotropic 0.15	0.15	0.15	0 , 20

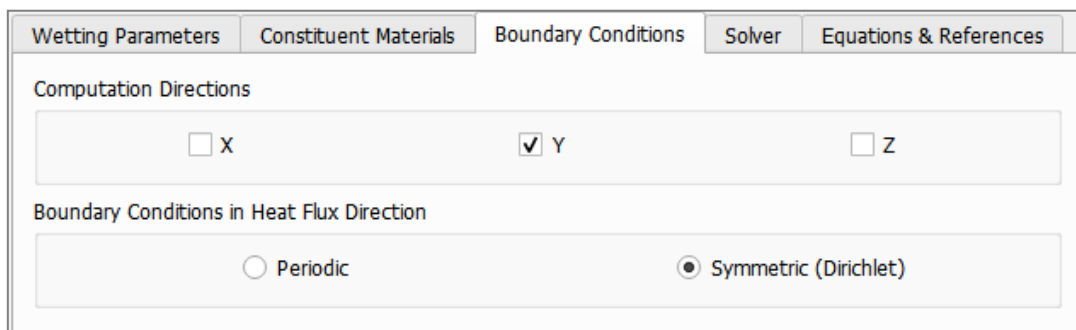
Next, set the **Invading Fluid** to be Electrolyte that invades the structure's pore space.



The 'Wetting Parameters' dialog box shows the 'Invading Fluid' set to 'Electrolyte...' and the 'Displaced Fluid' set to 'Air'.

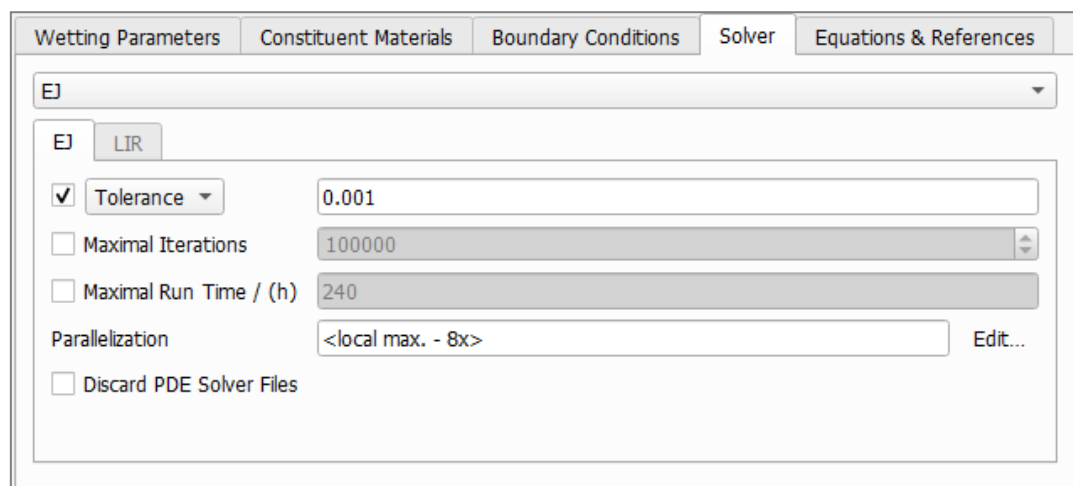
Now the electrolyte will be the wetting phase, that replaces the non-wetting phase (Air) in the simulation.

- Under the **Boundary Conditions** tab, deselect **Z** and instead choose **Y** as the computation direction, which is the through-plane direction of the separator. Set the **Boundary Conditions in Heat Flux Direction** to Symmetric (Dirichlet), since the structure is not periodic in Y-direction.



The 'Boundary Conditions' dialog box shows 'Computation Directions' with 'Y' selected and 'Z' deselected. Under 'Boundary Conditions in Heat Flux Direction', 'Symmetric (Dirichlet)' is selected.

- Finally, in the **Solver** tab, keep the default settings and click **OK** to close the dialog.

