GeoApps for GeoDict

User Guide

GeoDict release 2023

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GeoDict

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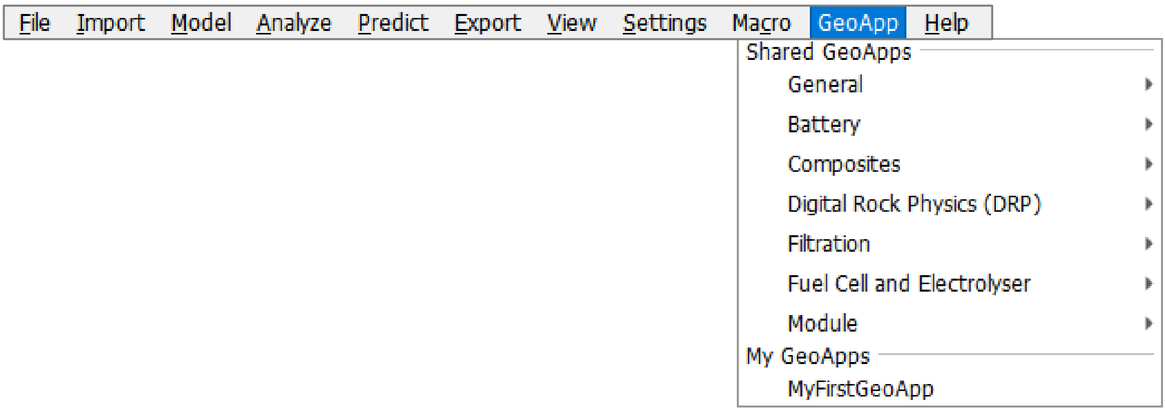
GeoApps for GeoDict 2023

GeoDict offers great automation possibilities to enhance productivity in the form of GeoApps. All steps done by the user in GeoDict are recorded in macros. The **GeoApp** menu in GeoDict gives access to several pre-defined macros for workflows that are often requested. Additionally, the user can add own recorded and edited parameter macros to create custom GeoApps for frequent workflows, as described on pages 93ff.

The **GeoApp** menu in the menu bar gives access to many **GeoApps**, grouped into **Shared GeoApps** and **My GeoApps**.



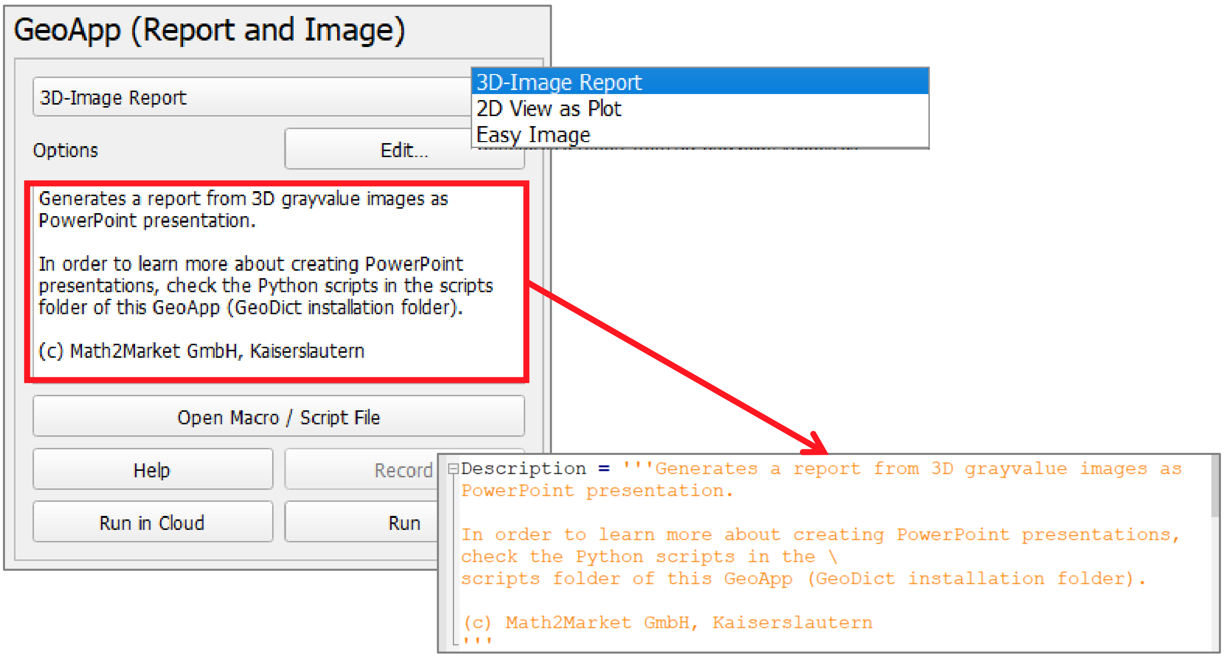
The **Shared GeoApps** are groups of apps delivered with GeoDict and, later, apps that the users create or modify to be shared with their colleagues.

- Compute tortuosities, create image reports and structures with the **General** GeoApps.
- Create electrodes with the **Battery** GeoApps.
- Create structures as glass-fiber enforced plastic and laminates with the **Composites** GeoApps.
- Run simulations on rocks with the **Digital Rock Physics** GeoApps, as for example quality control and nuclear magnetic resonance.
- Create particulate filters with the **Filtration** GeoApps.
- Generate fuel cell components with the **Fuel Cell and Electrolyser** GeoApps.
- Run **Module** specific GeoApps for several modules, which can also be found in the corresponding module sections.

Under **My GeoApps** is an example GeoApp provided by Math2Market and, later, the local GeoApps created by the user only for his/her private use. The **My GeoApps** are placed in the GeoDict settings folder as described on page 93.

Selecting one of the GeoApps groups opens the corresponding **GeoApp** module section, located left of the Visualization area. It contains a pull-down menu listing the available GeoApps for this particular GeoApp group.

GeoDict macros corresponding to the simulations are called and executed when the GeoApps are run. These macros are available in the **GeoApp** folder in the GeoDict installation folder. GeoApps may be opened with a text editor, to observe their syntax and the steps involved in the simulation and also be edited if the user has the privileges to change files in the GeoDict installation folder, which typically requires administrator privileges.



When selecting one of the available GeoApps, the description area displays a report about the app. In the corresponding GeoPy script, this report content can be found inside the apostrophes after **Description = ''' '''** and can be edited at any time after opening the script with a text editor. For the **3D-Image Report.py** app from the GeoApp module **General → Report and Image**, the text in the macro and the description area is shown above.

Click the **Options' Edit ...** button to edit the parameters of the macro.

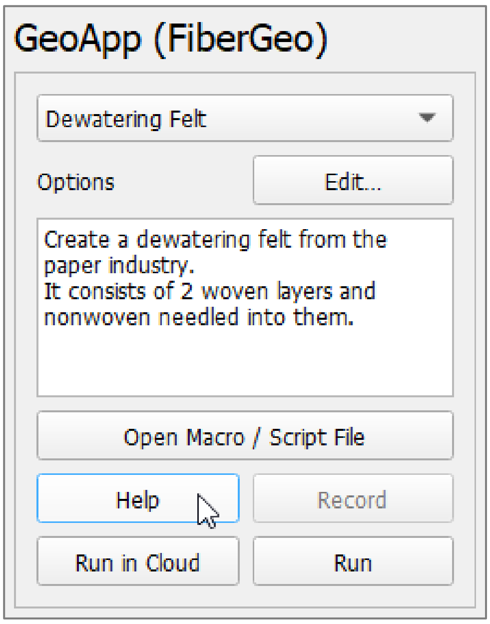
By clicking **Open Macro / Script File**, the macro file containing all steps for the app simulations can be accessed in a text editor. For detailed information about GeoPy and editing GeoDict macros refer to the GeoPy scripting handbook of this User Guide.

Clicking **Run** runs the app.

Click **Run in Cloud** to run it in the GeoDict cloud, see the High Performance Computing handbook of this User Guide for details. If interested in cloud simulations, contact Math2Market to apply for a GeoDict cloud license.

Module GeoApps are also contained in the corresponding modules and described in their User Guide handbooks.

Open the corresponding handbook by clicking **Help** in the GeoApp module section. In the example on the right, the **Help** button opens the FiberGeo handbook.



Shared GeoApps

The GeoApps delivered with GeoDict are described shortly in the following. Please ask support@math2market.de if you want to know more details about the specific parameters used in theses apps and the functionality they provide.

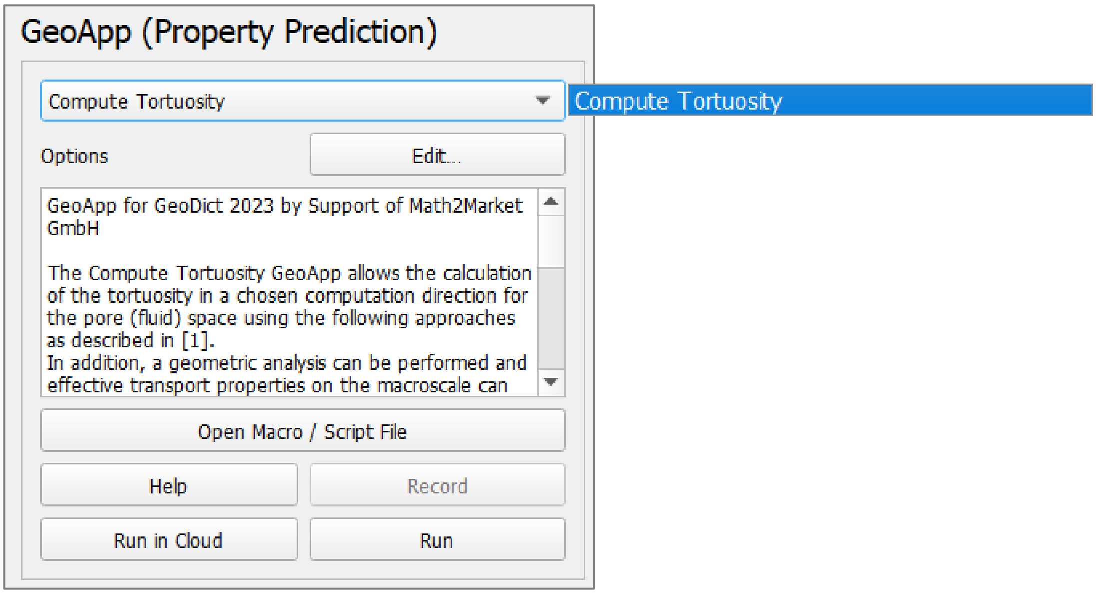
General

Three GeoApp - **General** are shipped with GeoDict.

- Use **Property Prediction** apps to compute physical properties.
- Save images and create PowerPoint reports with the **Report and Image** apps.
- Generate statistical twins with the **Structure Generation** apps.

Property Prediction

The **GeoApp (Property Prediction)** section contains the **Compute Tortuosity** app, selectable from the pull-down menu.



Compute Tortuosity

The **Compute Tortuosity** GeoApp calculates the tortuosity, for the pore space, in a chosen computation direction using different approaches.

Modules needed to run this GeoApp (depending on the selected options): PoroDict, MatDict, DiffuDict, ConductoDict, FlowDict, AddiDict

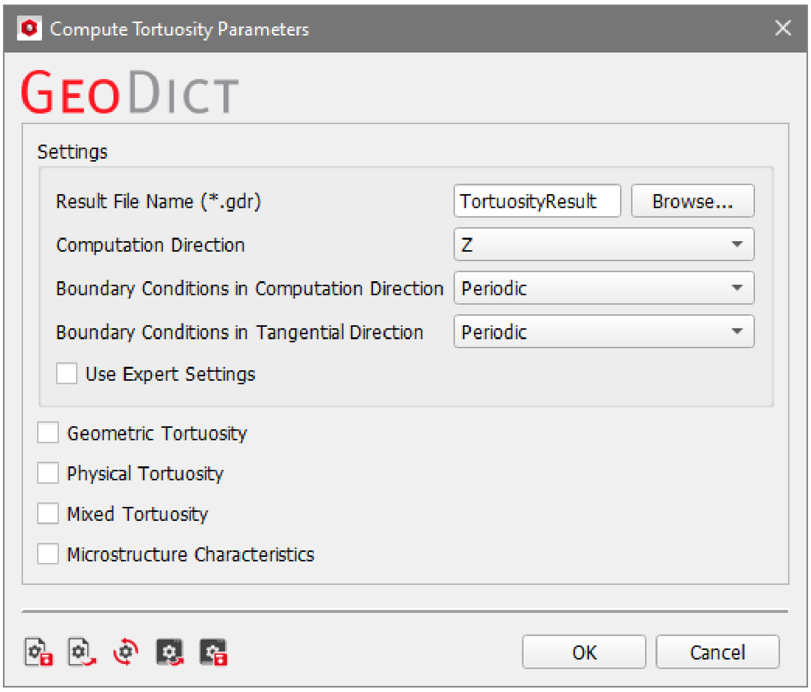
In addition, with the **Compute Tortuosity** app, a geometric analysis can be performed and effective transport properties on the macroscale can be predicted based on [1].

Generally, three different kinds of tortuosity can be computed:

- **Geometric Tortuosity**, which are directly derived from the microstructure

- **Physical tortuosity** or physics-based tortuosity, which are indirectly derived by transport mechanisms
- **Mixed Tortuosity**, which use a mixture determination from geometric analysis and physical transportation phenomena.

Clicking **Edit** opens the **Compute Tortuosity Parameters** dialog.



Select a **Result File Name** and the **Computation Direction** in the **Settings** panel. Also, the **Boundary Conditions in Computation Direction** and **Boundary Conditions in Tangential Direction** can be changed.

Then, choose which properties should be computed.

Two options are available for **Geometric Tortuosity**. These tortuosity are directly derived from the morphological characteristics of the analyzed structure and are well-defined by the structure only.

The general definition of the Geometric tortuosity is the comparison of the effective geometric pathlength L_{eff} to the shortest geometric pathlength L_0:

$$\tau = \frac{L_{eff}}{L_0} \tag{1}$$

The geometric tortuosity available are:

- **Geodesic Tortuosity** in PoroDict: Computing the mean geodesic tortuosity from the percolation pathway starting from every voxel in the inlet. I.e., the shortest path in pore space is compared to the direct path.
- **Percolation Tortuosity** in PoroDict: Computing the mean value of the percolation pathways with the 50 largest diameters. I.e., the length of the path of large particles (largest possible diameters) through the structure (median axis) is compared to the direct path.

Four options are available for **Physical tortuosity**. These tortuosities are indirectly derived and do not use the geometric path lengths:

$$\tau \neq \frac{L_{eff}}{L_0} \tag{2}$$

Physical tortuosities are determined using effective properties to deduce a tortuosity value indirectly. Therefore, microstructure effects as bottleneck-effects are included. A physical tortuosity is only meaningful if it bases on a transport phenomenon that is relevant to the simulated material. Thus, different tortuosities can be determined depending on the dominating transport mechanism: diffusion of molecules or ions, conductivity of electrons etc. For example, consider the effective diffusion of gas through a porous membrane in comparison to the self-diffusion of the gas. Then, the diffusion tortuosity is of interest [2]. GeoDict can output both, the value for the **tortuosity** τ and the value of the **tortuosity factor** κ by comparing the effective diffusion to self-diffusion:

$$\tau_{\text{indir,diff}} = \sqrt{\kappa_{\text{indir,diff}}} = \sqrt{\frac{\varepsilon}{D_{\text{rel}}}} \tag{3}$$

where ε is the porosity and D_{rel} the relative diffusivity due to the porous-media dependent part of the effective diffusion. GeoDict can output both, the value for the tortuosity τ and the value of the tortuosity factor κ. These numbers can be converted in each other by the general relation between τ and κ:

$$\tau = \sqrt{\kappa} \tag{4}$$

The available physical tortuosities are:

- **Diffusion Tortuosity** in DiffuDict: Diffusion as indirect, physical approach [3]. The tortuosity will be extracted from the DiffuDict **Laplace** and **Knudsen** Diffusion result files (GDR), respectively.
- **Conduction Tortuosity** in ConductoDict: **Electrical** and **Thermal** conductivity as indirect, physical approach [4]. The tortuosity will be extracted from the respective ConductoDict result file (GDR).

Five options are available for **Mixed Tortuosity.** The mixed tortuosities are derived from a mixed determination including the geometrical analysis of streamlines and pathways from simulations of diffusion, flow, advection, etc. The available mixed tortuosities are:

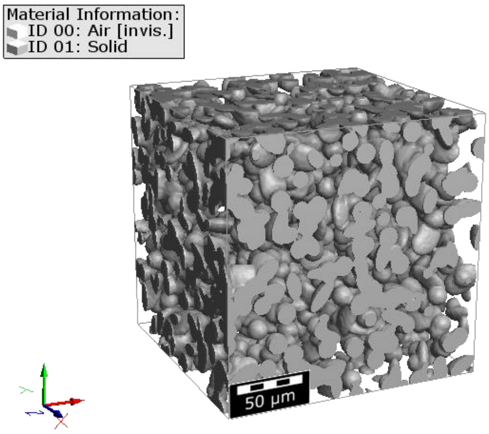
- **Tortuosity from Laplace Diffusion Flux** in DiffuDict [5]: The mean value of DiffuDict Laplace diffusion flux streamlines and/or the tortuosity is calculated based on the volume average of DiffuDict Laplace diffusion flux.
- **Tortuosity from Electrical Current Density and Thermal Heat Flux** in ConductoDict: The mean value of the streamline length of ConductoDict flow velocity streamlines and/or the tortuosity is calculated based on the volume average of ConductoDict flow velocity for thermal or electrical conductivity.
- **Tortuosity from Stokes Flow Velocity** in FlowDict [6]: The mean value of the streamline length of FlowDict Stokes flow velocity streamlines and/or the tortuosity is calculated based on the volume average of FlowDict Stokes flow velocity.
- **Tortuosity from Advection Particle Path Length** in AddiDict: Computing the mean value of the particle path length for advection.
- **Tortuosity from Particle Diffusion Path Length** in AddiDict: The mean value is calculated based on effective isotropic diffusivity.

Additionally, to the different tortuosities, the **Compute Tortuosity** GeoApp can calculate **Microstructure Characteristics**. Three options are available:

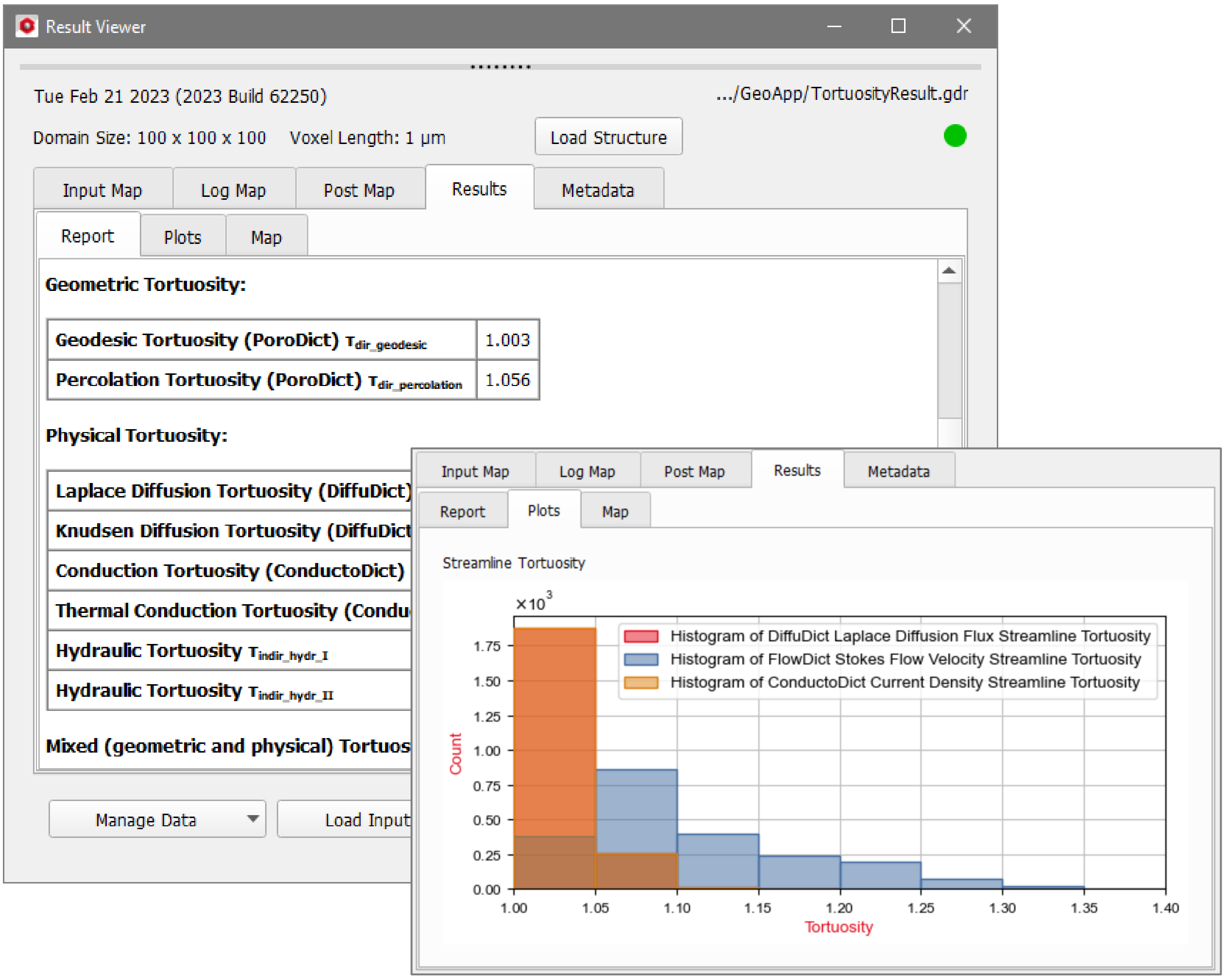
- **Characteristic Diameters** from **Granulometry** or **Porosimetry** in PoroDict: Computing D10, D50, and D90.
- **Surface Area** in MatDict: Specific surface area between pore space and solid materials.

The result file's Result Viewer opens when the **Compute Tortuosity** App finishes.

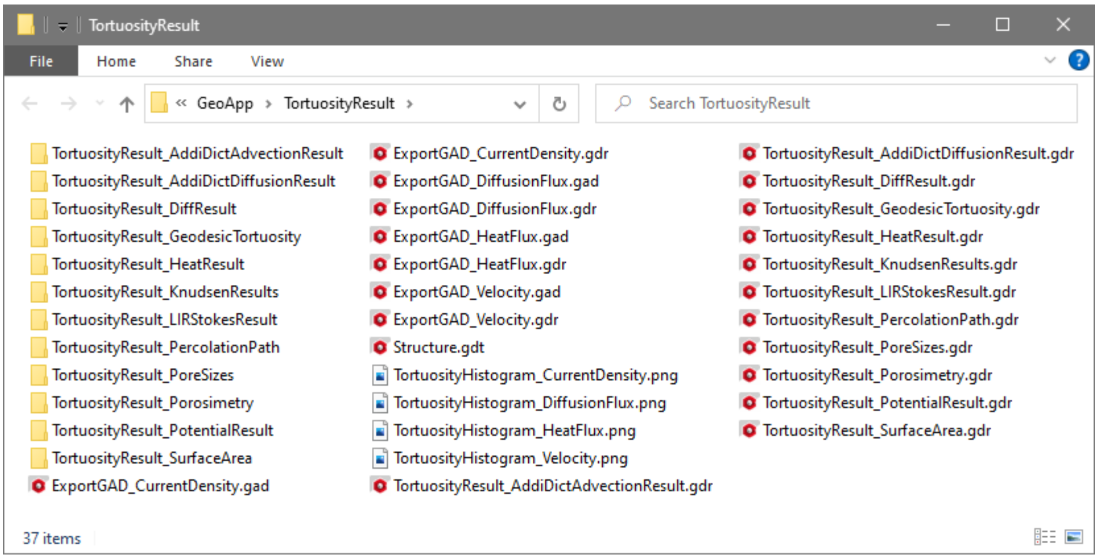
The result file provides detailed information about the formulas used to calculate the different tortuosities, the microstructure characteristics, the pore phase and transport properties, as well as those used to predict effective transport properties.



Depending on the selection in the **Compute Tortuosity Parameters** dialog, the results are given in tables. If the calculation of the tortuosity based on streamlines was selected, the evaluation of streamline length is shown as a **Streamline Tortuosity** plot.



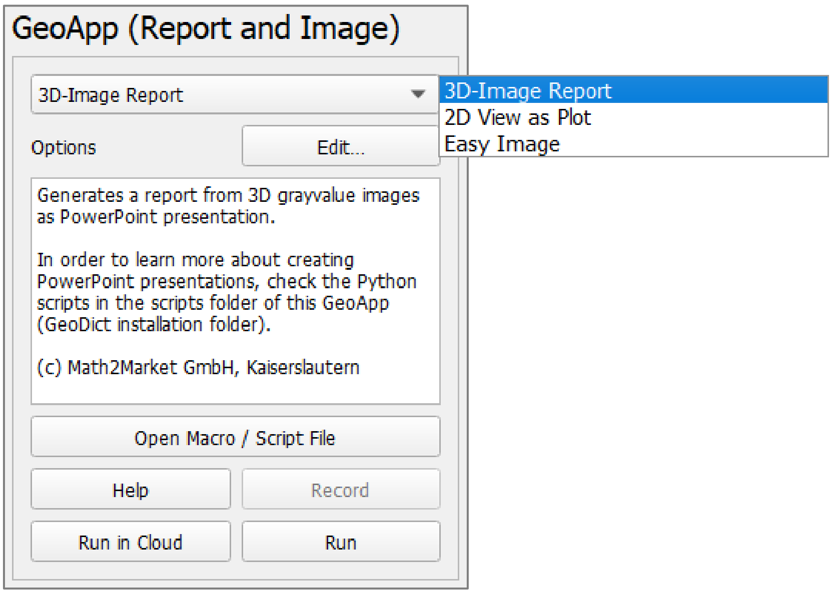
Additionally, the corresponding result folder contains the detailed GeoDict results corresponding to the respective simulations.



Report and Image

The **GeoApp (Report and Image)** section contains the following, selectable from the pull-down menu:

- **3D-Image Report:** generates a report from 3D gray value images as a PowerPoint presentation.
- **2D View as Plot**: saves the 2D view of the current structure as a plot.
- **Easy Image**: provides the possibility to create a variety of media materials, e.g., for the website, presentations, based on proofed presets**.**



3D Image Report

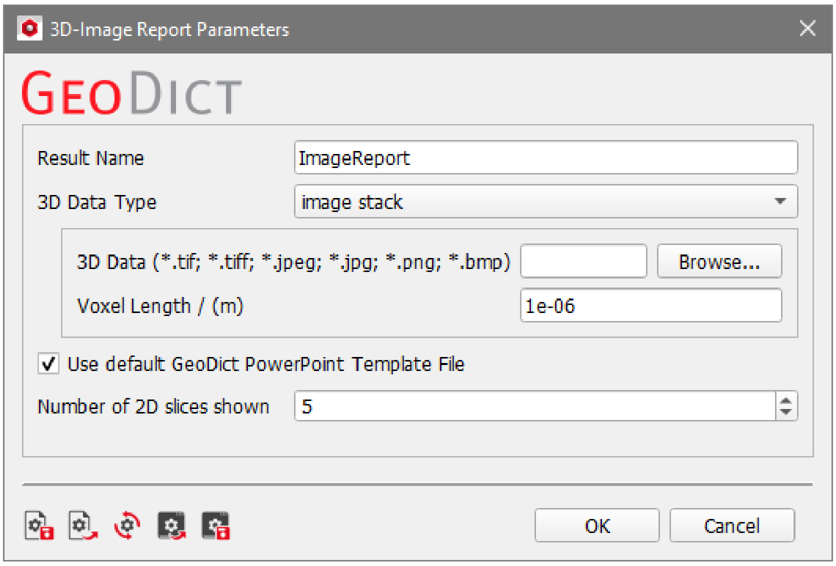
The **3D-Image Report** app generates a report from 3D gray value images as a PowerPoint presentation.

In order to learn more about creating PowerPoint presentations, refer to the GeoPy handbook of this User Guide or check the Python scripts in the scripts folder of this GeoApp (GeoDict installation folder).

Modules needed to run this GeoApp: ImportGeo-Vol

Clicking **Edit** opens the **3D-Image Report Parameters** dialog.

The input parameters include **Result Name**, **3D Data Type**, **Voxel Length**, **Use default GeoDict PowerPoint Template File**, and **Number of 2D slices shown**.

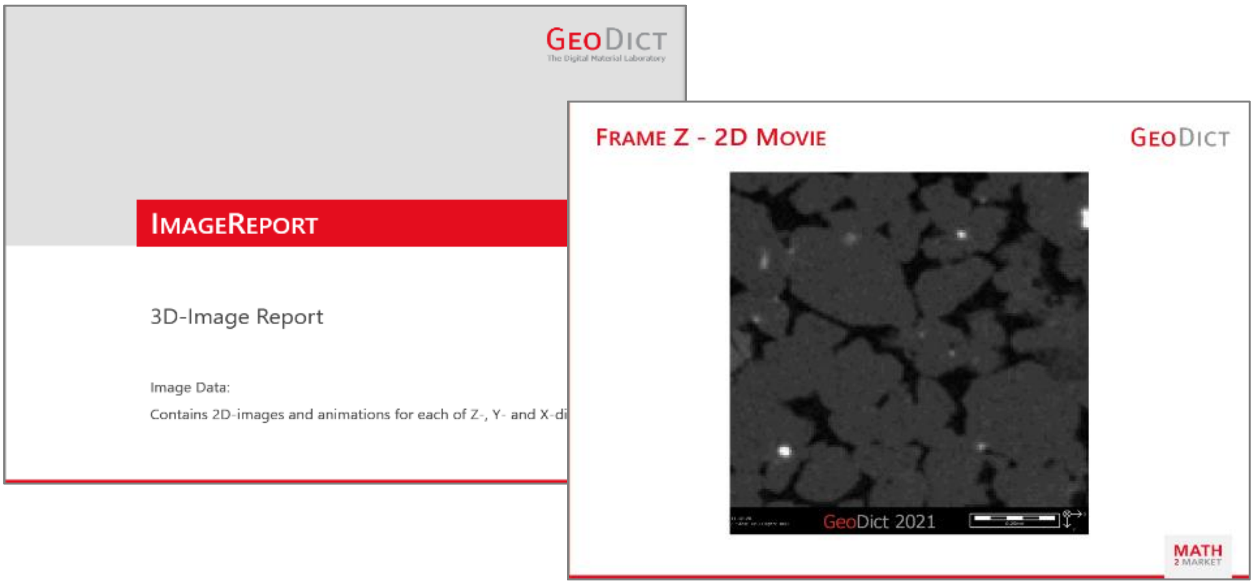


The detailed explanations of the parameters and how to customize the PowerPoint Template File are found in the GeoApp for 3D-Image PowerPoint reports tutorial. Also, helpful tooltips appear, when hovering the cursor over the parameters.

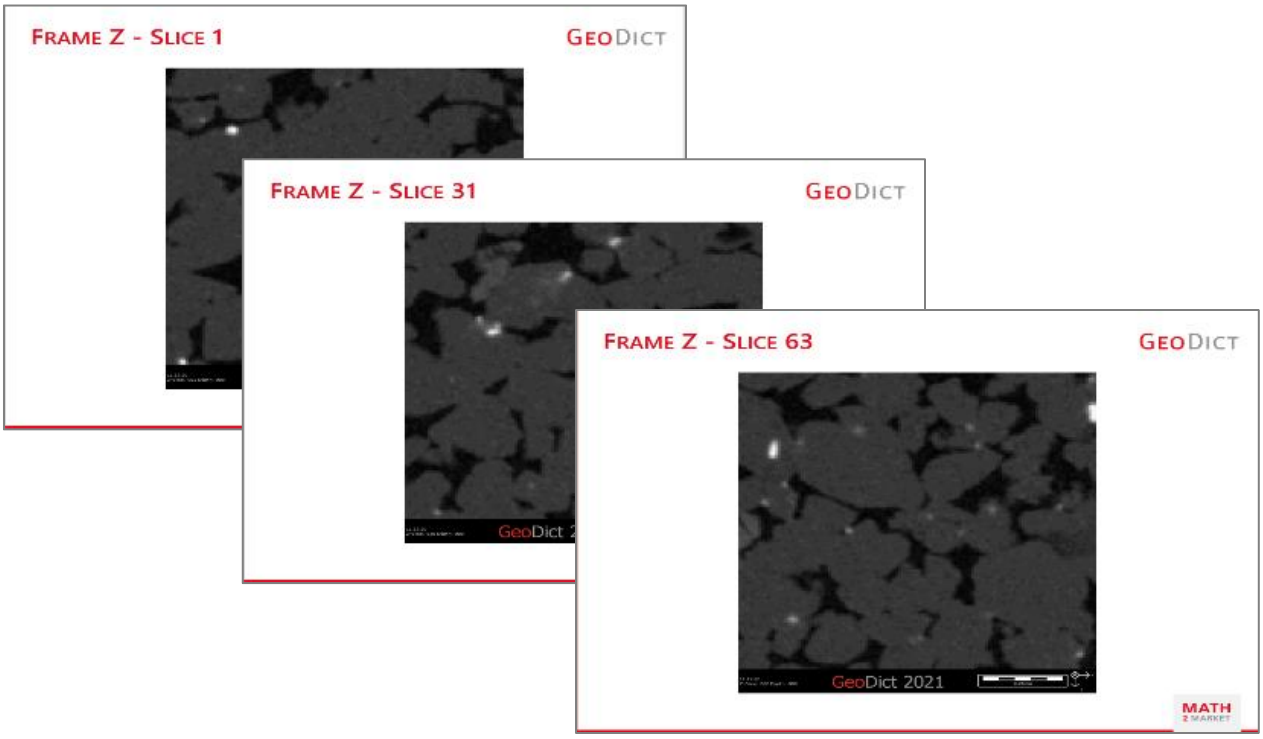
The parameters can be modified if needed. Otherwise, click **OK** to close the dialog, go back to the **GeoApp** section and click **Run**.

The PowerPoint report is found in the result folder after the GeoApp run is finished.

The presentation contains a title slide and, for each of the Z-, Y-, and X-Directions, the set amount of 2D image slices is included. Three 2D videos can be started by clicking the corresponding slide. The videos show the whole image data from this axis.



A careful examination of the PowerPoint presentation slides, running as a loop, may reveal previously unknown image artifacts.



2D View as Plot

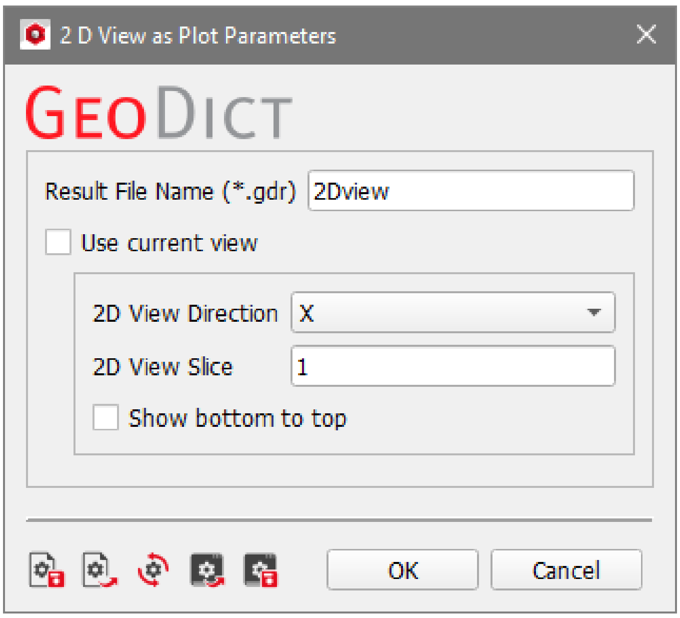
The **2D View as Plot** app saves the 2D visualization of the current structure as a plot. This plot is then contained in a GeoDict result file (*.gdr).

Modules needed to run this GeoApp: GeoDict Base

Clicking **Edit...** opens the **2D View as Plot Parameters** dialog.

Select a **Result File Name** fitting to the current project.

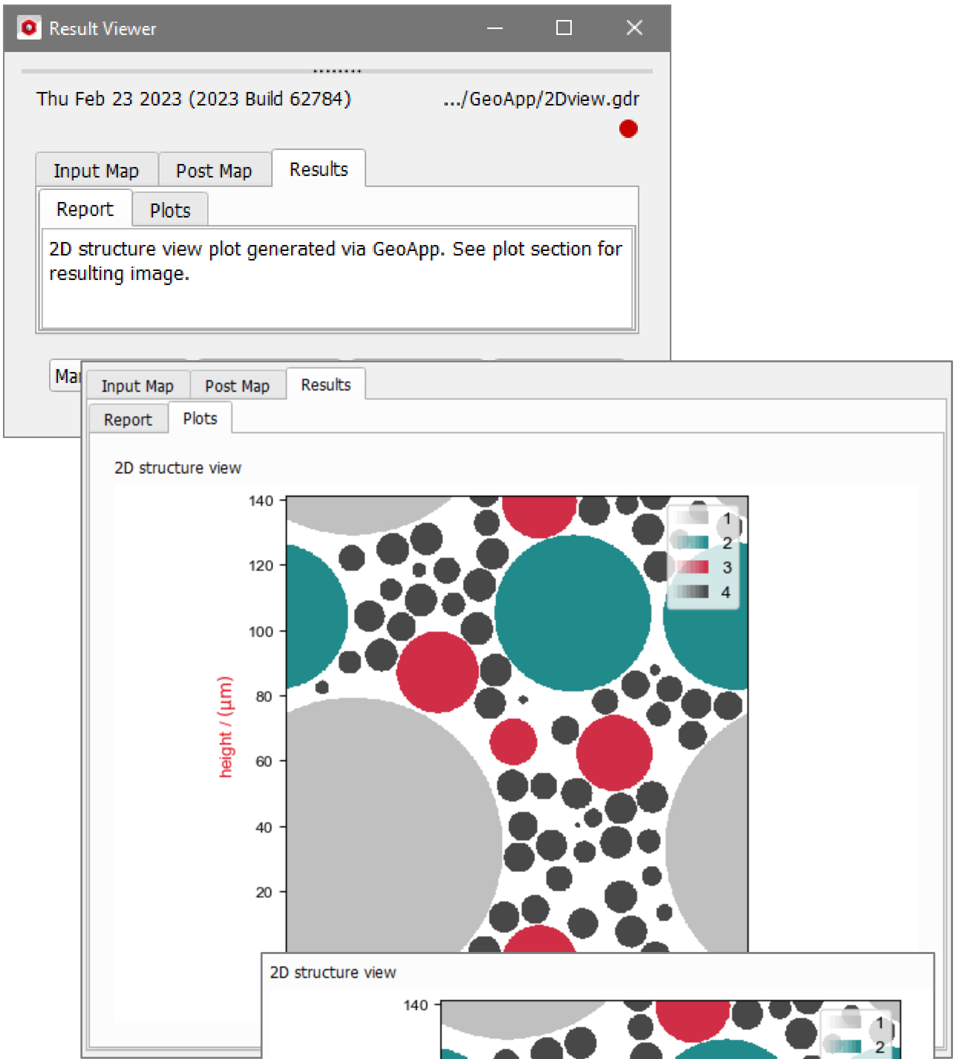
Check **Use Current View** to save a plot of the currently visualized 2D slice and view direction. Otherwise select the **2D View Direction**, the **2D View Slice** and choose whether to **Show bottom to top** or not.

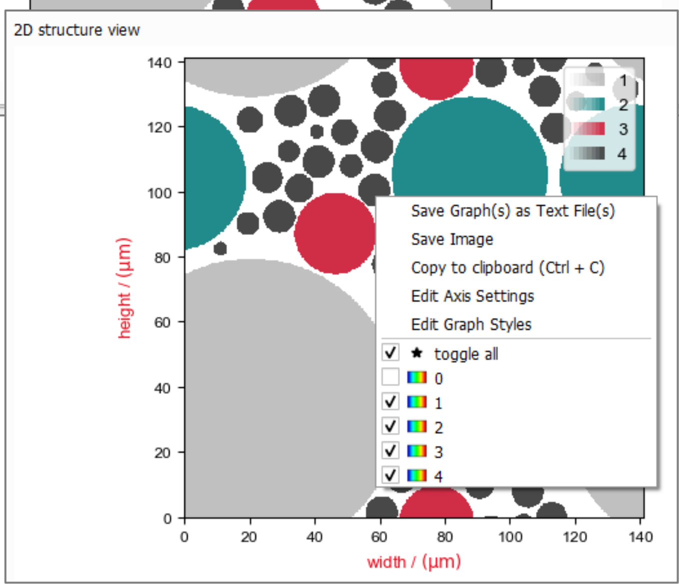


The parameters can be modified if needed. Otherwise, click **OK** to close the dialog, go back to the **GeoApp** section, and click **Run**.

When the image generation finishes, the **Result Viewer** of the result file (*.gdr) opens automatically.

The **Results** → **Report** tab only displays a short report and more graphical information is found in the **Result** → **Plots** tab. There, find the resulting image from the 2D structure view.





Right-clicking in the plot opens a dialog providing several options for post-processing, as described in the Result Viewer handbook of the User Guide.

The image also is saved as *.png in the corresponding result folder.

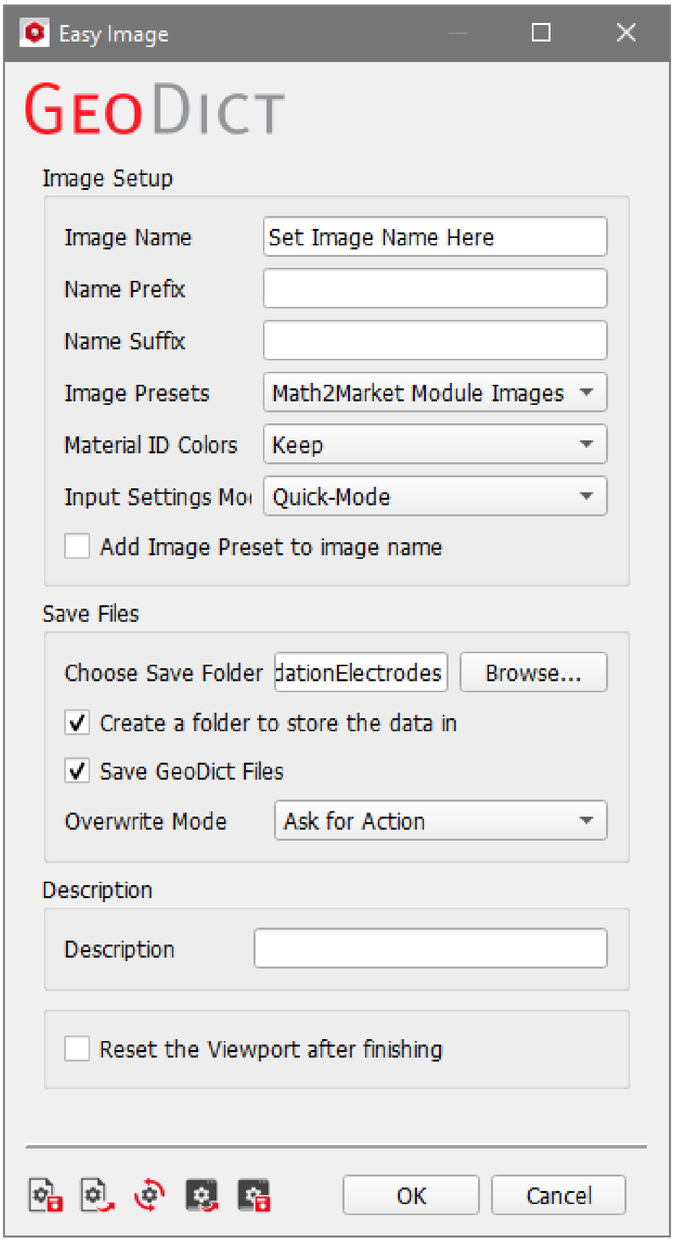
EASY IMAGE

The **Easy Image** app is designed to guide you through the steps of creating various media in an understandable way. It also saves the data needed to recreate the created media material.

Clicking **Run** opens the **3D-Image Report Parameters** dialog.

Modules needed to run this GeoApp: GeoDict Base

Here you set the basic settings, such as file naming, location and image preset selection. Tooltips describe these options in more detail.



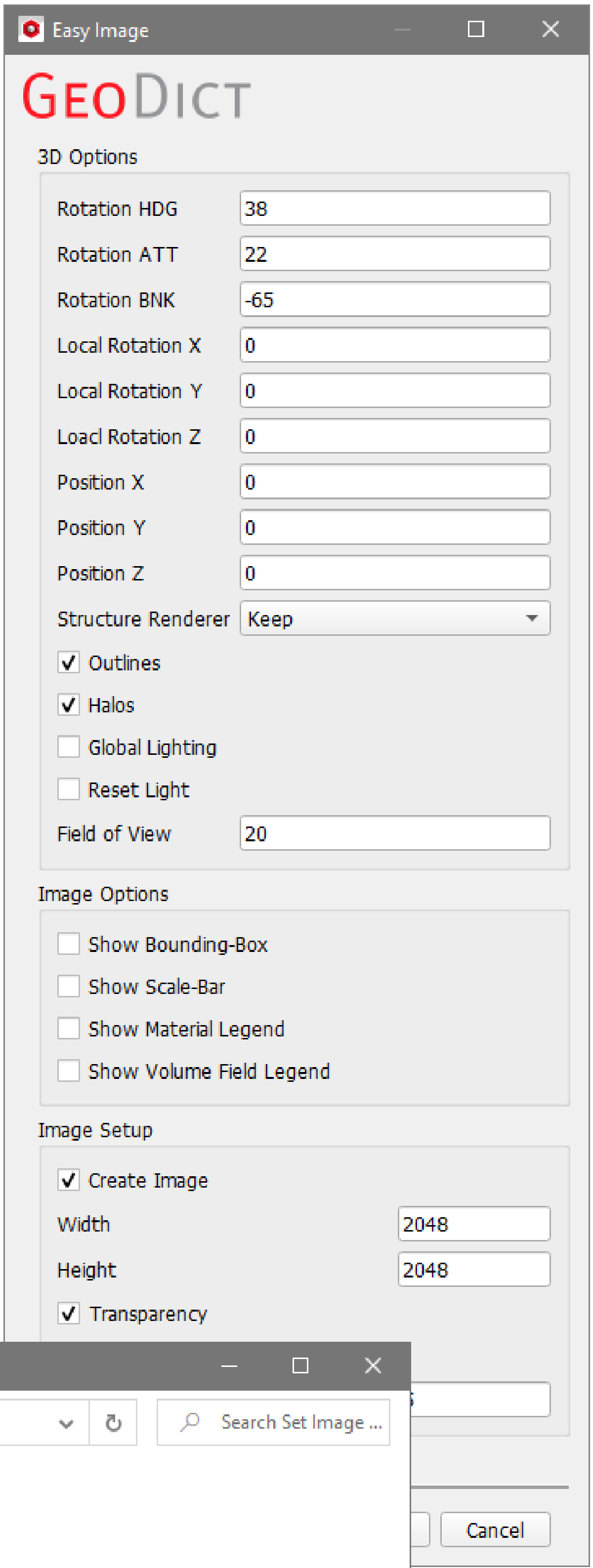
In the image presets, you can also select special modes, such as the split-by material preset. With this preset you can additionally save a video that visualizes the process of splitting.

