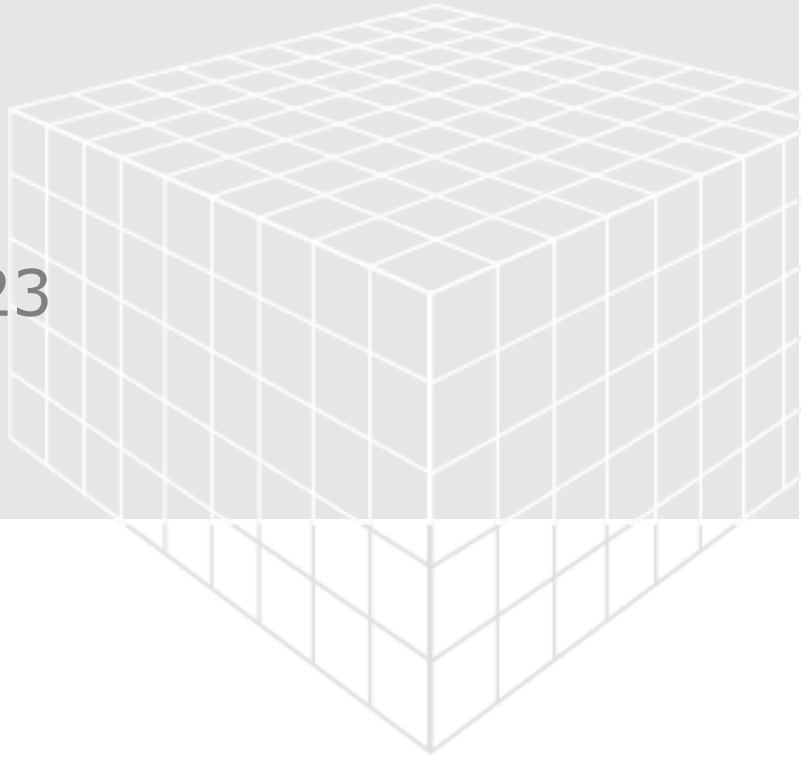
SatuDict



User Guide

GeoDict release 2023

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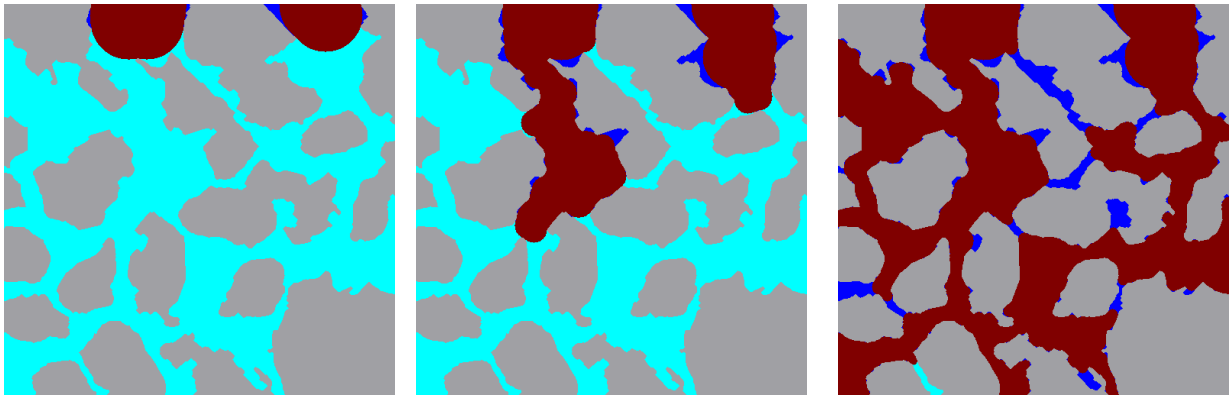
ASSESSING SATURATION-DEPENDENT MATERIAL PROPERTIES IN POROUS MEDIA

SatuDict is the GeoDict module for the computation of saturation-dependent material parameters in porous media. In many applications, the porous media is partly saturated, so that part of the pore space is filled with water and part with air, gas, or oil. Oil-water, water-air, or other two-phase systems are possible. Generally, one of the fluids preferably wets the media surfaces and is therefore called the **wetting** phase, whereas the other fluid, with less affinity for the media, is called the **non-wetting** phase. It is not unusual that water is the non-wetting phase.