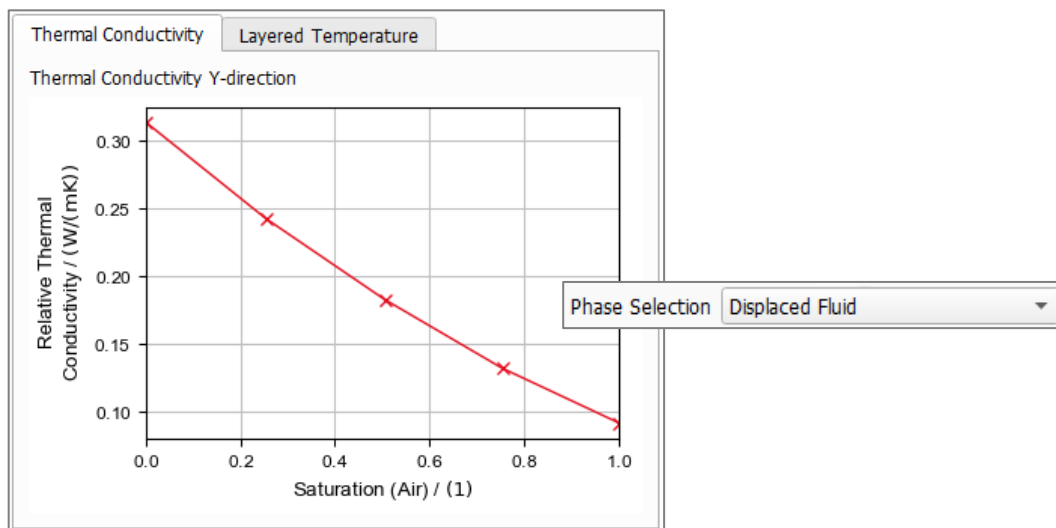
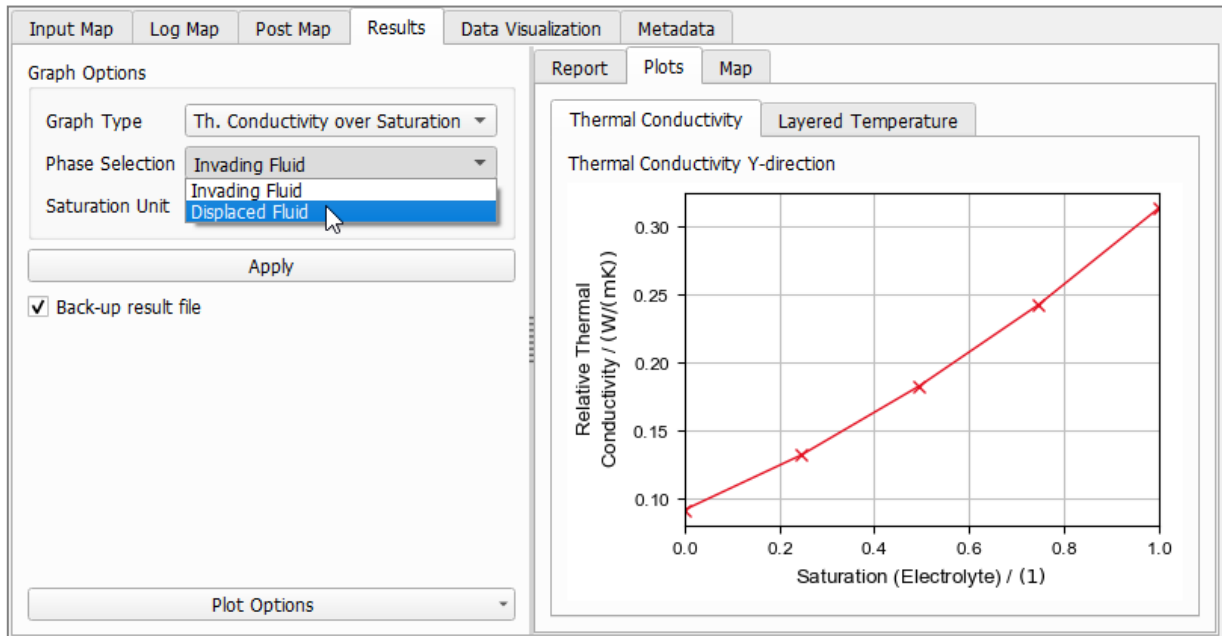


The 'Solver' dialog box shows the 'EJ' solver selected. The 'Tolerance' is set to 0.001, 'Maximal Iterations' to 100000, and 'Maximal Run Time / (h)' to 240. The 'Parallelization' is set to '<local max. - 8x>'. The 'Discard PDE Solver Files' checkbox is unchecked.

10. Click **Run** in the **SatuDict** section to start the computation. The computation took about 4 minutes on our machine with 8 cores.

When the computation has finished the Result Viewer of the **RelConductivity_300x300x300.gdr** result file opens.

In the **Graph Options** left from the **Results-Plots** subtab, select the **Phase** for the plot and click **Apply**. By default, the graph shows the increase in relative thermal conductivity with increasing saturation of the separator with electrolyte.



5. COMPUTING THE DEFORMED STRUCTURE FOR REV

Now, we want to study the changes of geometric properties and in separator-electrolyte interaction if the geometry of the separator is deformed. In battery-operating conditions a separator experiences deformation due to mechanical loads originating from expansions of the electrodes during charging and discharging.