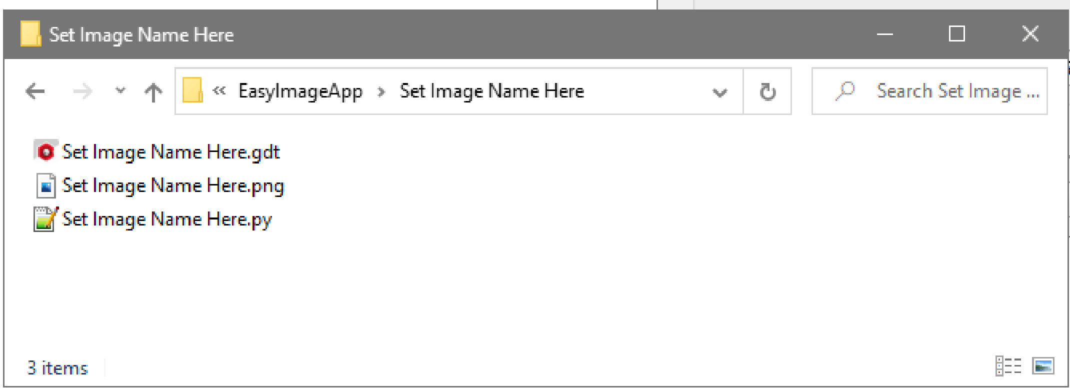
If you want to learn more about this, you can find a video tutorial here.

During image creation, additional dialogs help you to collect and save all necessary GeoDict files. Other dialogs let the user make adjustments to the image setup during image creation. On the right we see for example the Expert Mode dialog, which allows changes to the camera and visualization effects.

At the end of the image creation by the **Easy Image App**, you get a folder with the previously selected **Image Name**. **Name Prefix** and **Name Suffix** are applied only to the files stored in the folder. This way you can quickly and easily create multiple versions in the same place and not have to duplicate the necessary files.

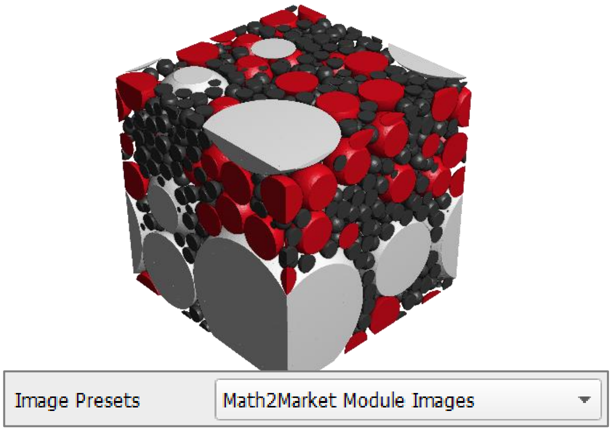
With all files in one place and the image settings saved as a Python macro, images can be reproduced quickly and easily.

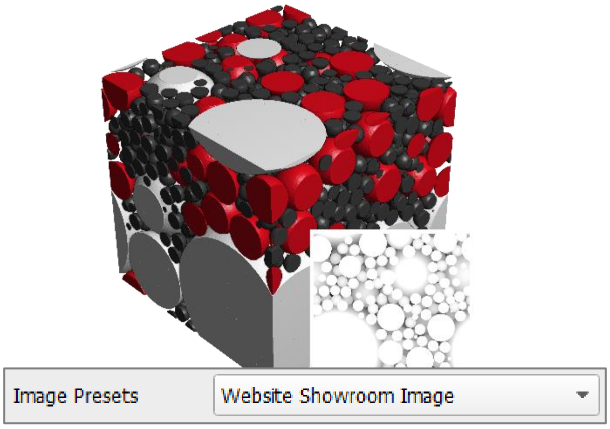


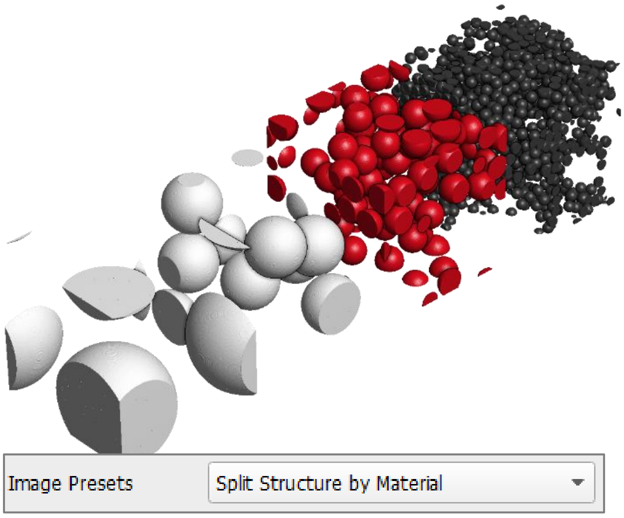


Here, three different **Image Presets** were used for the same structure, available on our website.

The **Material ID colors** were set to **GeoDict Highlight colors**. All other parameters were kept at default settings.



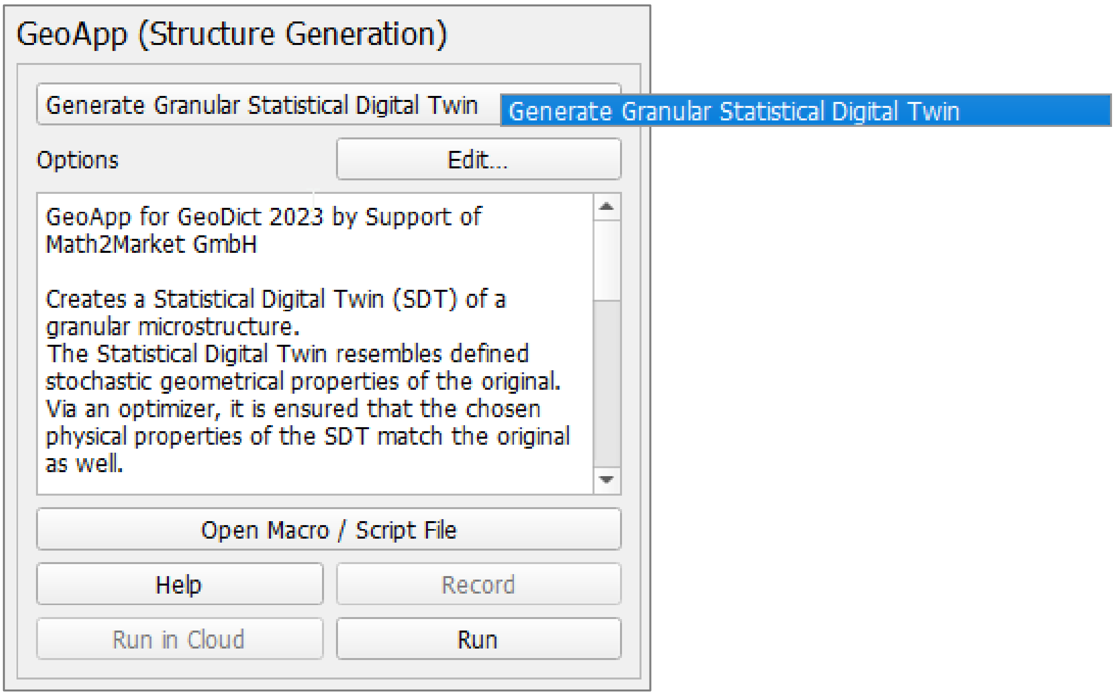




Structure Generation

The **GeoApp (Structure Generation)** section contains the following, selectable from the pull-down menu:

- **Generate Granular Statistical Twin:** creates a Statistical Digital Twin (SDT) of a granular microstructure.



Generate Granular Statistical Twin

The **Statistical Digital Twin** app uses stochastic geometric modelling on a grain-based distance field to generate a digital twin of a reference structure, combined with an optimization algorithm to iterate the twin to the target.

Modules needed to run this GeoApp: GrainGeo + PoroDict, MatDict, GrainFind, FlowDict, DiffuDict (depending on the settings)

Clicking **Edit** opens the **Generate Granular Statistical Digital Twin Parameters** dialog.

Define a **Result File Name** for the result file (*.gdr) and the result folder containing several intermediate information.

Structure Settings:

- Check **Use Current Structure as Reference** if the reference structure is the currently loaded structure in GeoDict. Uncheck to browse for the original structure instead.
- Check **Apply Domain Properties to Statistical Digital Twin**, to take the domain parameters of the reference structure for the twin. Uncheck to define other domain parameters.
- If **Apply Microstructure Properties to Statistical Digital Twin** is checked, the porosity of the reference structure is used. Uncheck to define another porosity.

Criteria to Match: Define the error function components from the list of physical properties. These structure properties will be matched by the twin as good as possible. Note that choosing none will be caught in the GeoApp.

Optimization Components: Define the sets of parameters to be used as optimization variables.

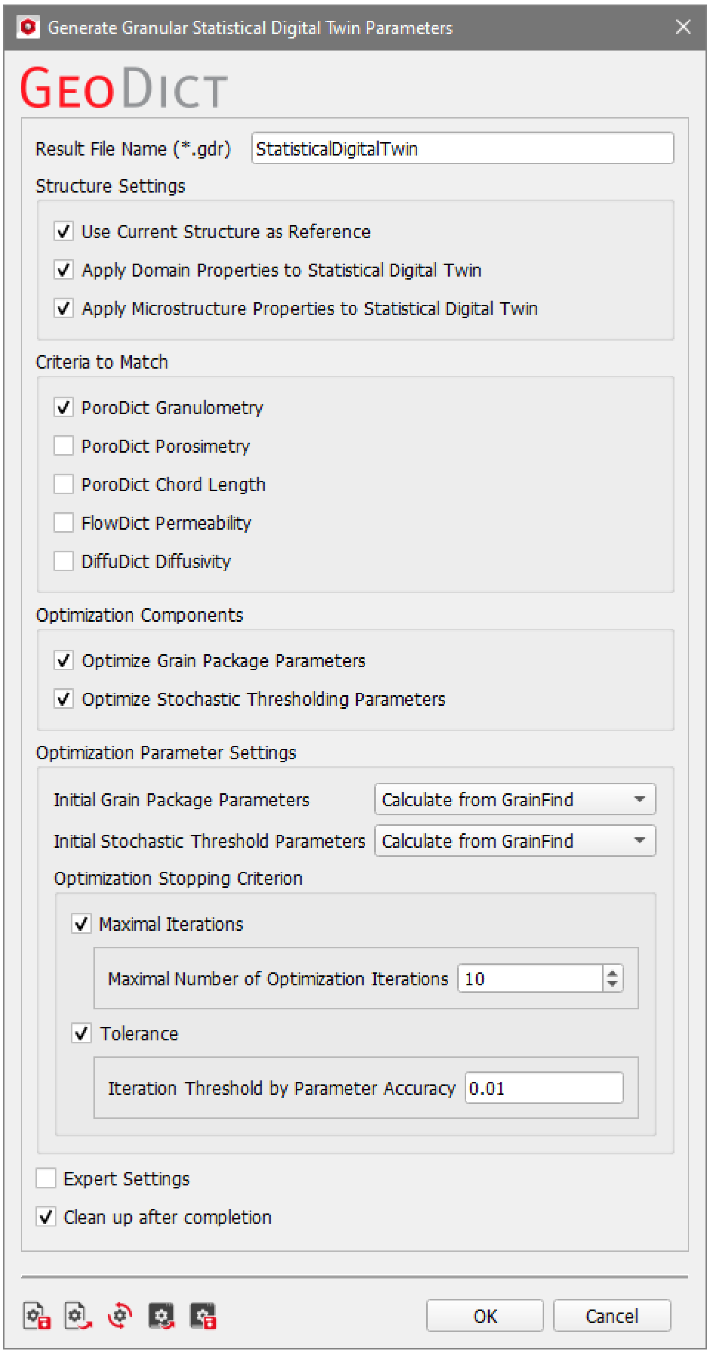
Optimization Parameter Settings: Set the initial parameter values for the optimization variables either manually or let them be determined from the reference structure by using GrainFind. Loading them from existing result files is not included, yet.

Optimization Stopping Criterion: Set the stopping criterion by choosing a maximal number of iterations or set a tolerance accuracy to reach. Note that choosing none or setting maximal iterations to 0 will perform one single run, only.

Expert Settings: These are special development parameter settings:

- **Grain Modeling** targets the initial grain package used for distance field generation. Here, the solid volume percentage, the maximal number of overlap removal steps, and the overlap removal threshold can be specified.
- **Distribution Type**: The generator for the initial grain package uses convex polyhedrons with enclosing ellipsoids. The distribution of these, even though specified with mean value (diaX/Y/Z) and standard deviation (diaSD), can be Gaussian or (more realistic) log-normal.
- **Aim Error**: In case of several percentages of error being fine, a certain amount of the error function can be removed (with zero being the minimum).

If checking **Clean up after completion** all intermediate results are deleted.



Clicking **Run** in the GeoApp section analyzes the reference structure and creates the statistical digital twin.

The *Nelder–Mead* method is a direct search method (based on function comparison) to find the minimum of an objective function in a multidimensional space. The method approximates a local optimum of a problem with n variables when the objective function varies smoothly and is unimodal. The method uses the concept of a simplex, which is a special polytope of n + 1 vertices in n dimensions. In each iteration, it extrapolates the behavior of the objective function measured at each test point in order to find a new test point and to replace one of the old test points with the new one. See the Wikipedia page and [13] for further details.

In each iteration step of the optimization method, a structure is generated based on the optimization parameters. This generation is done in three steps:

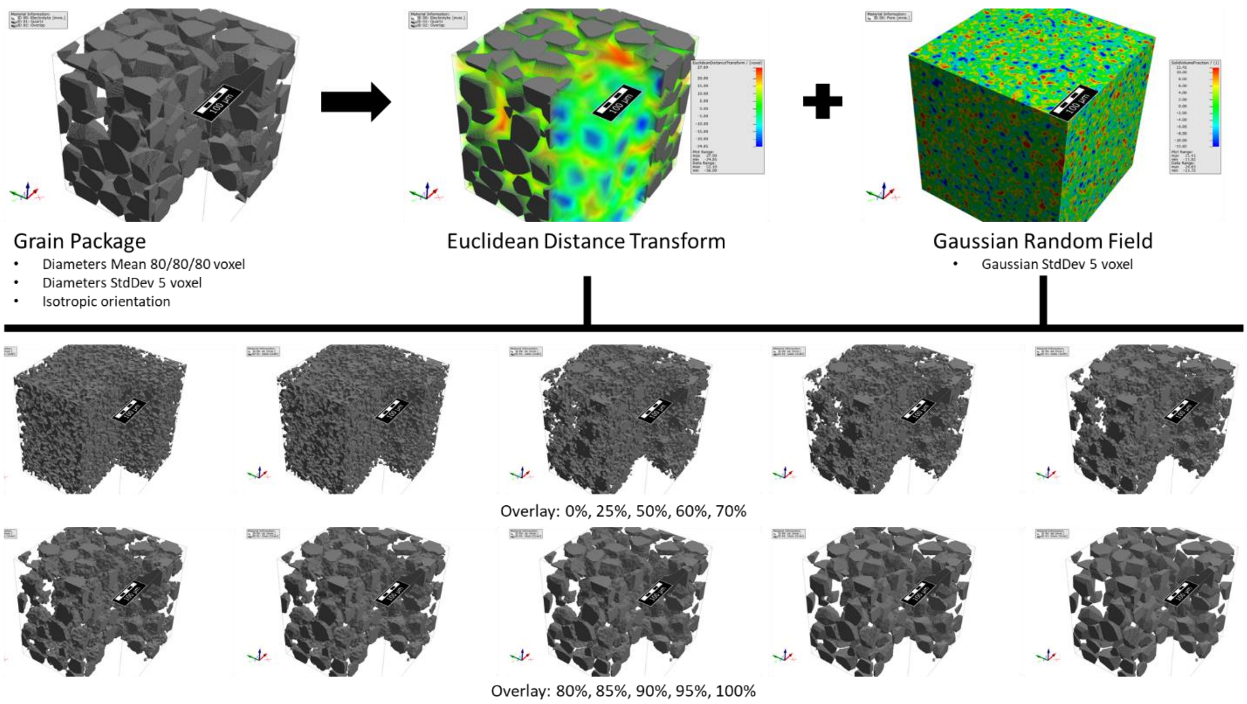
1. A package of grains is generated by GrainGeo **Create Grains**, targeting 50% porosity and removing overlap up to a certain degree. The grain generator uses convex polyhedrons with enclosing ellipsoids and shape orientation tensors based on the reference structure.
2. Based on this grain package, a Euclidean distance field is generated.
3. Using GrainGeo **Stochastic Field Thresholding**, an isotropic Gaussian Random Field is generated, overlayed with the Euclidean distance field and thresholded to reach the targeted porosity.

This results in two sets of parameters used to vary the structure generation:

- Optimize grain package parameters: grain mean values and size distribution standard deviation.
- Optimize stochastic thresholding parameters: overlay strength and standard deviation of the Gaussian random field.

Both sets of parameters can be chosen separately but must remain together as a set.

Overlay of a Gaussian random field with a Euclidean distance map is a new feature of Stochastic Field Thresholding, resulting in the grain package being visible. The figure below illustrates an example of different overlay strengths for a target with 30% solid volume percentage.



After generation, the structure is cleansed to remove artifacts.

In each iteration step of the optimization method, a scalar-valued error function is evaluated. For this, the generated structure is analyzed, and the results are compared with reference values from the reference structure.

The error function is a combination of several modules. Each error function component can be activated or deactivated. Several error measures are available as error function components:

- Using **PoroDict and MatDict Granulometry**:

  After running granulometry, the error in the pore diameter distribution and solid size distribution with respect to the reference structure is evaluated to reach a minimal mean relative difference sum of 5 percentile values each.

- Using **PoroDict Porosimetry**:

  After running porosimetry, the error in pore throat diameter distribution with respect to the reference structure is evaluated, to reach a minimal mean relative difference sum of 5 percentile values.

- Using **PoroDict Chord Length:**

  After calculating the chord length distribution of pore and solid phases, the error with respect to the reference structure is evaluated, to reach a minimal mean relative difference sum of 5 percentile values each.

- Using **FlowDict Permeability:**

  After calculating permeability, relative permeabilities differences can be evaluated.

  Each axis can be chosen separately, only main diagonal elements of the permeability tensor are compared.

- Using **DiffuDict Diffusivity:**

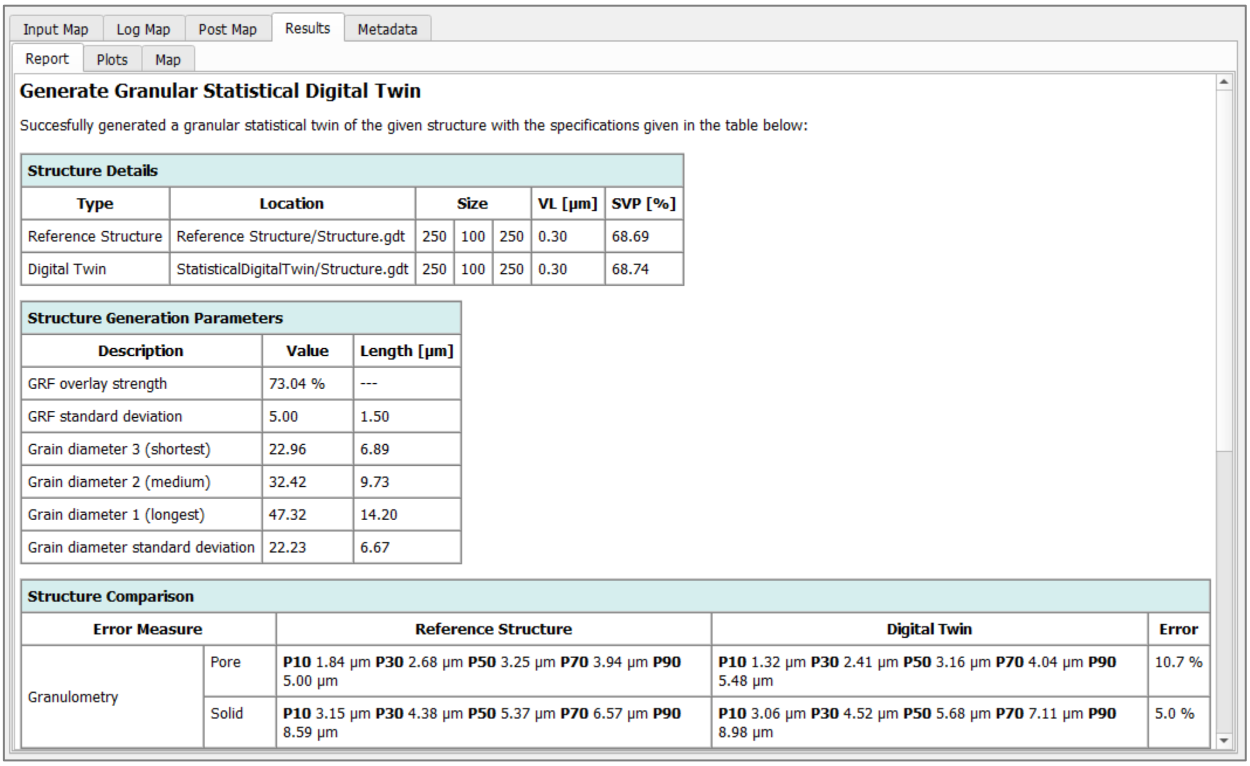
  After calculating the tortuosity from a diffusion experiment, the relative error is added as error component.

  Each axis can be chosen separately, only main diagonal elements of the tortuosity tensor are compared.

Note that choosing more than one error component will probably make the error function not unimodal anymore, resulting in the optimization solution being only a local extrema, not a global solution anymore. Be aware of the choice of initial parameter settings in this case.

Results

After the generation is finished, the corresponding result file is opened in the **Result Viewer**. The report tab provides information about the generation process.



Generate Granular Statistical Digital Twin

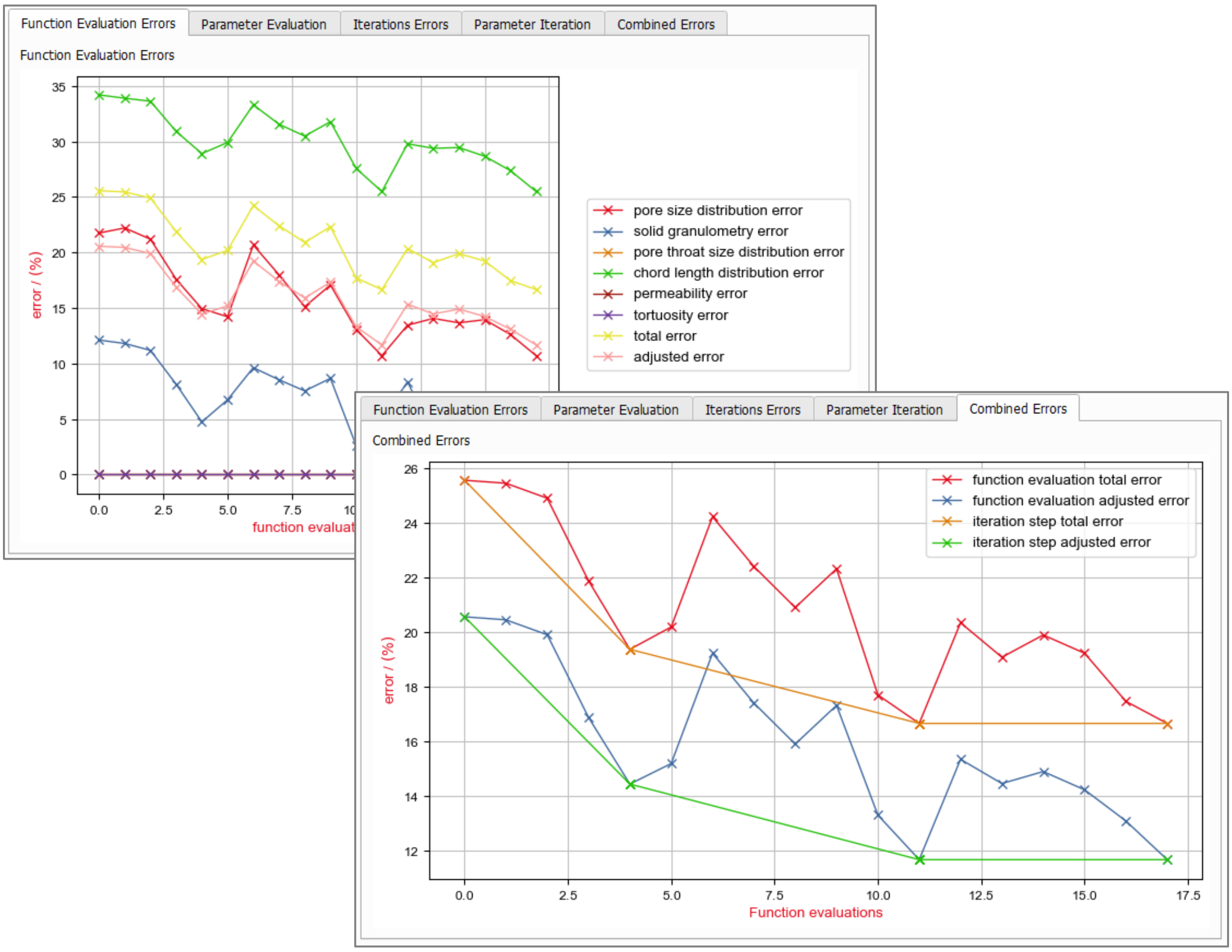
Succesfully generated a granular statistical twin of the given structure with the specifications given in the table below:

Structure Details						
Type	**Location**	**Size**			**VL [µm]**	**SVP [%]**
Reference Structure	Reference Structure/Structure.gdt	250	100	250	0.30	68.69
Digital Twin	StatisticalDigitalTwin/Structure.gdt	250	100	250	0.30	68.74

Structure Generation Parameters		
Description	**Value**	**Length [µm]**
GRF overlay strength	73.04 %	---
GRF standard deviation	5.00	1.50
Grain diameter 3 (shortest)	22.96	6.89
Grain diameter 2 (medium)	32.42	9.73
Grain diameter 1 (longest)	47.32	14.20
Grain diameter standard deviation	22.23	6.67

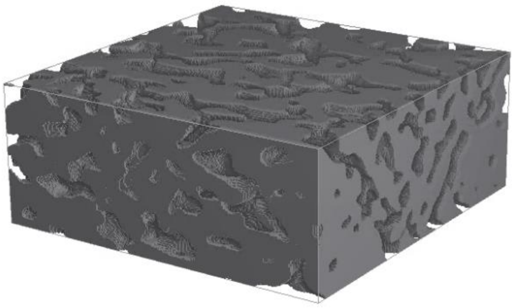
Structure Comparison				
Error Measure		**Reference Structure**	**Digital Twin**	**Error**
Granulometry	Pore	**P10** 1.84 µm **P30** 2.68 µm **P50** 3.25 µm **P70** 3.94 µm **P90** 5.00 µm	**P10** 1.32 µm **P30** 2.41 µm **P50** 3.16 µm **P70** 4.04 µm **P90** 5.48 µm	10.7 %
	Solid	**P10** 3.15 µm **P30** 4.38 µm **P50** 5.37 µm **P70** 6.57 µm **P90** 8.59 µm	**P10** 3.06 µm **P30** 4.52 µm **P50** 5.68 µm **P70** 7.11 µm **P90** 8.98 µm	5.0 %

Additionally, in the **Plots** tab find the **Function Evaluation Errors**, the **Parameter Evaluation**, the **Iteration Errors**, the **Parameter Iteration** and the **Combined Errors** visualized in 2D plots.

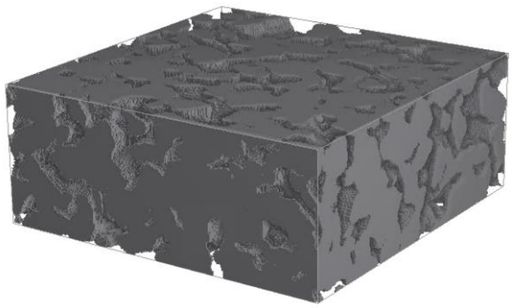


In the result folder, find the following:

- The analysis results of the **Reference Structure**.
- The analysis results of the final **Digital Twin**. Note that this implies the deletion of previous intermediate structures.
- The results generated in every last error function evaluation are contained in the **StructureOptimizationReport.txt**.
- The final statistical digital twin **Structure.gdt**.



Reference structure



Statistical Digital Twin

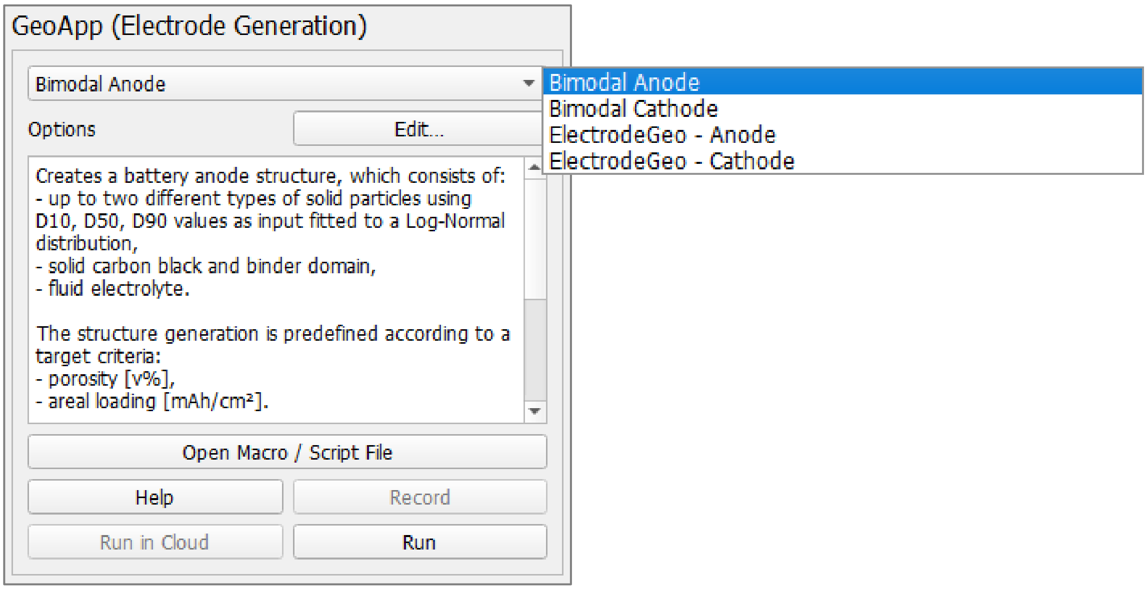
Battery

The GeoApp - **Battery** group contains the **Electrode Generation** GeoApp to create anodes and cathodes for a battery.

Electrode Generation

The **GeoApp (Electrode Generation)** section contains the following, selectable from the pull-down menu:

- **Bimodal Anode:** generates an anode structure, which consists of one or two types of solid elliptical particles with known grain size distributions, solid carbon black and binder domain (CBD) and fluid electrolyte.
- **Bimodal Cathode**: generates a cathode structure, which consists of one or two types of solid spherical particles with known grain size distributions, solid carbon black and binder domain (CBD) and fluid electrolyte.
- **ElectrodeGeo - Anode:** generates an anode from different materials.
- **ElectrodeGeo - Cathode:** generates a cathode from different materials.

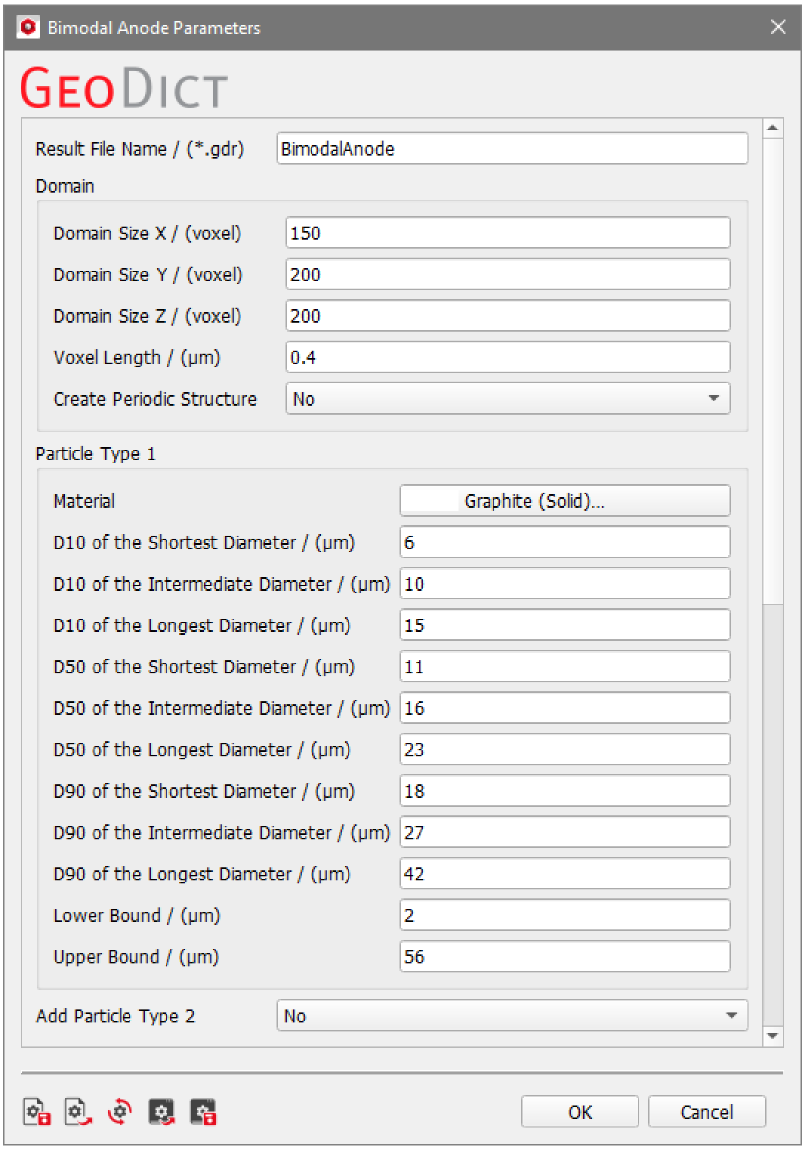


Bimodal Anode

The **Bimodal Anode** generates a battery anode structure, which consists of up to two types of solid elliptical particles, solid carbon black and binder domain (CBD) and fluid electrolyte – the constituent materials can be selected from the material database. The recipe of the anode considers the grain size distribution of the particles, the ratio between particle types, binder mass percentage and target porosity or target areal loading (mAh/cm²) of the anode.

Modules needed to run this GeoApp:
GrainGeo

Clicking **Edit...** opens the **Bimodal Anode Parameters** dialog.

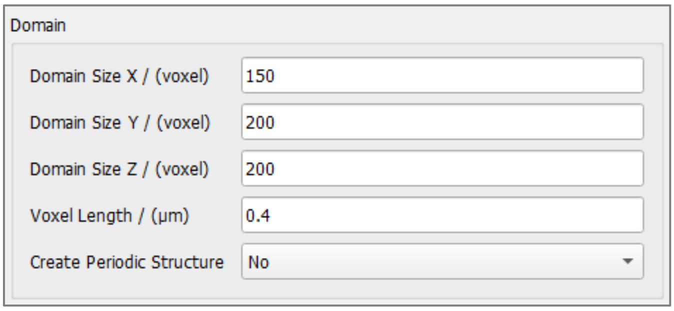


Enter a **Result File Name** for the bimodal anode.

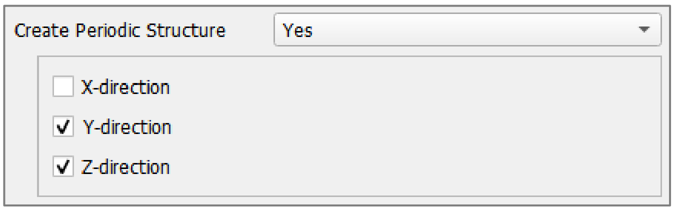
The anode parameters are organized into six groups.

Domain

Set the **Domain Size** in voxels for the X-, Y- and Z-direction and enter a **Voxel Length**.



The structures periodicity can be adjusted in each of the three directions.

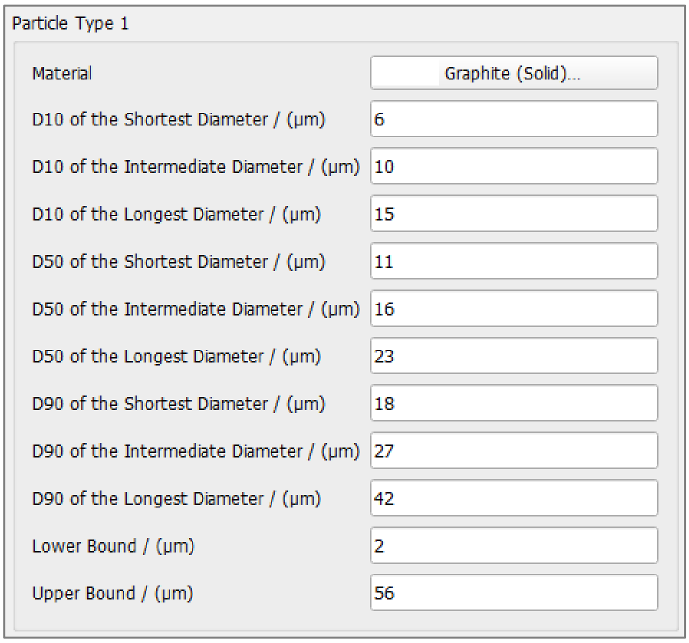


Particle Type 1

Select the **Material** for the active material for particle type 1.

Define the diameter distribution with D-values. **D-values** are specified separately for shortest, intermediate, and longest axis of particles: **D-10**, **D-50**, **D-90,** and fitted to Log-Normal distribution.

The **Lower** and **Upper Bounds** are also fitted to Log-Normal distribution but assigned once for all diameters within one particle type. They can be set as **D1-** and **D99**-values of corresponding measurements.

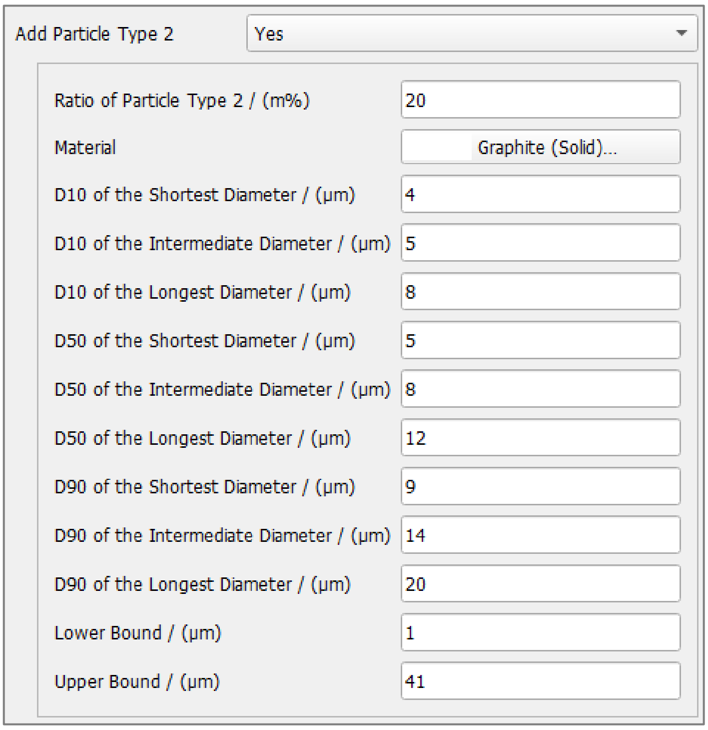


Add Particle Type 2

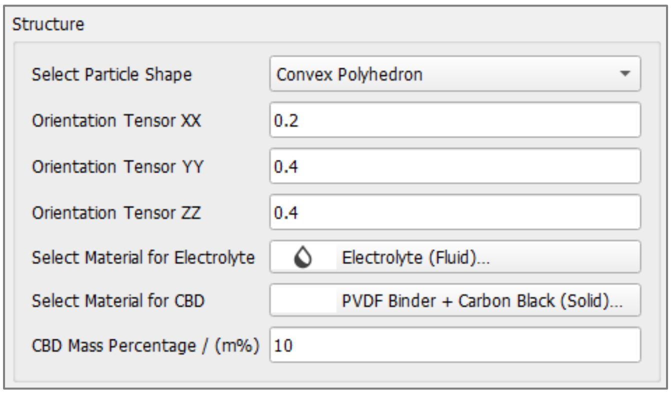
With **Add Particle Type 2**, a second active material can be added to the structure.

If **No** is used (default), an anode structure with one active material type is created.

If **Yes** is selected, the macro enables creating a bimodal structure, where **Ratio of Particle Type 2** is defined in **m%**, and grain size distribution can be predefined using their own **D-values**.



Structure

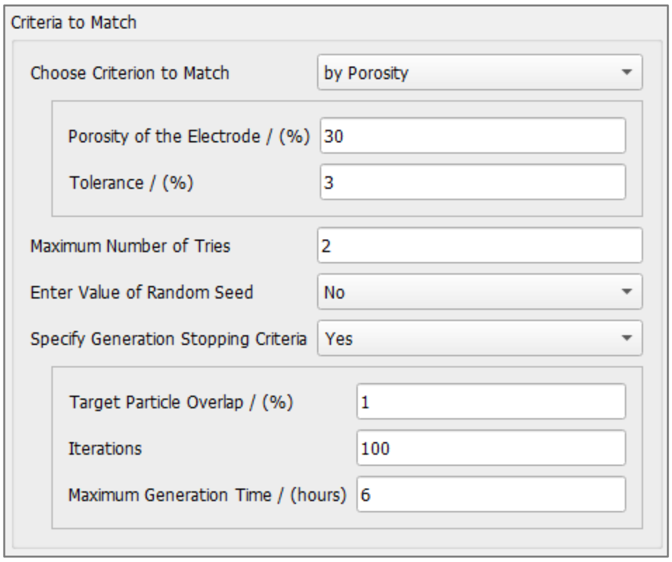


All particles in the structure can be generated either with **Ellipsoids** or with **Convex Polyhedrons** based on ellipsoids.

The **Orientation** of particles is specified by the main diagonal tensor orientation in the global coordinate system XYZ. Corresponding values of **Orientation Tensor XX**, **YY** or **ZZ** are set as the probabilities within ranges between 0 (a low probability) and 1 (a high probability). The sum of all three tensor components is 1.

Additionally, **Select Materials for Electrolyte** and **CBD** and define the **CBD Mass Percentage** in m%.

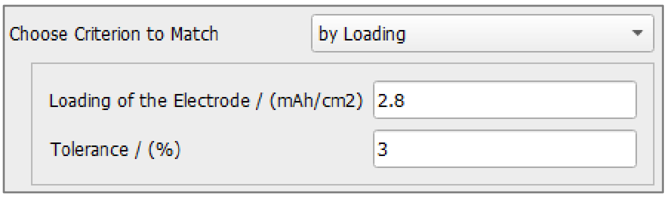
Criteria to Match



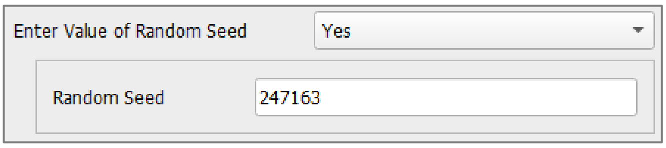
In addition, you can **Choose the Criterion to Match**. The default criterion is **by Porosity**, which allows to define the desired porosity of the electrode.

As an alternative, **by Loading** allows to define the desired areal loading of the electrode in mAh/cm^2.

In both cases, structure generation is repeated within **Maximum Number of Tries** until the desired porosity or areal loading is reached within a given **Tolerance** in **%**. If the target porosity or loading was not reached, GeoDict saves and displays the result of the last generation try.

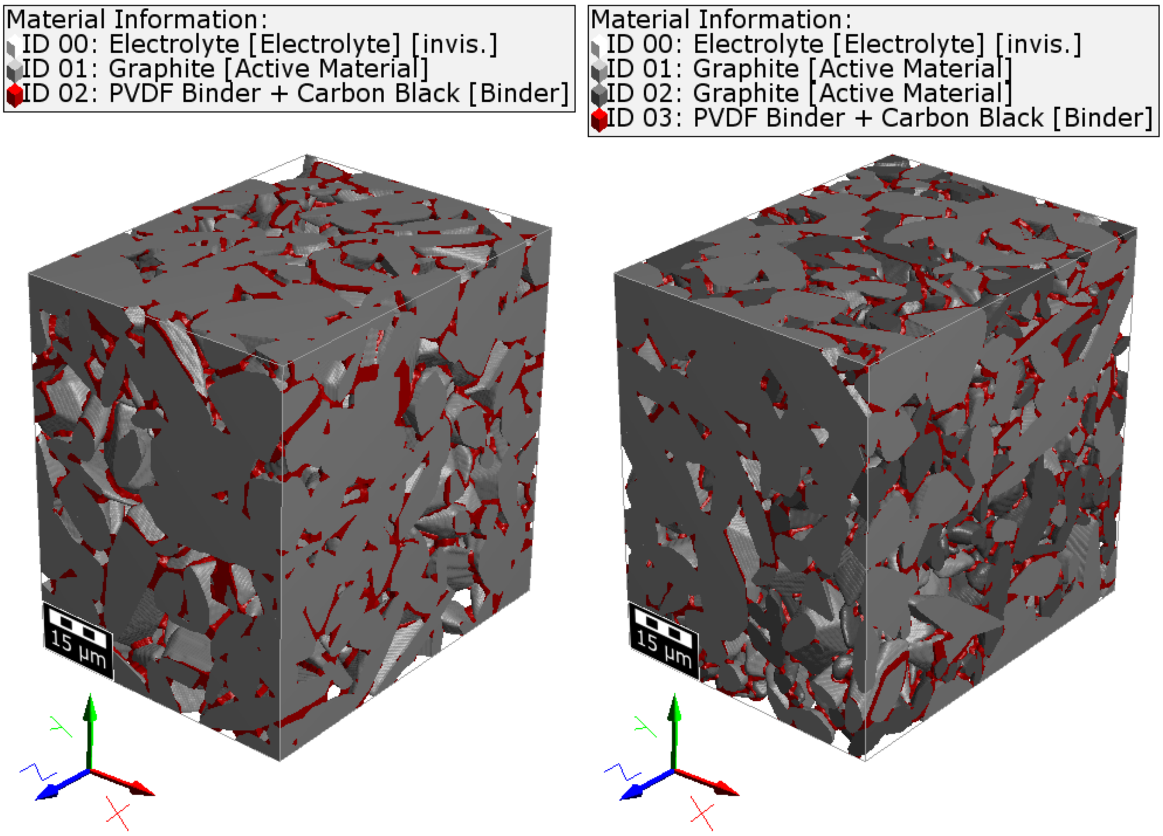


Enter Value of Random Seed: By default, the seed for generating the structure will be randomly chosen. If you choose **Yes**, you can enter a random seed manually. Entering the same **Random Seed** will result in an identical structure.