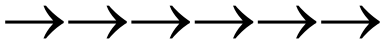
SatuDict can calculate the phase distribution for the two types of phase displacement, namely Drainage and Imbibition.

A **Drainage** displacement occurs where a **non-wetting** invading fluid enters the porous media and displaces a **wetting** fluid, which was saturating it.

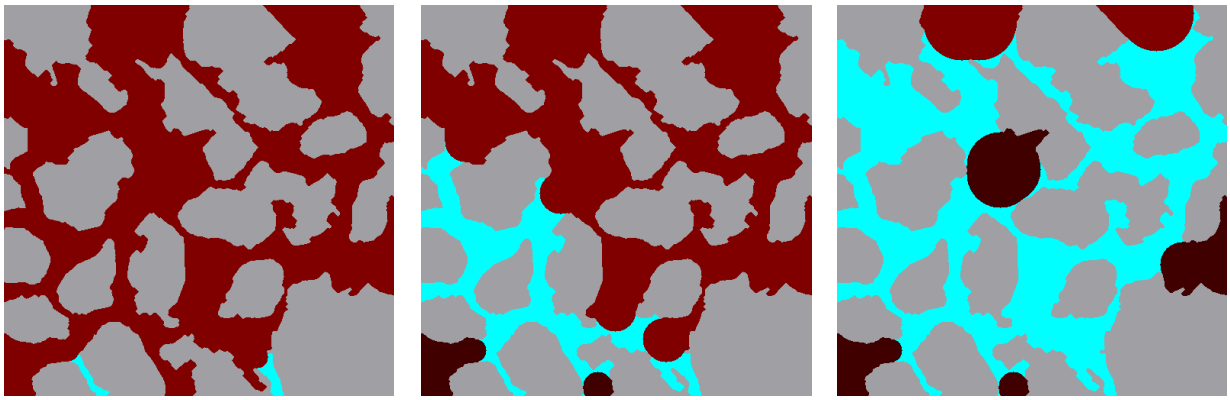


Material Information:
- ID 00: Water [Wetting Phase]
- ID 01: Quartz
- ID 02: Oil [Non-Wetting Phase]
- ID 03: Water [Residual Wetting Phase]

Drainage process

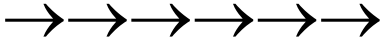


The opposite case, **Imbibition**, occurs when a **wetting** fluid invades the space around the material and the material surface, which had been occupied by a **non-wetting** fluid, displacing it.



Material Information:
- ID 00: Oil [Non-Wetting Phase]
- ID 01: Quartz
- ID 02: Water [Wetting Phase]
- ID 04: Oil [Residual Non-Wetting Phase]

Imbibition process



Not only the pore size, but also the connectivity of the phases to a phase reservoir determines the final distribution of the phases and has to be accounted for. After Drainage, a residue of the wetting phase (Residual Wetting Phase) or, after Imbibition, a residue of the non-wetting phase (Residual Non-Wetting Phase) can remain trapped in the porous media.

The mechanisms of the displacements in drainage and imbibition are quite different and the two cases should not be confused. Typically, in drainage the invading non-wetting fluid only enters a pore if the capillary pressure is equal to or greater than the threshold pressure of that pore. The threshold pressure corresponds to the capillary pressure in the narrowest part of the pore. However, in imbibition at low injection rate the invading wetting fluid enters the narrowest pores before any other pore is considered.

Pore Morphology Methods

SatuDict uses several **Pore Morphology** methods to determine the distribution of the two phases inside the porous media.

The **Quasi-Static Pore Morphology Method** [1] calculates the stationary distribution of wetting and non-wetting phases for a given capillary pressure and it is applicable when

- gravity and viscous forces are negligible compared to capillary forces,
- the material is homogeneous, i.e. there exists a well-defined contact angle between material surface and phase boundary, and
- only two-phase systems are considered.