The **GeoDict** module **ElastoDict** is used to compute the deformed structure under mechanical load. As simplification, we assume a linear elastic behavior of the separator. Depending on the material of the separator, this assumption might be too simple to describe the real deformation. Deformation with non-linear elastic behavior can be computed in **ElastoDict** as well.

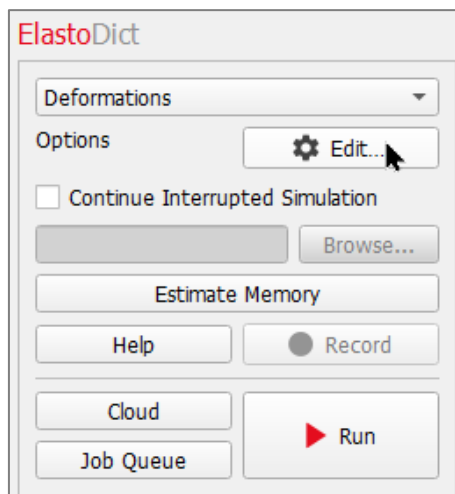
The runtimes for the computations of geometric properties and for the separator-electrolyte interaction on the 300x300x300 cropped segment are moderate. It is well possible to perform these computations on the whole structure. For the computation of the deformation of the separator, which is more time consuming, it is preferable to use the REV to run the computation.

We compute the deformed structure for a 5% and a 10% compression.

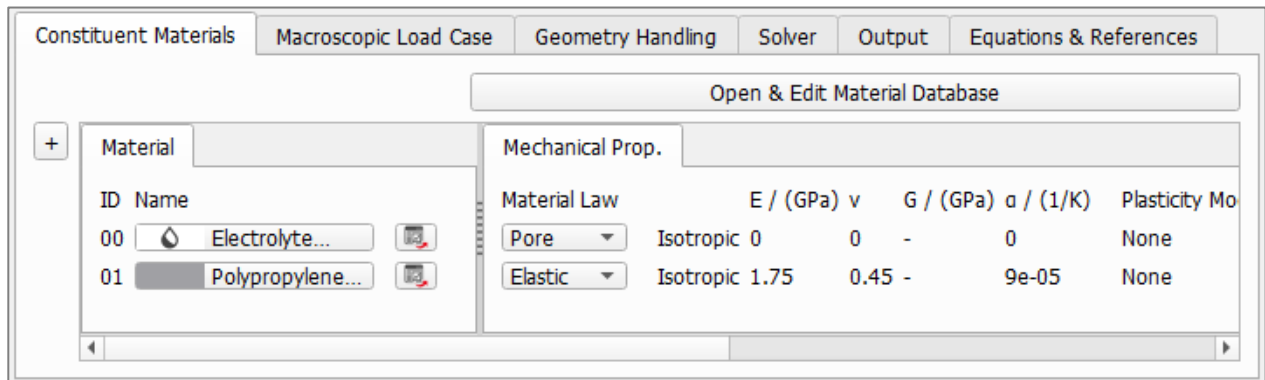
1. Select the **Results-User** folder as project folder as described on page 3.
2. To load the cropped segment of size 300x300x300 select **File** → **Open Structure (*.gdt, *.gad)...** and choose the **Celgard_PP1615_300_300_300.gdt** file from the project folder.



3. Select **Predict** → **ElastoDict** from the menu bar.
4. In the **ElastoDict** module section, select **Deformations** to compute a deformed geometry and click the **Edit** button to open the dialog for the solver options.