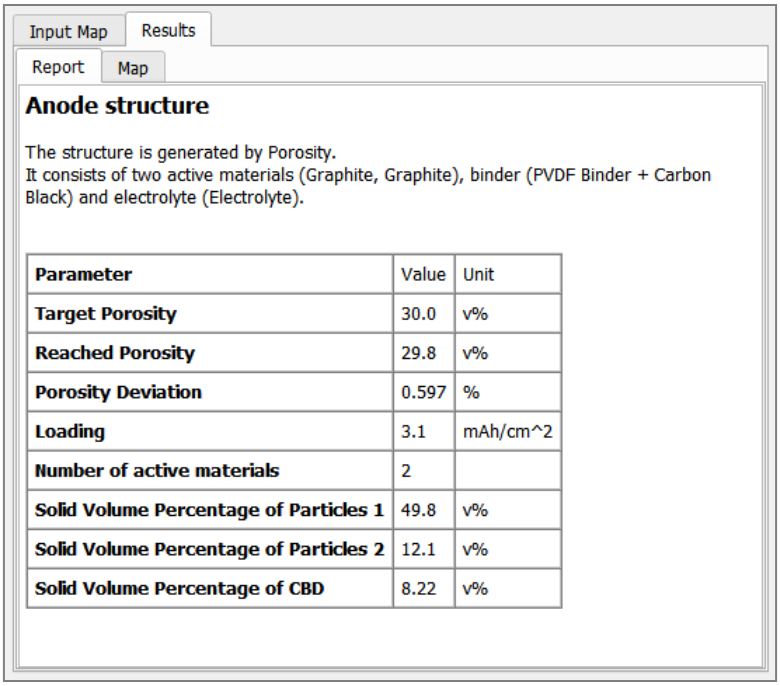
The parameters which **Specify Generation Stopping Criteria** for the particles creation are **Target Particle Overlap**, **Iterations** and **Maximum Generation Time**. They are active by default and can be changed if needed.

Clicking **Run** creates the anode.



In the figure above, on the left, a monomodal battery anode is shown, generated with the default settings. On the right, a bimodal battery anode is shown generated with the default settings.

The result file is opened in the **Result Viewer** when the generation is finished and the **Report** tab provides information about the structure generation.



Anode structure

The structure is generated by Porosity.
It consists of two active materials (Graphite, Graphite), binder (PVDF Binder + Carbon Black) and electrolyte (Electrolyte).

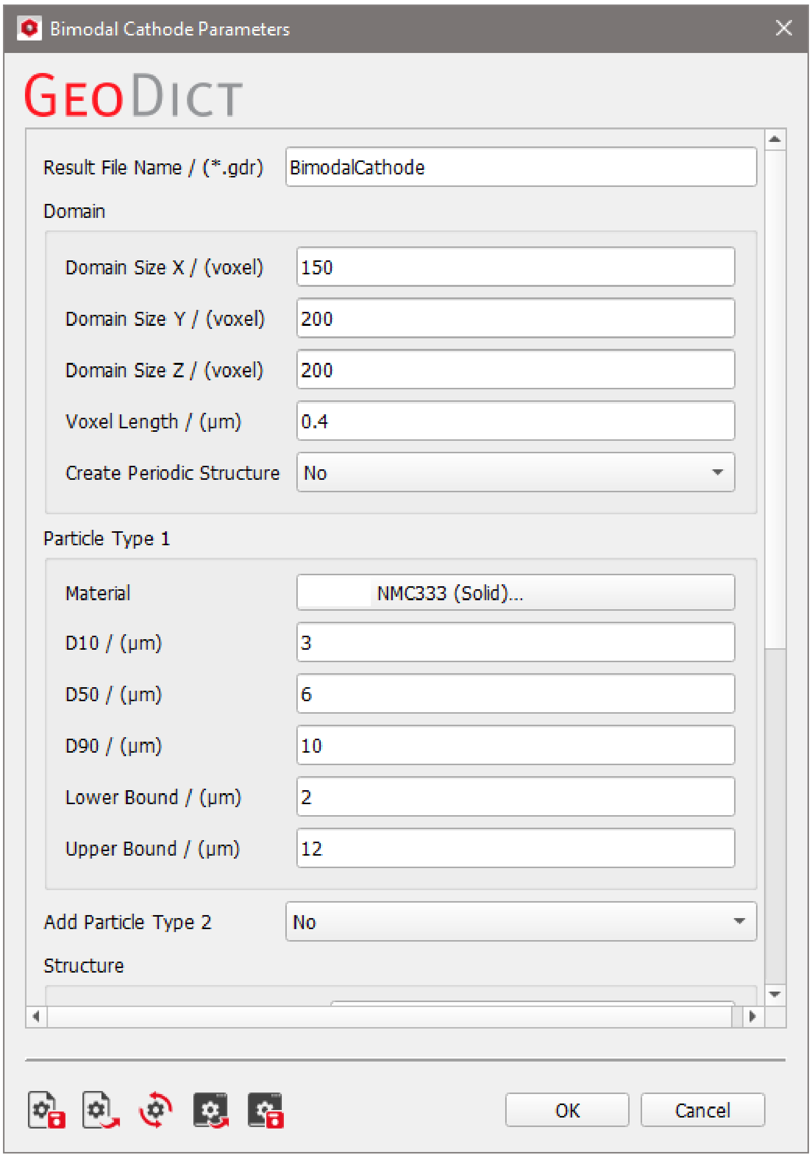
Parameter	Value	Unit
Target Porosity	30.0	v%
Reached Porosity	29.8	v%
Porosity Deviation	0.597	%
Loading	3.1	mAh/cm^2
Number of active materials	2	
Solid Volume Percentage of Particles 1	49.8	v%
Solid Volume Percentage of Particles 2	12.1	v%
Solid Volume Percentage of CBD	8.22	v%

BIMODAL CATHODE

The **Bimodal Cathode** generates a battery cathode structure, which consists of up to two types of solid spherical particles, solid carbon black and binder domain (CBD) and fluid electrolyte – the constituent materials can be selected from the material database. The recipe of the cathode considers the grain size distribution of the particles, the ratio between particle types, binder mass percentage and target porosity or target areal loading (mAh/cm²) of the cathode.

Modules needed to run this GeoApp:
GrainGeo

Clicking **Edit...** opens the **Bimodal Cathode Parameters** dialog.



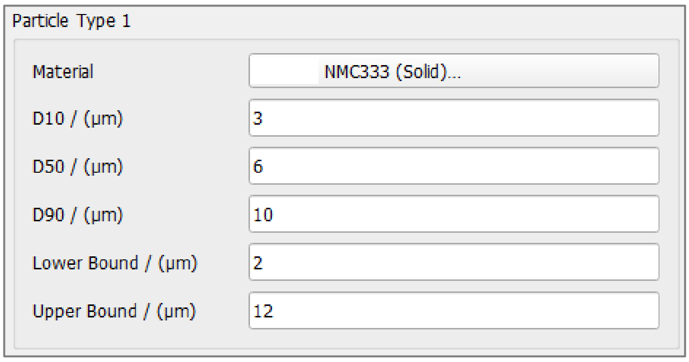
Enter a **Result File Name** for the cathode.

The cathode parameters are organized into six groups. For the **Domain** and **Criteria to Match** parameter groups refer to the Bimodal Anode described on page 21.

Particle Type 1

Select the **Material** for the active material for particle type 1.

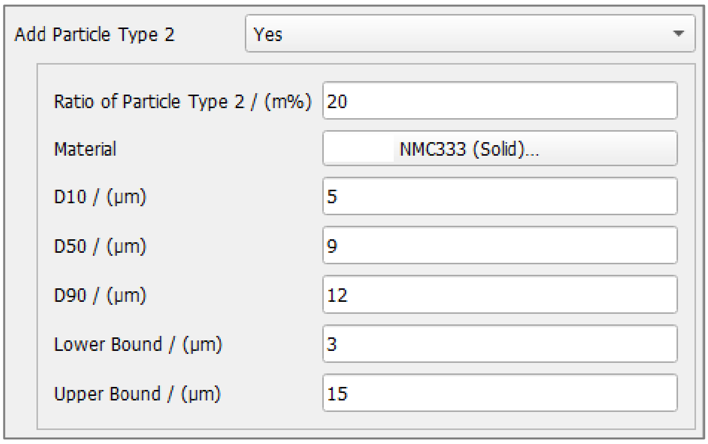
The **D-values D-10**, **D-50**, **D-90**, **Lower Bound** and **Upper Bound**, and fitted to Log-Normal distribution. The **Lower** and **Upper Bounds** can be set as **D1**- and **D99**-values of corresponding measurements.



Add Particle Type 2

With **Add Particle Type 2**, a second active material can be added to the structure. If **No** is selected (default), a cathode structure with one active material type is created.

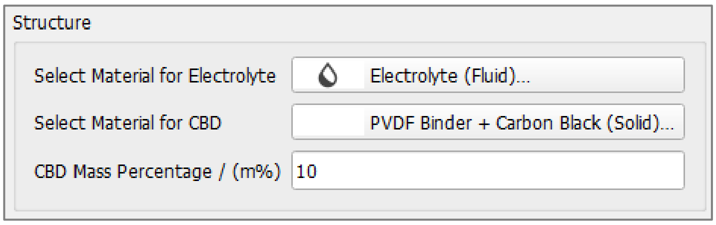
If **Yes** is selected, the macro enables creating a bimodal structure, where **Ratio of Particle Type 2** is defined in **m%**, and grain size distribution can be predefined using their own **D-values**.

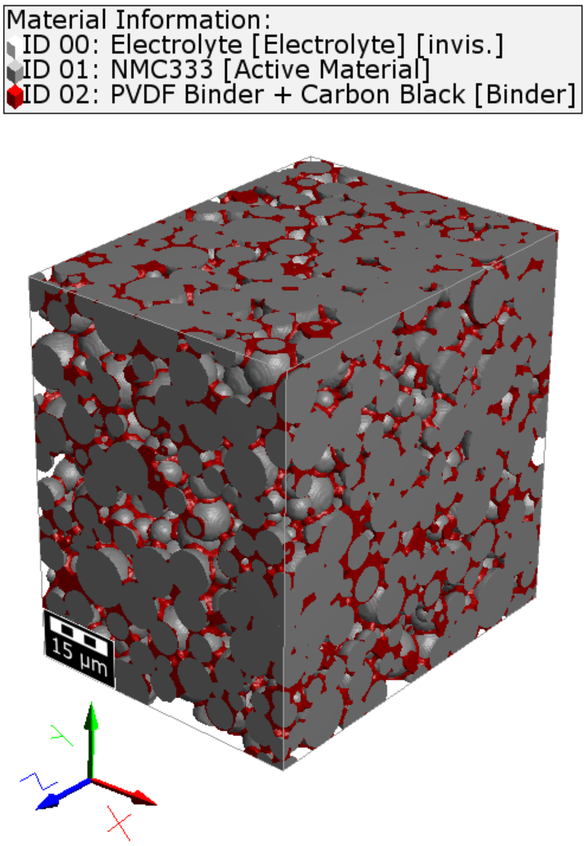


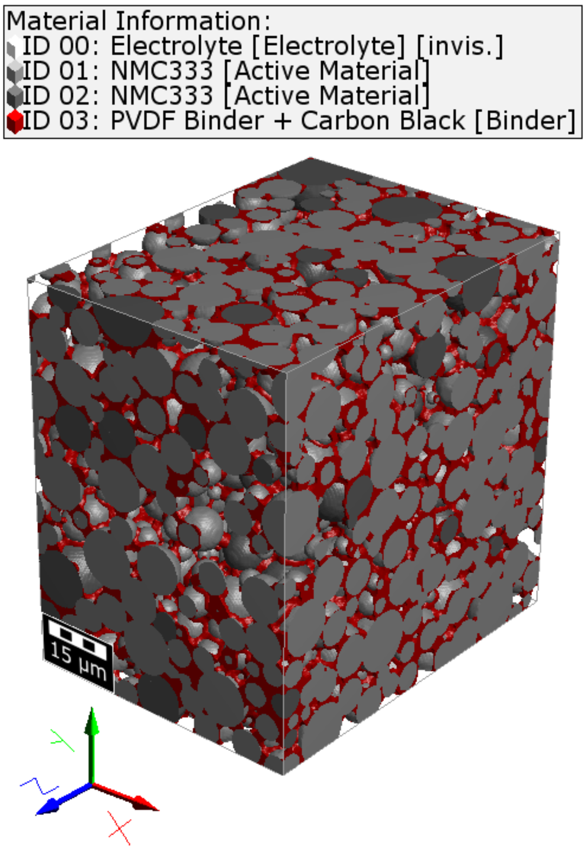
Structure

All particles in the structure will be spherical grains.

Select Materials for Electrolyte and **CBD** and define the **CBD Mass Percentage** in m%.







In the figure above, on the left, a monomodal battery cathode is shown, generated with the default settings. On the right, a bimodal battery cathode is shown generated with the default settings.

The result file is opened in the **Result Viewer** when the generation is finished, and the **Report** tab provides information about the structure generation.

Input Map | Results

Report | Map

Cathode structure

The structure is generated by Porosity.
It consists of two active materials (NMC333, NMC333), binder (PVDF Binder + Carbon Black) and electrolyte (Electrolyte).

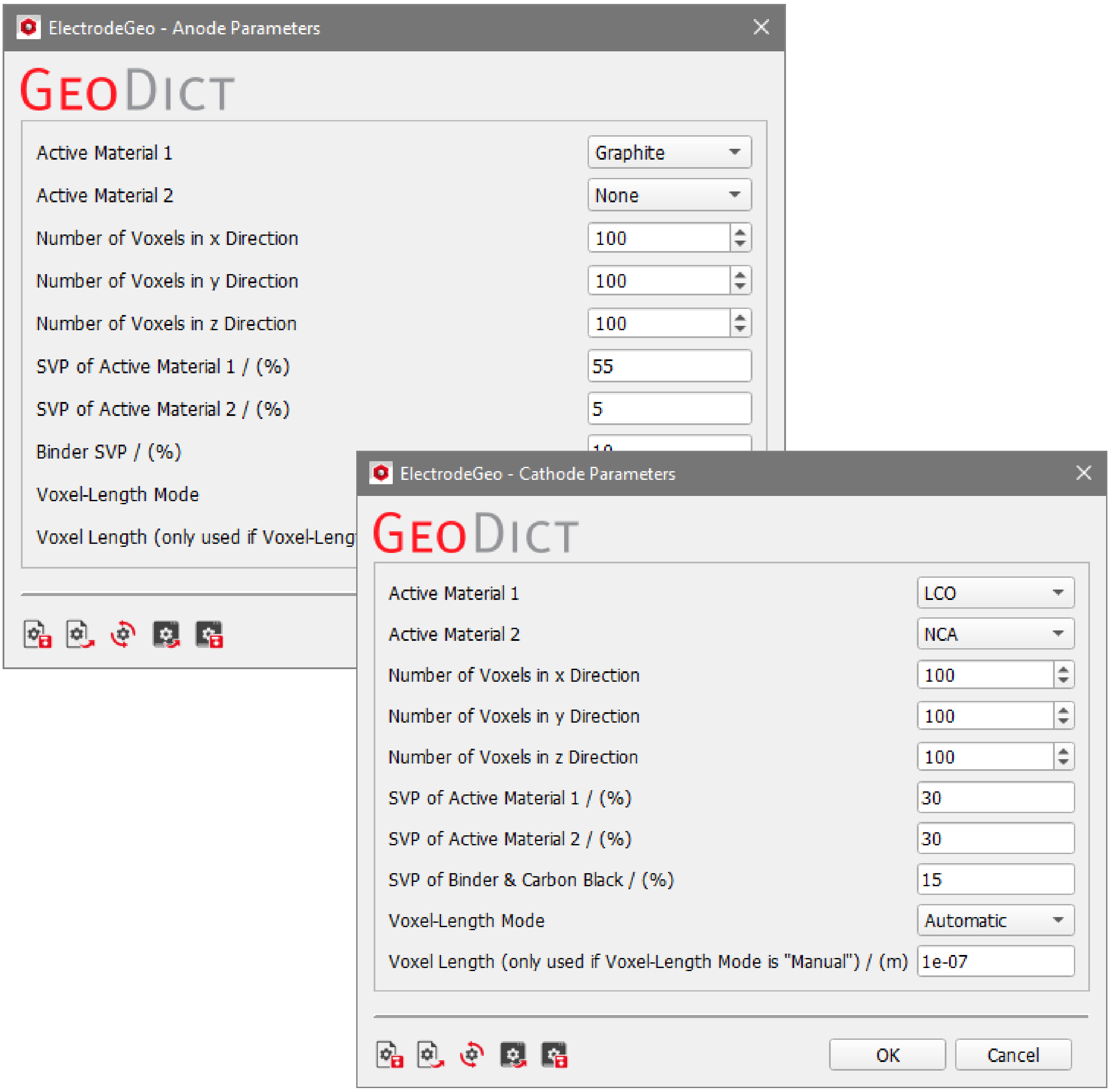
Parameter	Value	Unit
Target Porosity	30.0	v%
Reached Porosity	30.0	v%
Porosity Deviation	0.0394	%
Loading	3.15	mAh/cm^2
Number of active materials	2	
Solid Volume Percentage of Particles 1	44.1	v%
Solid Volume Percentage of Particles 2	10.9	v%
Solid Volume Percentage of CBD	14.9	v%

ElectrodeGeo - Anode and Cathode

The **ElectrodeGeo** apps generate anode and cathode according to the given materials and solid volume percentages.

Modules needed to run this GeoApp:
GrainGeo

Clicking **Edit...** opens the **ElectrodeGeo Parameters** dialog.



For both electrodes two active materials can be set. If only one active material is needed, set the second material to **None**.

For the cathode choose from the materials LCO, LMO, NCA and NMC.

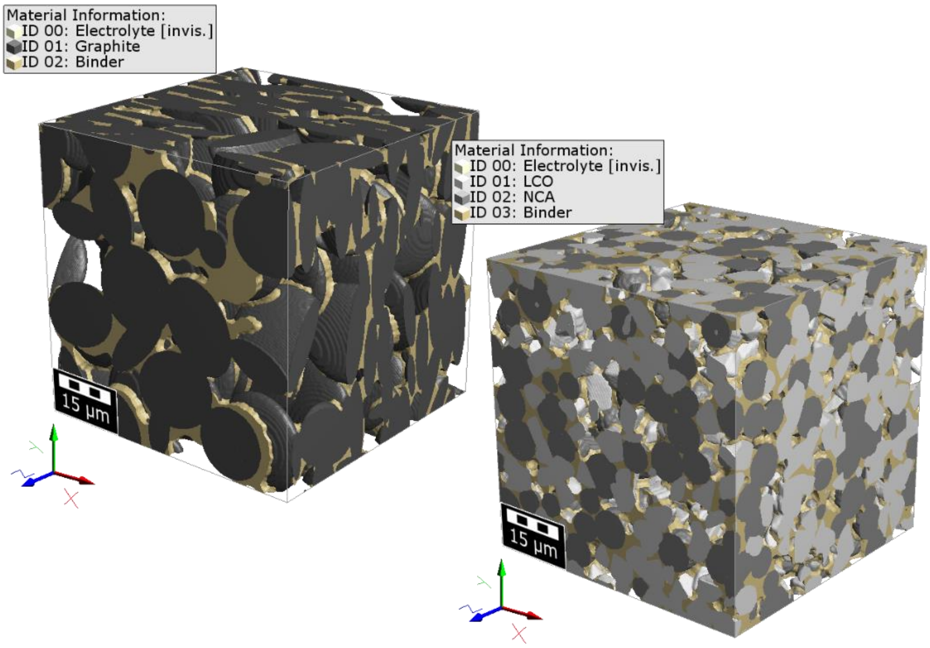
For the anode select between Graphite, Si and LTO.

Define the volume dimensions as **Number of Voxels** in the three directions.

Determine the solid volume percentages (**SVP**) for the active materials and the binder.

The voxel length can either be given manually or it can be set automatically fitting the other parameters.

Clicking **Run** creates the respective electrode.



In the figure above, on the left, an anode is shown, generated with the default settings. On the right, a cathode is shown generated with the default settings.

Composites

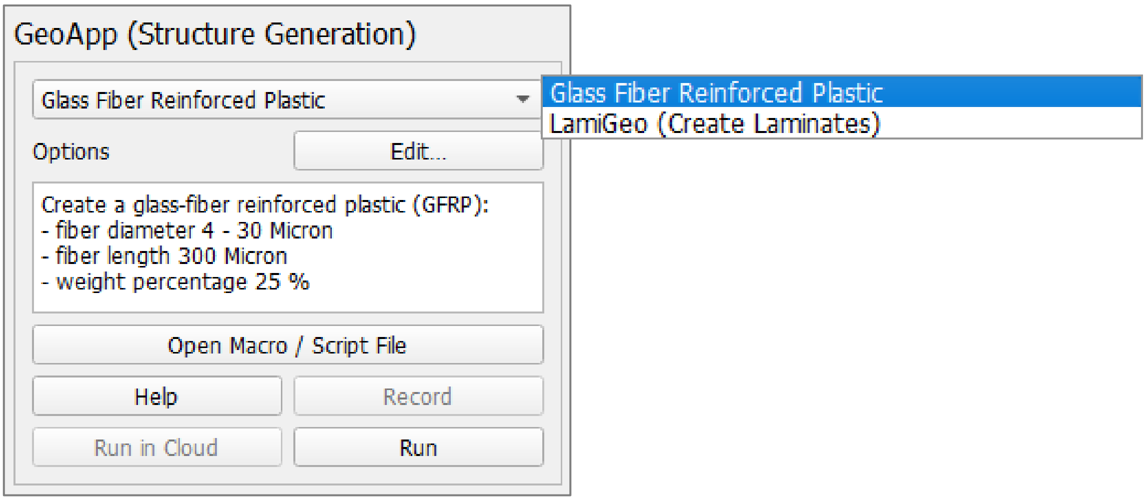
One GeoApp of the **Composite** group is shipped with GeoDict:

- Create composite structures with the **Structure Generation** apps.

Structure Generation

The **GeoApp (Structure Generation)** section contains the following, selectable from the pull-down menu:

- **Glass Fiber Reinforced Plastic:** generates a predefined fiber structure.
- **LamiGeo**: generates a model of a multi-layer laminate composite.

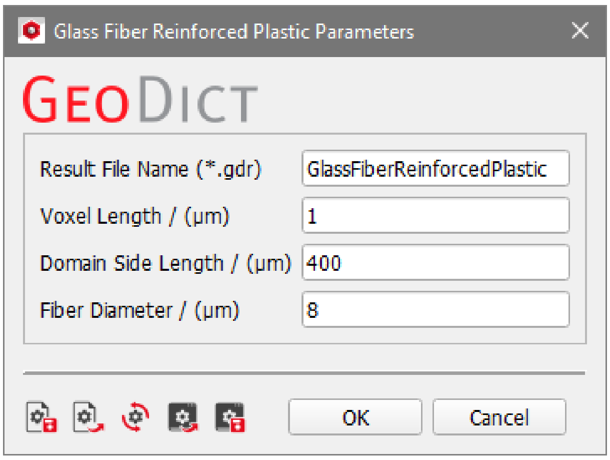


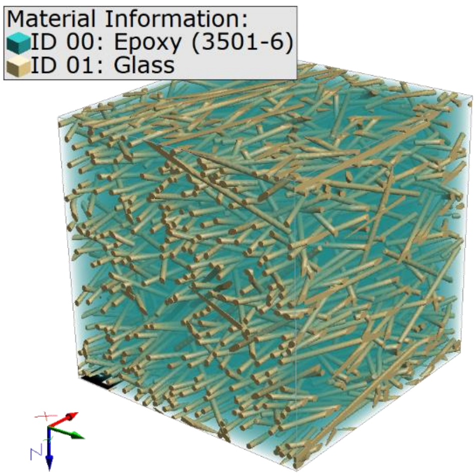
Glass Fiber Reinforced Plastic

The **Glass Fiber Reinforced Plastic** app generates a predefined fiber structure.

Modules needed to run this GeoApp:
FiberGeo

Clicking **Edit...** opens the **Glass Fiber Reinforced Plastic Parameters** dialog.

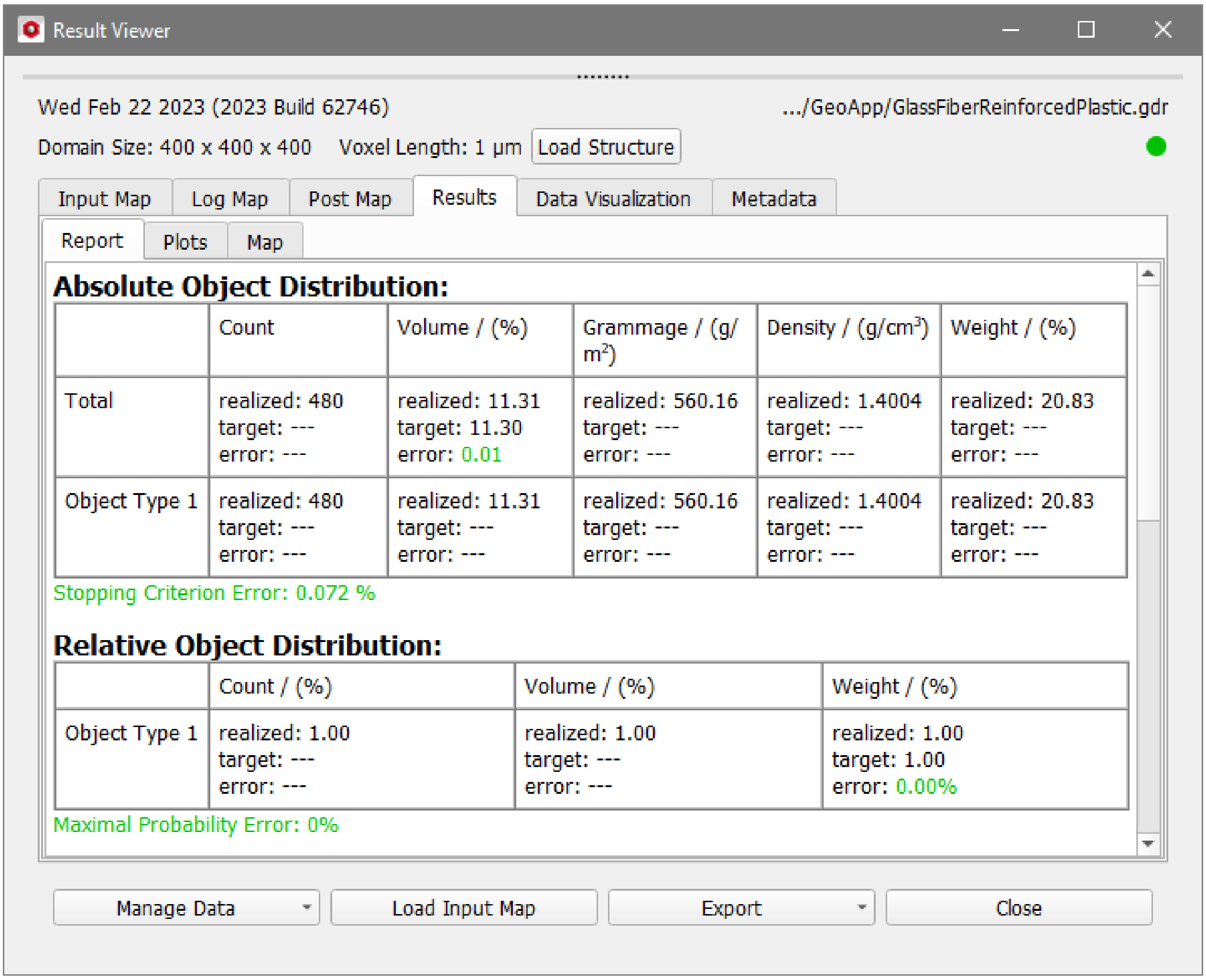




Define the **Result File Name**, the **Voxel Length**, the **Domain Length** for all three dimensions and the **Fiber Diameter**.

Clicking **Run** creates the plastic structure.

When the structure generation finishes, the **Result Viewer** of the FiberGeo result file (*.gdr) opens automatically.

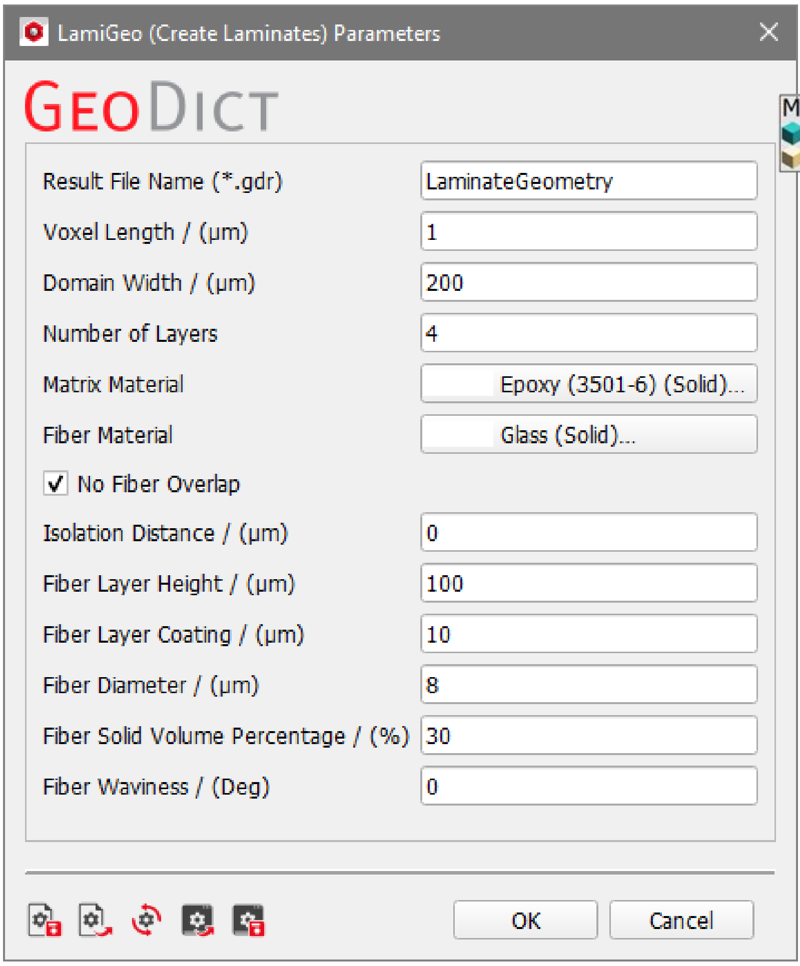


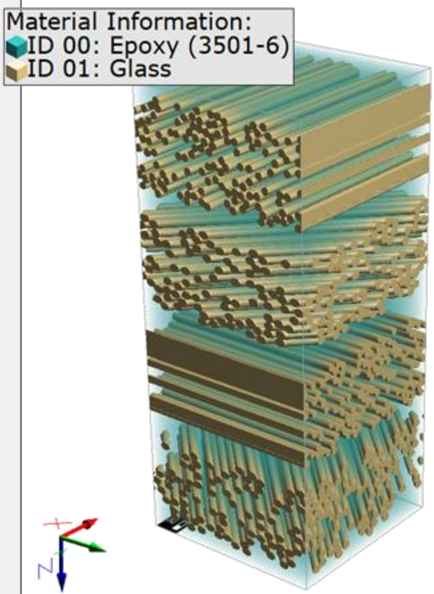
LamiGeo (Create Laminates)

The **LamiGeo** app generates a laminate structure.

Modules needed to run this GeoApp:
FiberGeo

Clicking **Edit...** opens the **LamiGeo Parameters** dialog.





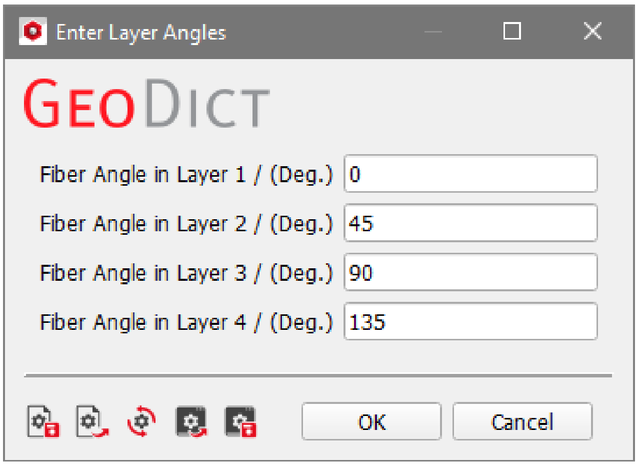
Define the following parameters:

- **Result File Name**,
- **Voxel Length**,
- **Domain Width** in X- and Y-direction,
- **Number of Layers**,
- **Matrix Material**,
- **Fiber Material**,
- if the overlap should be removed (**No Fiber Overlap**) or not,
- **Isolation Distance**, in case the overlap is removed,
- **Fiber Layer Height** for each layer,
- how much **Fiber Layer Coating** should be generated in Z-direction around the fibers,

- **Fiber Diameter**,
- **Fiber Solid Volume Percentage** within the layers without the coating,
- and the **Fiber Waviness** as angle around the fiber orientation direction, where positive values lead to slightly curved fibers.

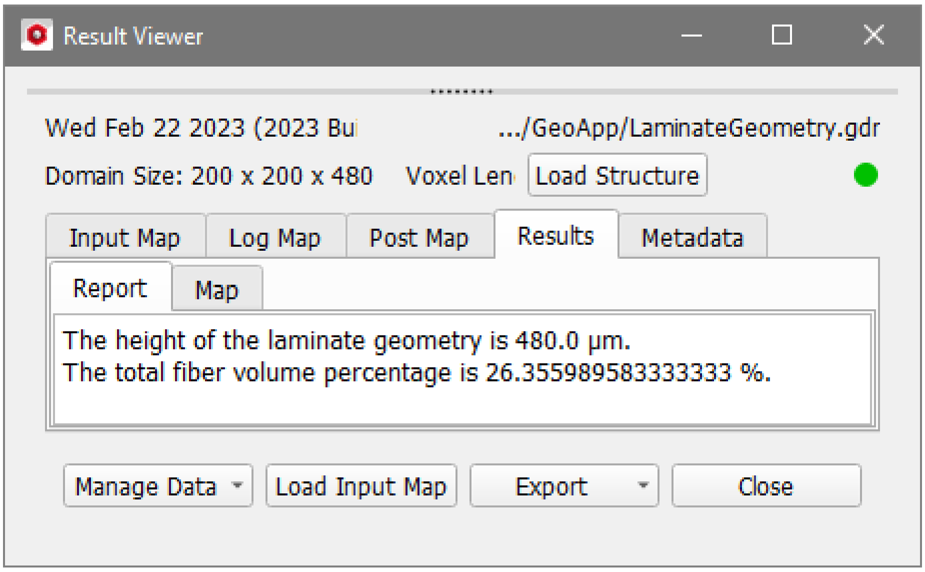
Clicking **Run** creates the plastic structure.

Then, the **Enter Layer Angles** dialog appears where the **Fiber Angles** in the defined layers can be given.



When the structure generation finishes, the **Result Viewer** of the result file (*.gdr) opens automatically.

The **Results** → **Report** tab displays a short report about the resulting structure.



Digital Rock Physics (DRP)

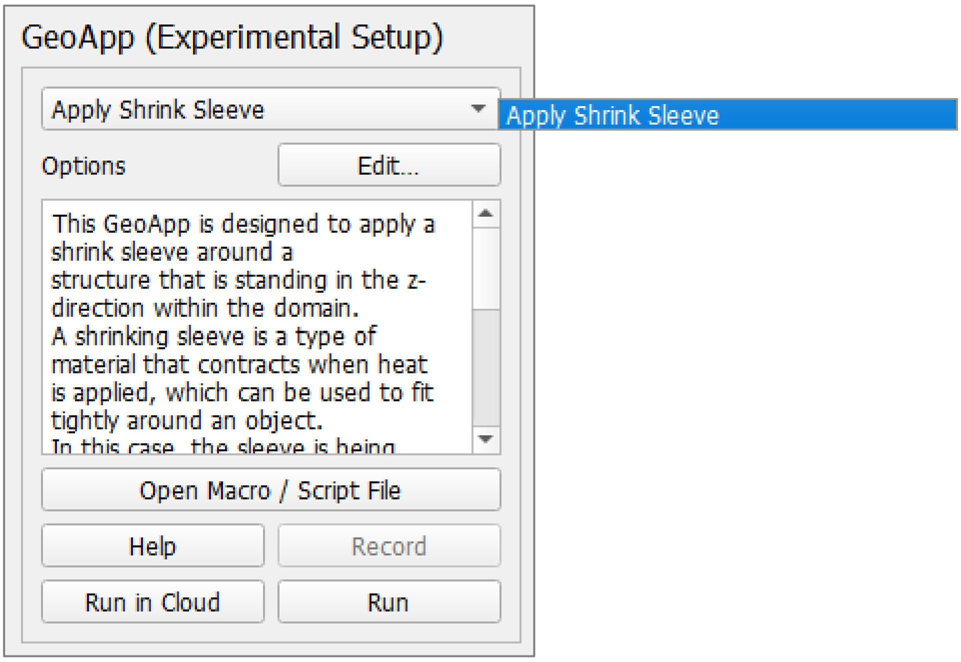
Six **Digital Rock Physics (DRP)** GeoApp modules are shipped with GeoDict:

- Use **Experimental Setup** to prepare your structure for further simulations.
- Run **Nuclear Magnetic Resonance** experiments on rock structures.
- Run a **Quality Control** on a sandstone.
- Simulate **Reactive Flow** by executing mineral dissolution and/or precipitation.
- Run an entire **Routine Core Analysis** workflow.
- Simulate **Two-Phase Flow**.

Experimental Setup

The **GeoApp (Experimental Setup)** section contains the following, selectable from the pull-down menu:

- **Apply Shrink Sleeve:** Apply a shrink sleeve around a structure that is oriented in Z-direction.

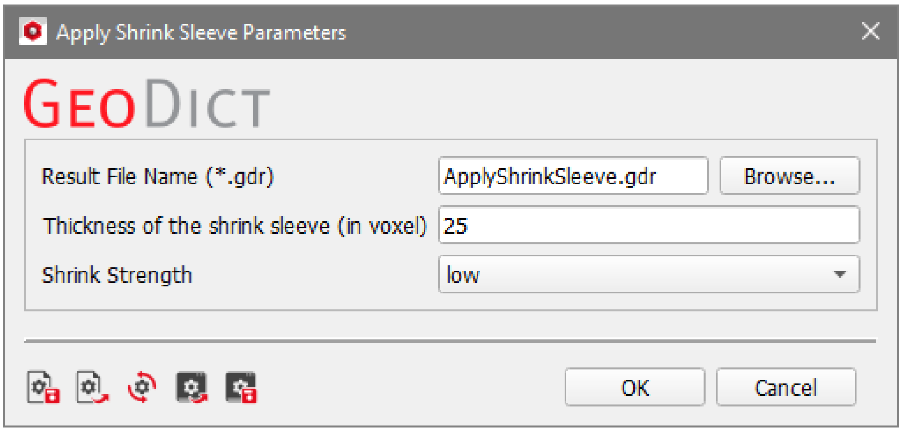


Apply Shrink Sleeve

A shrink sleeve is a material that tightens when heat is applied. The **Apply Shrink Sleeve** app simulates this behavior by adding a layer of a different material ID around a structure. This allows to separate the pore space inside a structure from the pore space on the outside. This is especially helpful when processing cylindrical structures, e.g. core samples. The structure needs to be oriented vertically, i.e. in the Z-direction.

Modules needed to run this GeoApp: GeoDict Base

After loading a 3D structure, clicking **Edit** for the **Apply Shrink Sleeve** app opens the **Apply Shrink Sleeve Parameters** dialog.



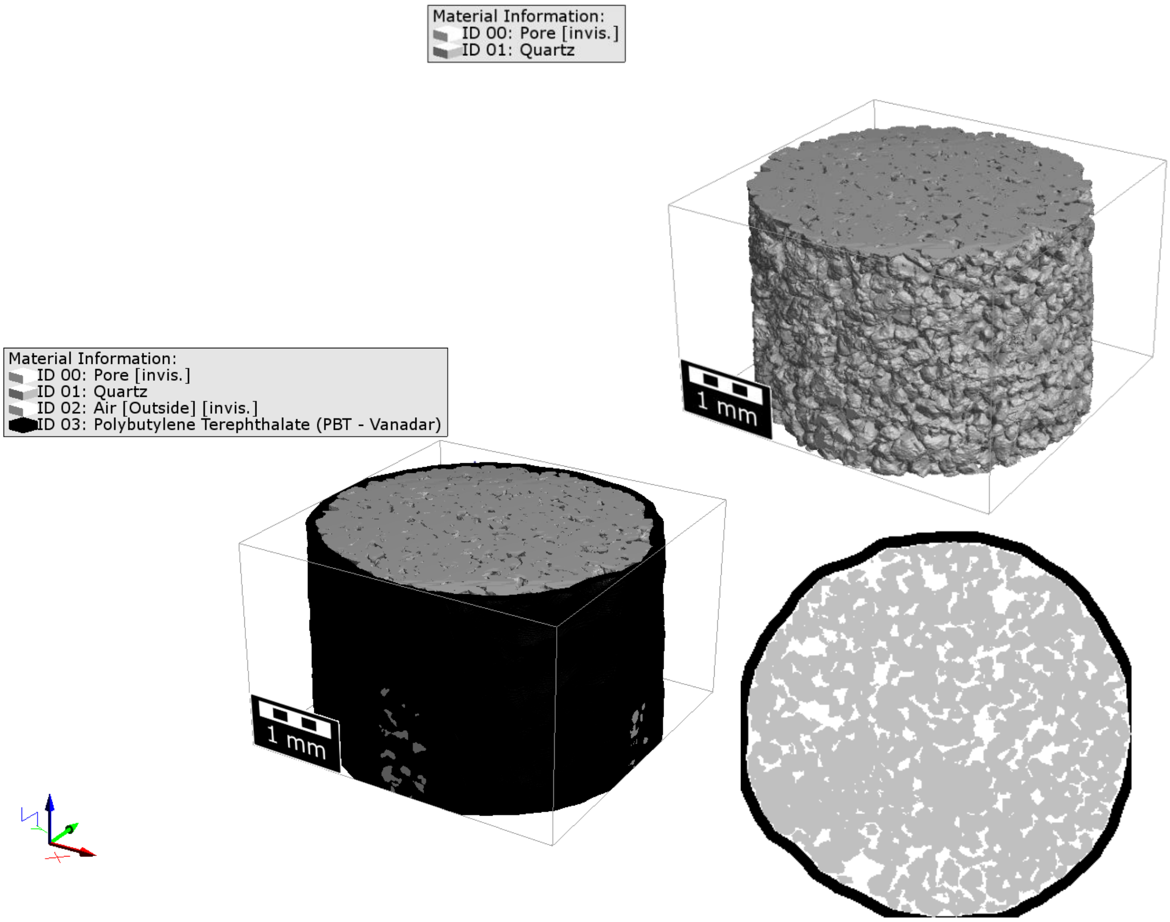
Three parameters can be edited. First enter a **Result File Name**.

The **Thickness of the shrink sleeve (in voxel)** defines the thickness of the applied layer.

The **Shrink Strength** can be selected as **low**, **medium** or **high**. For a high shrink strength the added shrink sleeve is very tight around the structure. This means that pores at the outside of the solid material might also be filled with the coating material of the shrink sleeve.

Click **OK** to close the dialog, go back to **GeoApp** section, and click **Run**. After the run is finished the Result Viewer opens. The structure with the applied shrink sleeve is shown in the visualization area and saved in the project folder with the same name as the result file.

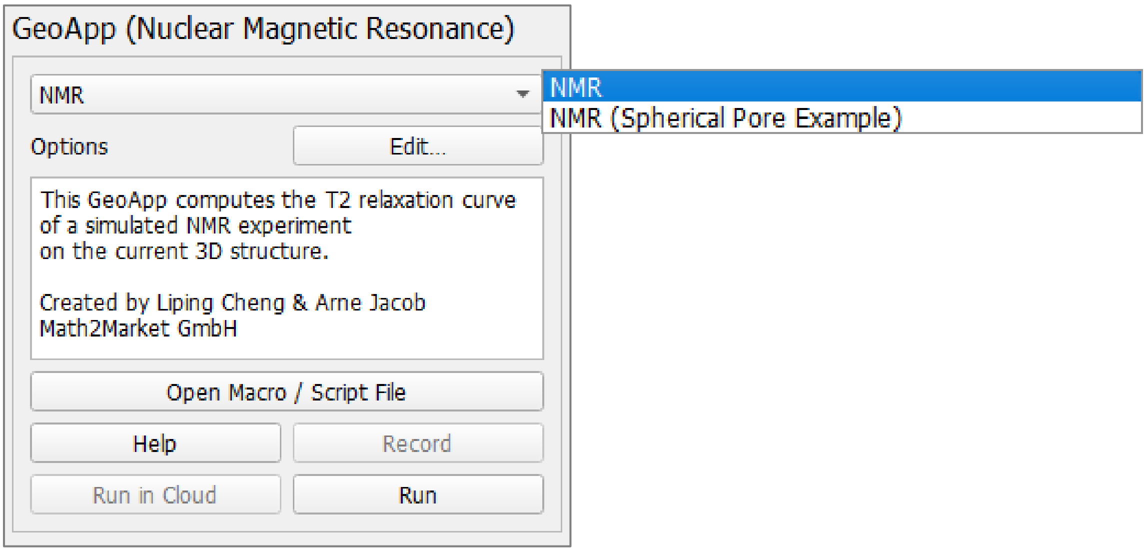
Below, the result for a medium shrink strength is shown for a Gildehauser sandstone [15] in 3D and in 2D visualization.



Nuclear Magnetic Resonance

The **GeoApp (Nuclear Magnetic Resonance)** section contains the following, selectable from the pull-down menu:

- **NMR:** run an NMR experiment on the current structure.
- **NMR (Spherical Pore):** run an NMR experiment on a spherical pore.