For such systems, the pore space accessible to the non-wetting phase is given by the Young-Laplace equation, where σ is the surface tension, α the contact angle, p_c is the capillary pressure and r defines the minimum radius of accessible pores. Thus, the problem is reduced to a purely geometrical problem,

$$r = \frac{2\sigma}{p_c}\cos(\alpha) \qquad (1)$$

The contact angle α can be different at each solid phase inside the porous medium [2] and, thus, variable wettability can be incorporated.

The Quasi-Static Pore Morphology Method has the drawback, that for a drainage simulation, the whole structure is filled instantly after the invading fluid passed the narrowest pore throat. For an imbibition simulation, the whole structure is filled instantly, if the invading wetting phase filled the biggest pore. Since GeoDict 2021, the **Dynamic Pore–Morphology Method** is therefore available in SatuDict. It allows for a dynamic simulation of the drainage and imbibition processes, even with non-monotonic capillary pressure curves. Like this, the capillary pressure can drop down during a drainage simulation when the non-wetting phase passes a pore-throat. During an imbibition simulation, the capillary pressure is not monotonically decreasing, but can rise again, when the wetting phase passes a big pore. Even without the option of non-monotonic capillary pressure curves selected, several intermediate steps are computed for the same pressure value, to avoid instant filling of the whole structure.

With this new method, for imbibition processes, additionally, thin wetting layers can be considered by modified connectivity checks. Wetting residuals near the invading wetting phase front are always treated as connected. The distance from the invading wetting front considered for this modification is user-defined and constant during the simulation.

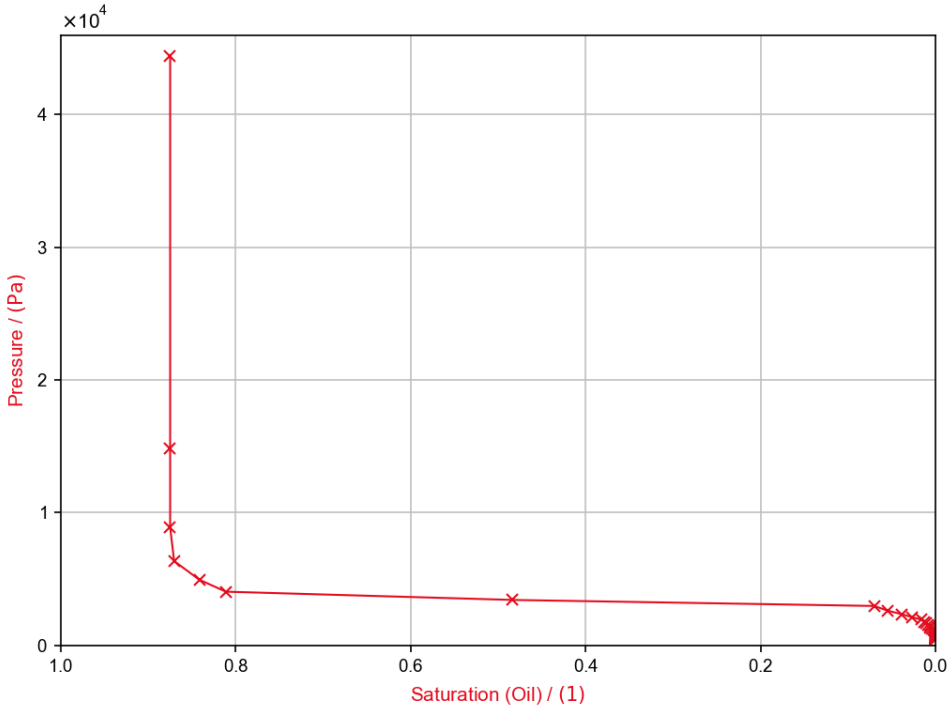
In the following, an example of the resulting capillary pressure curve of a drainage simulation with all three methods is shown below.

Quasi-Static Pore Morphology Method

With this method, the capillary pressure for a drainage simulation is monotonically increasing. At each simulation step, the capillary pressure is increased by a fixed value. This leads to the effect that large pores beyond small pore throats are filled at once when the pressure is high enough to pass the pore throat.