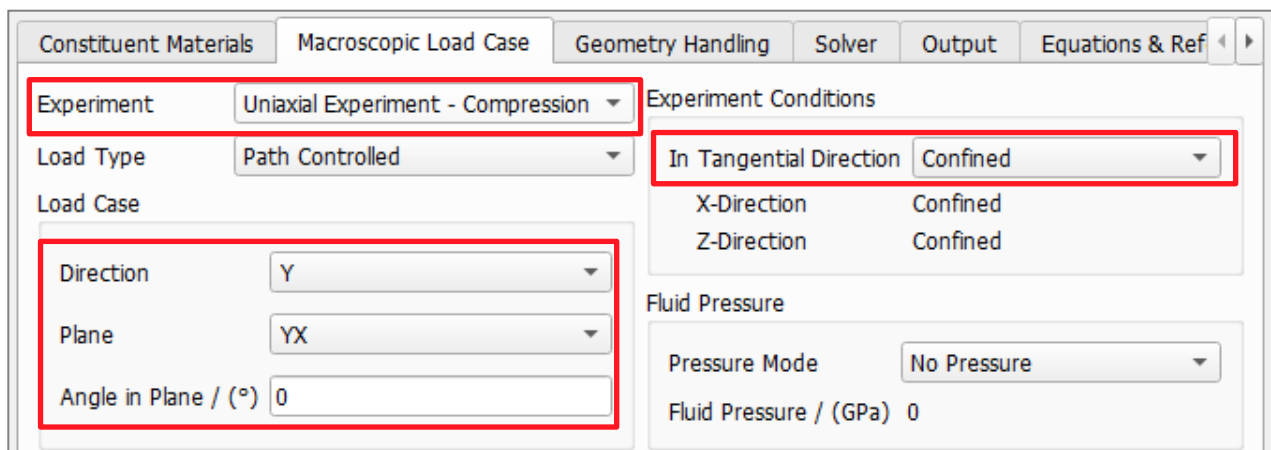
5. The **Constituent Materials** tab shows information on the structure materials. The mechanical properties of Polypropylene are taken from the material database. During deformation, the fluid filling the pore space (Electrolyte) can leave the separator and, therefore, it is not relevant for the computation of deformations.



6. In the **Macroscopic Load Case** tab, the parameters for the deformation need to be defined. First, set the **Experiment** to Uniaxial Experiment – Compression.

Then, define the **Load Case**: Since the **Y-Direction** is the through-plane of the separator, and the separator is compressed by the expansion of the electrodes, define the load in Y-direction.

Next, define the **Experiment Conditions**: In **Tangential direction**, use **Confined** experiment conditions, since the separator structure continues in X-direction and Z-direction, and the segment chosen for the computation cannot extend freely in these directions during compression.



In the table at the bottom left of this tab, define to compress the structure by **5%** and to apply the whole strain in one step. There are two possibilities to achieve this. The first method is to change the **Number of Rows** to 1 and enter 1 for **Time**, 5 for **Strain** and 0 for **Temp. Change**.

In this case, the first option is fast and easy. But if we want to have many and more complicated steps, the table can be changed by editing the **Predefined Shape** on the right. With the choice of **Linear** for **Shape**, the compression is linear. Thus, it is not necessary to apply the load in several steps. Set the **Magnitude** to 5% and the **Length** and **Number of Steps** to 1. Clicking **Apply** automatically updates the table.

Load TableLoad Graph

	Time / (s)	Strain / (%)	Temp. Change
1	1	5	0

Number of Rows

1

Load...

Save...

Predefined Shape

Shape

Linear

Magnitude / (%)

5

Temperature Change / (K)

0

Length / (s)

1

Number of Steps

1

Apply

Finally, choose **Mixed** boundary conditions, i.e., symmetric boundary conditions in the load direction and periodic boundary conditions in the other directions. In the load direction the structure is not periodic, therefore symmetric boundary conditions should be used here.

Boundary Conditions

☐ Periodic
☐ Symmetric
☒ Mixed

- Keep the built-in default settings for the **Geometry Handling**, **Solver** and **Output** tabs.

Constituent MaterialsMacroscopic Load CaseGeometry HandlingSolverOutputEquations & References

Geometry Update

Deformation Type

Without Geometric Nonlinearity

☐ Calculate on Deformed Geometry

☐ Keep Volume Fraction of Deformed Geometry

Geometry Update

All

Update Geometry Each n-th Step

1

Resampling

Maintain Volume

☐ Enable Object Tracking (*.g32)

Constituent MaterialsMacroscopic Load CaseGeometry HandlingSolverOutputEquations & References

Simulation Stopping Criterion

Tolerance

0.0001

☐ Maximal Iterations

1000

☐ Maximal Run Time / (h)

240

Method

Intermediate (Memory Efficient Conjugate Gradient)

Parallelization

<local max. - 8x>

Edit...

☐ Use Downsampling

Downsampling Factor

2

Composite Voxels

Laminate Theory

☐ Write Deformation Data to File (slower but less memory)

Orientation Mode for Anisotropic Materials

Use Orientation from Analytic Objects (gad)

Constituent Materials Macroscopic Load Case Geometry Handling Solver Output Equations & References

Write Steps

☒ Write All Steps

Write Result Fields (*.das) for Each n-th Step

Deformed Geometry

☒ Write Deformed Geometry

☐ Write Volume Fields for Deformed Geometry

☐ Write Volume Fractions for Deformed Geometry

☐ Allow Restart for Deformation Simulations

Write Volume Field

Displacement: ☐ X ☐ Y ☐ Z Check All Uncheck All

Stress: ☐ XX ☐ YY ☐ ZZ ☐ YZ ☐ XZ ☐ XY ☒ Von Mises

Strain: ☐ XX ☐ YY ☐ ZZ ☐ YZ ☐ XZ ☐ XY ☒ Von Mises

☒ Material State Variables

☐ Export VTK File (*.vti)

8. Enter **DeformationResult_5%_300x300x300.gdr** as result file name and click **OK** to close the dialog.

Click **Run** in the **ElastoDict** section. Note that the computation takes some minutes. On our machine with 8 cores it took about 30 minutes. Instead, you can also load the result from the **Results-M2M** folder inside the tutorial folder.