NMR

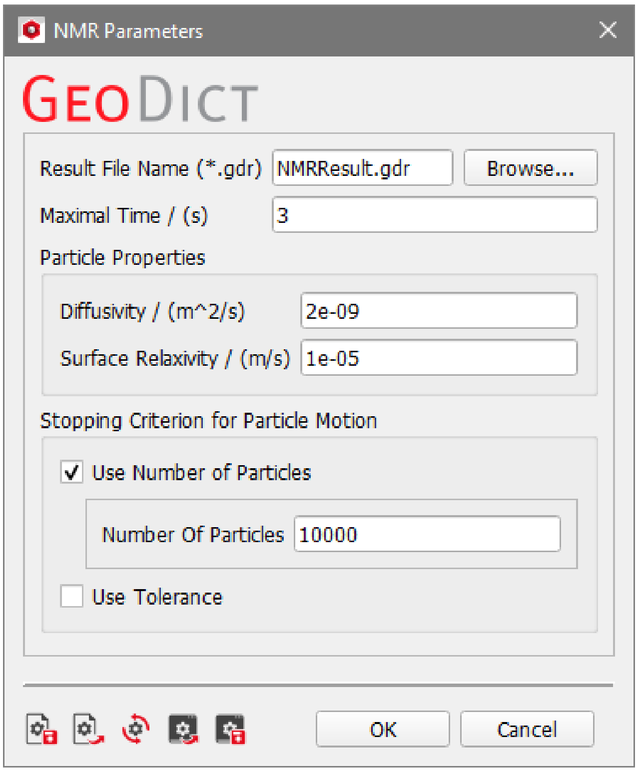
The **NMR** app computes the T2 relaxation curve of a simulated NMR experiment on the current 3D structure. Thus, it is used for general NMR simulation purposes, while the **NMR (Spherical Pore)** app creates a close pore structure and simulates on it.

Modules needed to run this GeoApp: AddiDict

After loading a 3D structure, clicking **Edit** for the **NMR** app opens the **NMR Parameters** dialog. The predefined parameters are the same as those for the **NMR (Spherical Pore)** app. Modify them according to the desired NMR expriment and start the simulation.

Tooltips describe the parameter options.

Two NMR simulation examples, one for a Bentheim sandstone and the other for an Obernkirchen sandstone, are found in the NMR tutorial.



NMR (Spherical Pore)

The **NMR (Spherical Pore)** app generates a spherical pore and computes the T2 relaxation curve of a simulated NMR experiment. The results can be compared to the known analytical solution.

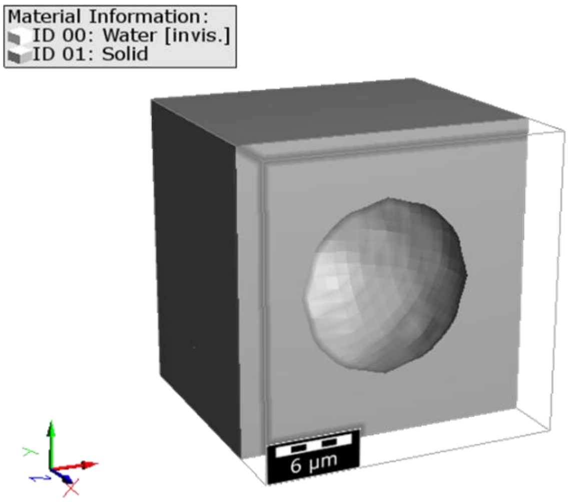
Modules needed to run this GeoApp: AddiDict

Clicking **Edit...** opens the **NMR (Spherical Pore) Parameters** dialog. The input parameters include **Result File Name**, **Maximal Time**, **Diffusivity**, **Surface Relaxivity**, **Number of Particles** and **Tolerance**.

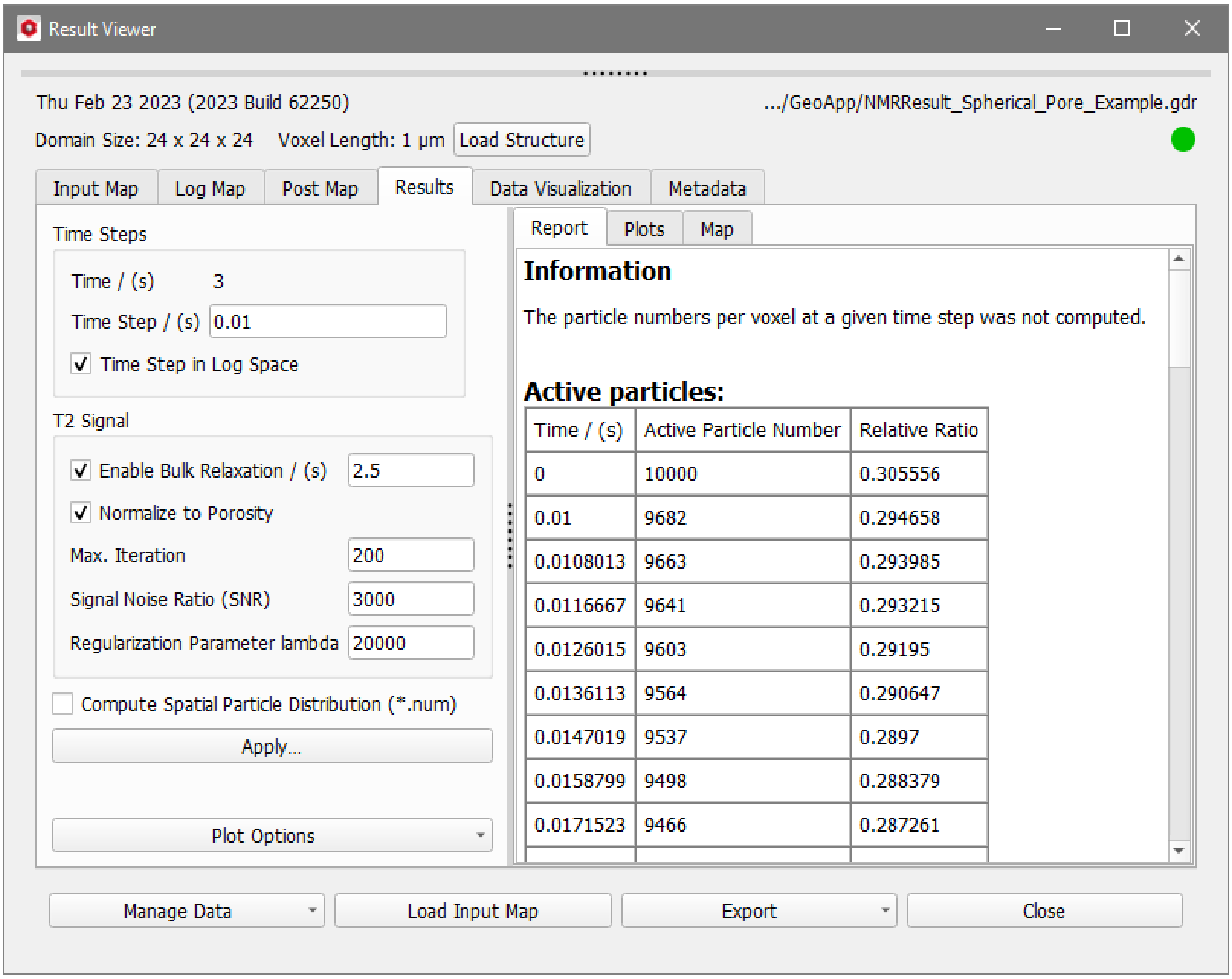
Tooltips describe the parameter options and detailed explanations of the parameters are found in the tutorial [Random-walk method to simulate T2 of NMR](#).

The parameters can be modified if needed. Otherwise, click **OK** to close the dialog, go back to **GeoApp** section, and click **Run**.

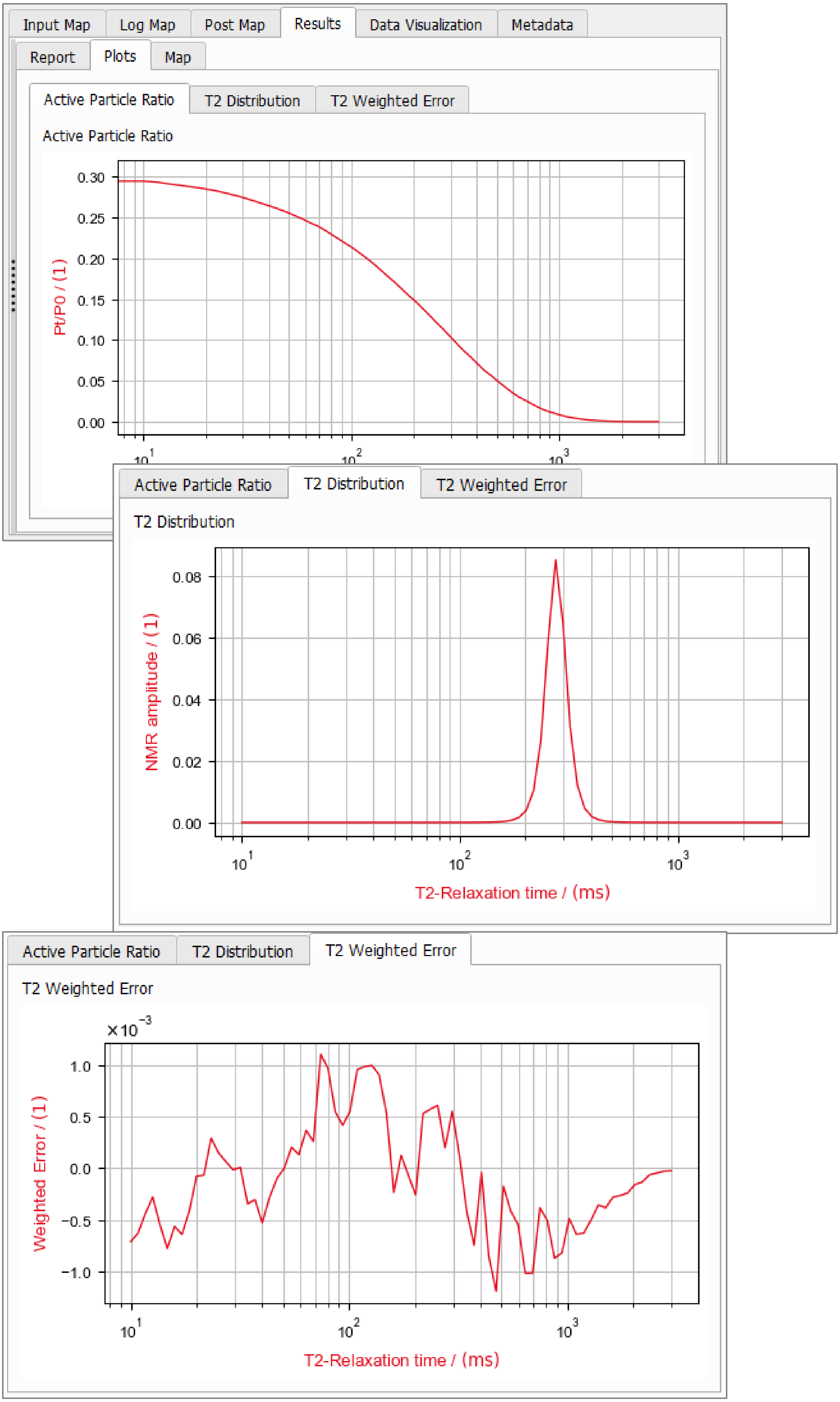
When the simulation finishes, the **Result Viewer** of the result file (*.gdr) opens automatically, and in the Visualization area a hollow cube with a spherical pore is shown; here clipped in Z-direction.



The **Results** → **Report** subtab of the **Result Viewer** shows the table for the number of **Active particles** and the resulting relative ratio vs. the simulation time.



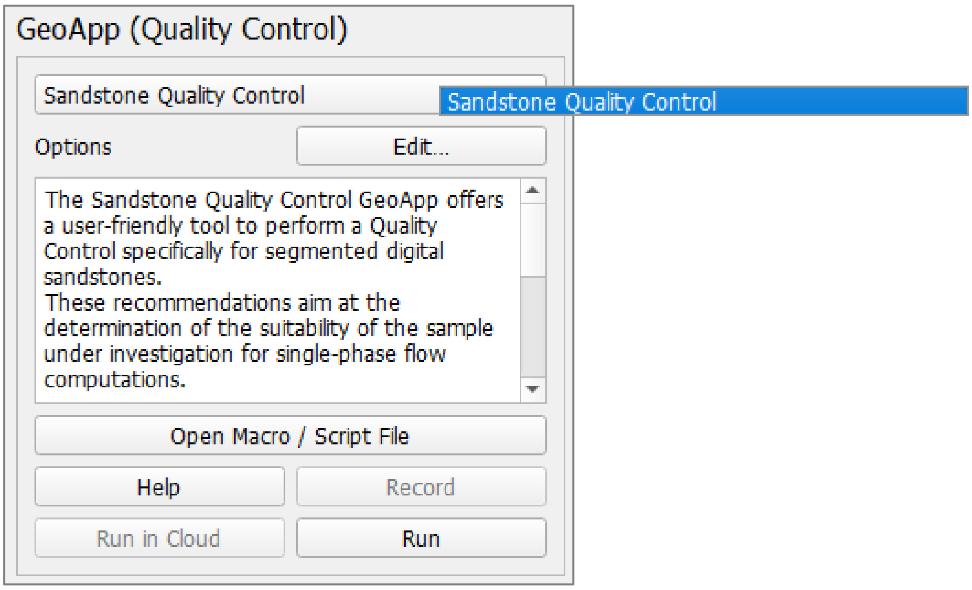
In the **Results** → **Plots** subtab, the plot of **Active Particle Ratio**, corresponding to the values of the Active particles table, the plot of **T2 Distribution**, and **T2 Weighted Error** are shown. For more details on the results, refer to the NMR tutorial.


Input Map
Log Map
Post Map
Results
Data Visualization
Metadata
Report
Plots
Map
Active Particle Ratio
T2 Distribution
T2 Weighted Error
Active Particle Ratio
Pt/P0 / (1)
0.30
0.25
0.20
0.15
0.10
0.05
0.00
10^1
10^2
10^3
T2 Distribution
NMR amplitude / (1)
0.08
0.06
0.04
0.02
0.00
T2-Relaxation time / (ms)
T2 Weighted Error
×10^-3
Weighted Error / (1)
1.0
0.5
0.0
−0.5
−1.0
T2-Relaxation time / (ms)

Quality Control

The **GeoApp (Quality Control)** section contains the following, selectable from the pull-down menu:

- **Sandstone Quality Control**: run a quality control on the current structure.



Sandstone Quality Control

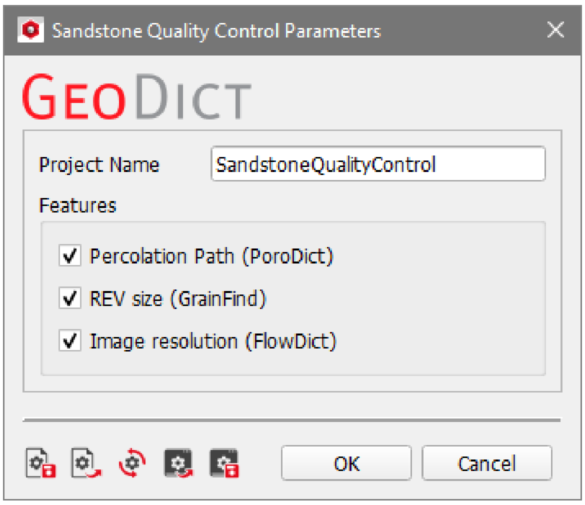
Segmented 3D digital images require a quality check. Therefore, we implemented the **Sandstone Quality Control** app to offer a user-friendly tool to perform a Quality Control specifically for segmented digital sandstone rocks based on methods and findings published by [10] and [11]. These recommendations aim at the determination of the suitability of the sample under investigation for single-phase flow computations.

Parts of the following Quality control recommendations may also be considered for other rock types and further samples.

Modules needed to run this GeoApp: PoroDict, GrainFind, and/or FlowDict

Clicking **Edit** opens the **Sandstone Quality Control Parameters** dialog.

An online workshop for this feature (amongst others) is available from here.



The usage of all the three available features is recommended (as long as the given modules are available):

- The **Percolation Path** feature investigates the pore throat resolution, which affects the computed permeability. Saxena et al. (2018) recommend a resolution of 10 voxels to sufficiently resolve pore throats for single-phase flow computations that predict the absolute permeability. For the usage of our flow solvers, we recommend a resolution of at least 4 voxels. Below 4 voxels, the runtime might increase significantly, and the permeability prediction may become inaccurate.

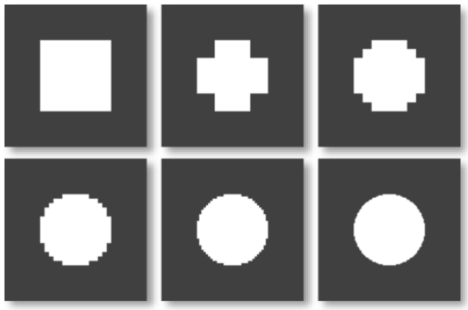
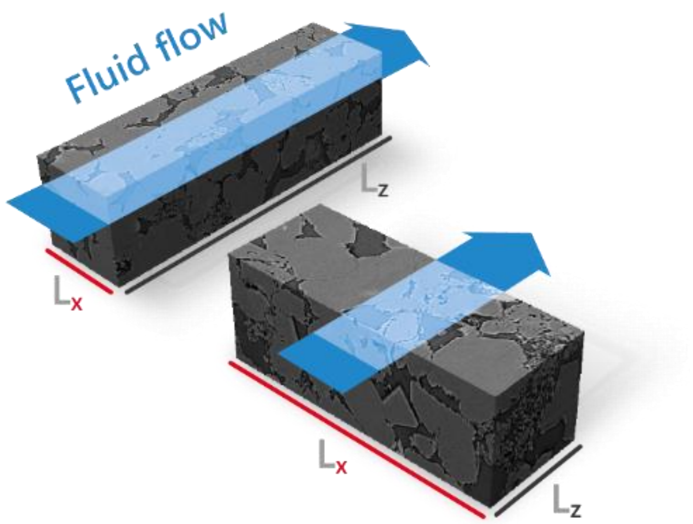


Figure 1.

Schematic representation of tubes resolved at varying voxel diameter highlighting the significant effect of the pore throat resolution on the permeability that may be predicted by numerical solvers.

- The **REV Size** considers the **R**epresentative **E**lementary **V**olume that is required to compute an absolute permeability that is representative for the rock formation under investigation. In general, an REV may be defined as a rock volume large enough that properties under investigation are insensitive to changes in rock volume and in boundary conditions of numerical tools. Saxena et al. (2018) recommend considering the ratio of the (smallest) structure length to the effective grain diameter:



$$L_{structure} > 5 * d_{Grains} \tag{5}$$

- The **Image Resolution** feature applies sample porosity and roughly approximated permeability (with a short computational runtime) to check if the acquired image resolution is suitable for single-phase flow computations. The applied workflow is based on findings published by [11] upon consideration of a large sandstone database.

Curves in **Figure 2** depict the permeability that can be computed by Stokes solvers – at minimum – based on segmented porosity, image voxel size, and numerics. The permeability of the sample (red cross) should be above the numerical minimum (red cure). Otherwise, we recommend acquiring an image of higher resolution.

If porosity and permeability are known a priori, we recommend using the additional curves as a suggestion for a suitable image resolution.

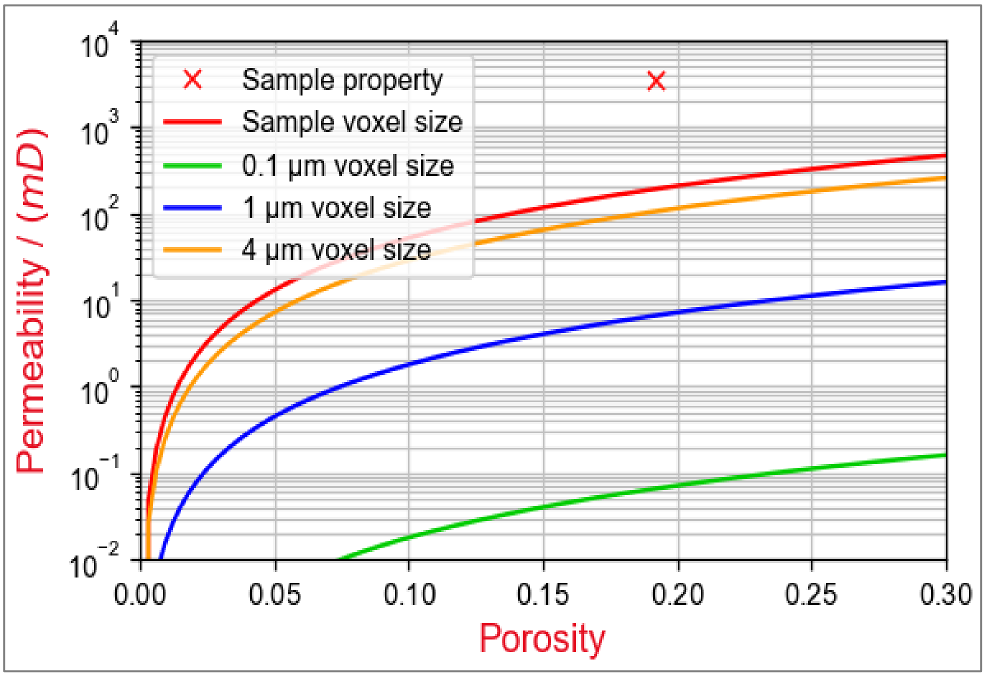
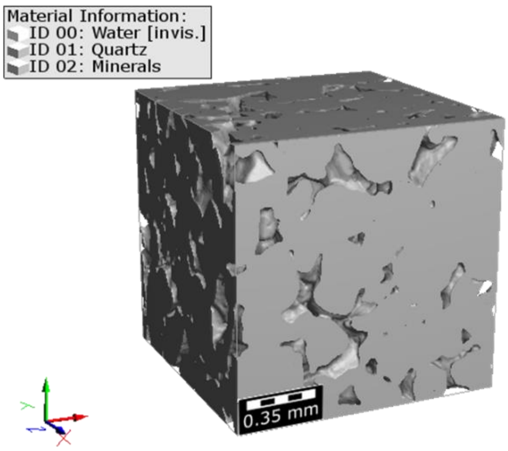


Figure 2.

Result for a Workshop geometry (dimensions: 256³). The <u>red curve</u> shows the minimum permeability computable for this sample. The <u>red cross</u> shows a computed permeability, which is far above the numerical minimum (red curve) and thus the <u>image resolution is fine</u>, from this perspective.

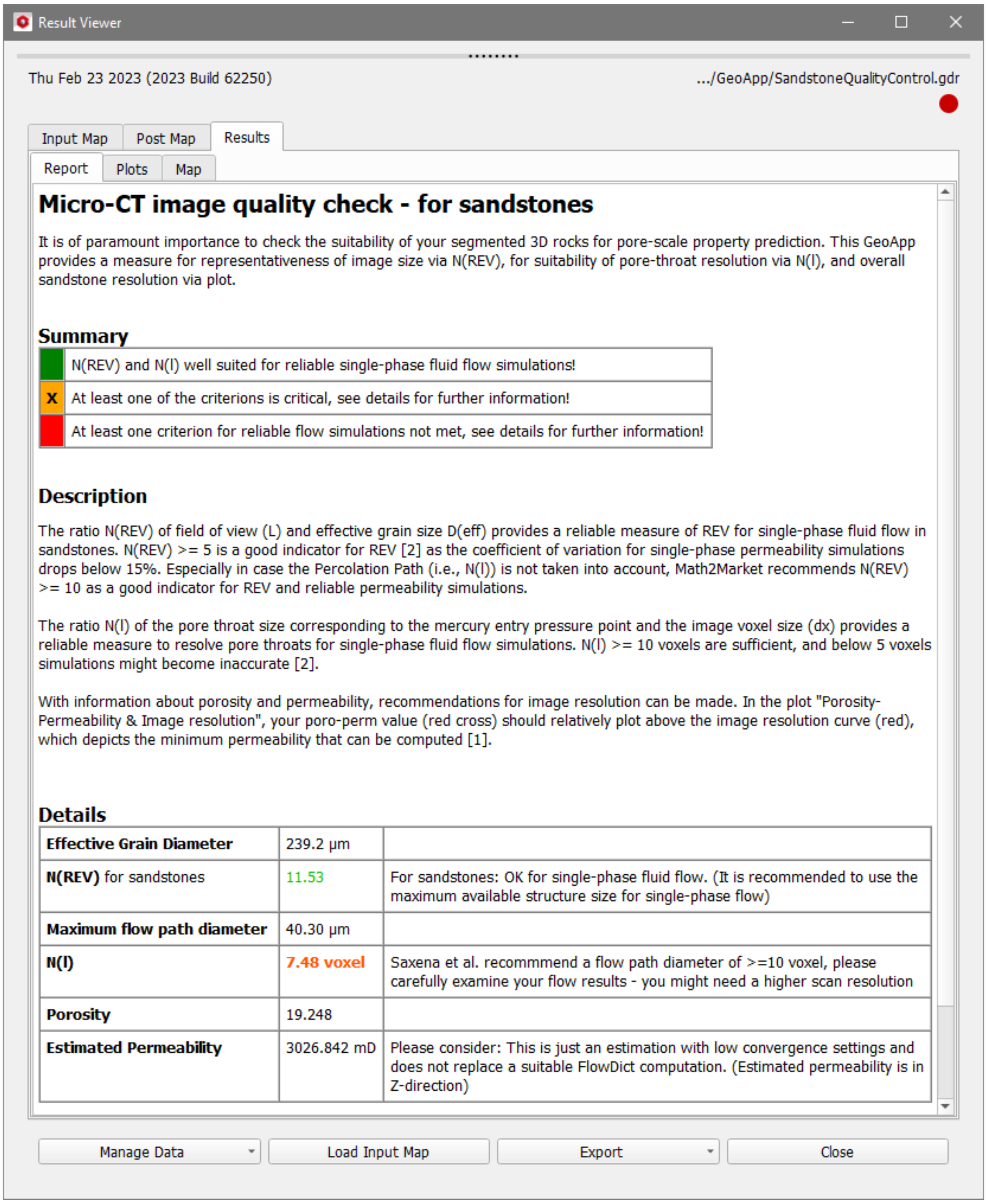
The parameters can be modified if needed, otherwise click **OK** to close the dialog. Go back to GeoApp GUI and click **Run**.

When the simulation finishes, the **Result Viewer** of the result file (*.gdr) opens automatically.



The **Results** → **Report** subtab (*below*) of the Result Viewer shows the results of the quality control.

The resolution is displayed in orange in the table, but observing the plot under the **Results** → **Plots** tab shows, that in this case, the image resolution is fine, as explained in **Figure 2**.



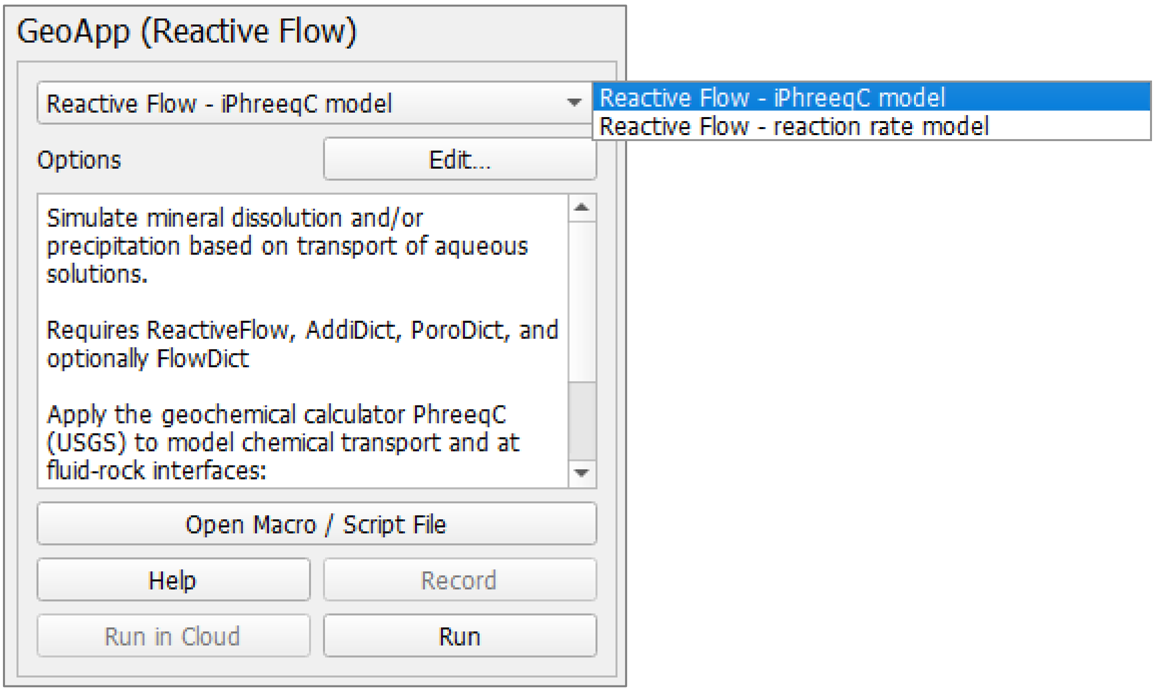
Reactive Flow

The **GeoApp (Reactive Flow)** section contains the following, selectable from the pull-down menu:

- **Reactive Flow – iPhreeqC model:** Simulate mineral dissolution and/or precipitation based on transport of aqueous solutions.
- **Reactive Flow – reaction rate model:** Execute mineral-specific dissolution and precipitation reactions on particle-mineral collisions.

In addition, we have a **pH-based Model**, currently available only on request. This reactive flow model computes Mineral dissolution due to acid injection. The reactivity is controlled by a user-defined pH value and particle-rock collisions based on the approach of [8], see also our dedicated technical report [12].

These GeoApps are applicable to many different research and business topics such as "CO_2 sequestration", "Acidizing treatments" and further applications such as "Nuclear Waste Storage", "Environmental Remediation", and "Hydrogen Underground Storage".



Reactive Flow – iPhreeqC model

The **Reactive Flow – iPhreeqC Model** app computes dissolution and precipitation of mineral phases during continuous inflow of reactants (e.g., acid) and predicts:

- Permeability reduction & enhancement (porosity-permeability relationship)
- 4D rock alteration: automated generation of animations that enable visual determination of the precipitation and dissolution patterns in addition to the analysis via various plots that are generated automatically.
- Chemical transport in the geometry, determined on the voxel scale

Modules needed to run this GeoApp: AddiDict,
optionally: FlowDict, PoroDict

For solving **Reactive Flow** for the various application areas, the geochemical calculator PhreeqC (USGS) is coupled to GeoDict to compute geochemical transport and mineral dissolution / precipitation based on the Lagrangian Transport method.

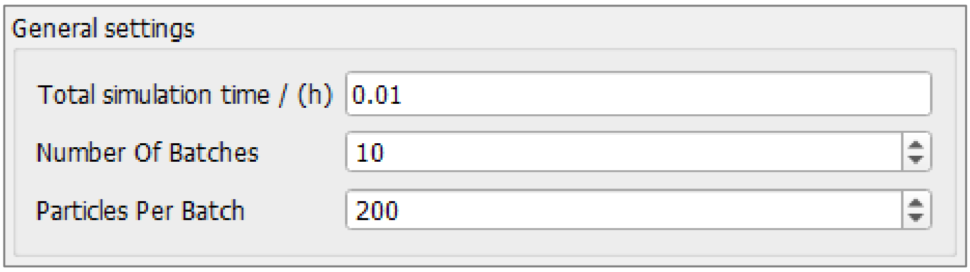
Clicking **Edit** opens the **Reactive Flow Parameters** dialog.

Choose a **Result Name** for the resulting GeoDict result file (*.gdr) and the corresponding result folder.

The parameters are organized into five groups.

General settings

For the **General Settings** define the **Total simulation time**, the **Number of Batches** and the **Particles per Batch** for the reaction rate simulation. During each batch first the flow is computed if the current and relative porosity change is larger than 1%. Then, the transport is computed and finally the reactions at water-rock interfaces are computed. Fewer particles decrease the accuracy of the simulation and thus, improve the performance. Using more particles increases the accuracy while leading to longer runtimes. As a rule of thumb, it is sufficient to use the number of pore voxels at the inflow boundary (approx. nx*ny*porosity). Feel free to decrease that number for ~linearly improved performance at a relatively lower cost of accuracy.

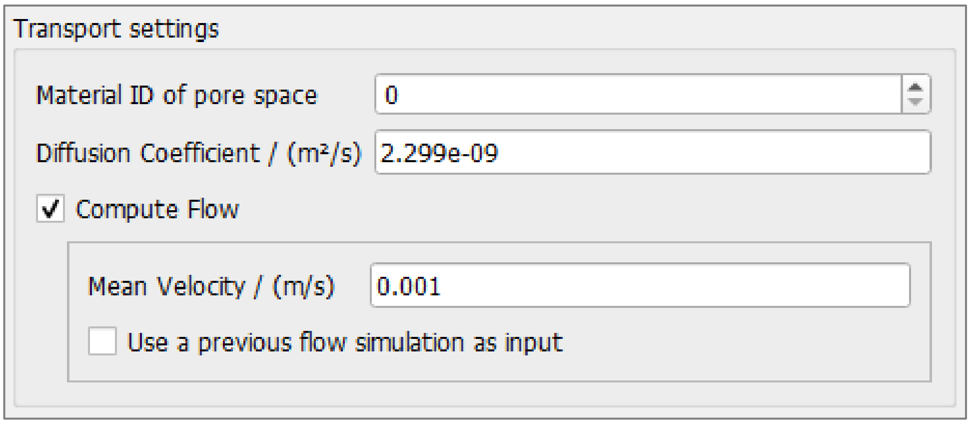


Transport settings

The Reactive transport experiment is based on advection-diffusion-reaction or diffusion-reaction. In both cases the transport is computed along the Z-axis.

Select the **Material ID of pore space** and set the **Diffusion Coefficient.** This coefficient affects the inflow fluid transport paths according to the Brownian motion. Default is the self-diffusion coefficient of pure water at 25°C.

Select **Compute Flow** if a reactive flow experiment should be performed by computing the flow field regularly. This requires a FlowDict license. Define the **Mean Velocity**. Instead, a previous flow simulation can be used as input, which is especially beneficial in case of restarting simulations in large geometries.



Geochemical Model

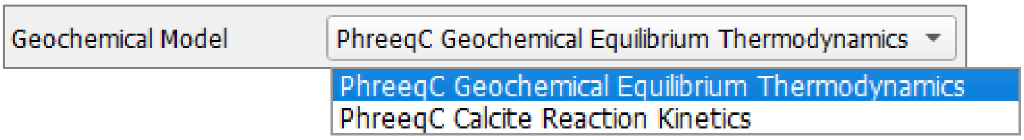
Two **Geochemical Models** can be selected for the simulation.

You do not need a separate PhreeqC installation to run this reactive flow model. But, we recommend to install PhreeqC, get used with the software and set up your geochemistry therein in advance. Please make sure to check your setup for reactive mineral phases and to balance the electrical charge.

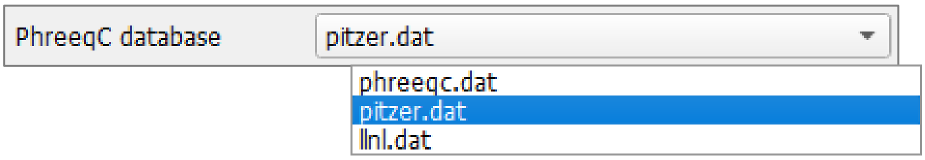
Please visit https://www.usgs.gov/software/phreeqc-version-3 for more information.

PhreeqC Geochemical Equilibrium Thermodynamics (PGET) calculates reactions based on the input of aqueous fluids by employing the geochemical calculator PhreeqC.

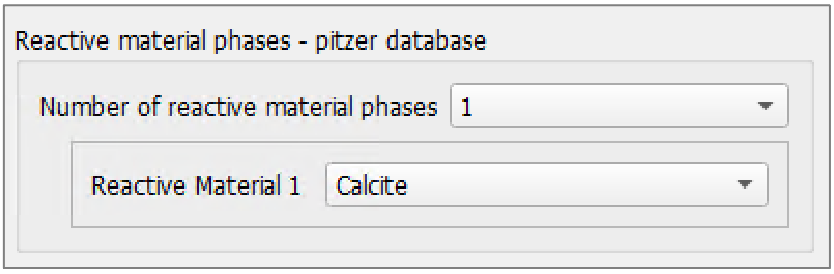
PhreeqC Calcite Reaction Kinetics (PCRK) calculates kinetic reations with calcite as the reactive mineral phase and based on the input of aqueous fluids by employing the geochemical calculator PhreeqC The database (phreeqc.dat) for calcite kinetics is however limited to ambient conditions.



For PGET select a **PhreeqC database**. The databases are located in the app folder within the GeoDict installation folder and can be adjusted or replaced. This may require administrator rights. For reservoir conditions with high pressure, temperature and salinity the **pitzer.dat** database is recommended. For most other setups the **phreeqC.dat** should work well. Additionally, the **llnl.dat** (Lawrence Livermore National Laboratory) is available, which contains the highest number of mineral phases. Note that we have not included all the approx. 2000 mineral phases considered by the llnl.dat database. Feel free to contact us if you're missing a specific mineral phase.



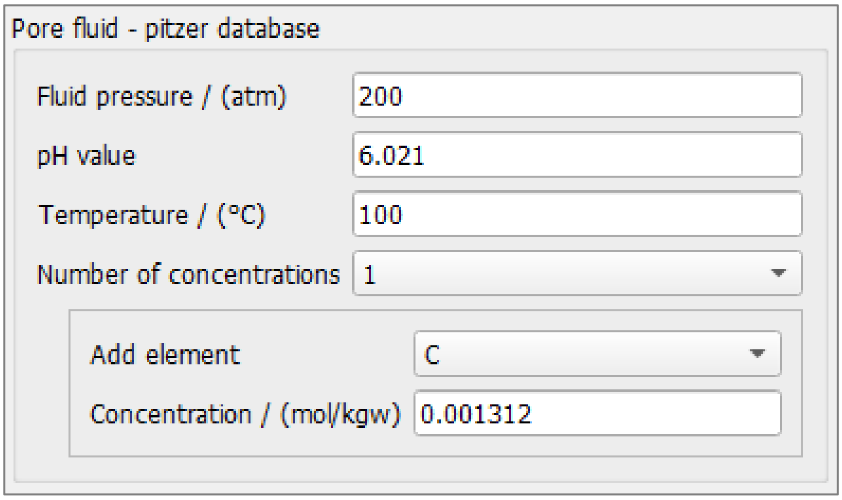
Define the **Number of reactive material phases** and select each **Reactive Material** from the pul-down menu. The chosen mineral phases will be dissolved and / or precipitated based on PhreeqC calculations. The available materials depend on the selected database.



Set the **Fluid pressure**, **pH value**, and **Temperature**. For pressure and temperature, values are limited to the ranges specified for the corresponding database. Subsequently, set the **Number of concentrations** for both the pore fluid (formation fluid) and the inflow fluid (injected fluid). For each concentration, select the **Added element** and enter a **Concentration** value in mol per kg water (mol/kgw), which is the default PhreeqC unit.

PhreeqC calculates with element concentrations and converts these into the respective molecules for further geochemical calculations. This requirement is well in line with hydrogeochemical fluid analysis, so the user interface is designed towards these factors.

Note: Please make sure to equilibrate your fluids in advance (e.g., via PhreeqCI). This includes an electric charge balance for both fluids and an equilibrium of the pore fluid w.r.t. the reactive materials (mineral phases) selected above. Note that future GeoDict developments will aim at a simplified user experience in this context.

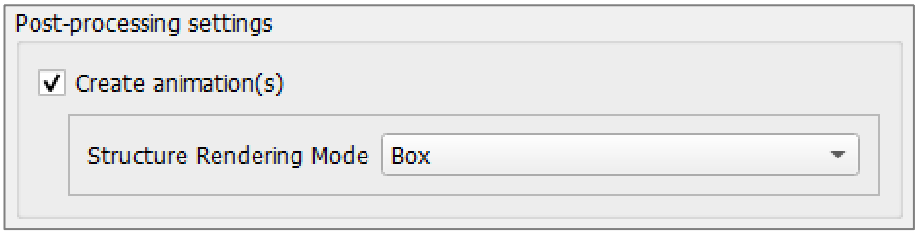


Post-Processing settings

Decide if the structure changes during the reactive flow simulation should be animated in a video by selecting or deselecting **Create animations**. In case of a geochemical model including PhreeqC calculations additionally pore fluid animations are created. Animations have a default length of 10s each. They are especially smooth in case of an increased number of batches.

Note that for an improved visibility of geochemical transport w.r.t. the inflow fluid a transparency is introduced for the initial pore fluid concentration.

For the animation select if the structure should be rendered with **Box**, **GPU** or **Smooth** renderer.



Expert settings

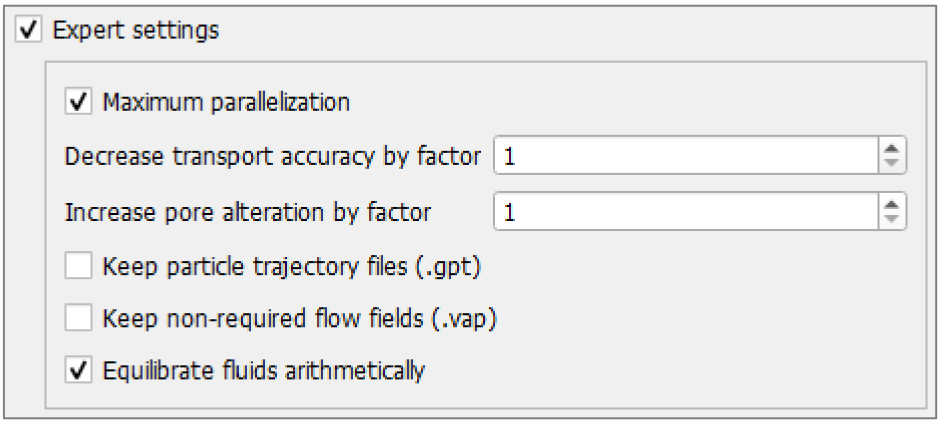
The available **Expert settings** include **Parallelization**, defining the factor for **Decreased transport accuracy** and **Increased pore alteration**, selecting to **Keep particle trajectory files** and **non-required flow fields** and deciding to **Equilibrate fluids arithmetically** or not.

A decreased transport accuracy improves the geochemical performance at the cost of transport accuracy. The value shouldn’t be increased above 1 unless there is no other option left.

Note: Increase pore alteration increases the reaction time beyond the transport time. This option allows you to compute reactions at time scales beyond s / min / h. Technically, the computed volume of dissolved / precipitated mineral phase is scaled by the given factor. It is thus recommended to first calculate a reasonable value. This could be exercised via PhreeqC. As an alternative, you could run test simulations in small structures and investigate the fraction of minerals altered at voxel surfaces as stored in the corresponding volume file (e.g., *SolidFractions01.gvf*) in your result folder.

By default, some non-required files are deleted from your result folder during the reactive flow simulation to save disk space. You may deactivate this behavior by checking the **Keep** options.

Finally, **Equilibrate fluids arithmetically** significantly improves the performance by reducing the overall amount of PhreeqC calculations for the geochemical transport.



The parameters can be modified as needed. Once finished with defining your individual setup, click **OK** to close the dialog, go back to **GeoApp** section and click **Run**.

When the simulation finishes, the **Result Viewer** of the result file (*.gdr) opens automatically. The results show Number of Batches, Total Simulation Time, Total Reaction Time, and Delta Porosity in the **Results** → **Report** tab.

Multiple result plots are found under the **Results** → **Plots** tab, depending on your setup: Porosity-permeability, Porosity, Porosity gradient (in flow direction), Reaction rate, Damkoehler number (Da), Péclet number (Pe), and PeDa number (product of Pe and Da).

In the following, see some sample visualizations that are generated automatically depending on your post-processing settings and stored in your result folder as images and (*.mp4) animation:

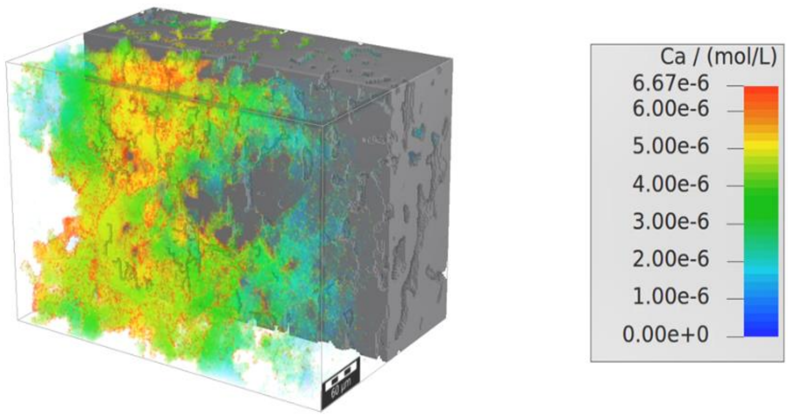


Figure 1.

Digital Reactive Flow Experiment considering the entire aqueous geochemistry here showing an intermediate result of a digital kinetically-controlled acidizing treatment of a Grosmont carbonate rock ([9]) upon inflow of a hydrochloric acid at pH 5.5

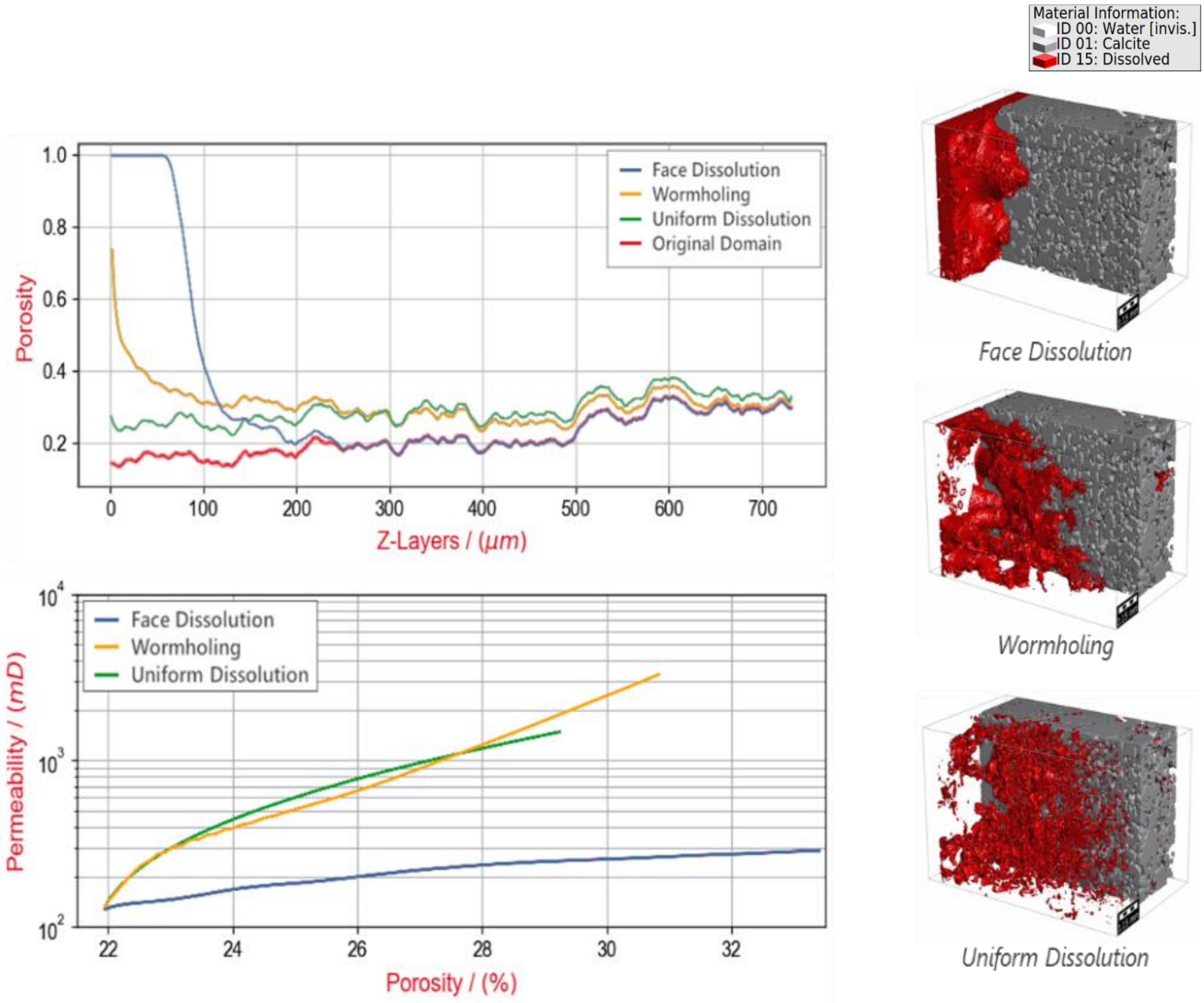


Figure 2.

Simulation of acidizing treatment in the digital Grosmont carbonate rock of Andrä et al. (2013) using different injection velocities and the same geochemical setup, which results in three main different Dissolution regimes upon usage of the reaction-rate model or pH-based model to dissolve the calcite at computed particle-rock collisions.

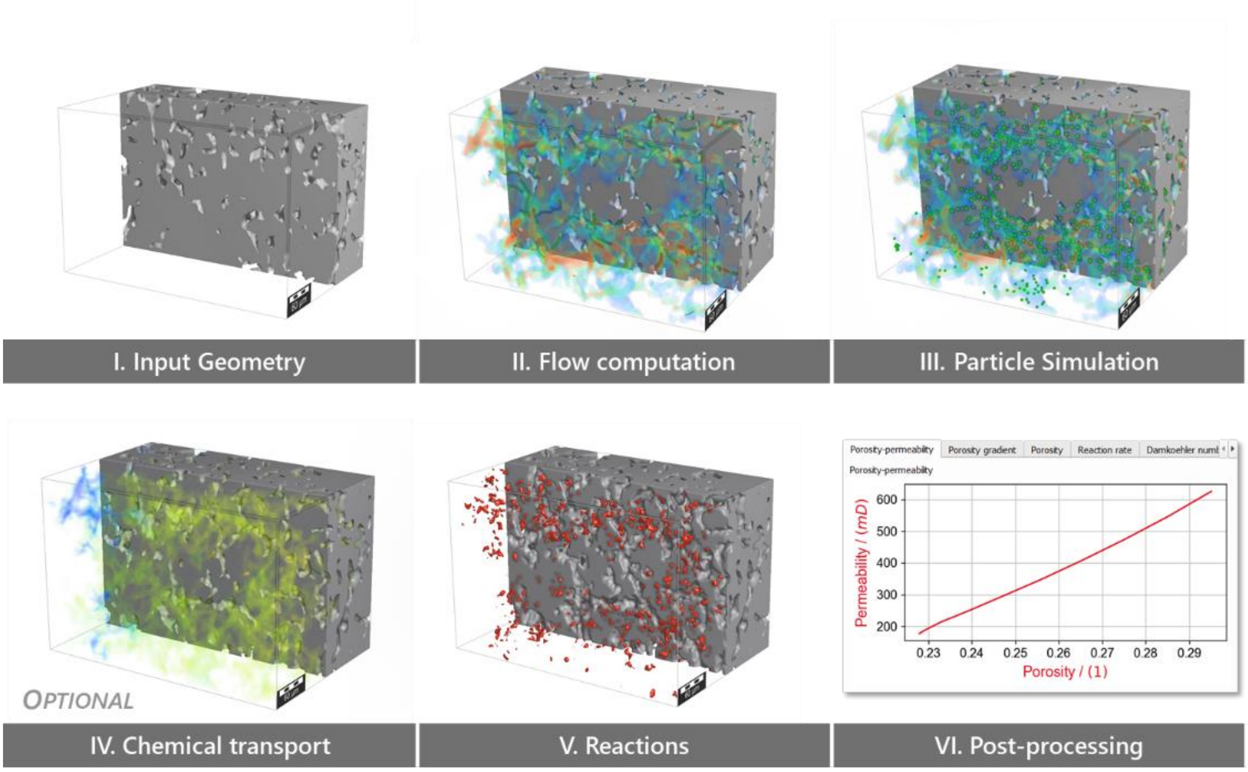


Figure 3.

The general workflow for Reactive Flow modeling in GeoDict 2023.
Step IV is only considered upon usage of the PhreeqC models.

Reactive Flow – Reaction Rate Model

The **Reactive Flow – Reaction Rate Model** app computes dissolution and precipitation of mineral phases during continuous inflow of reactants (e.g., acid) and predicts:

- Permeability reduction & enhancement (porosity-permeability relationship)
- 4D rock alteration: automated generation of animations that enable visual determination of the precipitation and dissolution patterns in addition to the analysis via various plots that are generated automatically.
- Chemical transport in the geometry, determined on the voxel scale

Modules needed to run this GeoApp: AddiDict,
optionally: FlowDict, PoroDict

Clicking **Edit** opens the **Reactive Flow Parameters** dialog.

Choose a **Result Name** for the resulting GeoDict result file (*.gdr) and the corresponding result folder.

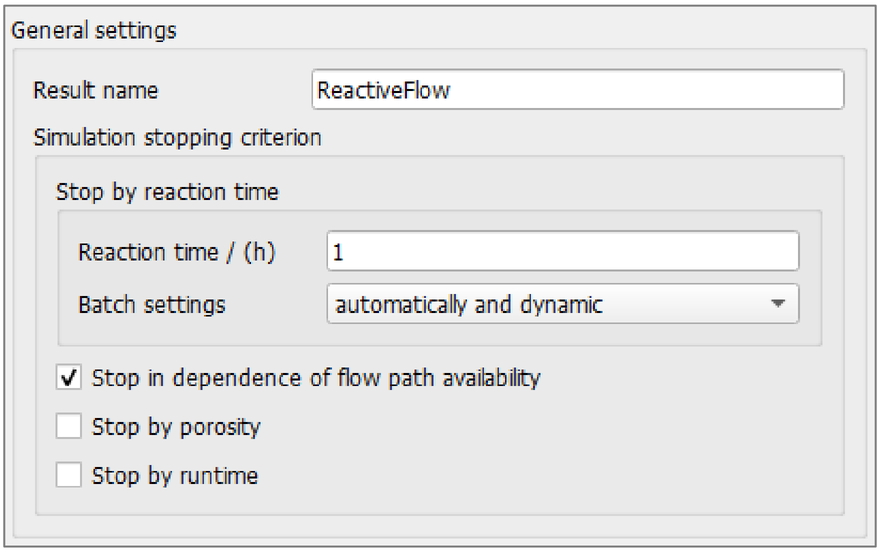
The parameters are organized into five groups.

General Settings

Define the **Result name** for the result file and the folder containing the results.

Enter the **Reaction time** after which the simulation should stop and choose the desired **Batch settings** from the pull-down menu. **Automatically and dynamic** is based on reaction time and geometry. If selected, the number of particles is chosen dynamically. For **manual** batch settings the number of particles per batch and the number of batches from which the time per batch is calculated must be defined manually.

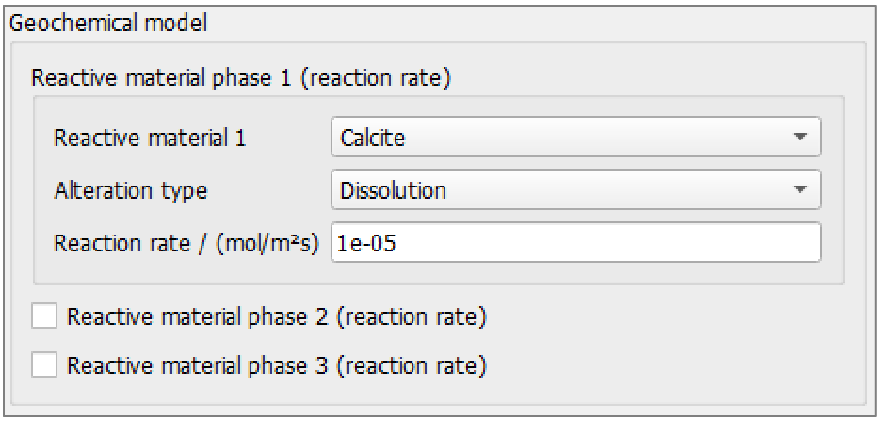
Additional stopping criterions are **in dependance of flow path availability**, reaching a given **porosity** and reaching a given **runtime**.



Geochemical Model

Select a **Reactive Material** from the pull-down menu and set the **Alteration type**. The material can be dissolved or precipitated.

Define the global **Reaction rate** of the reactive material phase. This reaction rate is prerequisite for each batch.

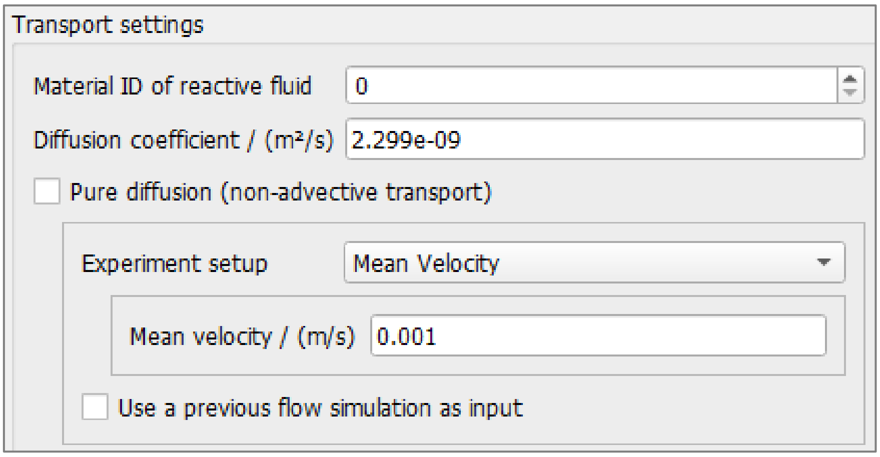


Up to three material phases can be defined for the reaction rate. For material 2 and 3 the alteration type is always dissolution.

Transport settings

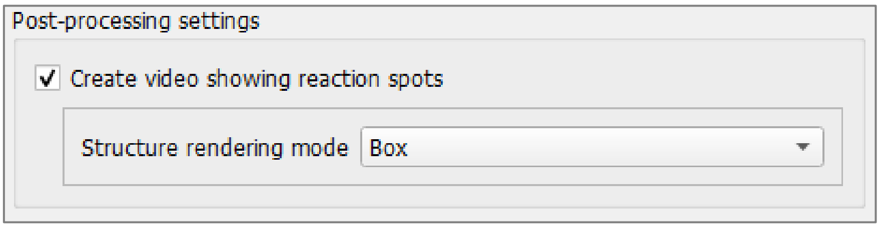
Select the **Materal ID of reactive fluid** and enter a **Diffusion coefficient** as described for the PhreeqC app on page 45.

If the transport should be computed from **Pure diffusion**, select the corresponding checkbox. Otherwise, select, depending on the **Experiment setup** or reservoir system select **Mean Velocity**, **Pressure Drop** or **Flow Rate** as input parameter. Enter the according value below.



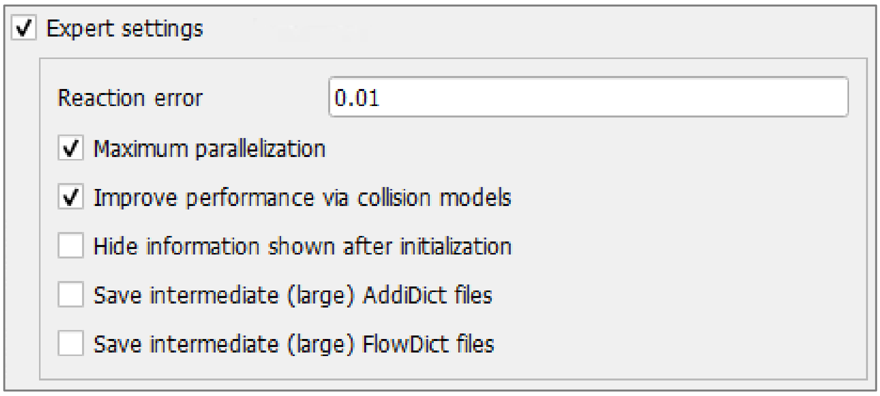
Post-processing settings

If **Create video** is selected, the structure changes are animated with dissolution and precipitation locations highlighted in red, while the solid matrix is made invisible in the front half.



Expert settings

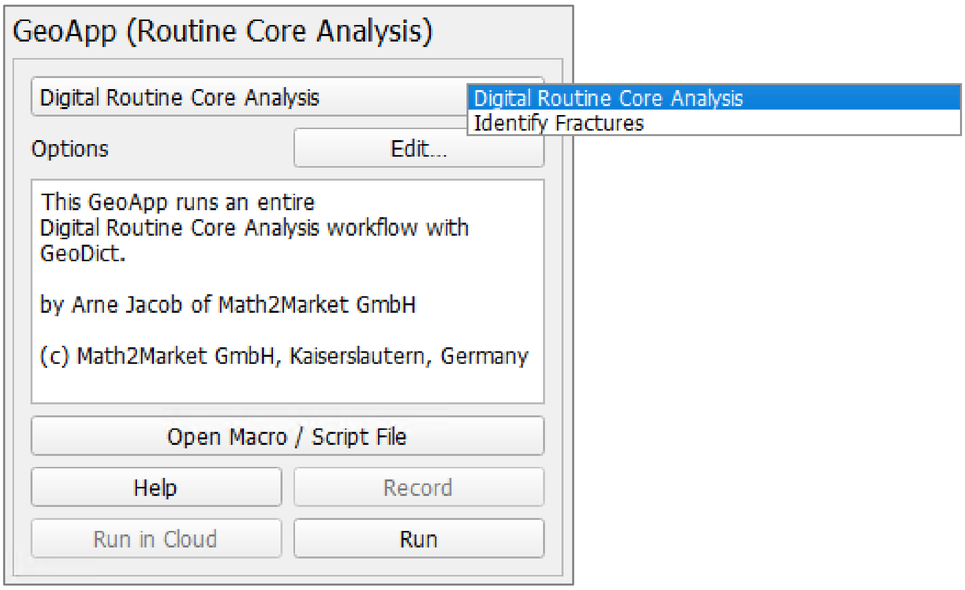
The **Expert settings** include **Reaction error**, **Parallelization**, **Improve performance via collision models**, **Hide information shown after initialization**, **Save intermediate AddiDict** and **FlowDict files**.



Routine Core Analysis

The **Routine Core Analysis** GeoApp section contains the following GeoApps, selectable from the pull-down menu:

- **Digital Routine Core Analysis:** run an entire digital routine core analysis workflow.
- **Identify Fractures**: analyze the pore morphology and segment the chosen material into fractures, small and large pores.



Digital Routine Core Analysis

The **Digital Routine Core Analysis** app runs an entire digital routine core analysis workflow with the chosen properties. Additionally, a PowerPoint presentation is saved which contains images and data from the structure and the selected properties.

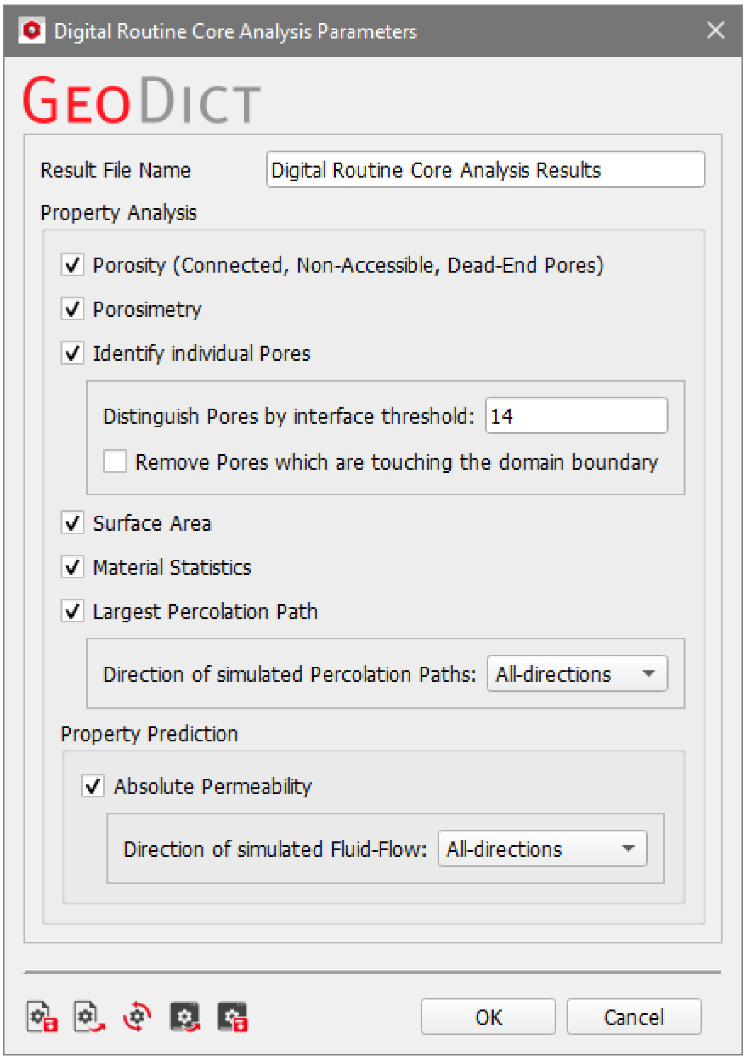
Modules needed to run this GeoApp:
PoroDict, FlowDict

Clicking **Edit...** opens the **Digital Routine Core Analysis Parametes** dialog.

Define the **Result File Name** for the result file and the result folder where all results will be stored into.

Decide if the app should

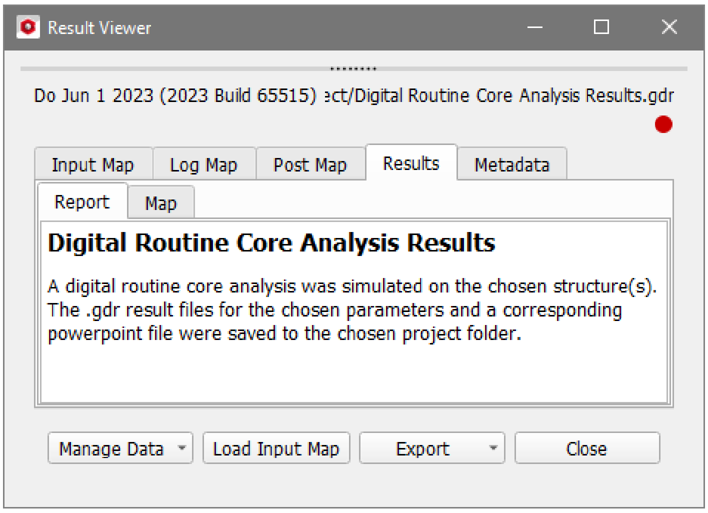
- compute the **Porosity**,
- determine the **Porosimetry**,
- **Identify individual Pores**,
- estimate the **Surface Area**,
- compute the **Material Statistics**,
- determine the **Largest Percolation Path** in the chosen directions or
- compute the **Absolute Permeability** in the chosen directions.



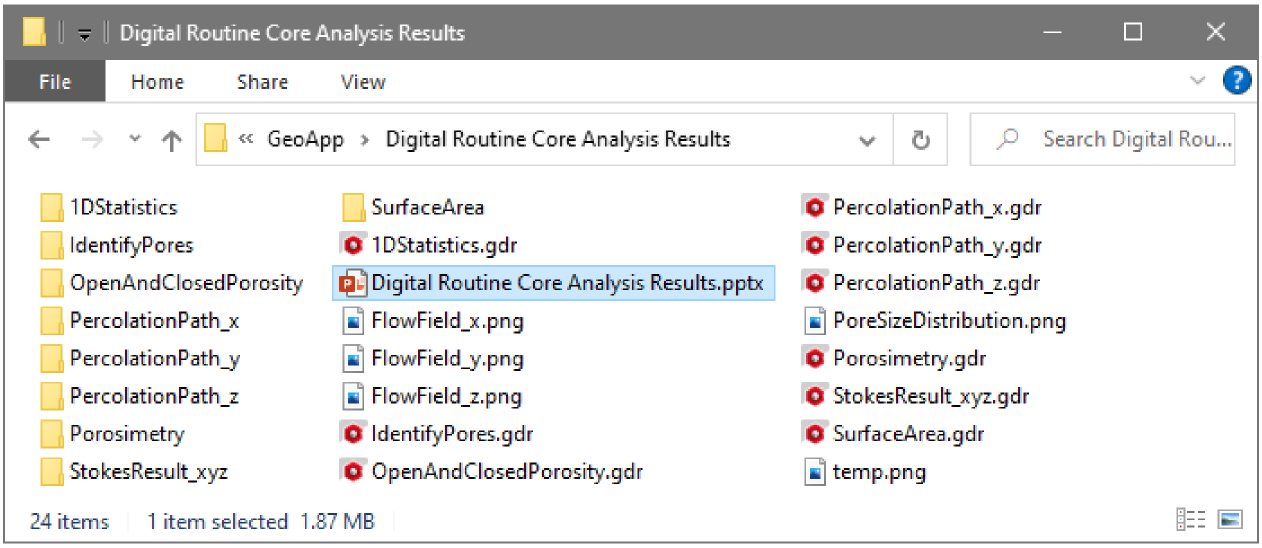
Clicking **Run** starts the digital routine core analysis.

When the simulation finishes, the **Result Viewer** of the result file (*.gdr) opens automatically.

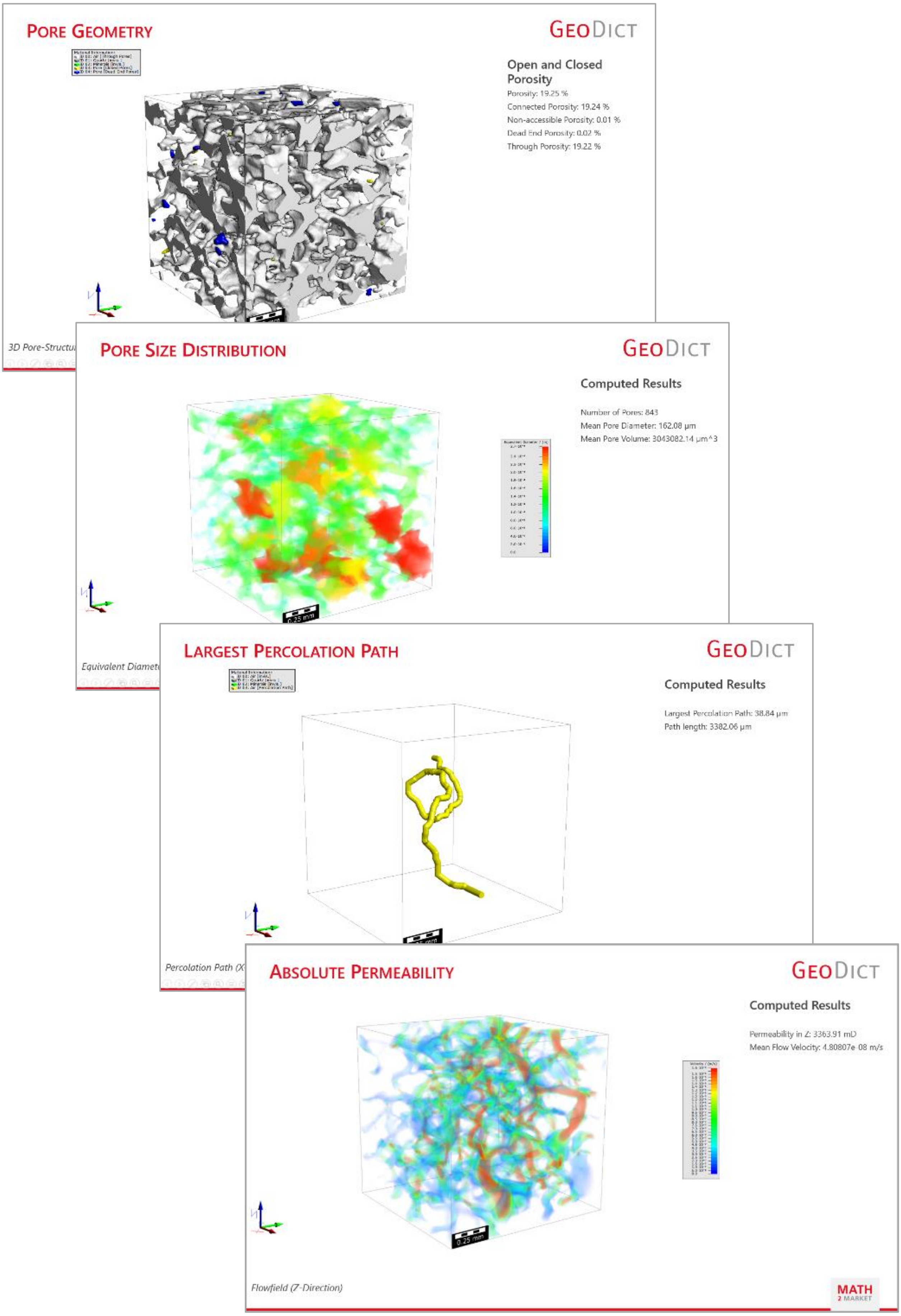
The result files of the chosen property computations are available in the corresponding folder. Up to nine different result files are available: OpenAndClosedPorosity.gdr, Porosimetry.gdr, IdentifyPores.gdr, SurfaceArea.gdr, 1DStatistics.gdr, PercolationPath_x.gdr, PercolationPath_y.gdr, PercolationPath_z.gdr, and StokesResult_xyz.



Additionally, a PowerPoint report can be found in the result folder between the other results.



Depending on the selected options, the PowerPoint report shows a structure overview, the pore geometry, the pore size distribution, the largest percolation path and the absolute permeability in the selected directions.


Pore Geometry
GeoDict
Open and Closed Porosity
Porosity: 19.25 %
Connected Porosity: 19.24 %
Non-accessible Porosity: 0.01 %
Dead End Porosity: 0.02 %
Through Porosity: 19.22 %
3D Pore-Structu
Pore Size Distribution
GeoDict
Computed Results
Number of Pores: 843
Mean Pore Diameter: 162.08 µm
Mean Pore Volume: 3043082.14 µm^3
0.25 mm
Equivalent Diamet
Largest Percolation Path
GeoDict
Computed Results
Largest Percolation Path: 38.84 µm
Path length: 3382.06 µm
Percolation Path (X
Absolute Permeability
GeoDict
Computed Results
Permeability in Z: 3363.91 mD
Mean Flow Velocity: 4.80807e-08 m/s
0.25 mm
Flowfield (Z-Direction)
MATH 2 MARKET

Identify Fractures

The **Identify Fractures** app analyzes the pore morphology and segments the chosen Material ID into fractures, small and large pores. The macro applies multiple runs of **Identify Pores** and the corresponding **Identify Pores Post Processing** to distinguish between pores and fracture phase.

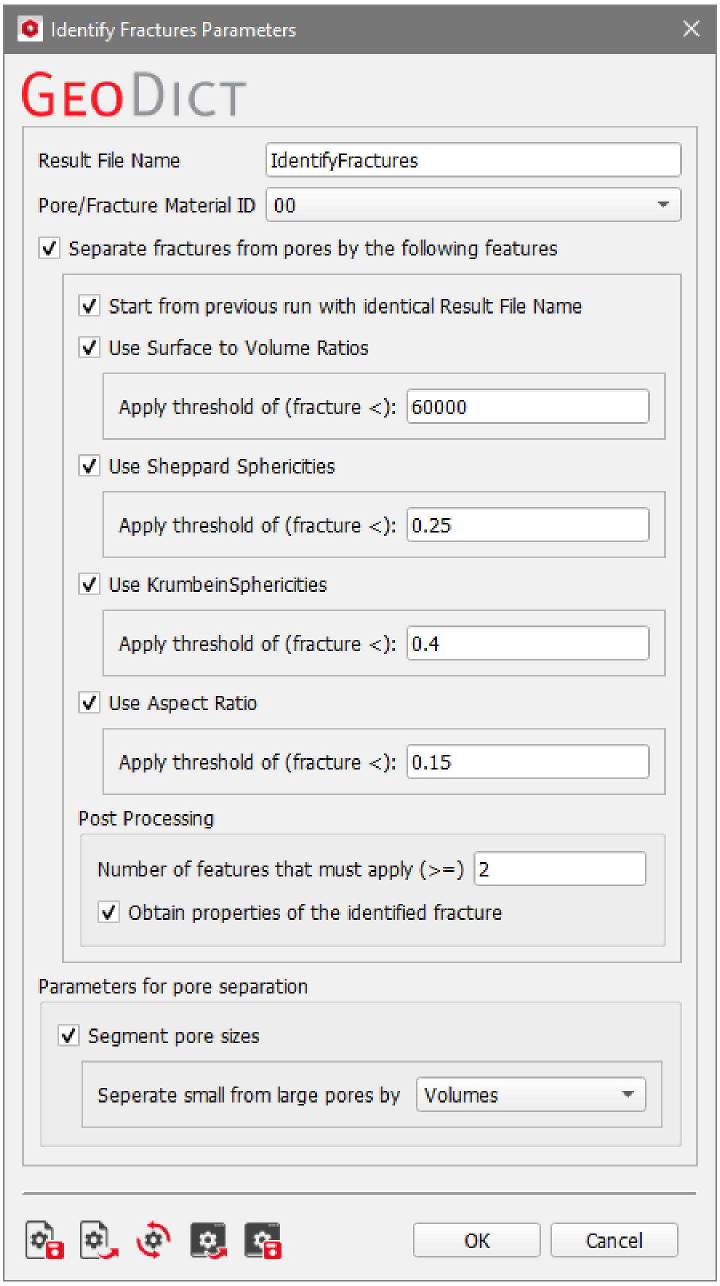
Modules needed to run this GeoApp: PoroDict

Clicking **Edit...** opens the **Identify Fractures Parameters** dialog.

There are two main features of the **Identify Fractures** app.

The first main feature **Separate fractures from pores by the following features** segments the selected **Pore/Fracture Material ID** into fracture and pore phase.

The second main feature **Segment pore sizes** allows the differentiation between small and large pores. When both features are activated, the differentiation of the pore sizes will be performed only on the pore phase, not on the fracture phase.

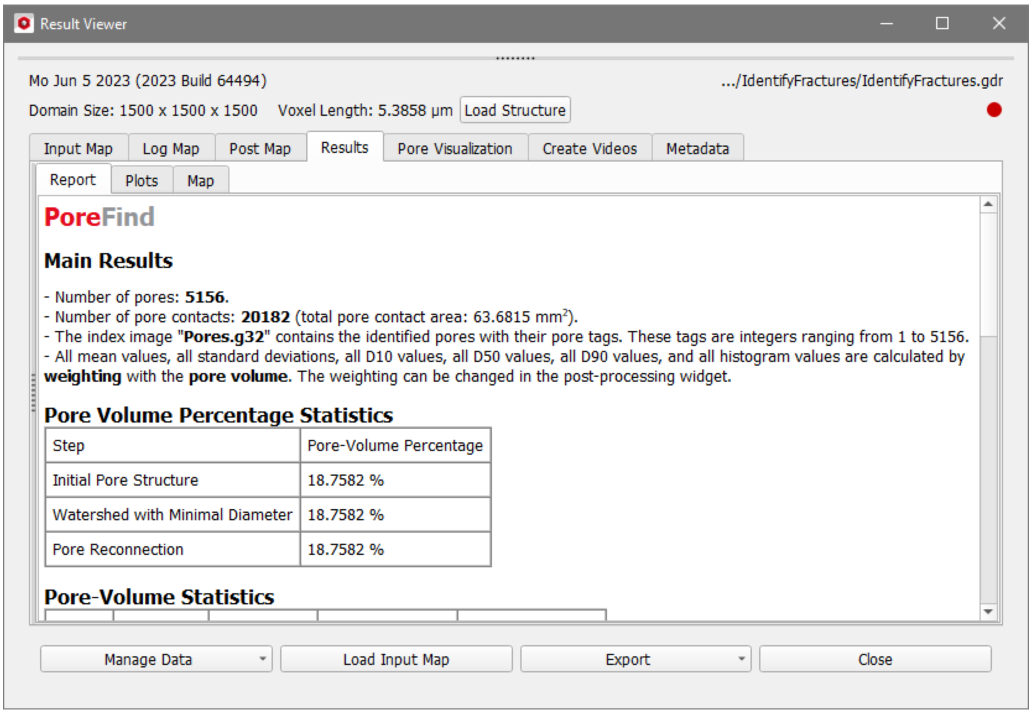


For the fracture identification, the chosen threshold values consider void space in a structure as a fracture if the values are below a chosen threshold for each parameter. The parameters can be modified if needed. The default threshold values may already segment fractures correctly. To improve the result, adjust the threshold values accordingly to the current structure. In the **Post Processing** section, the **Number of features that must apply** to identify a fracture phase can be chosen. The number must always be smaller or equal to the number of activated features. When **Obtain properties of the identified fracture** is activated, an additional instance of **Identify Pores** is executed on the previously identified fractures.

If **Identify Fractures** was executed on a structure but the segmentation needs to be improved, the app should be re-executed to obtain the best result iteratively. That can be done by re-executing the app with different values until a sufficient result is achieved. To save time, activate **Start from previous run with identical Result File Name**. This skips the first **Identify Pores** instance and uses the previously created *.gdr to execute **Post Processing**.

Click **OK** to close the dialog, go back to the **GeoApp** section, and click **Run**.

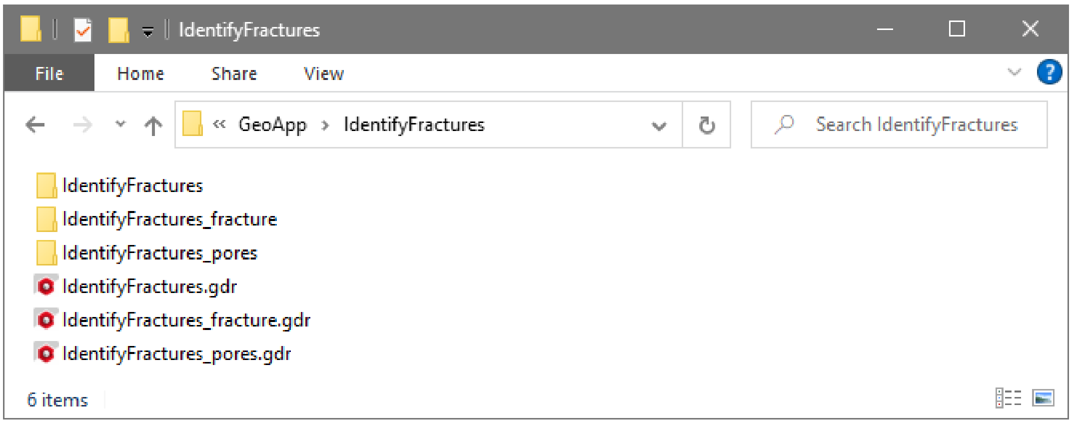
When the macro run is finished, and the checkbox of **Obtain properties of the identified fracture** is checked, the **Result Viewer** of the result file (*.gdr) opens automatically. Find the results in the **Results** → **Report**, **Results** → **Plots** and **Pore Visualization** tabs. The result file is created with **PoroDict** → **Identify Pores**. Thus, for detailed information about the result file content refer to the PoroDict handbook.



Three result files and result folders are generated and can be found in the project folder.

The prefix is based on the chosen Result File Name (default is **IdentifyFractures**). The **IdentifyFractures** folder contains the results of the **Identify Pores** instance which was executed on the structure. The thresholding of the fractures by features, which can be performed with the script, is executed on the contained **IdentifyFractures.gdr**. When **Obtain properties of the identified fracture** is activated, the **IdentifyFractures_fracture** folder contains results of the respective **Identify Pores** run. When **Segment pore sizes** is activated, the pores in the structure are segmented by their **Volume** or **Equivalent diameters**.

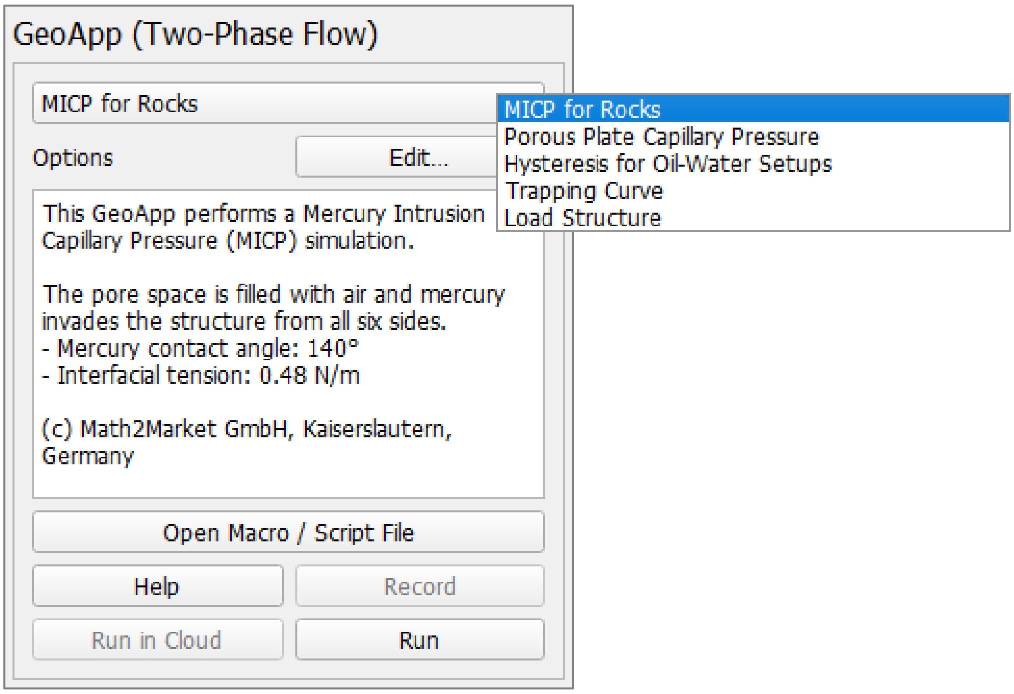
In this case, the folder **IdentifyFractures_pores** is created which contains the **Identify Pores** run performed on the pores.



Two-Phase Flow

The **GeoApp (Two-Phase Flow)** section contains the following, selectable from the pull-down menu:

- **MICP for Rocks:** perform a Mercury Intrusion Capillary Pressure (MICP) simulation.
- **Porous Plate Capillary Pressure:** run a Porous Plate Capillary Pressure (PPCP) simulation.
- **Hysteresis for Oil-Water Setups:** predict a Capillary Pressure Hysteresis Cycle in an oil-water setup.
- **Trapping Curve:** creates a trapping curve for the currently loaded structure and given contact angle.
- **Load Structure:** Load a structure file and adjust material IDs and colors

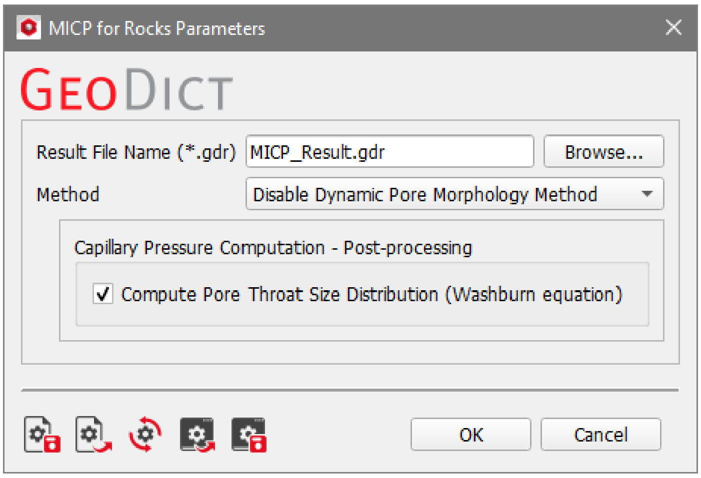


MICP for Rocks

The **MICP for Rocks** app performs a Mercury Intrusion Capillary Pressure (MICP) simulation.

Modules needed to run this GeoApp: SatuDict

Clicking **Edit...** opens the **MICP for Rocks** dialog.



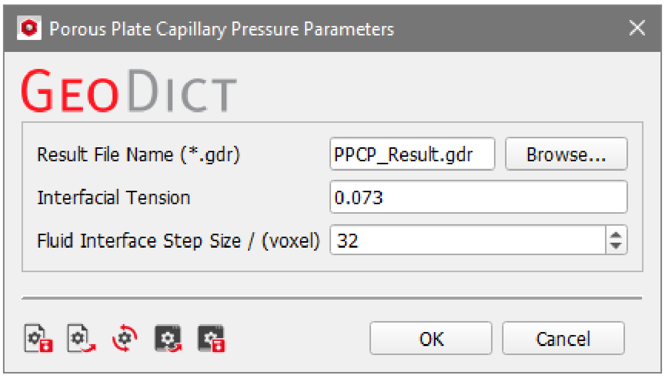
Find a description and examples in the SatuDict handbook.

Porous Plate Capillary Pressure

The **Porous Plate Capillary Pressure** app fills the pore space of the current structure with water. Then, air invades the structure from all but one side. The face in Z- direction is connected to a porous plate. The Porous Plate Capillary Pressure app is similar to the MICP app, but here air displaces water.

Modules needed to run this GeoApp: SatuDict

Clicking **Edit...** opens the **Porous Plate Capillary Pressure Parameters** dialog.



Enter the **Result File Name** for the generated GeoDict result file (*.gdr) and the corresponding result folder.

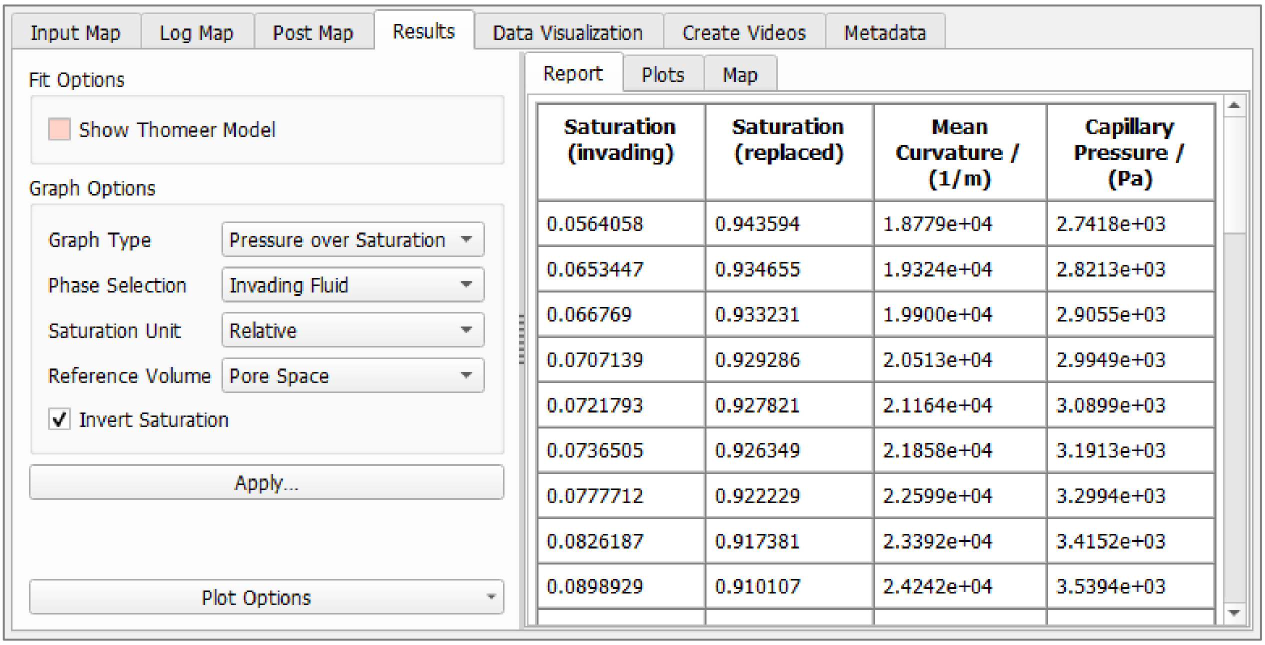
Two parameters can be defined.

Set the **Interfacial Tension** in N/m between water and air. The given default value refers to the value at 20°C for an air contact angle of 140°. The air contact angle cannot be changed.

The **Fluid Interface Step Size** determines the range of voxels that can be maximally saturated within one pressure step. Lower values might increase the runtime and the number of saturation steps significantly, but give a more realistic development of the saturation process.

Clicking **Run** runs the capillary pressure simulation. The pore space is filled with water then air invades the structure from all sides except of Z-.

After the simulation is finished, the result file is opened in the **Result Viewer**. Refer to the SatuDict handbook for more details regarding the results.



Saturation (invading)	Saturation (replaced)	Mean Curvature / (1/m)	Capillary Pressure / (Pa)
0.0564058	0.943594	1.8779e+04	2.7418e+03
0.0653447	0.934655	1.9324e+04	2.8213e+03
0.066769	0.933231	1.9900e+04	2.9055e+03
0.0707139	0.929286	2.0513e+04	2.9949e+03
0.0721793	0.927821	2.1164e+04	3.0899e+03
0.0736505	0.926349	2.1858e+04	3.1913e+03
0.0777712	0.922229	2.2599e+04	3.2994e+03
0.0826187	0.917381	2.3392e+04	3.4152e+03
0.0898929	0.910107	2.4242e+04	3.5394e+03

Hysteresis for Oil-Water Setups

The **Hysteresis for Oil-Water Setups** app predicts a capillary pressure hysteresis cycle in an oil-water setup with primary drainage, spontaneous and forced imbibition and, if selected, secondary drainage.