9. The **Result Viewer** of the result file opens automatically at the end of the computations.

Input Map Log Map Post Map Results Strain/Stress Visualization Create Videos Metadata

Report Plots Map

Coordinate system

The coordinate system of the experiment is aligned with the coordinate axis in GeoDict.

Average strain

Time / (s)	Temp. Change / (°C)	XX / (%)	YY / (%)	ZZ / (%)	YZ / (%)	XZ / (%)	XY / (%)	VonMises / (%)	Hydrostatic / (%)
0	0	0	0	0	0	0	0	0	0
1	0	4.1303e-09	4.9999	0	0.44275	0	0.68302	5.19489	-1.66664

Average stress

Time / (s)	Temp. Change / (°C)	XX / (GPa)	YY / (GPa)	ZZ / (GPa)	YZ / (GPa)	XZ / (GPa)	XY / (GPa)	VonMises / (GPa)	Hydrostatic / (GPa)
0	0	0	0	0	0	0	0	0	0
1	0	0.0071766	0.045878	0.017503	6.3411e-05	3.3985e-05	8.8383e-05	0.0347101	-0.0235191

10. Now, we run a second deformation simulation with strain of 10% instead of 5%. For this, in the **ElastoDict** section click **Edit** again and in the **Macroscopic Load Case** tab change the strain to 10% and the **Result File Name** to **DeformationResult_10%_300x300x300.gdr**. Click **OK** to close the dialog and

Run to run the deformation simulation. On our machine with 8 cores, it took about 30 minutes.

The screenshot shows a software window with two tabs: 'Load Table' and 'Load Graph'. The 'Load Table' tab is active, displaying a table with three columns: 'Time / (s)', 'Strain / (%)', and 'Temp. Change'. The first row contains the values '1', '1', and '10' respectively. The 'Predefined Shape' section on the right has a 'Shape' dropdown set to 'Linear', and input fields for 'Magnitude / (%)' (10), 'Temperature Change / (K)' (0), 'Length / (s)' (1), and 'Number of Steps' (1). There are 'Load...', 'Save...', and 'Apply' buttons at the bottom.

Time / (s)	Strain / (%)	Temp. Change
1	1	10

11. For both computations (5% and 10%), the deformed structures can be loaded in **GeoDict**. Choose **Load** for the Deformed Geometry under the **Strain/Stress Visualization** tab of the Result Viewer.

The screenshot shows the 'Strain/Stress Visualization' tab in the 'Results' section of a software interface. It features a 'Time Step / (s)' dropdown set to '1'. Below this, under 'Step 1', there are three rows: 'Deformed Geometry (*.gdt)' with a 'Load' button, 'Deformed Solution File (*.das)' with the text 'unavailable', and 'Solution File (*.das)' with a 'Load' button. A mouse cursor is hovering over the 'Load' button for 'Deformed Geometry'.

The undeformed (left) and deformed geometry (middle 5%, right 10%) are shown in the following image.