Modules needed to run this GeoApp: SatuDict

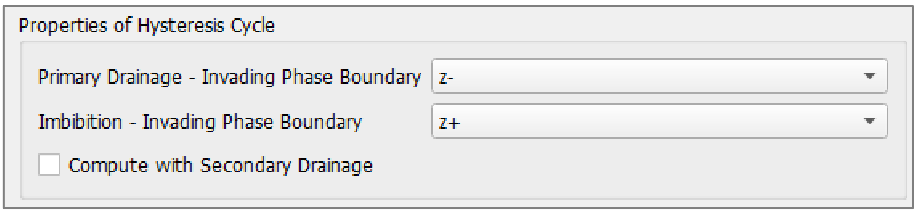
Clicking **Edit...** opens the **Hysteresis for Oil-Water setups Parameters** dialog.

Select a **Result File Name** fitting to the current project.

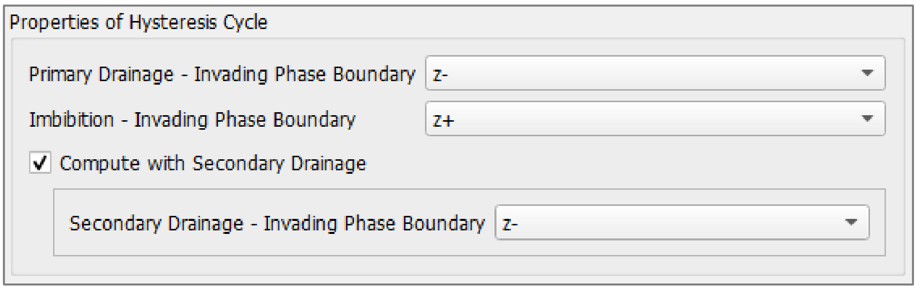
The parameters are organized into three groups.

Properties of Hysteresis Cycle

Define the **Properties of Hysteresis Cycle**. Set the **Primary Drainage – Invading Phase Boundary** side and the **Imbibition – Invading Phase Boundary** side.



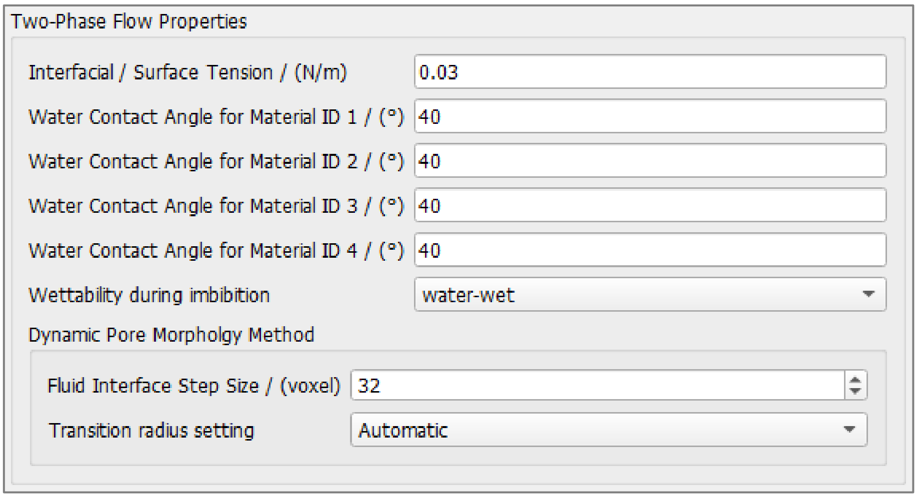
Select if also **Secondary Drainage** should be considered in the computation and choose the invading phase boundary for it.



Two-Phase Flow Properties

Set the **Two-Phase Flow Properties**.

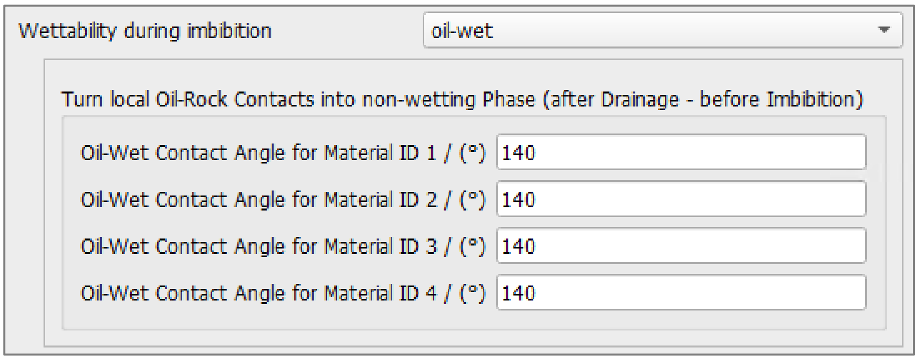
Define the **Interfacial /Surface Tension** in N/m between the two material phases water and oil. At the beginning the structure is filled with water and all solids are water-wet. For up to four solid materials the **Water Contact Angle** can be set. During the primary drainage simulation oil enters the structure. The contact angle of the solids to the oil is 180° - Water Contact Angle.



After the primary drainage, the wettability of the solids may change for the imbibition and secondary drainage. The **Wettability during imbibition** can be selected from the pull-down menu.

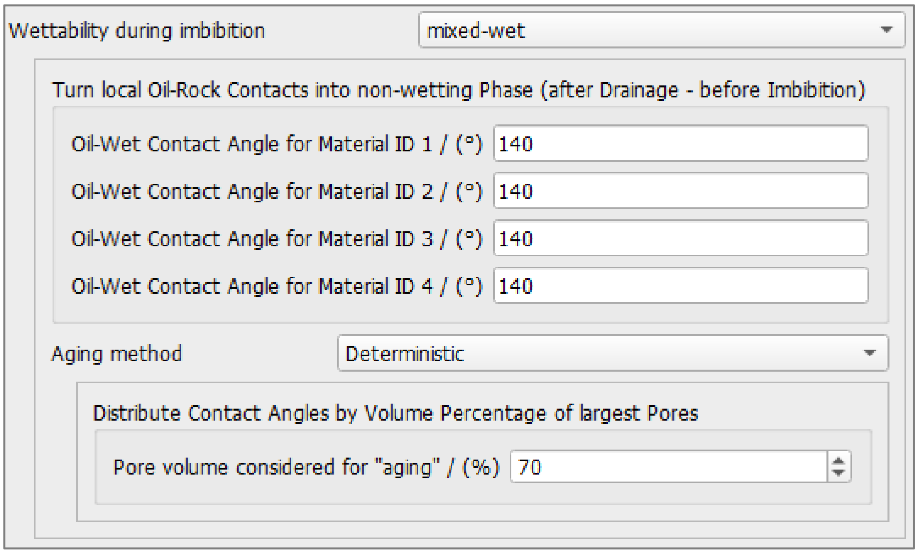
If **water-wet** is chosen, nothing changes after the primary drainage and all solid surfaces remain water-wet. For **mixed-wet** the wettability only changes locally after the primary drainage. If **oil-wet** is selected, the wettability changes globally after primary drainage. All solid surfaces that are covered by oil change from water-wet surfaces to oil-wet surfaces. They are then non-wetting against water.

In the case of a changing wettability, the new contact angles for the oil-rock contacts must be defined. Again, for up to four solid material IDs the **Oil-Wet Contact Angles** can be defined.

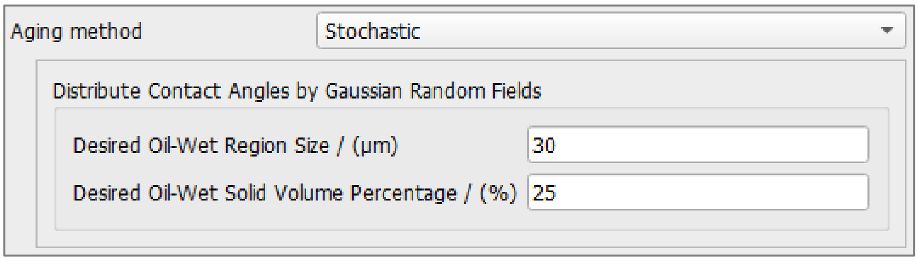


For a **mixed-wet** set-up also the distribution of the oil-wet solids must be specified. First, select an **Aging Method** and then set the corresponding parameters. The aging method introduces which surfaces change their wettability after the primary drainage and before the imbibition.

For a **Deterministic** aging method, the wettability is changed at surfaces in large pores and in contact with the invading oil. The **Pore volume considered for aging** defines the limit for the material reassignments to oil-rock surfaces in large pores. A geometric pore size distribution is applied to determine the pore space that allows consideration of oil-wet surfaces with adjusted contact angles. For example, a value of 70% means that the largest 70% of the pores is changed from water-wet to oil-wet. A higher percentage leads to more contact material changes and an increased saturation change during forced imbibition, while the saturation changes during spontaneous imbibition is decreased.



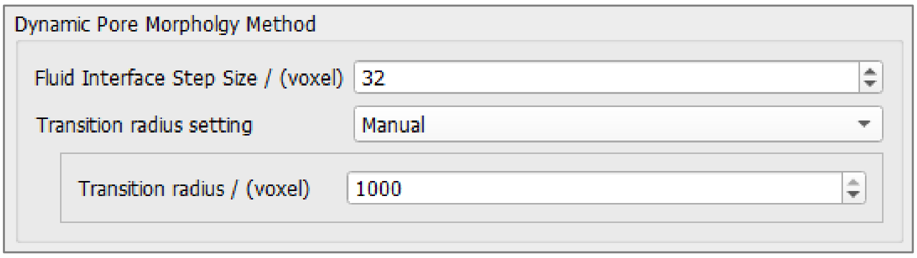
A **Stochastic** aging method distributes the wettability changes using Gaussian random fields. Define the **Desired Oil-Wet Region Size**, being the standard deviation for the applied Gaussian distribution. Additionally enter the **Desired Oil-Wet Solid Volume Percentage**.



Define the **Dynamic Pore Morphology Method** parameters.

The **Fluid Interface Step Size** defines how many voxels the computed fluid interface can move in each step. Lower values might increase the runtime significantly.

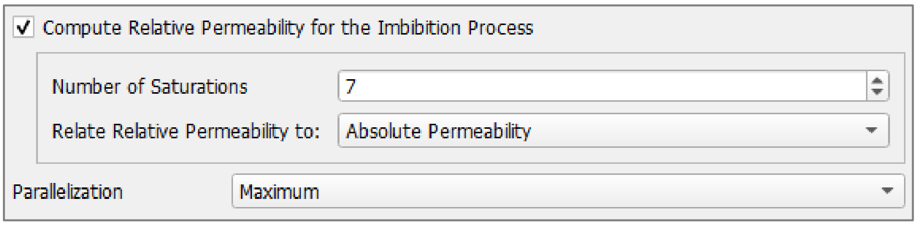
The imbibition starts with the spontaneous imbibition part. At some point, defined by the transition radius, the imbibition changes from spontaneous to forced. For the **Transition radius setting Automatic** this point is determined automatically. For a **Manual Transition Radius** define the sphere radius at which the dynamic transition from spontaneous to forced occurs. The meniscus of the water-front can be interpreted as a part of a circle. If this circle has a radius larger than the transition radius, the meniscus flips over, and the forced imbibition applies. This parameter is experimental. Examine the results carefully, especially if contact angles close to 90°are chosen.



Others

To compute the relative permeability during the imbibition check **Compute Relative Permeability for the Imbibition Process**. Define the **Number of Saturations** for which to compute the relative permeability. The default number of 7 means that for seven different saturations of the structure the permeability is computed. Increase the number to obtain more data points on the relative permeability curve. **Relate the Relative Permeability** to **Absolute Permeability**, where the permeability of the whole pore space is used as reference permeability, or to the **Oil Permeability at irreducible Water Saturation**, where the water trapped after the primary drainage is treated as solid. In this case only the pore space occupied by oil is used to compute the reference permeability.

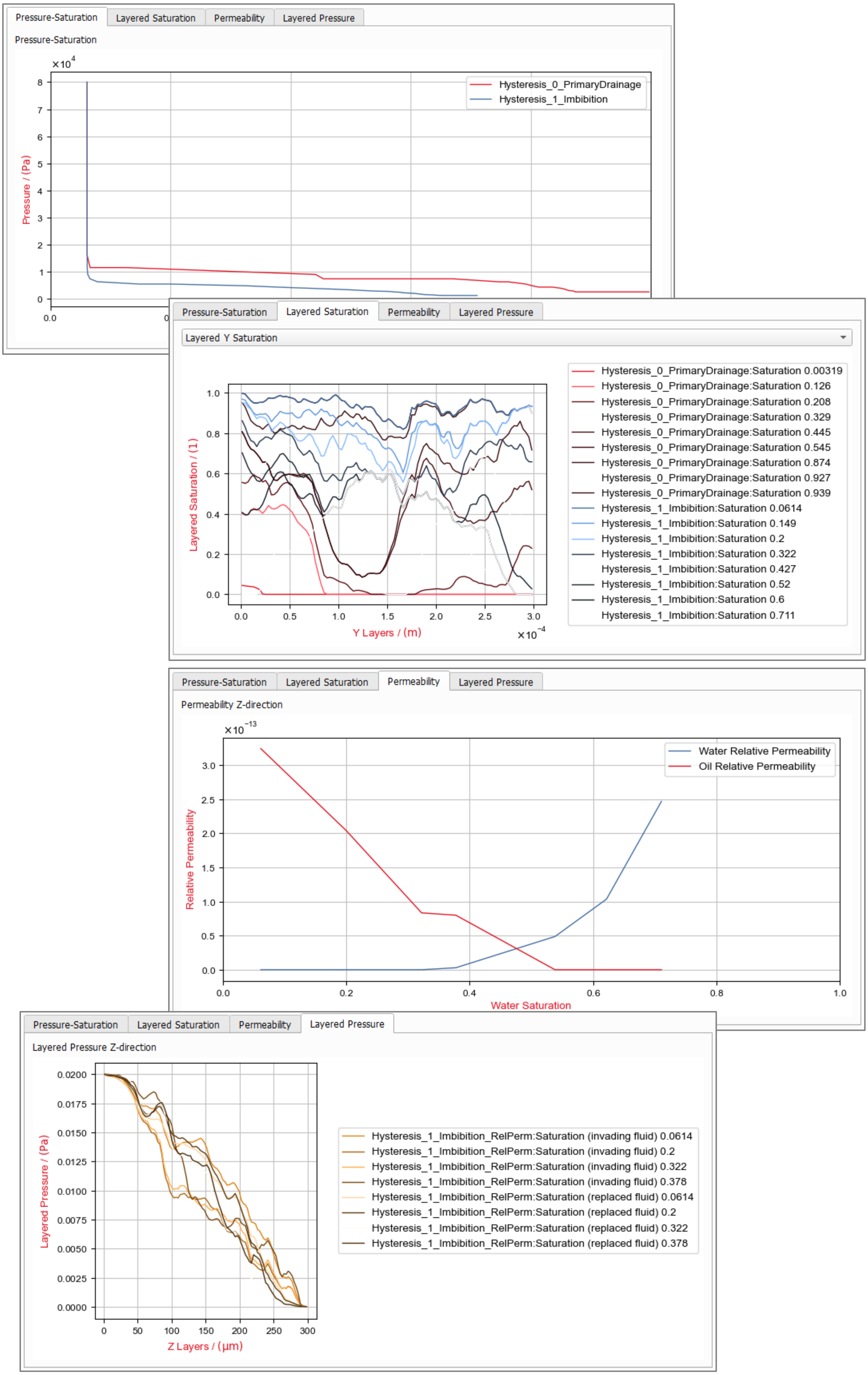
Finally, determine the **Parallelization** for the execution. Either use the maximal available or maximal licensed number of cores or enter a value **Manually**.



Click **OK** to save the settings made. Clicking **Run** performs the hysteresis simulation.

When the simulation finishes, the result file opens in the **Result Viewer** automatically.

The **Results** → **Plots** tab contains plots for **Pressure Saturation**, **Layered Saturation**, **Permeability** and **Layered Pressure**.

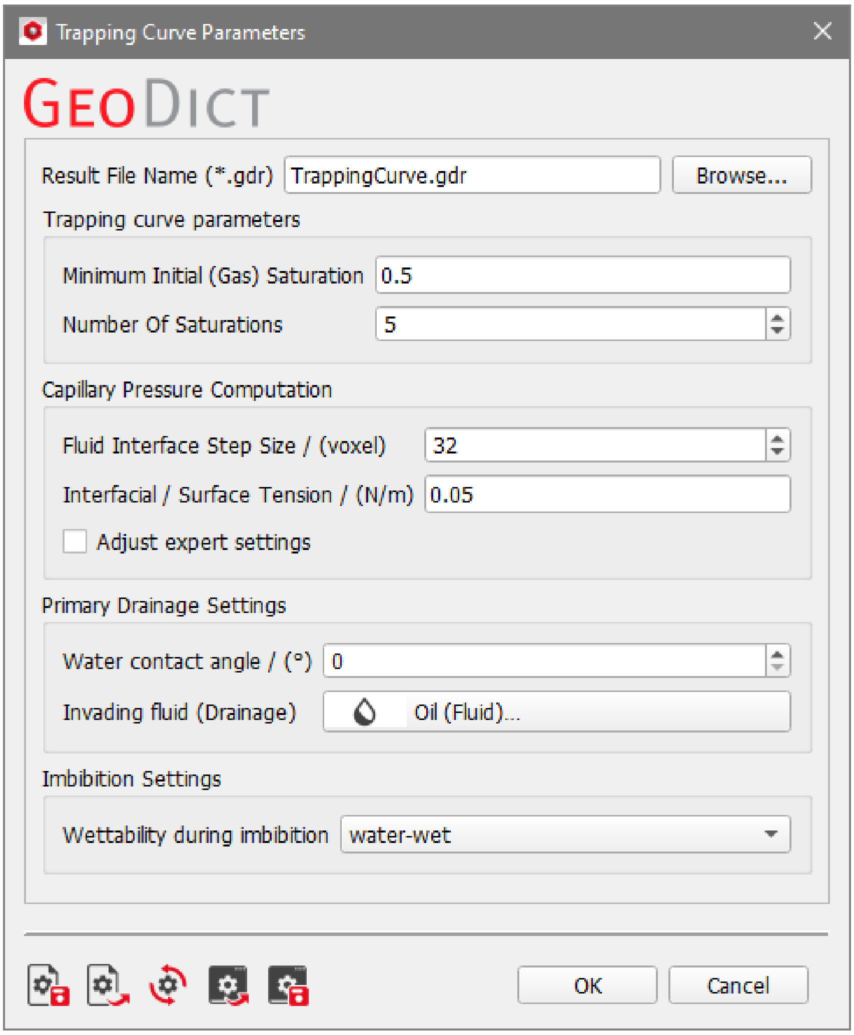

Pressure-Saturation
Layered Saturation
Permeability
Layered Pressure
Pressure-Saturation
Pressure / (Pa)
Hysteresis_0_PrimaryDrainage
Hysteresis_1_Imbibition
Layered Y Saturation
Layered Saturation / (1)
Y Layers / (m)
Hysteresis_0_PrimaryDrainage:Saturation 0.00319
Hysteresis_0_PrimaryDrainage:Saturation 0.126
Hysteresis_0_PrimaryDrainage:Saturation 0.208
Hysteresis_0_PrimaryDrainage:Saturation 0.329
Hysteresis_0_PrimaryDrainage:Saturation 0.445
Hysteresis_0_PrimaryDrainage:Saturation 0.545
Hysteresis_0_PrimaryDrainage:Saturation 0.874
Hysteresis_0_PrimaryDrainage:Saturation 0.927
Hysteresis_0_PrimaryDrainage:Saturation 0.939
Hysteresis_1_Imbibition:Saturation 0.0614
Hysteresis_1_Imbibition:Saturation 0.149
Hysteresis_1_Imbibition:Saturation 0.2
Hysteresis_1_Imbibition:Saturation 0.322
Hysteresis_1_Imbibition:Saturation 0.427
Hysteresis_1_Imbibition:Saturation 0.52
Hysteresis_1_Imbibition:Saturation 0.6
Hysteresis_1_Imbibition:Saturation 0.711
Permeability Z-direction
Relative Permeability
Water Saturation
Water Relative Permeability
Oil Relative Permeability
Layered Pressure Z-direction
Layered Pressure / (Pa)
Z Layers / (µm)
Hysteresis_1_Imbibition_RelPerm:Saturation (invading fluid) 0.0614
Hysteresis_1_Imbibition_RelPerm:Saturation (invading fluid) 0.2
Hysteresis_1_Imbibition_RelPerm:Saturation (invading fluid) 0.322
Hysteresis_1_Imbibition_RelPerm:Saturation (invading fluid) 0.378
Hysteresis_1_Imbibition_RelPerm:Saturation (replaced fluid) 0.0614
Hysteresis_1_Imbibition_RelPerm:Saturation (replaced fluid) 0.2
Hysteresis_1_Imbibition_RelPerm:Saturation (replaced fluid) 0.322
Hysteresis_1_Imbibition_RelPerm:Saturation (replaced fluid) 0.378

Trapping Curve

The **Trapping Curve** app predicts a capillary pressure hysteresis cycle and creates a trapping curve for the currently loaded structure and given contact angle. Initially the pore space is filled with water. Then a primary drainage with a chosen invading fluid is computed. For a chosen number of saturation steps a secondary imbibition with water is computed.

Modules needed to run this GeoApp: SatuDict

Clicking **Edit...** opens the **Trapping Curve Parameters** dialog.



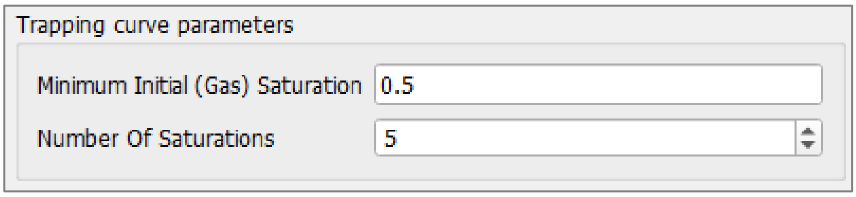
The parameters are organized in four groups.

Trapping curve parameters

Set the **Minimum Initial (Gas) Saturation** to determine the trapping curve from fully gas-saturated pore volume down to the given value between 0 and 1.

Define the **Number of Saturations**, i.e. the number of imbibitions calculated for the trapping curve.

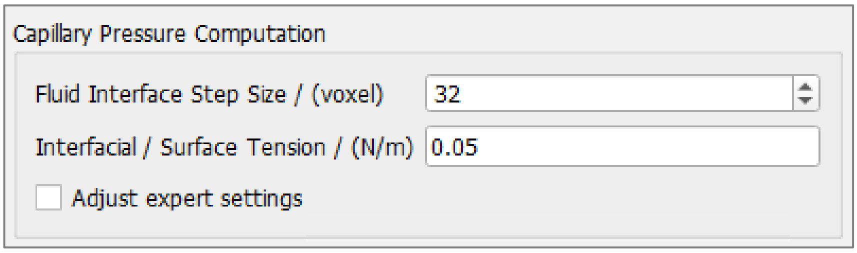
The starting saturations of the invading fluid for the imbibition are distributed between the value entered in Minimum Initial Saturation and 1.



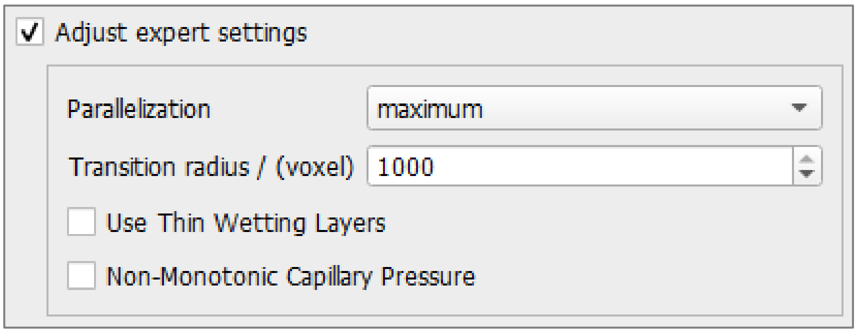
Capillary Pressure Computation

Define the **Fluid Interface Step Size** for the corresponding capillary pressure method. The **Fluid Interface Step Size** determines the range of voxels that can be maximally saturated within one pressure step. Note, that lower values might increase the runtime significantly.

Set the **Interfacial / Surface Tension** between the invading and the replaced fluid.

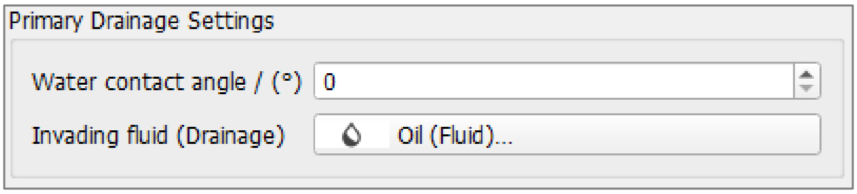


The available expert settings include **Parallelization**, **Transition radius**, and if **Thin Wetting Layers** and **Non-Monotonic Capillary Pressure** should be applied. Refer to the SatuDict handbook for a detailed explanation of these saturation experiment parameters.



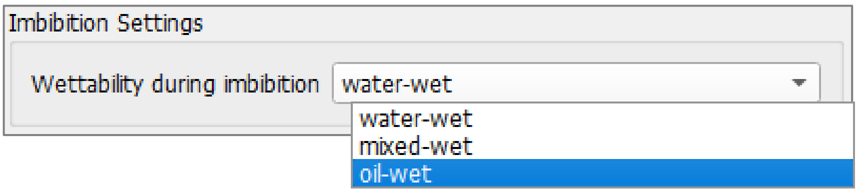
Primary Drainage Settings

By default, the initial pore fluid is water. Enter the **Water contact angle** that is used for the primary drainage computation. Select the **Invading fluid** for the primary drainage from the material database.



Imbibition Settings

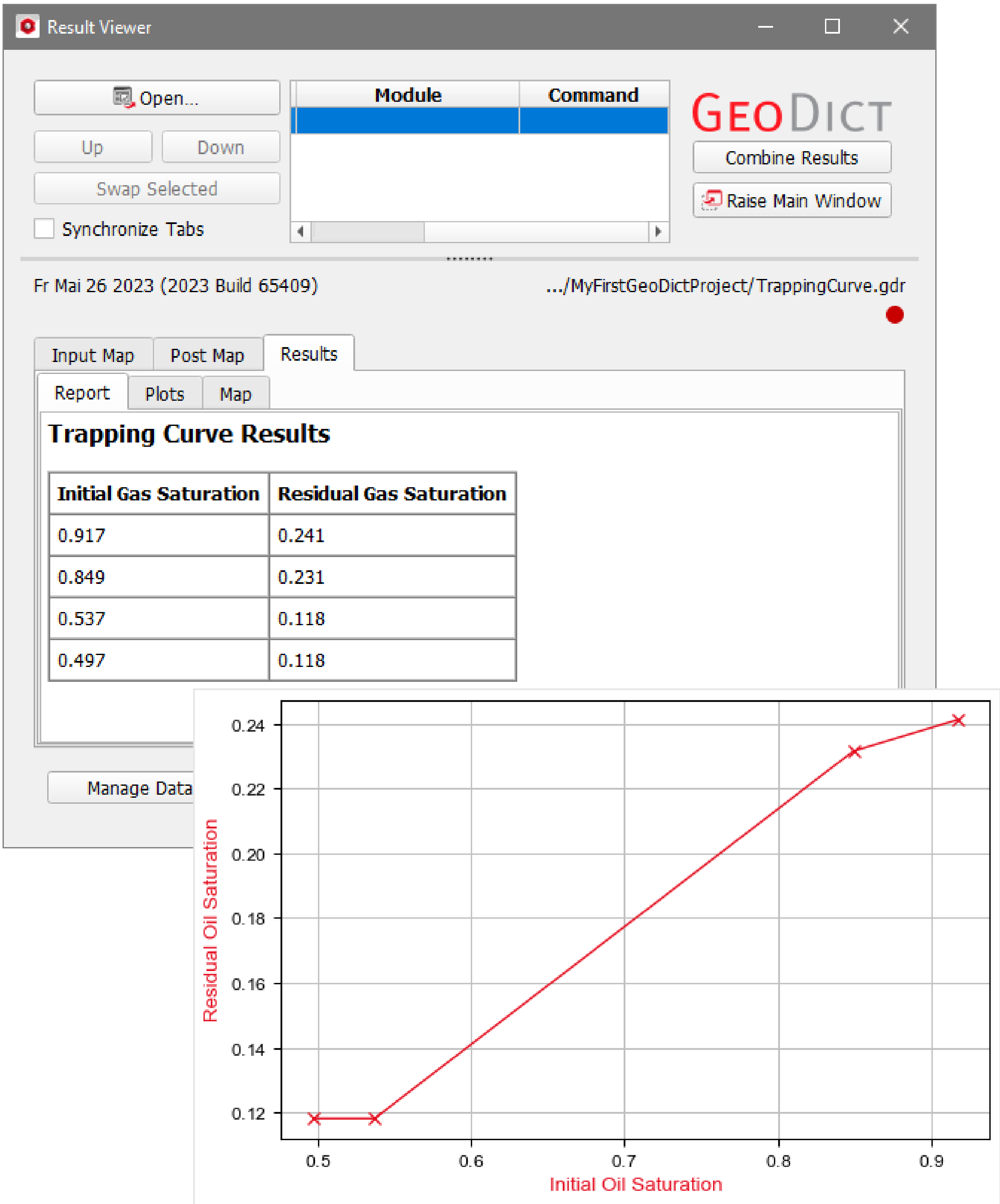
Set the **Wettability during imbibition** as explained for the **Hysteresis** app on page 64. Note, that here oil-wet means that the solid surfaces covered with the invading fluid (not necessarily oil) change their wettability.



Clicking **Run** creates the trapping curve.

When the simulation finishes, the result file opens in the **Result Viewer** automatically.

The **Results → Report** subtab of the Result Viewer shows a table with the saturation of the invading fluid at the beginning of the imbibition (**Initial Gas Saturation**) and after the imbibition (**Residual Gas Saturation**). These values are also plotted in a **Trapping curve** available in the **Plots** subtab.



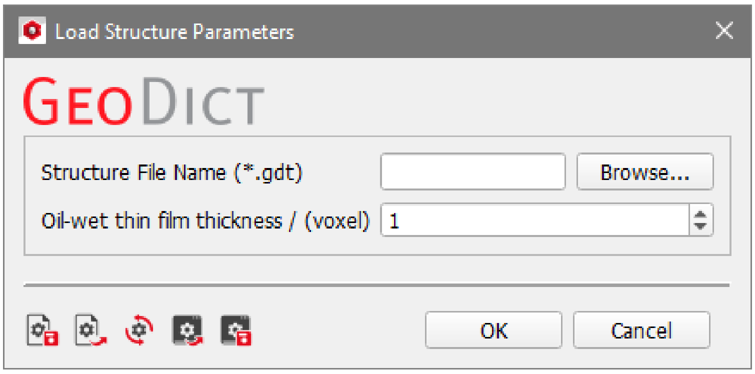
Load Structure

The **Load Structure** app loads a chosen structure file (*.gdt) and adjusts the material IDs and material colors. The app is dedicated to adjust the visualization after mixed-wettability setup simulations were performed.

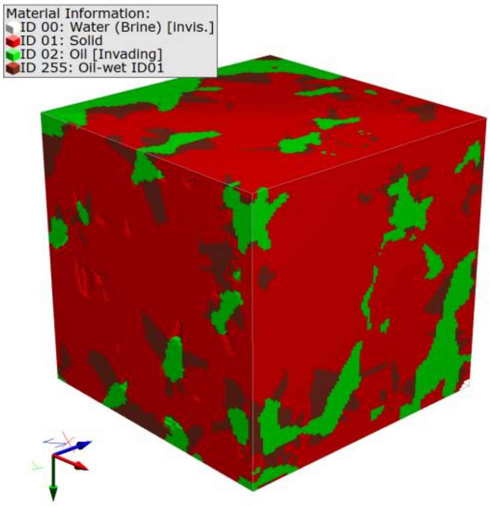
Modules needed to run this GeoApp: GeoDict-Base

Clicking **Edit...** opens the **Load Structure Parameters** dialog.

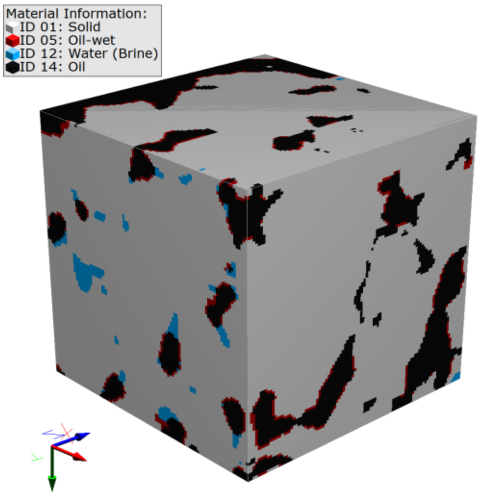
Browse for the structure to load and set the **Oil-wet thin film thickness**. This adjusts oil-wet materials to thin films for a representative structure appearance.



Clicking **Run** loads the structure to GeoDict with materials assigned and colored fitting to a forced imbibition set-up.



Structure loaded with **File → Load Structure** and default material colors applied



Structure loaded with the **Load Structure** GeoApp and material colors changed

Filtration

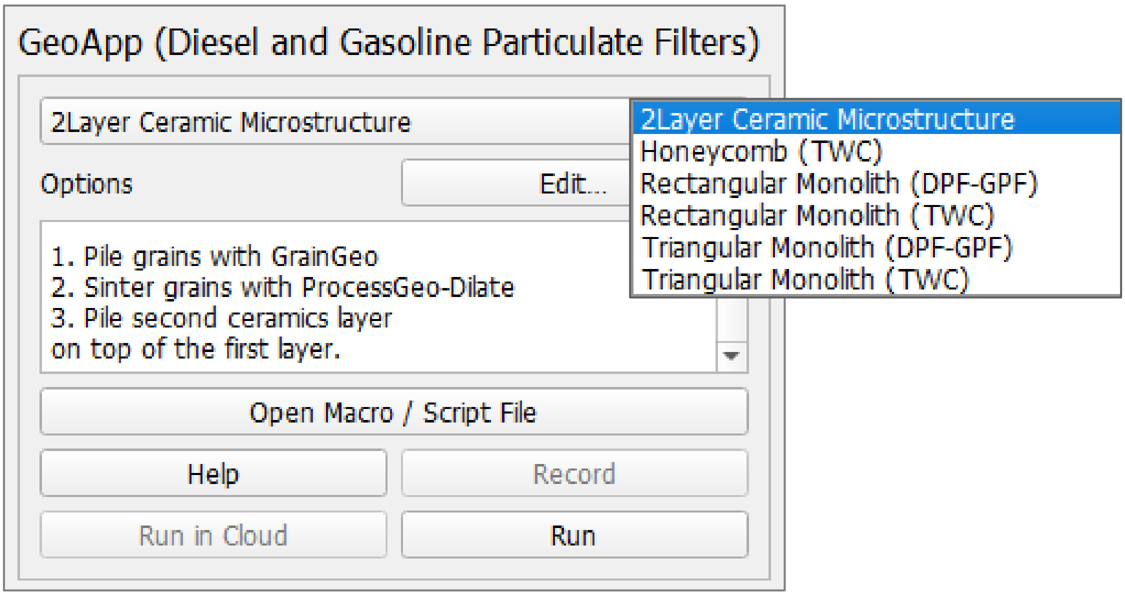
Two **Filtration** GeoApp modules are shipped with GeoDict:

- Create **Diesel and Gasoline Particulate Filter** structures.
- Create complete filters and optimize pleats with the **Filter and Pleat Optimization** apps.

Diesel and Gasoline Particulate Filter

The **GeoApp (Diesel and Gasoline Particulate Filters)** section contains the following, selectable from the pull-down menu:

- **2Layer Ceramic Microstructure:** create a two-layer ceramic.
- **Honeycomb (TWC):** create a three-way catalyst monolith hexagonal combs.
- **Rectangular Monolith (DPF-GPF):** create a Diesel Particulate Filter / Gasoline Particulate Filter with rectangular combs, which are partly closed.
- **Rectangular Monolith (TWC):** create a three-way catalyst monolith with rectangular combs.
- **Triangular Monolith (DPF-GPF):** create a Diesel Particulate Filter / Gasoline Particulate Filter with triangular combs, which are partly closed.
- **Triangular Monolith (TWC):** create a three-way catalyst monolith with triangular combs.

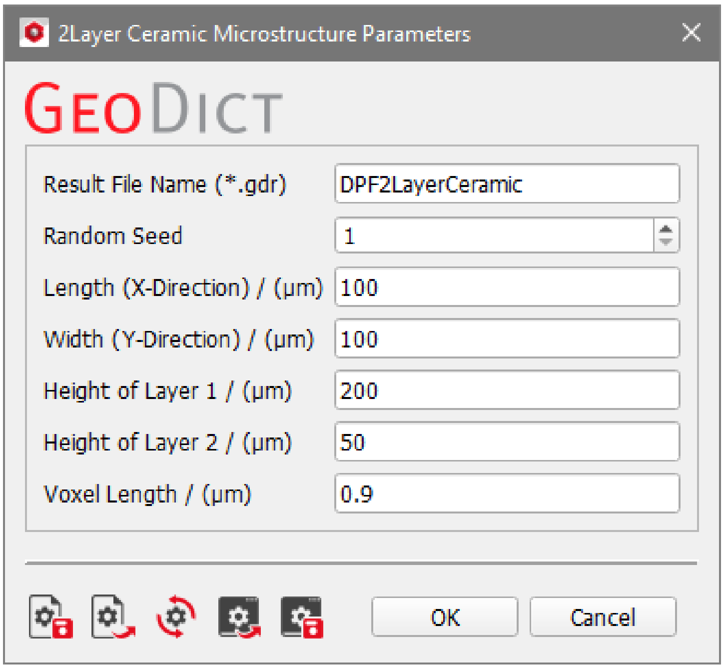


2Layer Ceramic Microstructure

The **2Layer Ceramic Microstructure** app generates a two-layer ceramic to be used as a diesel particulate filter.

Modules needed to run this GeoApp:
GrainGeo

Clicking **Edit…** opens the **2Layer Ceramic Microstructures Parameters** dialog.



Define the **Result File Name**, the **Random Seed**, the **Length** in X-direction, the **Width** in Y-direction, the **Height** of both layers and the **Voxel Length**.

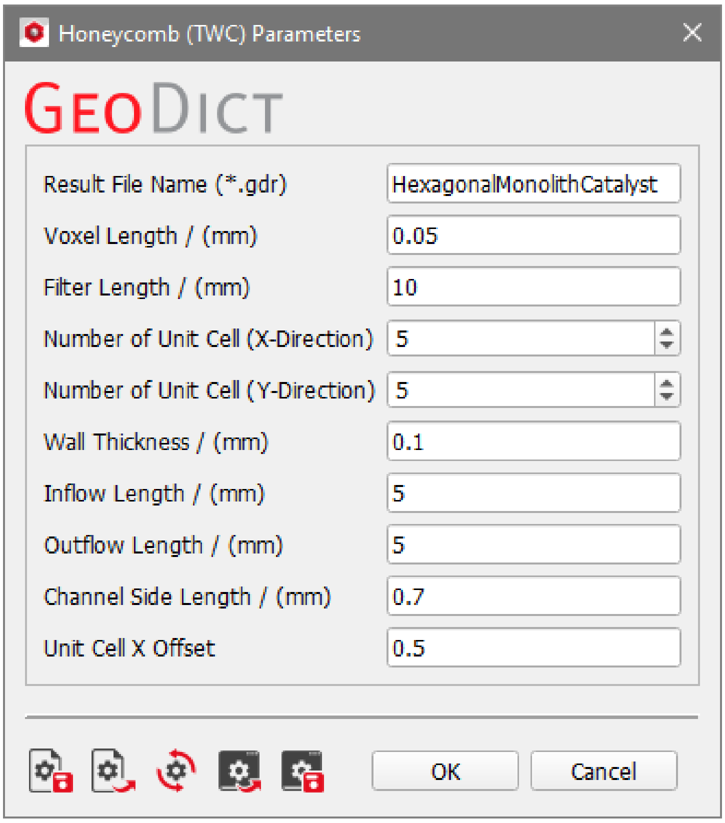
Clicking **Run** creates the two-layer ceramic.

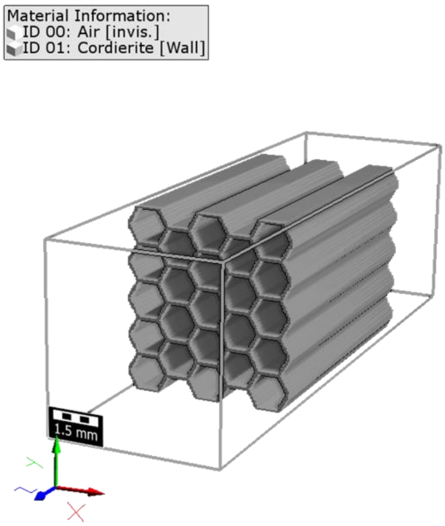
Honeycomb (TWC)

The **Honeycomb (TWC)** app generates a three-way catalyst monolith hexagonal combs.

Modules needed to run this GeoApp:
GridGeo

Clicking **Edit...** opens the **Honeycomb (TWC) Parameters** dialog.





Define the following parameters:

- **Result File Name**,
- the **Voxel Length**,
- the **Filter Length** in Z-direction without inflow and outflow region,
- the **Number of Unit Cells** in X- and Y-direction,
- the **Wall Thickness**,
- the **Inflow Length**, defining an inflow region,
- the **Outflow Length**, defining the outflow region,
- the **Channel Side Length**, for the hexahedron sides,
- and the **Unit Cell X Offset** defining the cell positions in X-direction.

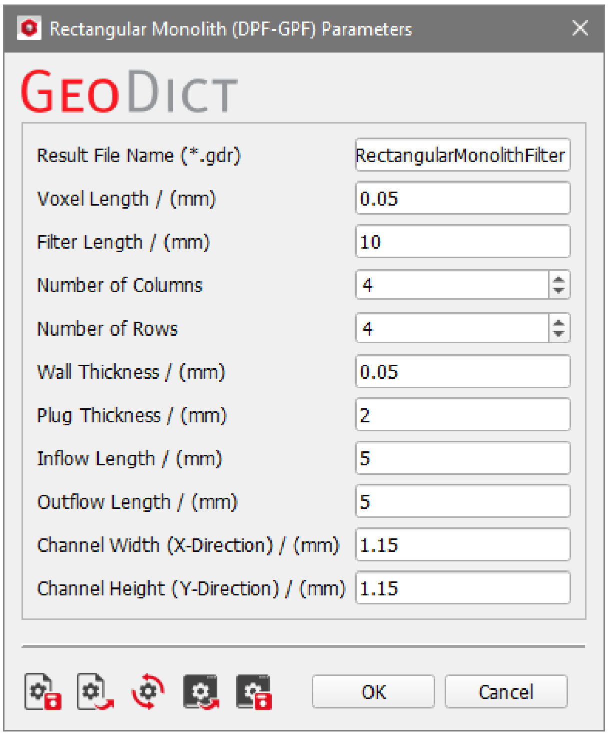
Clicking **Run** creates the honeycomb.

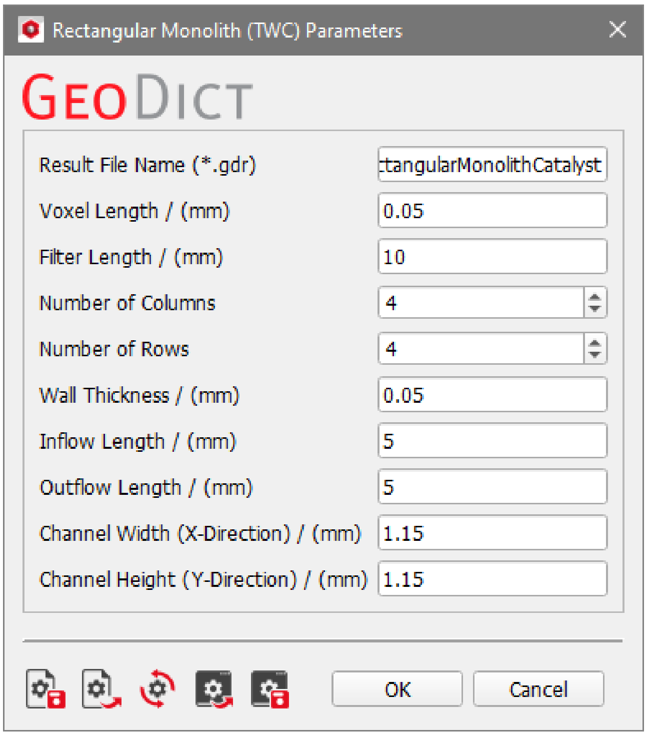
Rectangular Monolith (DPF-GPF) and (TWC)

The **Rectangular Monolith** apps generate a Diesel Particulate Filter / Gasoline Particulate Filter with rectangular combs. For the DPF-GPF variant, part of the pores are closed.

Modules needed to run this GeoApp: GridGeo

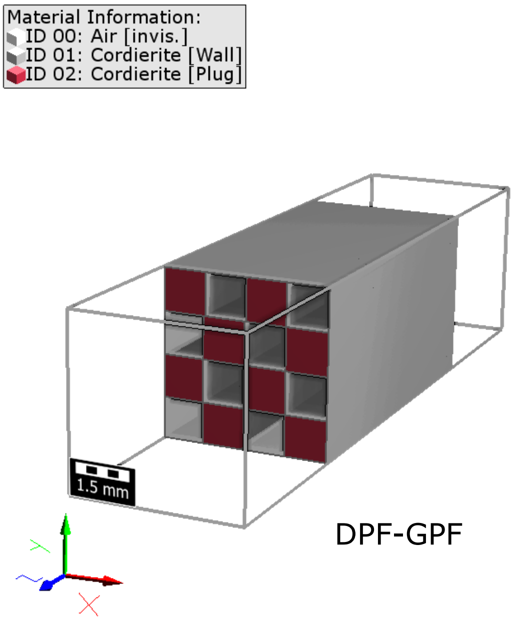
Clicking **Edit…** opens the **Rectangular Monolith Parameters** dialog.

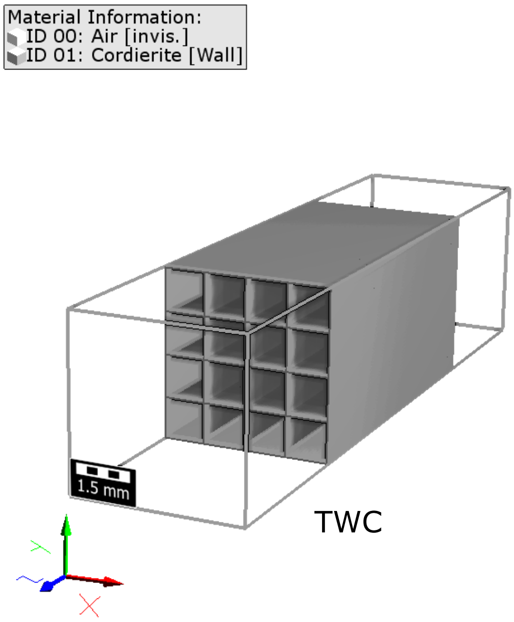




Define the **Result File Name**, the **Voxel Length**, the **Filter Length**, the **Number of Columns** and **Rows**, the **Wall Thickness**, the **Inflow Length**, the **Outflow Length**, the **Channel Width** and **Height**.