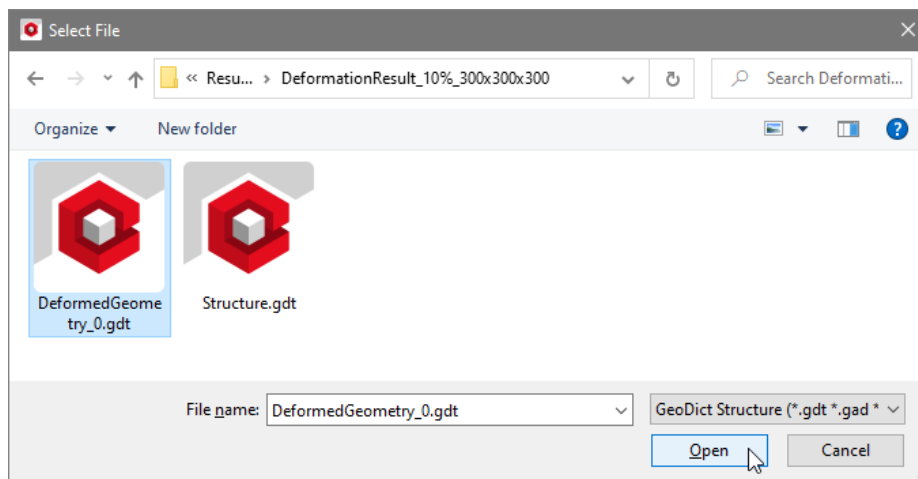


6. COMPUTING PROPERTIES OF DEFORMED STRUCTURE

Now, we compute the geometric properties and the thermal conductivity dependent on the separator saturation with electrolyte again for the deformed structures and compare them with those of the undeformed structure.

Since the computations are the same as shown above in the second and fourth section (page [12](#) and [26](#)), we explain here only how to access the deformed structure and how to compare the results in the **GeoDict** Result Viewer. If only interested in some of the results, only compute the desired properties or load them from the **Results-M2M** folder.

1. Select the **Results-User** folder as project folder, as described on page [3](#).
2. Open one of the deformed structures by clicking **File → Open Structure (*.gdt, *.gad)...** in the menu bar and browse to the result folders of the **ElastoDict** computations
 - **DeformationResult_5%_300x300x300** for the 5% deformation **or** the
 - **DeformationResult_10%_300x300x300** for the 10% deformation.
3. Open the file **DeformedGeometry_0.gdt**. Since the deformation was computed in one step, there is only one file for the deformed geometry available in the folder.



4. Rerun the computations of
 - geometric properties as shown in **2.1 Porosity** on page [12](#),
 - and transport properties as in **2.2 Diffusion and tortuosity** on page [14](#),
 - as well as the computation of **thermal conductivity** dependent on the saturation of the separator with electrolyte as shown in Unit 4 on page [26](#).

Add the suffix **_Def5%** or **_Def10%** to the name of the result file, respectively.

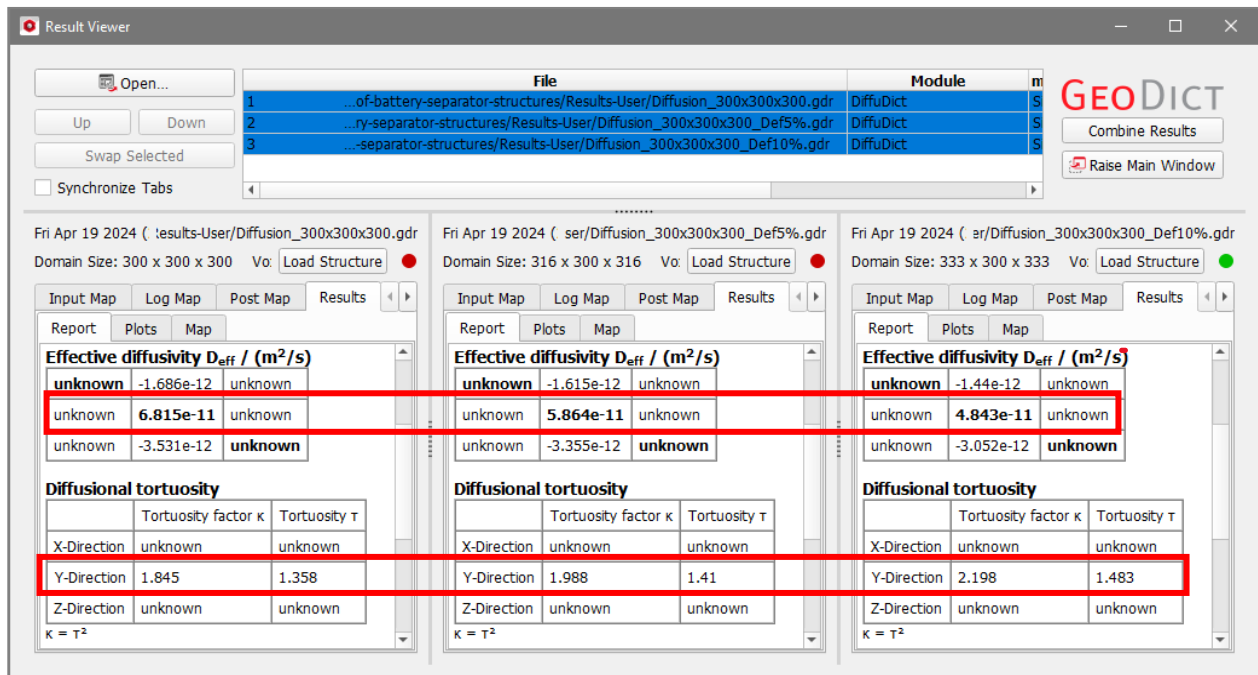
StructureInformation_300x300x300.gdr,
StructureInformation_300x300x300_Def5%.gdr and
StructureInformation_300x300x300_Def10%.gdr.

In the following screenshot, they are shown in the order of increasing deformation, from left to right. The result for the undeformed structure is shown on the left, the one for 5% deformation in the middle, and the one for 10% deformation on the right.



6.2 DIFFUSION AND TORTUOSITY COMPARISON

In the same way, the tortuosity and the diffusivity can be compared as well from the results of the **DiffuDict** computations (**Diffusion_300x300x300*.gdr**).

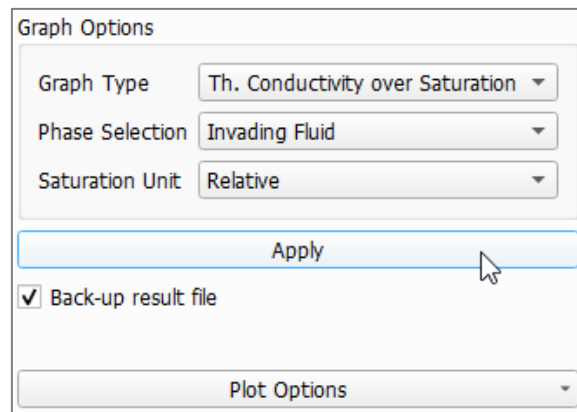


The diffusivity in the pore space filled with electrolyte decreases with increasing compression of the separator. In the same way, the geometric tortuosity of the structure increases. The reason for both is the decreased porosity due to the compression, which makes it more difficult to find a way through the structure.

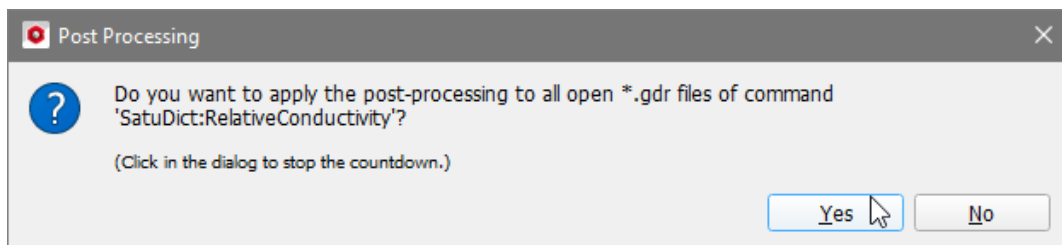
6.3 THERMAL CONDUCTIVITY COMPARISON

Next, we investigate the thermal conductivity changes for different electrolyte wetting levels of the structure under compression.

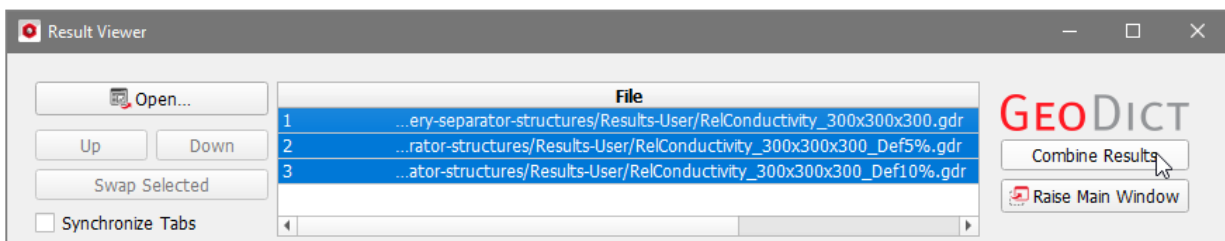
1. Open the result files of all three computations of relative thermal conductivity by clicking **File** → **Open Results** in the menu bar, selecting the result files, and clicking **Open (RelConductivity_300x300x300*.gdr)**.
2. In the Result Viewer that opens with all three result files, select them all. The results are shown now side-by-side in the Result Viewer.
3. To ensure to have the same plot settings for all three result files, in the **Graph Options** select **Invading Fluid** for **Phase Selection** and click **Apply**.