Clicking **Run** creates the rectangular monolith.



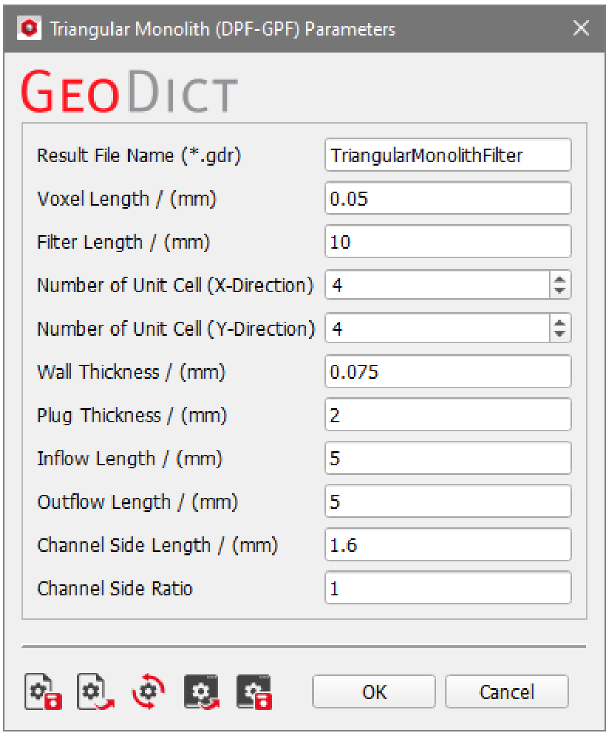


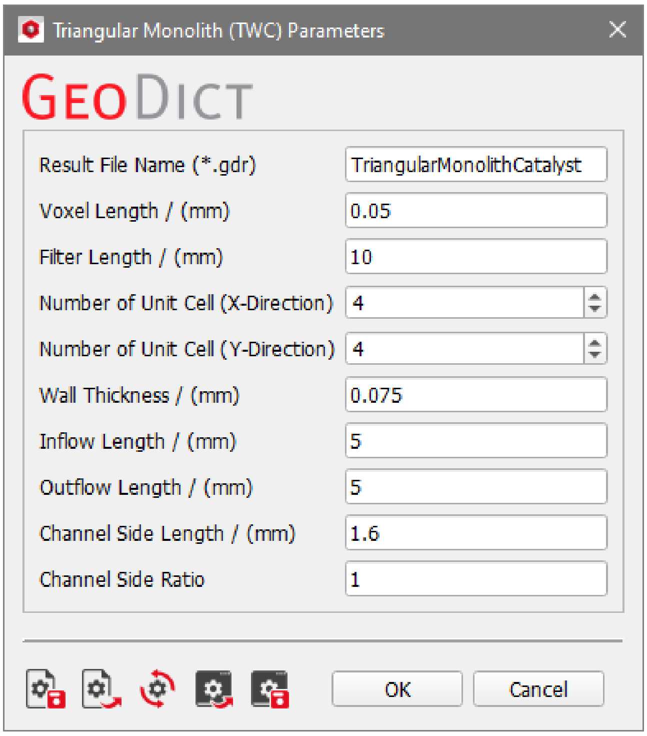
Triangular Monolith (DPF-GPF and TWC)

The **Triangular Monolith** apps generate a Diesel Particulate Filter / Gasoline Particulate Filter with triangular combs. For the DPF-GPF variant, part of the pores are closed.

Modules needed to run this GeoApp: GridGeo

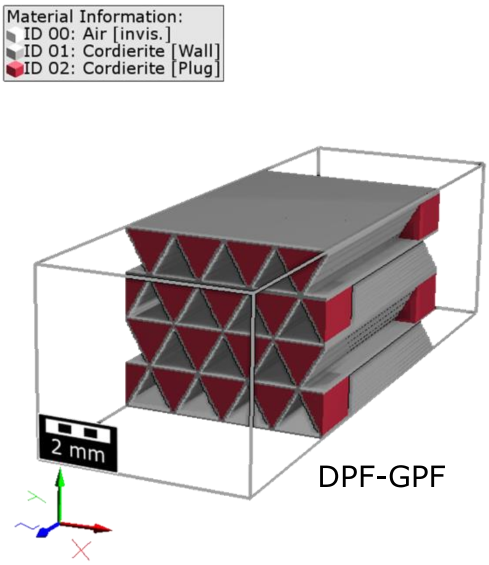
Clicking **Edit...** opens the **Triangular Monolith Parameters** dialog.

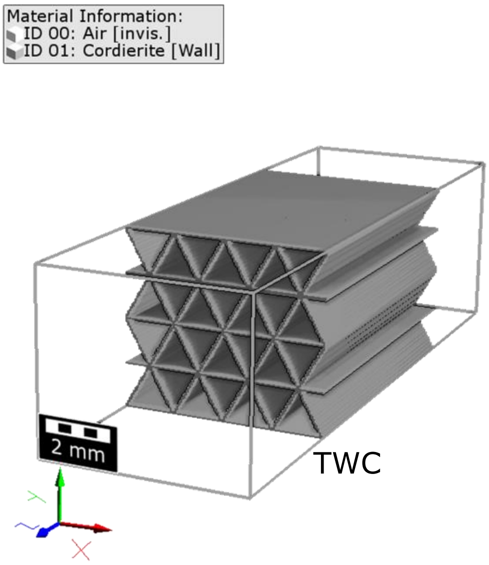




Define the **Result File Name**, the **Voxel Length**, the **Filter Length**, the **Number of Unit Cells** in X- and Y-direction, the **Wall Thickness**, the **Plug Thickness**, the **Inflow Length**, the **Outflow Length**, the **Channel Side Length** and **Side Ratio**.

Clicking **Run** creates the rectangular monolith.

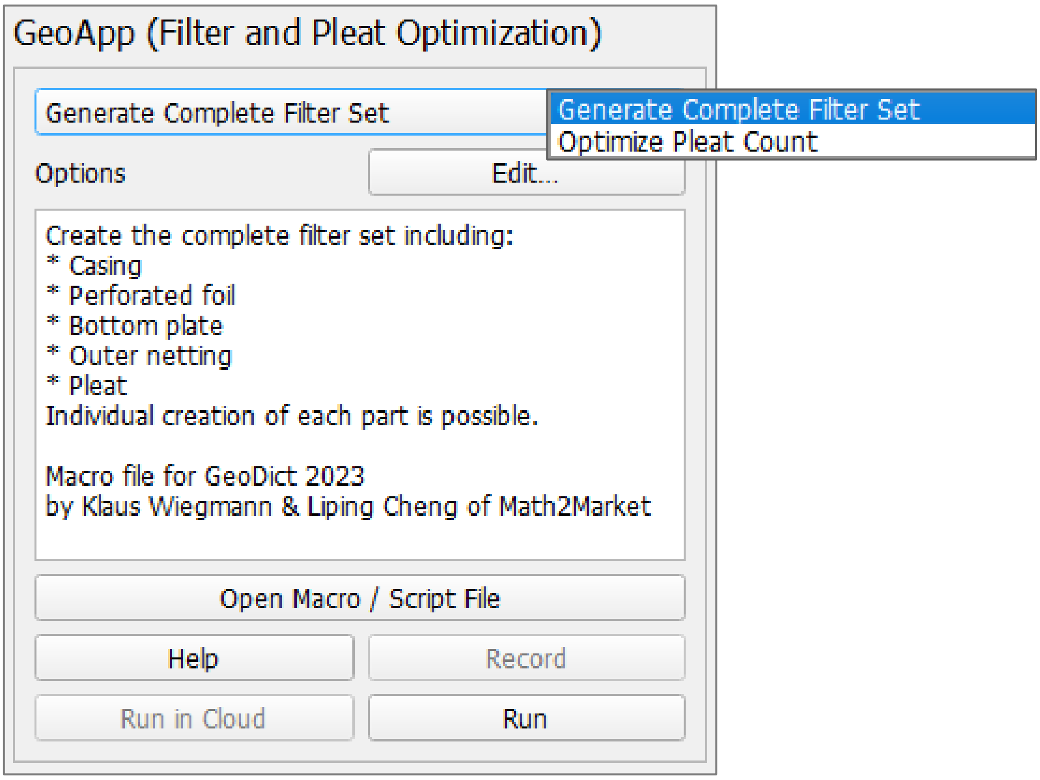




Filter and Pleat Optimization

The **GeoApp (Filter and Pleat Optimization)** section contains the following, selectable from the pull-down menu:

- **Generate Complete Filter Set:** create a complete filter with casing, foil, plates, netting and pleats.
- **Optimize Pleat Count:** optimize the number of pleats in a pleat filter.



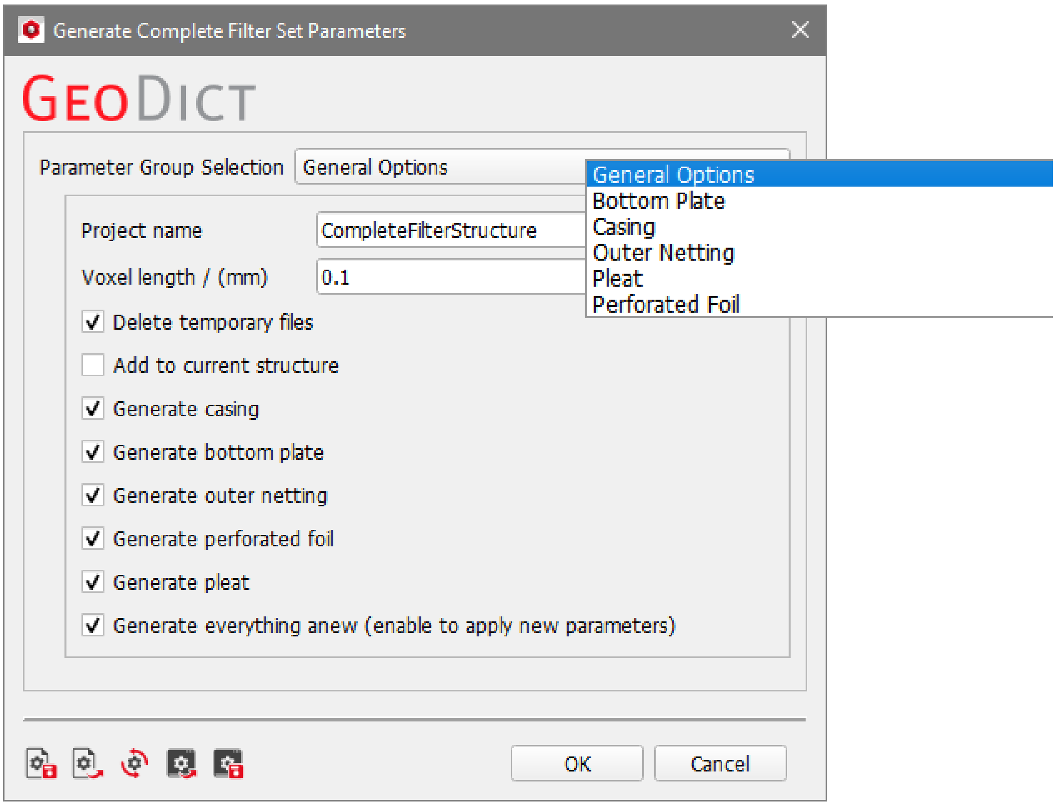
Generate Complete Filter Set

The **Generate Complete Filter Set** app generates an individual complete filter including casing, perforated foil, bottom plate, outer netting and pleat. It is also possible to only generate any subset of these filter parts.

Modules needed to run this GeoApp: PleatGeo

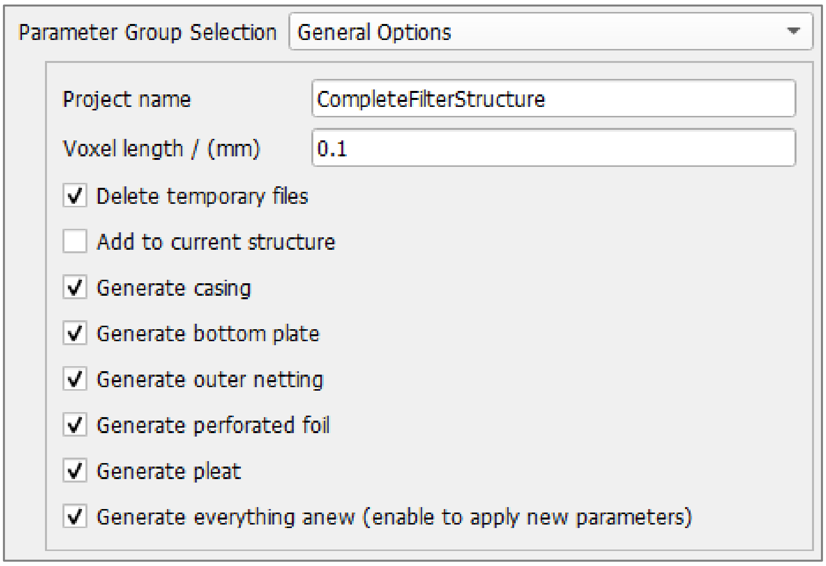
Clicking **Edit...** opens the **Generate Complete Filter Set Parameters** dialog.

The parameters are organized in six groups, available through the **Parameter Group Selection**.



General Options

In the **General Options** group specify a **Project name** for the folder containing all the results and the **Voxel Length** for the filter set.



Check **Delete temporary files** to delete intermediate results after the filter generation.

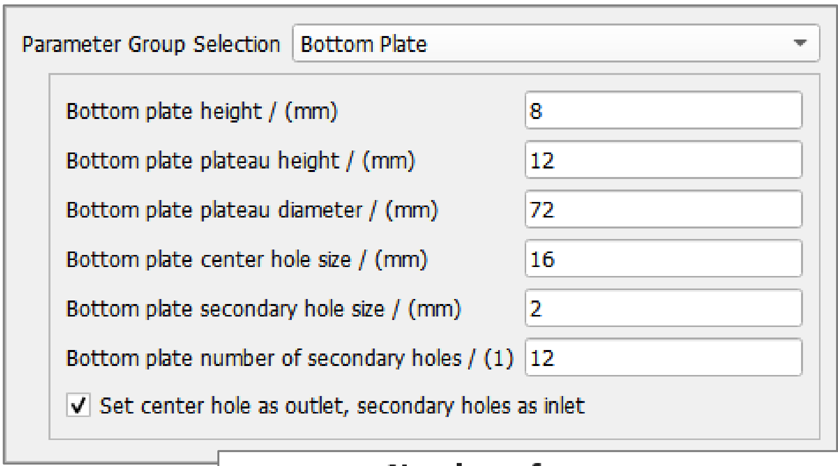
Check **Add to current structure**, if a filter structure is already loaded in GeoDict and needs some more components as for example a casing.

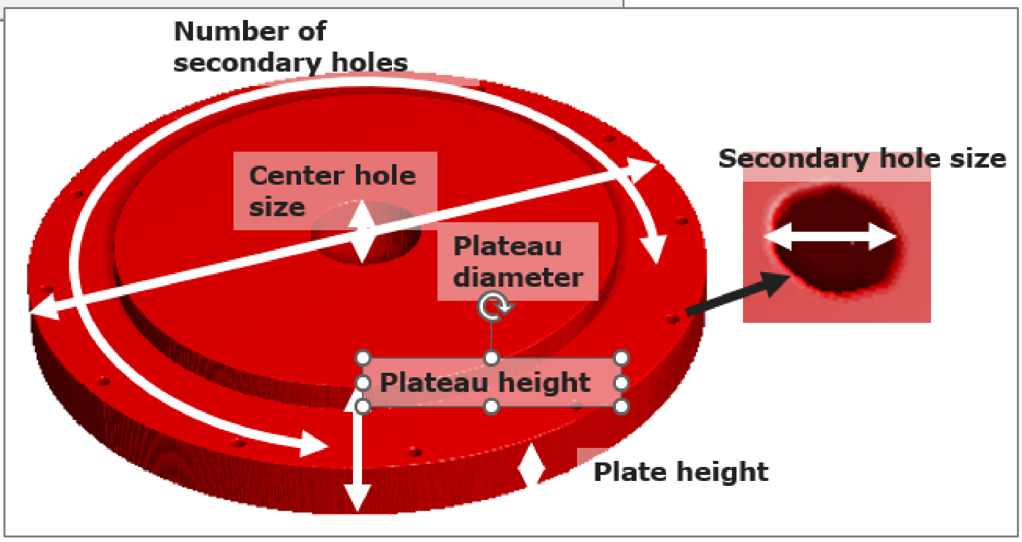
Decide which parts of the filter set should be generated. The possible filter parts are **casing**, **bottom plate**, **outer netting**, **perforated foil** and **pleat**. Define the corresponding parameters for each filter part in the respective parameter group available from the pull-down menu for **Parameter Group Selection**.

Enable **Generate everything anew (enable to apply new parameters)** if a completely new filter should be generated. If not checked, the GeoApp expects the corresponding filter parts to be in the folder specified by **Project name**.

Bottom Plate

Define the **Bottom Plate** parameters.





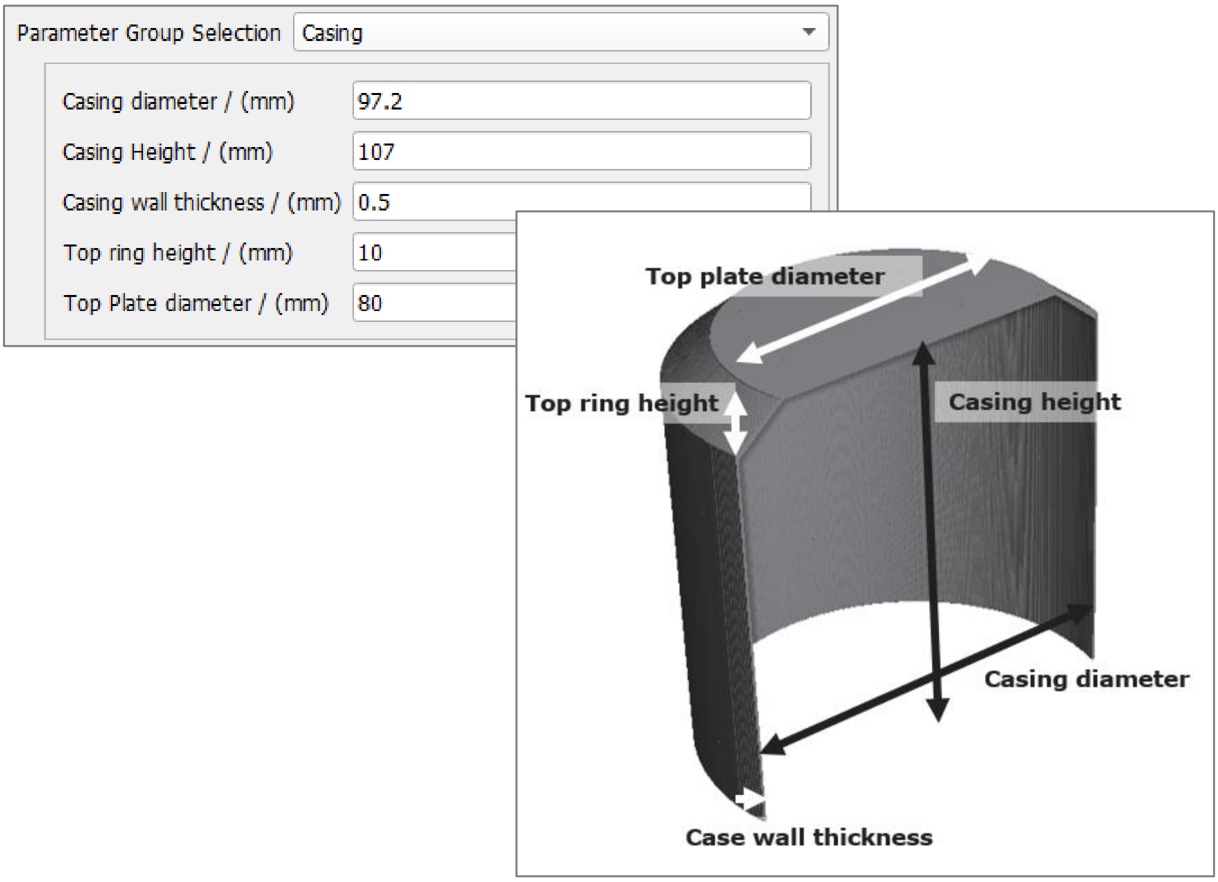
When checking **Set center hole as outlet, secondary holes as inlet**, the pore space in the holes will be set to a new material ID to define it as inlet and outlet for simulations. If simulating for example a flow experiment on the structure, the fluid then will enter the filter through the small holes in the outer circle of the bottom plate and, after passing the other filter parts, leave the filter again through the bigger hole in the middle.

Learn more about the flow experiment in the FlowDict handbook.

Otherwise, the holes are defined as material ID 00, like all other pore voxels in the structure.

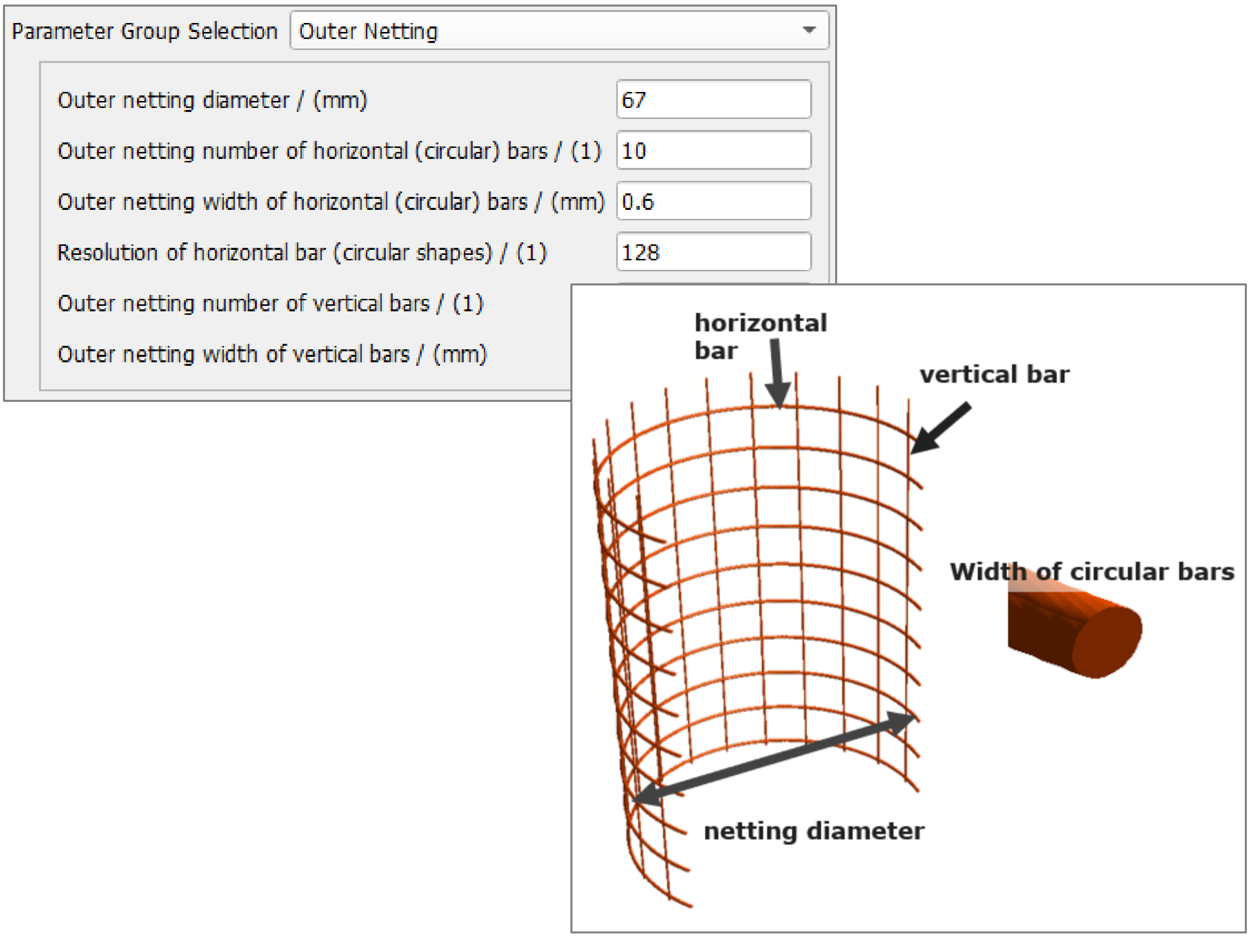
Casing

Define the parameters for the applied **Casing**.



Outer Netting

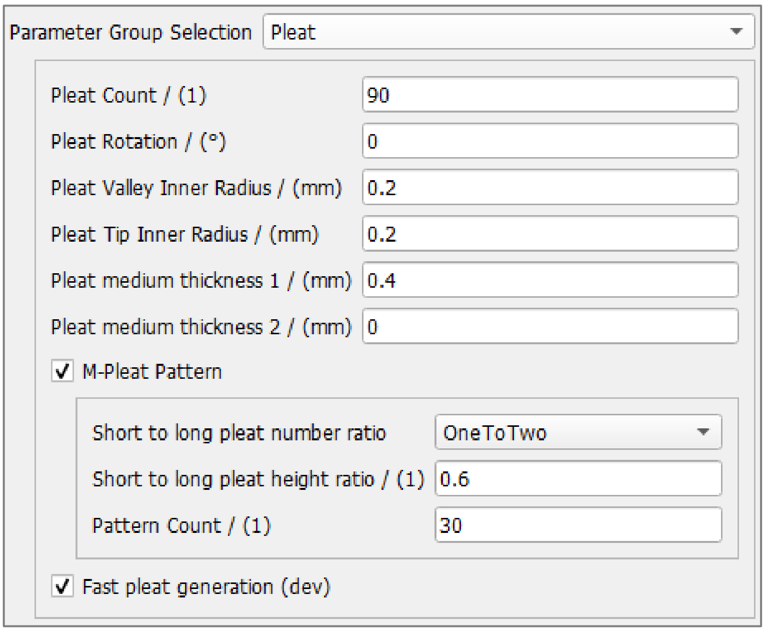
Define the **Outer Netting** parameters.

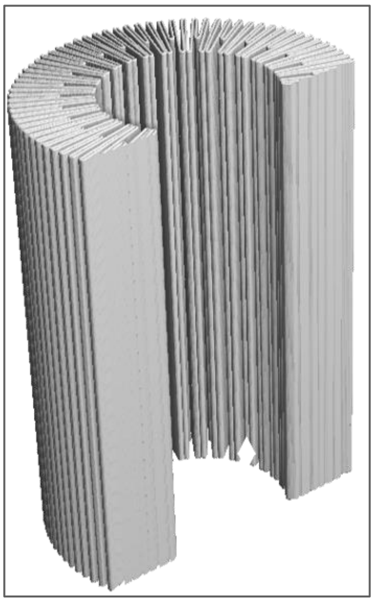


The **Resolution of horizontal bar** defines the resolution of the circular shape, i.e. a higher resolution results in a smoother circular shape of the horizontal bars. The resolution determines the number of points calculated in order to approximate a circle.

Pleat

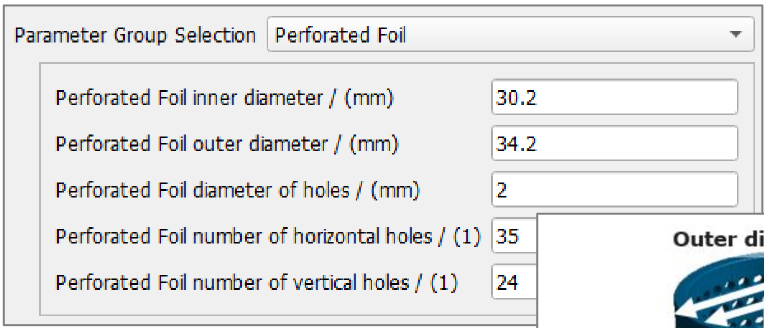
Define the **Pleat** parameters. For the pleat parameters refer to the PleatGeo handbook.

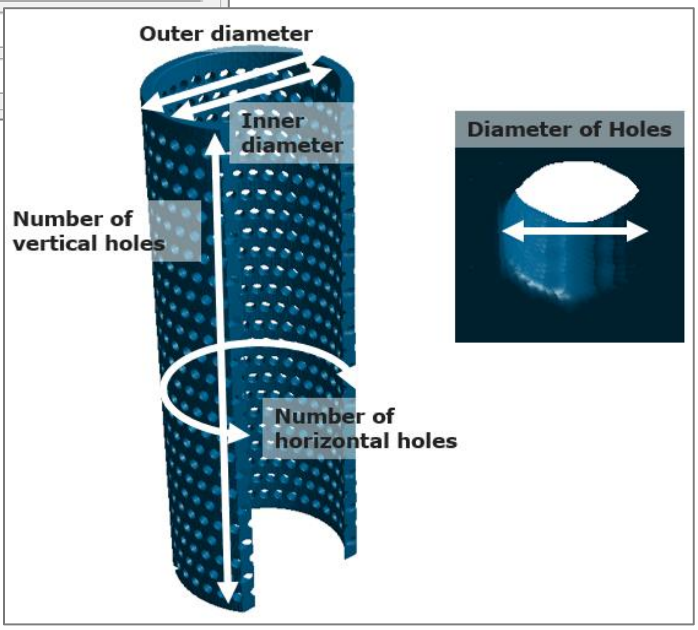




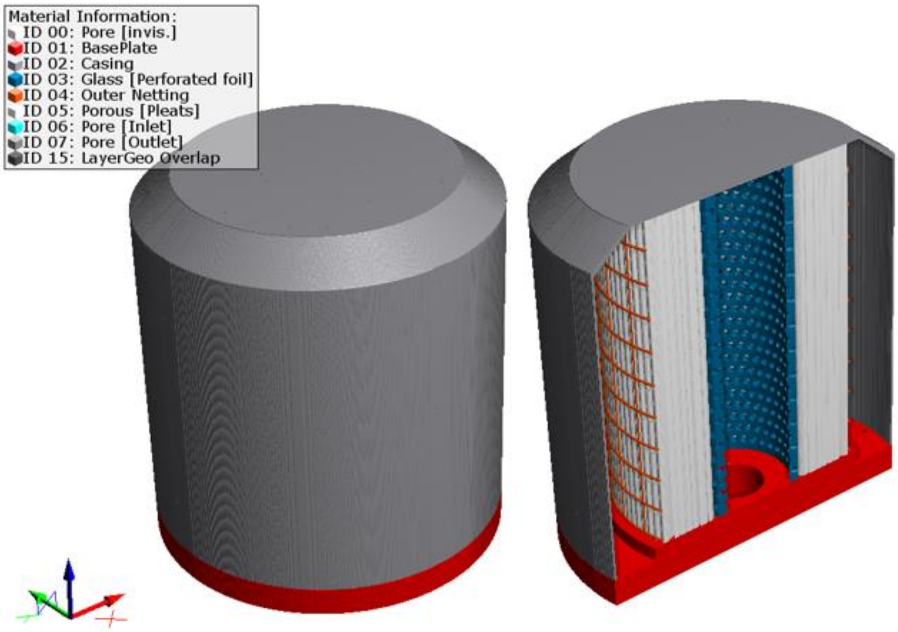
Perforated Foil

Define the **Perforated Foil** parameters.





Clicking **Run** creates the filter set including the selected components.

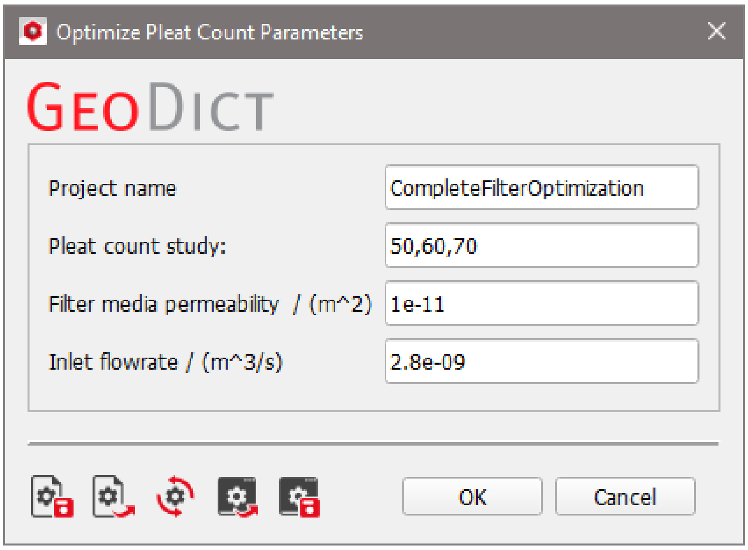


Optimize Pleat Count

The **Optimize Pleat Count** app generates a complete filter with different numbers of pleats and runs a flow experiment on them.

Modules needed to run this GeoApp: PleatGeo, FlowDict

Clicking **Edit…** opens the **Optimize Pleat Count Parameters** dialog.

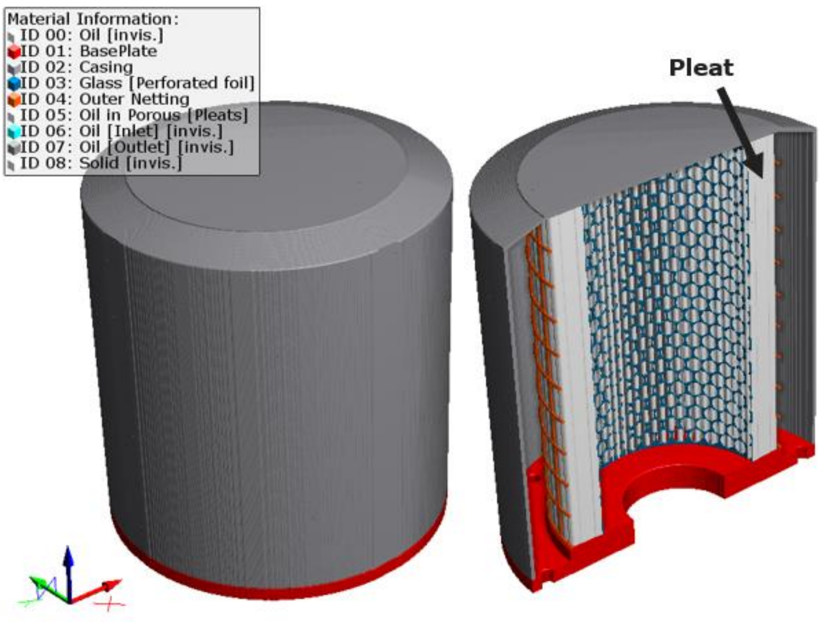


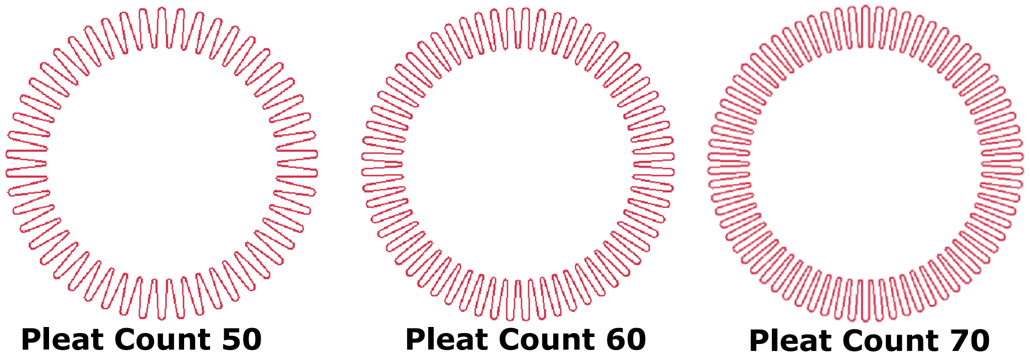
Choose a **Project name** for the folder containing all results from the experiment.

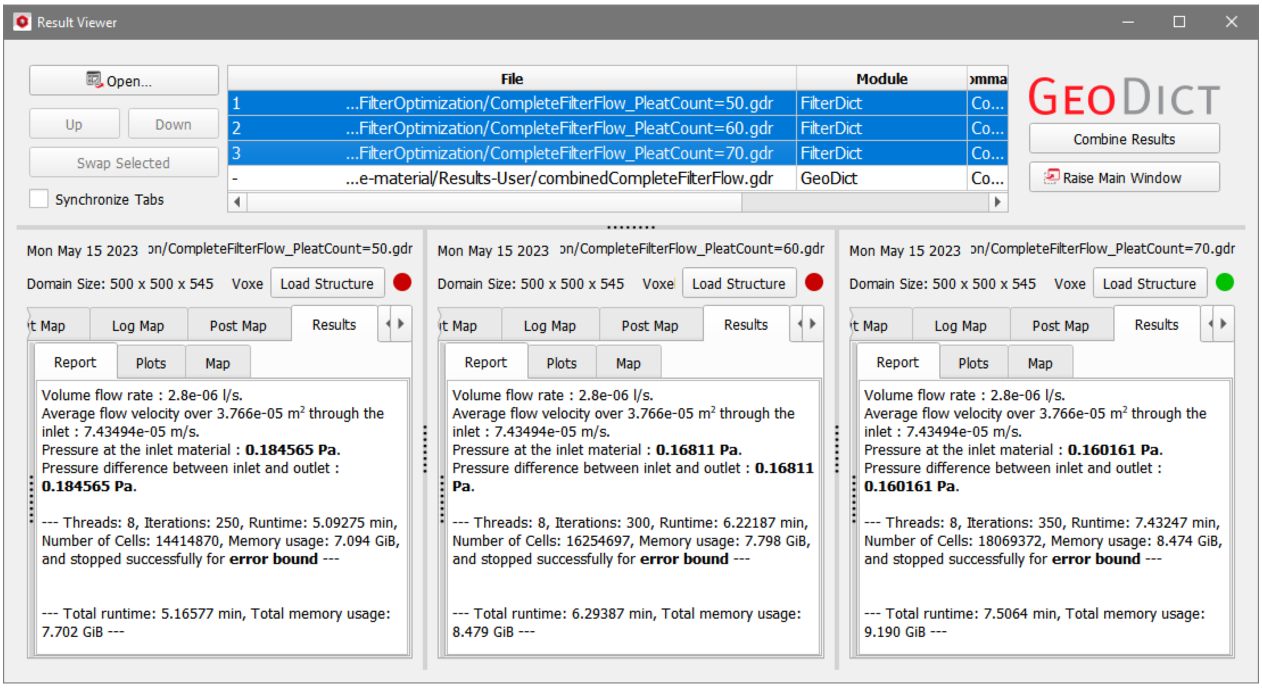
Enter the **Pleat Counts** to **study** as a comma-separated list.

Determine the **Filter media permeability** in m² and the **Inlet flowrate** in m³/s.

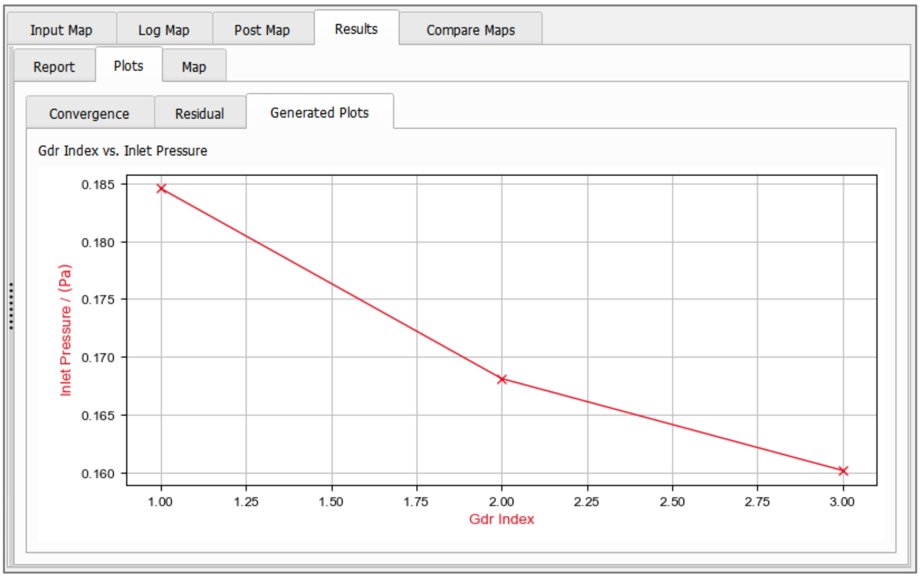
Clicking **Run** starts the pleat count study. When the experiments are finished, the FlowDict results corresponding to the given pleat counts are loaded to the **Result Viewer** and combined into one result file. By default, the pleat counts 50, 60 and 70 are examined, resulting in three result files. To learn more about the FlowDict results, refer to the FlowDict handbook. The generated complete filters are generated as described for the **Generate Complete Filter Set** app on page 77.







In the combined result file, the desired results can be plotted in customized plots, as described in the Result Viewer handbook. By default, the **Plots** tab contains the **Convergence**, the **Residual** and the **Generated Plots**. The last tab shows the **Inlet Pressure** for each flow result.



Fuel Cell and Electrolyser

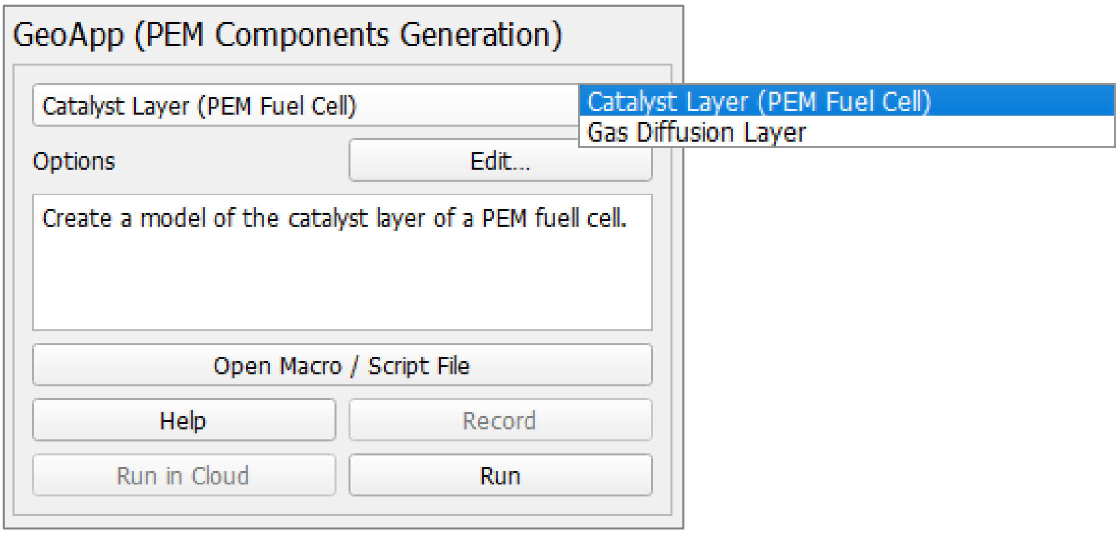
Two GeoApp **- Fuel Cell and Electrolyser** are shipped with GeoDict:

- Run a **PEM Components Generation**.
- Create **SOFC Components.**

PEM Components Generation

The **GeoApp (PEM Components Generation)** section contains the following, selectable from the pull-down menu:

- **Catalyst Layer (PEM Fuel Cell):** create a model of the catalyst layer of a PEM fuel cell.
- **Gas Diffusion Layer:** create a gas diffusion layer of a PEM fuel cell.



Catalyst Layer (PEM Fuel Cell)

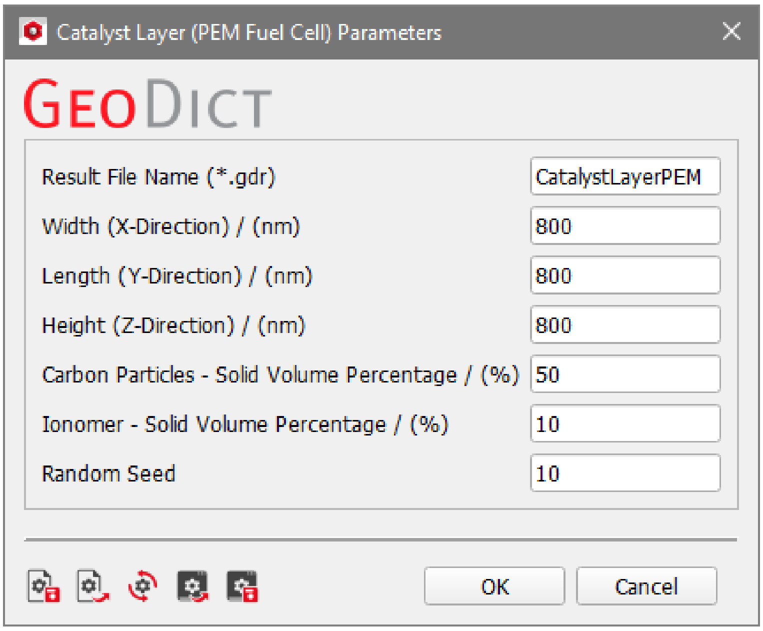
The **Catalyst Layer (PEM Fuel Cell)** app creates a model of the catalyst layer of a PEM fuel cell.

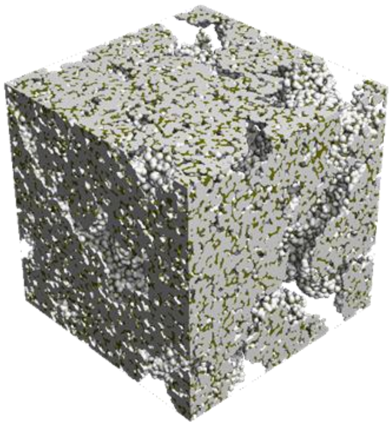
Modules needed to run this GeoApp:
GrainGeo

Clicking **Edit...** opens the **Catalyst Layer (PEM Fuel Cell) Parameters** dialog.

Define the **Result File Name**, the **Domain Size** in the three directions, the **Carbon Particles – Solid Volume Percentage**, the **Ionomer – Solid Volume Percentage** and the **Random Seed**.

Clicking **Run** creates the catalyst layer.