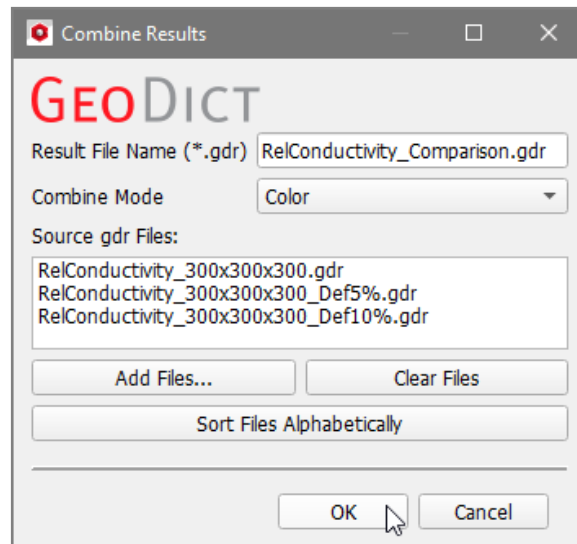
In the dialog that opens, choose **Yes** to apply the post-processing settings to all three result files (*.gdr) simultaneously.



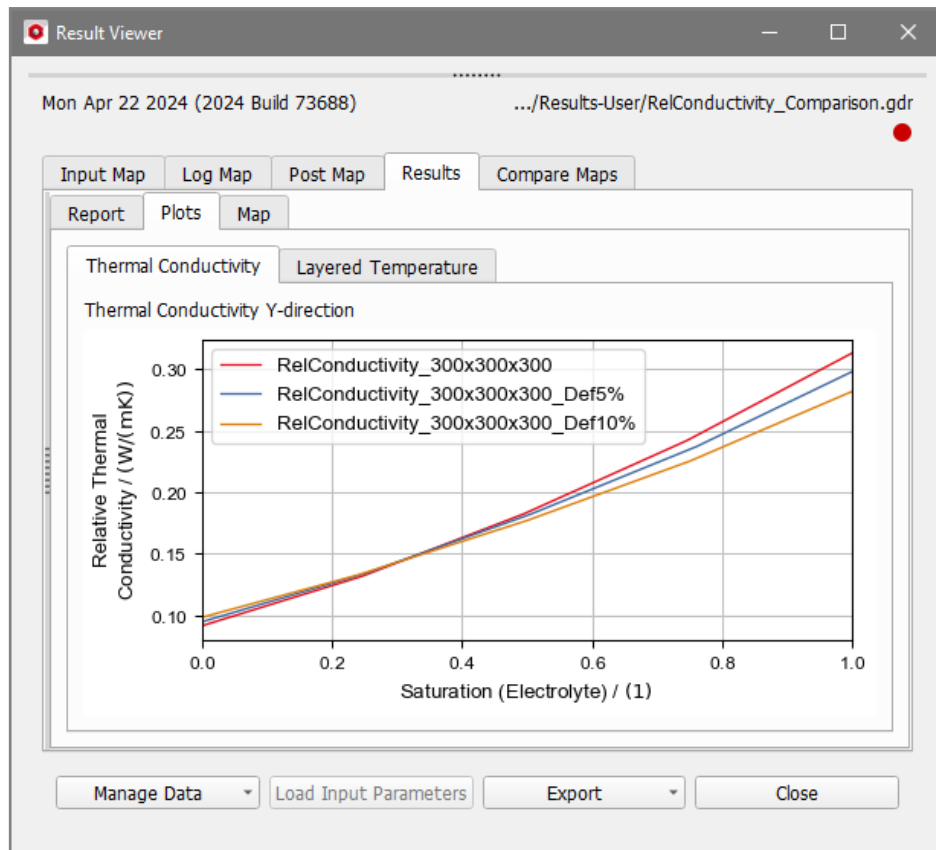
4. For an easier comparison of the three curves, click **Combine Results** in the top right of the result viewer.



5. Change the **Result File Name** to **RelConductivity_Comparison.gdr** in the opening dialog and click **OK**.



6. In the **Results** tab, select the **Plots** subtab. The thermal conductivity, dependent on the saturation of the separator with electrolyte, is shown for the structure before and after deformation in a single plot.



The thermal conductivity decreases at high saturation rates if the structure is compressed. The reason is the decrease in porosity when the structure is compressed (see porosities for the deformed structures). Since the electrolyte has a higher conductivity compared to polypropylene, the overall conductivity decreases when less electrolyte is contained in the separator.

SUMMARY

In this tutorial, the capabilities of GeoDict for digital analysis and design of Li-ion battery separators are shown.

- The geometric and transport properties of a segmented FIB-SEM scan of a Celgard® PP1615 separator are calculated. Specifically, the porosity, tortuosity and connectivity as well as the effective diffusivity are determined.
- The simulations show changes in the thermal conductivity of the microstructure with electrolyte wetting.
- The structure is then mechanically deformed and the influence of the deformation on the above-mentioned parameters is monitored.

REFERENCES

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