Gas Diffusion Layer

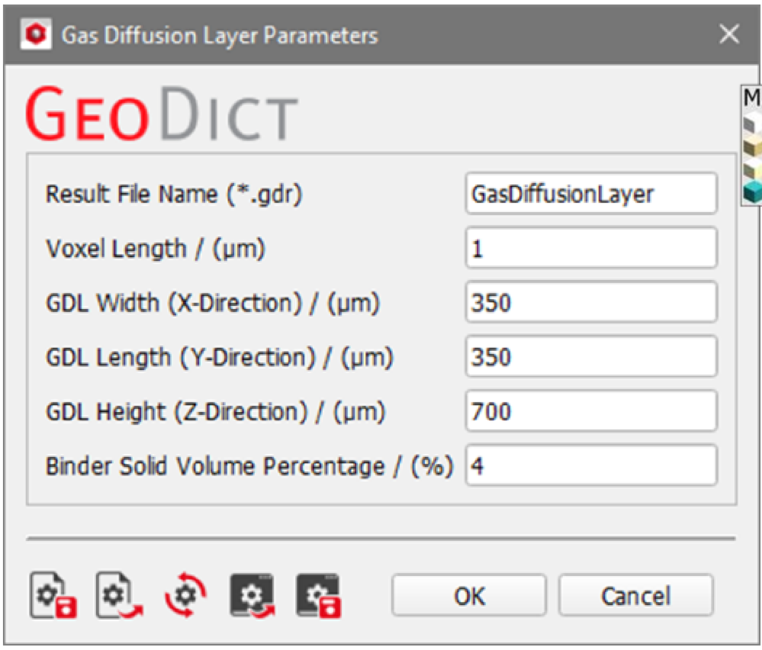
The **Gas Diffusion Layer** app creates a gas diffusion layer of a PEM fuel cell.

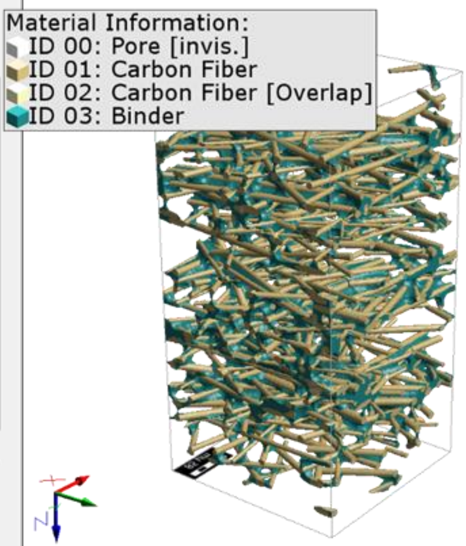
Modules needed to run this GeoApp:
FiberGeo

Clicking **Edit...** opens the **Gas Diffusion Layer Parameters** dialog.

Define the **Result File Name**, the **Voxel Length**, the **GDL Width, Length** and **Height** and the **Binder Solid Volume Percentage**.

Clicking **Run** creates the diffusion layer.

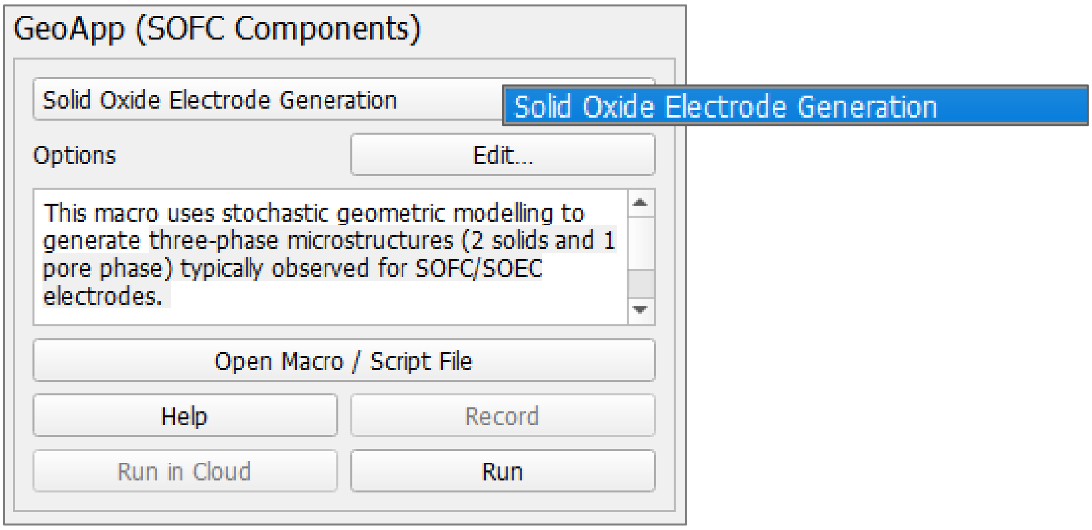




SOFC Components

The **GeoApp (SOFC Components)** section contains the following, selectable from the pull-down menu:

- **Solid Oxide Electrode Generation:** generate three-phase microstructures typically observed for SOFC/SOEC electrodes.



Solid Oxide Electrode Generation

The **Solid Oxide Electrode Generation** app uses stochastic geometric modelling to generate three-phase microstructures (2 solids and 1 pore phase) typically observed for SOFC/SOEC electrodes. It generates two independent Gaussian random fields to facilitate a bi-gaussian random field. This two-dimensional field is thresholded into three phases according to the specified volume fractions and contact angles, where the latter determine the wetting behavior of the phases. The approach is based on work of Philip Marmet [14].

Modules needed to run this GeoApp: FiberGeo or GrainGeo

Click **Edit** to open the **Solid Oxide Electrode Parameters** dialog.

The input parameters include **Result File Name**, **Gaussian Random Field Settings**, **Material Phases**, and **Expert Settings**.

Check **Generate Gaussian Random Fields** to generate two Gaussian random fields (GRF). Define the volume dimensions for the solid oxide electrode and the two GRFs. Standard deviation and random seed can be different for the two Gaussian random field phases.

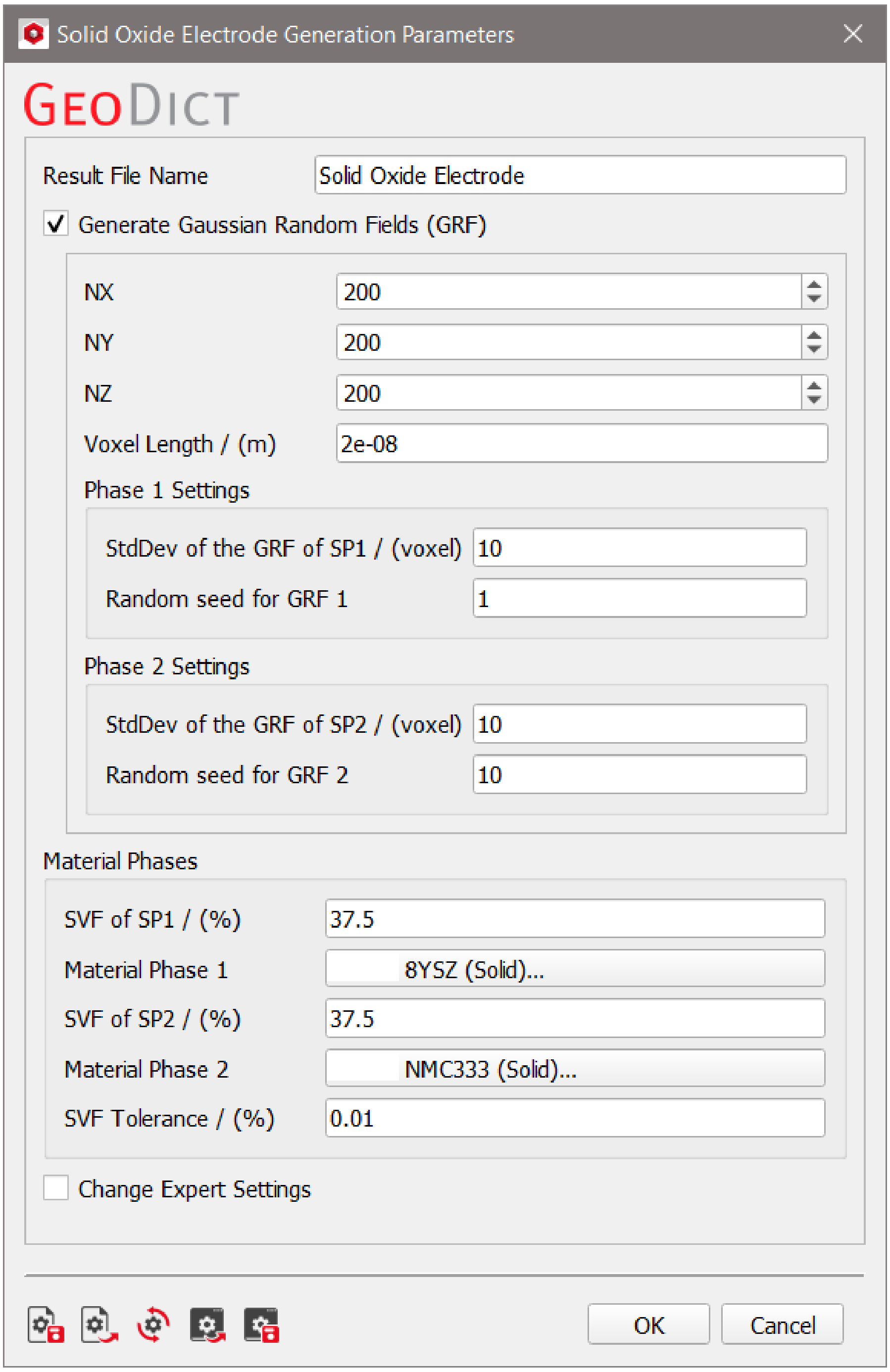
If rerunning the app for the same volume dimensions and the same random fields, uncheck **Generate Gaussian Random Fields** and browse for the two GRF result files in the solid oxide electrode result folder. They are loaded and analyzed for the new electrode generation. If not already present, they are copied into the result folder for the current electrode generation.

By using the same GRF for different Solid Volume Fractions, compositions of phase 1 and 2, as well as contact angles between the phases, large parameter studies can be done quickly and highly computational efficient.

The two GRFs represent two solid phases. Each phase has its own solid volume fraction (**SVF of SP1** and **SP2**) for the resulting electrode. Note that the sum of the two solid phases must be less than 100%. The remaining percentages specify the porosity of the electrode structure.

Click on the material box for **Material Phase 1** or **Phase 2** to define the materials for the two phases.

The solid volume fraction tolerance (**SVF Tolerance**) specifies how close the generation process has to approximate the target values.

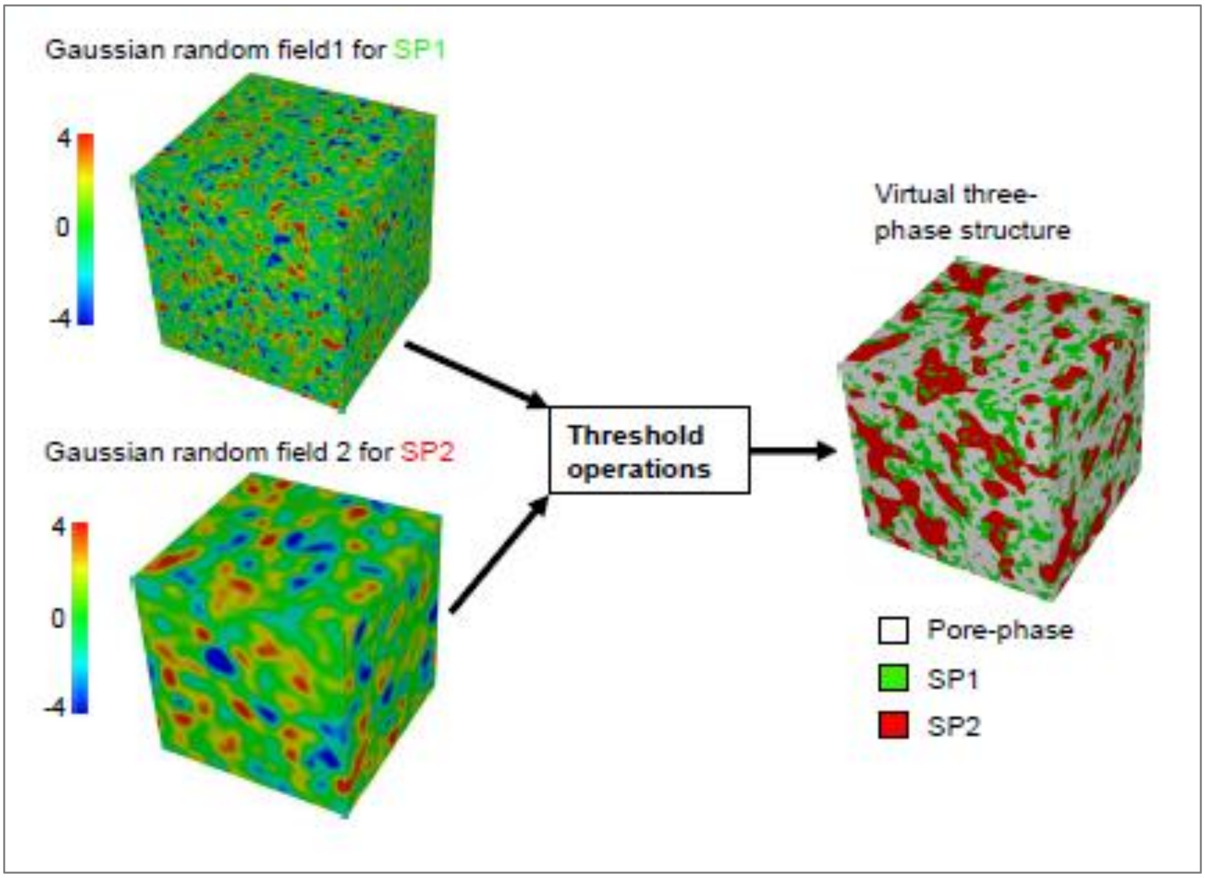


Check **Change Expert Settings** to

- **Adopt phase interface smoothing**: applies a Gaussian filter to the previously generated or loaded GRFs. This way, the phase boundaries created by stochastic field thresholding are sharpened.

- **Change threshold angle parameters:** The thresholding angles between the three resulting phases can be set. Their setting differentiates the two solid phases between wetting and non-wetting behavior. The values are optional and have commonly used defaults (neutral wetting behavior). See the section below for further details.
- **Smoothing of the final result:** To dilute the boundary between two phases, a smoothing based on voxels is applied. Dilation is used to coat neighboring voxels from another material. Doing this vice-versa between two phases, the boundary is smoothed. For this purpose, the dilation between two of the three phases can be stated. Note that at least one pair of phases needs to have a dilation radius >0 for any smoothing to commence.

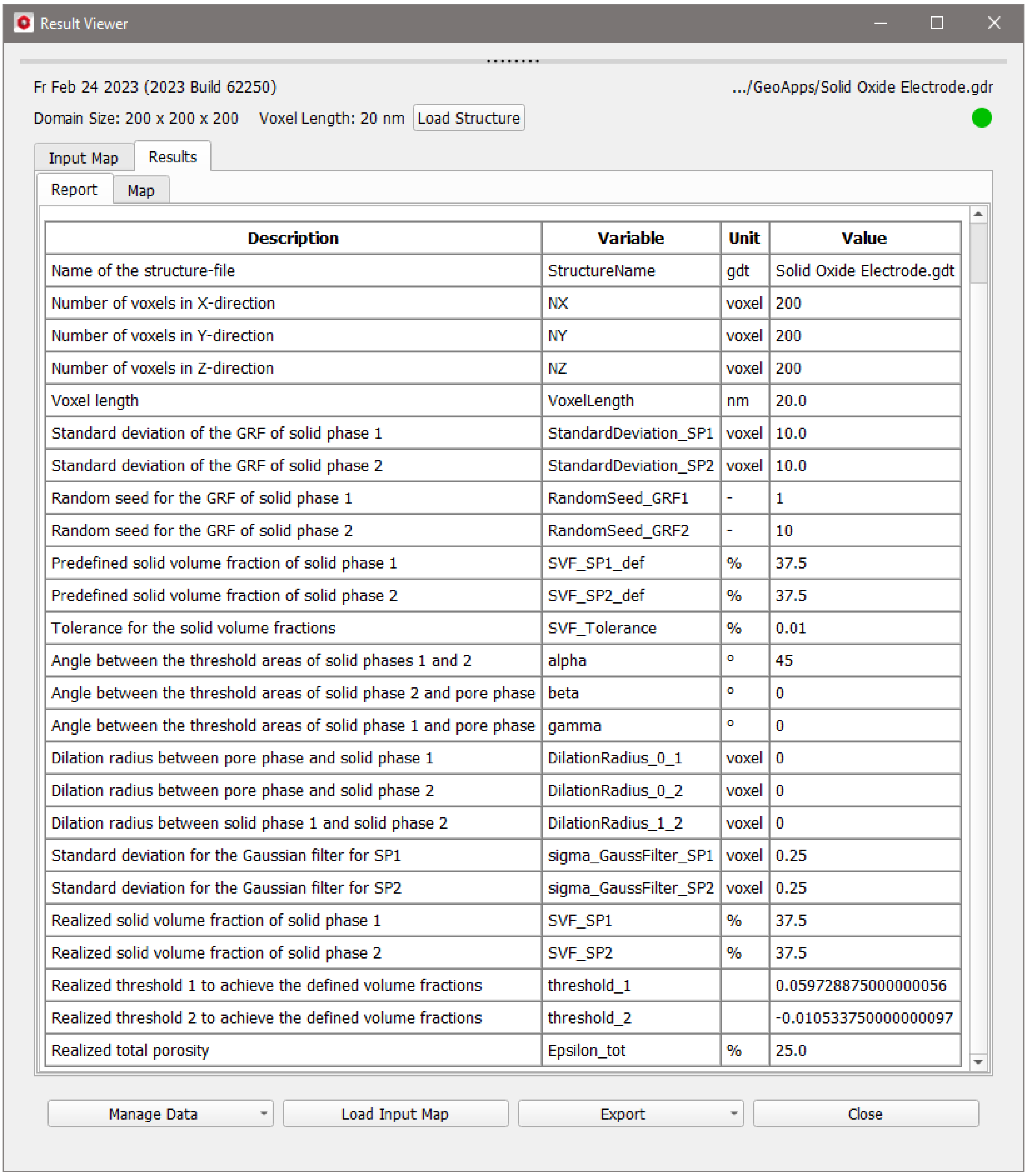
The figure below illustrates the virtual structure generation with pluri-Gaussian random fields. Two GRFs are combined with threshold operations to achieve three phases with defined phase volume fractions and wetting behavior.



Clicking **Run** starts the solid oxide electrode generation.

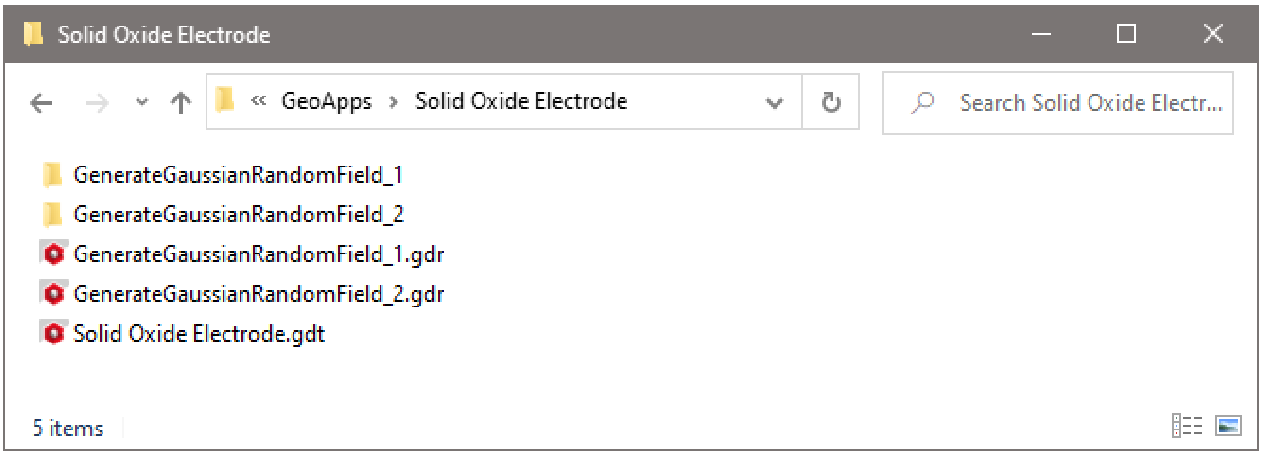
When the structure generation finishes, the **Result Viewer** of the result file (*.gdr) opens automatically.

The **Results** → **Report** tab displays a report about the resulting structure.



Description	Variable	Unit	Value
Name of the structure-file	StructureName	gdt	Solid Oxide Electrode.gdt
Number of voxels in X-direction	NX	voxel	200
Number of voxels in Y-direction	NY	voxel	200
Number of voxels in Z-direction	NZ	voxel	200
Voxel length	VoxelLength	nm	20.0
Standard deviation of the GRF of solid phase 1	StandardDeviation_SP1	voxel	10.0
Standard deviation of the GRF of solid phase 2	StandardDeviation_SP2	voxel	10.0
Random seed for the GRF of solid phase 1	RandomSeed_GRF1	-	1
Random seed for the GRF of solid phase 2	RandomSeed_GRF2	-	10
Predefined solid volume fraction of solid phase 1	SVF_SP1_def	%	37.5
Predefined solid volume fraction of solid phase 2	SVF_SP2_def	%	37.5
Tolerance for the solid volume fractions	SVF_Tolerance	%	0.01
Angle between the threshold areas of solid phases 1 and 2	alpha	°	45
Angle between the threshold areas of solid phase 2 and pore phase	beta	°	0
Angle between the threshold areas of solid phase 1 and pore phase	gamma	°	0
Dilation radius between pore phase and solid phase 1	DilationRadius_0_1	voxel	0
Dilation radius between pore phase and solid phase 2	DilationRadius_0_2	voxel	0
Dilation radius between solid phase 1 and solid phase 2	DilationRadius_1_2	voxel	0
Standard deviation for the Gaussian filter for SP1	sigma_GaussFilter_SP1	voxel	0.25
Standard deviation for the Gaussian filter for SP2	sigma_GaussFilter_SP2	voxel	0.25
Realized solid volume fraction of solid phase 1	SVF_SP1	%	37.5
Realized solid volume fraction of solid phase 2	SVF_SP2	%	37.5
Realized threshold 1 to achieve the defined volume fractions	threshold_1		0.059728875000000056
Realized threshold 2 to achieve the defined volume fractions	threshold_2		-0.010533750000000097
Realized total porosity	Epsilon_tot	%	25.0

The generated solid state electrode structure is shown in the visualization area of GeoDict and the result folder contains the GRFs and the electrode structure file.



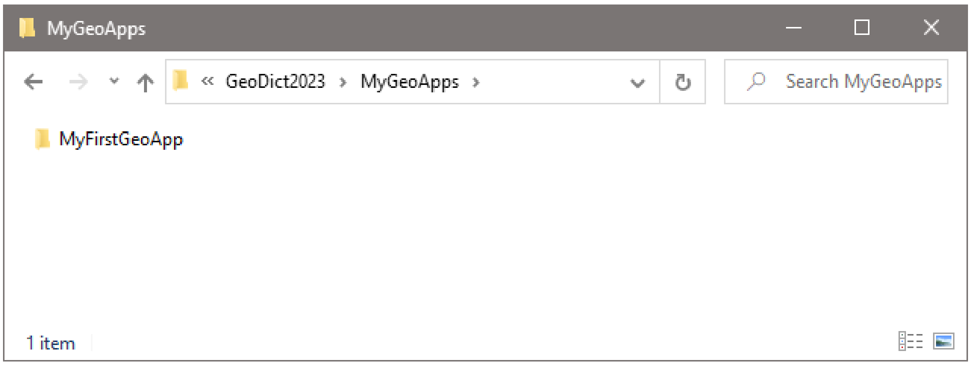
Adding custom GeoApps

There are two possibilities to add custom GeoApps. They can either be added locally without administrator rights or for all users by the system administrator.

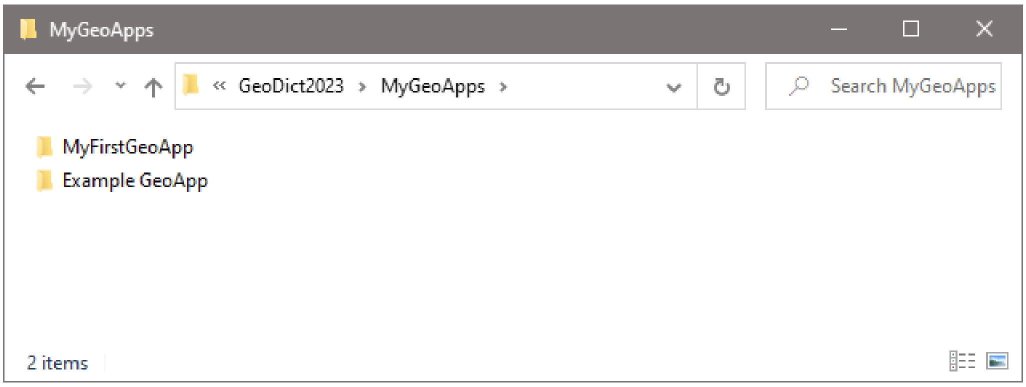
Locally adding custom GeoApps

To only locally add a custom GeoApps for one user, browse for the **MyGeoApps** folder in the GeoDict settings folder. For Windows this is located under **C:\Users\Username\GeoDict2023\MyGeoApp**.

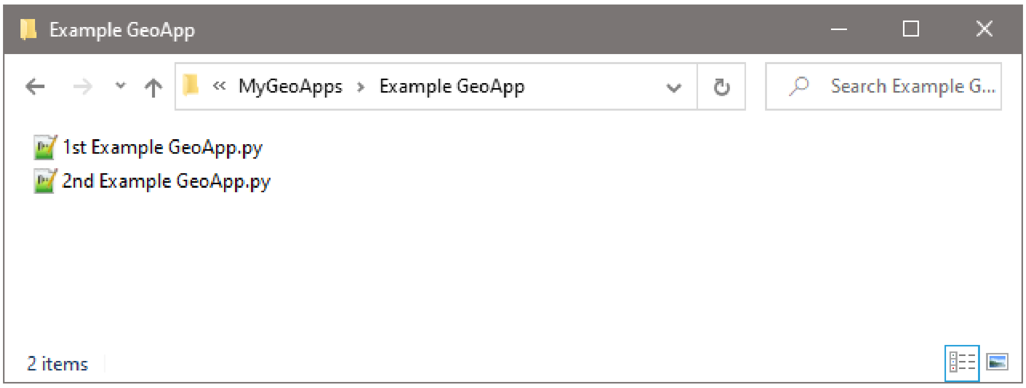
By default, this folder only contains the example **MyFirstGeoApp,** but additional apps may be placed there by the user and would then be available for this user after restarting GeoDict.



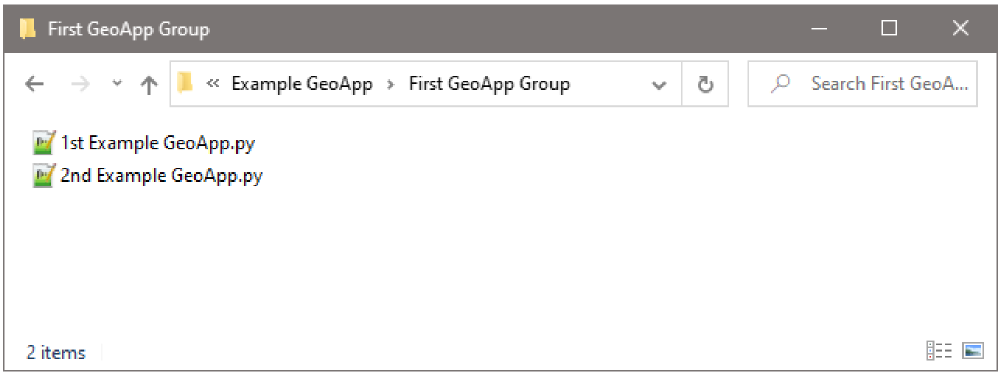
Therefore, create a new folder inside the **MyGeoApps** folder. In the example below, the **Example GeoApp** folder is added. The name of this folder will be displayed later under the GeoApp menu in the GeoDict Graphical User Interface (GUI).



In the new folder, place the GeoPy files that will be selectable from the pull-down menu in the new GeoApp. Here, for example, the two scripts: **1st Example GeoApp.py** and **2nd Example GeoApp.py.**

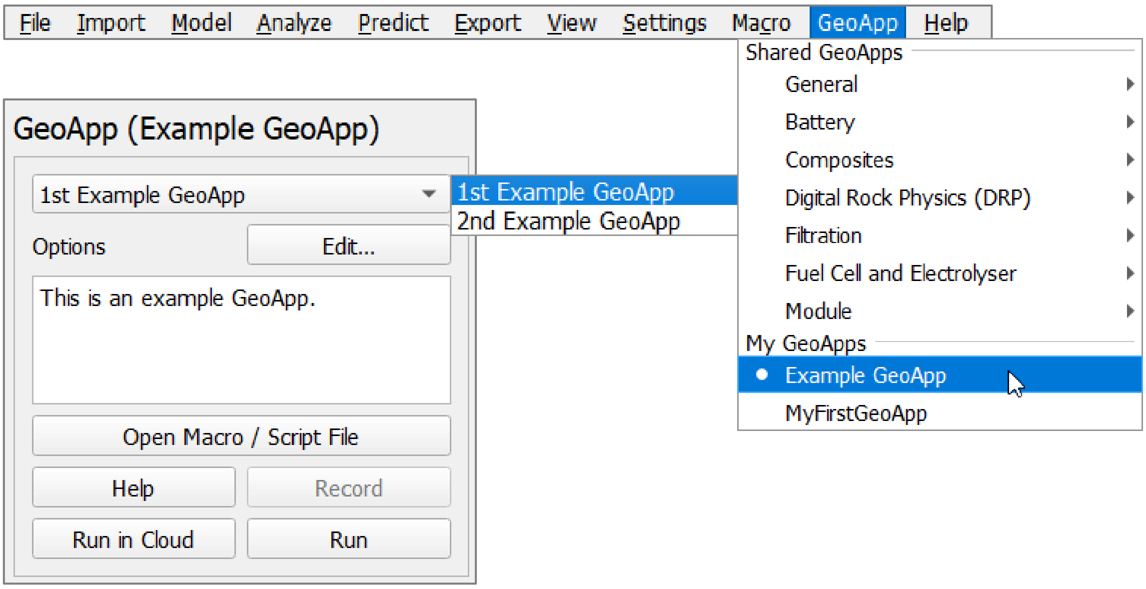


Alternatively, the GeoApps scripts can be grouped into subfolders.

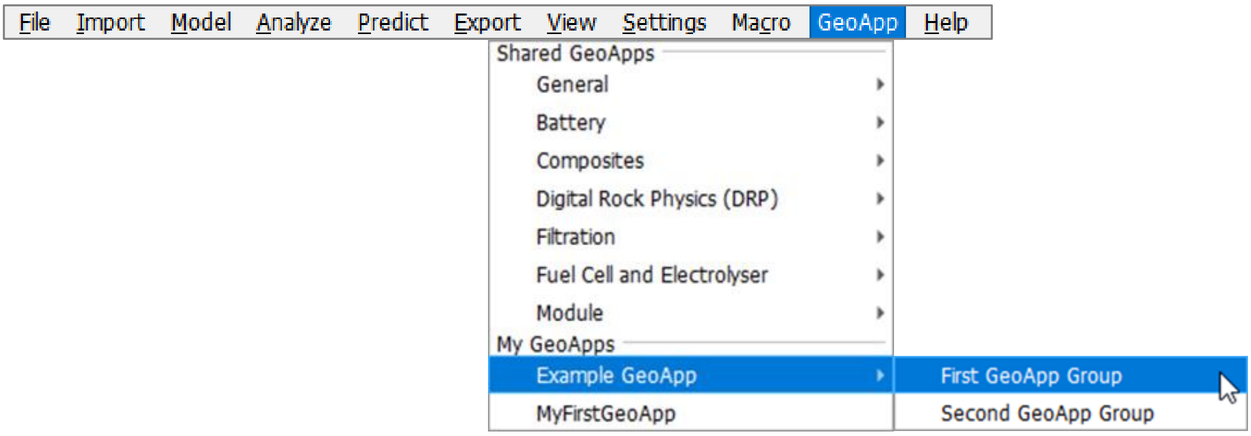


How to create a GeoPy file containing parameters accessible from the GeoDict GUI is described in the GeoPy scripting handbook of this User Guide.

After restarting GeoDict, the new app will be available from the GeoApp menu. If selected, in the GeoApp section the new apps are displayed in the **My GeoApps** section and can be edited and run as described on pages 1ff.



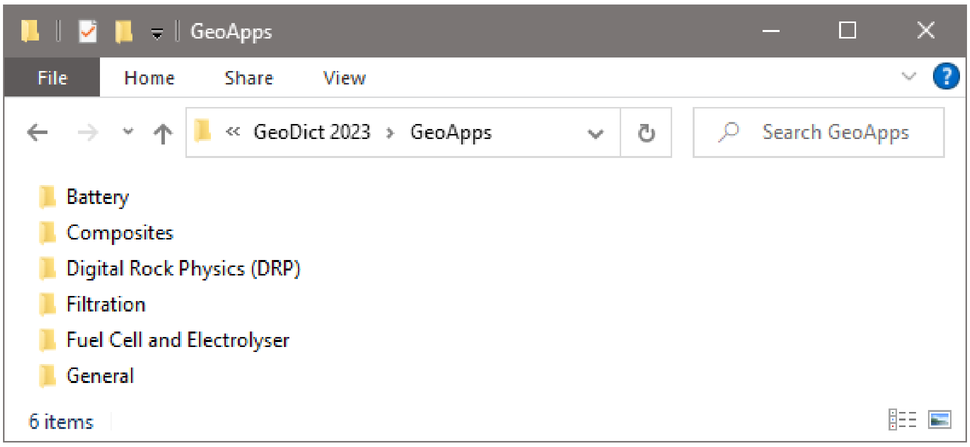
If organizing the GeoPy files in groups the GeoApp menu looks as follows:



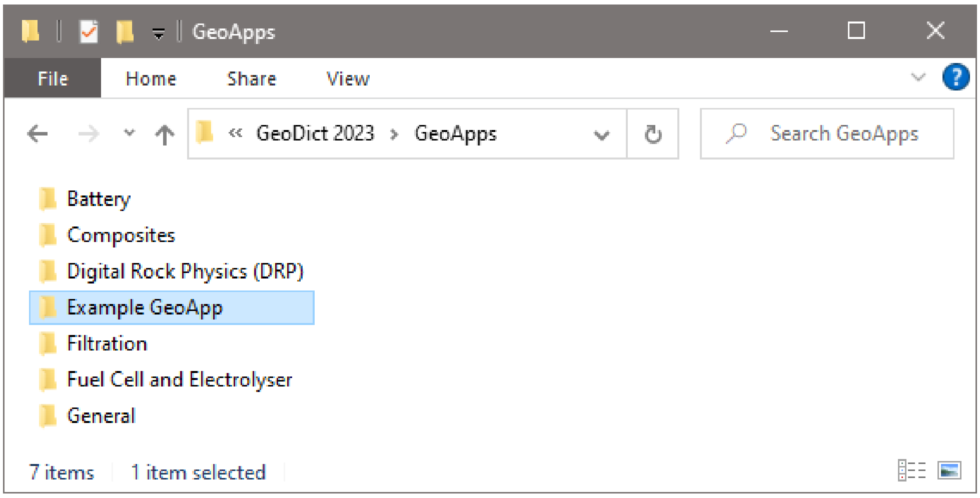
GLOBALLY ADDING CUSTOM GEOAPPS

The GeoApps are stored in the **GeoApps** folder included in the GeoDict installation folder. The **Module** specific apps are located in the corresponding module folders e.g., the GeoApps for FiberGeo are to be found in the **FiberGeo** folder in the GeoDict installation folder.

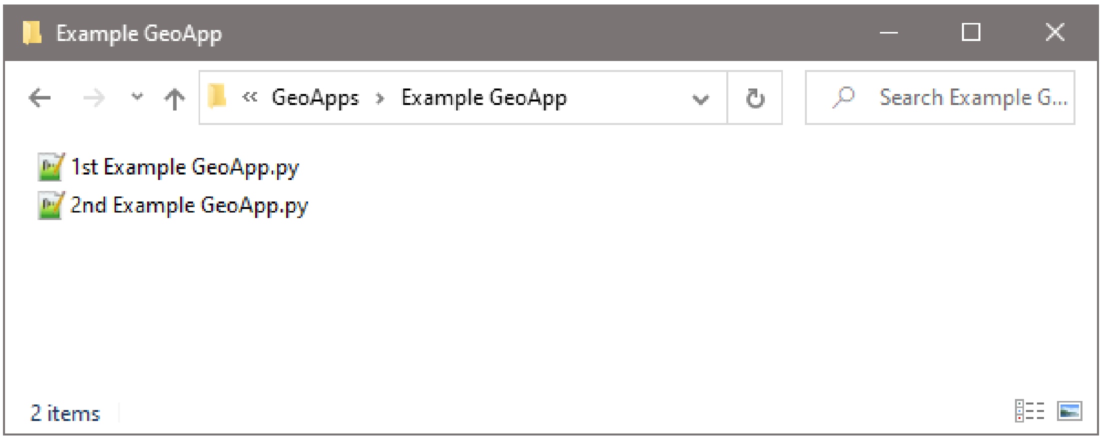
Below, the apps that are located in the installation folder **C:\Program Files\Math2Market GmbH\GeoDict 2023\GeoApps** are shown. Five **GeoApp** groups are included in the standard installation package, but additional apps may be placed there by the **system administrator** making them available for all users.



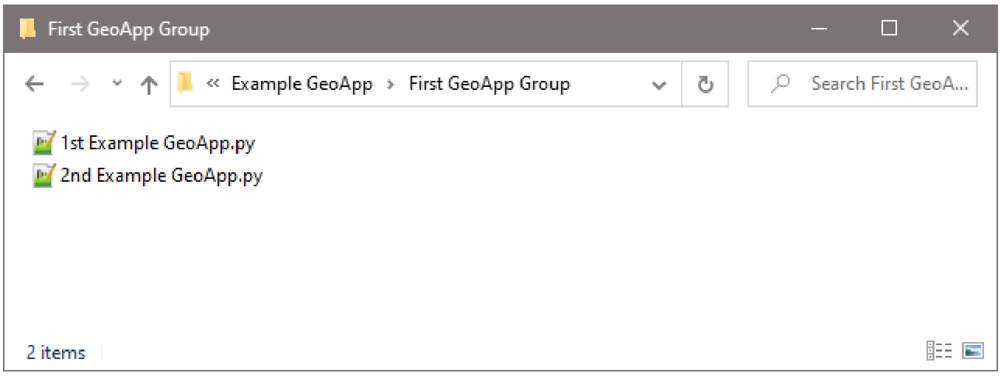
Therefore, create a new folder inside the **GeoApp** folder. In the example below, the **Example GeoApp** folder is added. The name of this folder will be displayed later under the GeoApp menu in the GeoDict Graphical User Interface (GUI).



In the new folder, place the GeoPy files that will be selectable from the pull-down menu in the new GeoApp. Here, for example, the two scripts: **1st Example GeoApp.py** and **2nd Example GeoApp.py.** How to create a GeoPy file containing parameters accessible from the GeoDict GUI is described in the GeoPy scripting handbook of this User Guide.

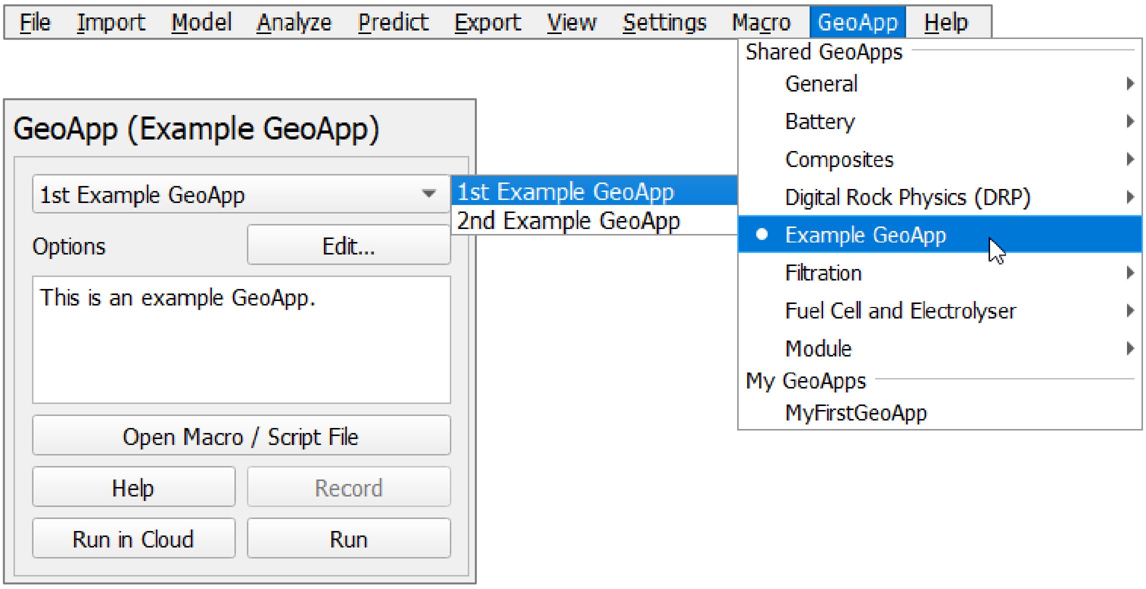


Alternatively, the GeoApps scripts can be grouped into subfolders.

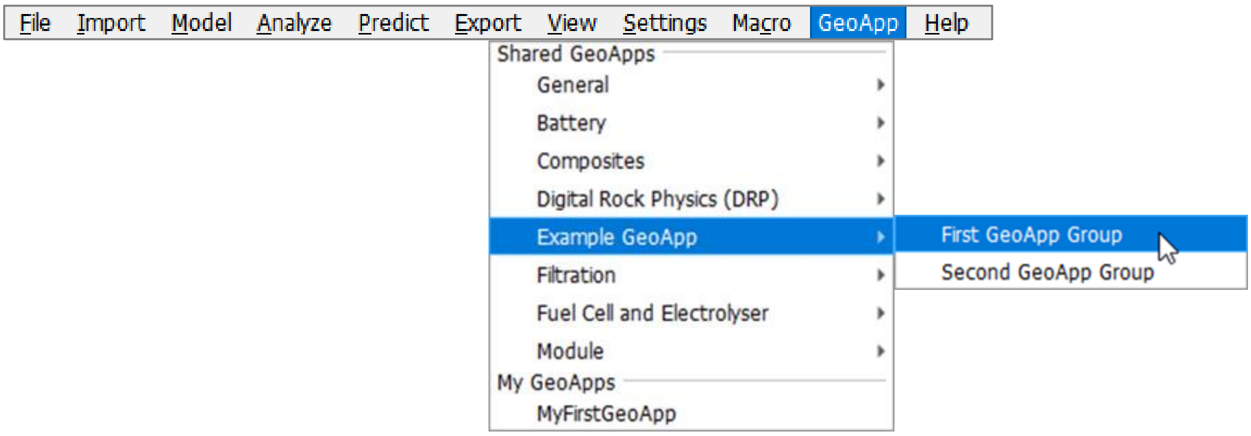


If thematical fitting to one of the existing GeoApp categories, the custom app can of course also be placed there.

After restarting GeoDict, the new app will be available from the GeoApp menu. If selected, in the GeoApp section the new apps are displayed in the **Shared GeoApps** section and can be edited and run as described on pages 1ff.



If organizing the GeoPy files in groups the GeoApp menu looks as follows:


File
Import
Model
Analyze
Predict
Export
View
Settings
Macro
GeoApp
Help
Shared GeoApps
General
Battery
Composites
Digital Rock Physics (DRP)
Example GeoApp
Filtration
Fuel Cell and Electrolyser
Module
My GeoApps
MyFirstGeoApp
First GeoApp Group
Second GeoApp Group

References

[1] L. Holzer, D. Wiedenman, B. Münch, L. Keller, M. Prestat, Ph. Gasser, I. Robertson and B. Grobéty, The influence of constrictivity on the effective transport properties of porous layers in electrolysis and fuel cells, Journal of Materials Science 48 (2013): 2934-2952.

[2] L. Cheng, J. Becker and B. Planas, DiffuDict User Guide, https://doi.org/10.30423/userguide.geodict2022-diffudict

[3] N. Epstein, On tortuosity and the tortuosity factor in flow and diffusion through porous media, Chemical engineering science 44.3 (1989): 777-779.

[4] W.J. Ullman, R.C. Aller, Diffusion coefficients in nearshore marine sediments, Limnology and Oceanography 27.3 (1982): 552-556.

[5] F. L. Tye, Tortuosity, Journal of Power Sources 9 (1983): 89-100.

[6] A. Duda, Z. Koza and M. Matyka, Hydraulic tortuosity in arbitrary porous media flow, Phys. Rev. E 84 (2011): 036319.

[7] L.N. Plummer, T.M.L. Wigley and D.L. Parkhurst, The kinetics of calcite dissolution in CO 2 -water systems at 5 degrees to 60 degrees C and 0.0 to 1.0 atm CO 2, American Journal of Science 278 (2) (1978): 179-216

[8] J.P. Nunes, M.J. Blunt and B. Bijeljic, Pore-scale simulation of carbonate dissolution in micro-CT images, Journal of Geophysical Research: Solid Earth 121 (2016): 558–576

[9] H. Andrä, N. Combaret, J. Dvorkin, E. Glatt, J. Han, M. Kabel, Y. Keehm, F. Krzikalla, M. Lee, C. Madonna, M. Marsh, T. Mukerji, E. H. Saenger, R. Sain, N. Saxena, S. Ricker, A. Wiegmann, X. Zhan, Digital rock physics benchmarks—Part I: Imaging and segmentation, Computers & Geosciences 50 (2013): 25-32

[10] N. Saxena, R. Hofmann, F.O. Alpak, S. Berg, J. Dietderich, U. Agarwal, K. Tandon, S. Hunter, J. Freeman and O.B. Wilson, References and benchmarks for pore-scale flow simulated using micro-CT images of porous media and digital rocks, Advances in Water Resources, 109 (2017): 211- 235

[11] N. Saxena, A. Hows, R. Hofmann, F.O. Alpak, J. Freeman, S. Hunter and M. Appel, Imaging and computational considerations for image computed permeability: Operating envelope of Digital Rock Physics, Advances in Water Resources, 116 (2018): 127-144

[12] T. Cvjetkovic, J.-O. Schwarz, L. Cheng, J. Becker, S. Linden and A. Wiegmann, Simulation of Reactive Transport Processes: Acidizing Treatments in Carbonate Reservoirs, Report No. M2M-2018-02, https://doi.org/10.30423/report.m2m-2018-02, Math2Market GmbH

[13] J. Brownlee, How to Use Nelder-Mead Optimization in Python, Machine Learning Mastery (2021) https://machinelearningmastery.com/how-to-use-nelder-mead-optimization-in-python/

[14] P. Marmet et al, Stochastic microstructure modeling of SOFC electrodes based on a pluri-Gaussian approach, in development (2022)

[15] S. Berg, R. Armstrong, and A. Wiegmann, Gildehauser Sandstone, *Digital Rocks Portal* (2018) https://www.digitalrocksportal.org/projects/134

https://doi.org/10.30423/userguide.geodict

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