For an imbibition simulation, the capillary pressure is monotonically decreasing. At each simulation step, the capillary pressure is decreased by a fixed value. This leads to the effect, that small pores beyond big pore bodies are filled at once when the capillary pressure is small enough.

Both effects are visible in the capillary pressure curve and responsible for large saturation jumps. Thus, there are sometimes too less computed saturation points in the saturation range between 20% and 80%. In the example shown below, only one saturation point is computed between a saturation of 20% and 80%.

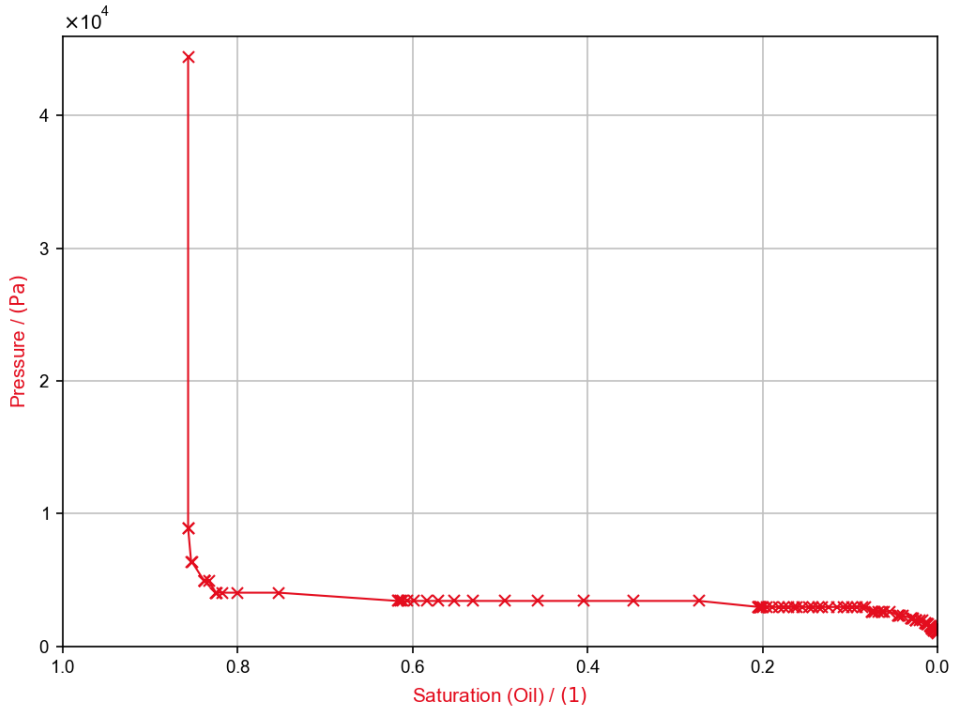


This method is useful for the prediction at which capillary pressure the breakthrough occurs and provides detailed information about fluid distributions for high and low saturated structures. If the detailed fluid distribution at a broad range of saturations is of interest, this method should not be used anymore. However, for structures with a layered distribution of pore sizes, the method provides detailed fluid distributions. E.g. if pores are large at the top and getting smaller toward the bottom and a drainage process is simulated from top to bottom.

Dynamic Pore-Morphology Method with monotonic capillary pressure

For drainage simulations, the capillary pressure is monotonically increasing. At each simulation step, the capillary pressure may be increased or it can stay the same.

For imbibition simulations, the capillary pressure is monotonically decreasing.



This method avoids large saturation jumps and provides many intermediate saturation steps. The interface between the two fluids is displaced by a small (interface) step size, defined in the Solver parameters. The method tries to move the interface according to this parameter. In the example shown, also in the range between 20% and 80% saturation, some intermediate saturation steps are computed and the wetting fluid invades without big jumps.

This method predicts a more accurate fluid movement compared to the quasi-static pore morphology method. The performance of the method was increased for the last service packs of GeoDict 2021 and the runtimes with GeoDict 2022 are similar with the quasi-static method.

This method should be used if a detailed fluid distribution at a broad range of saturations is of interest.

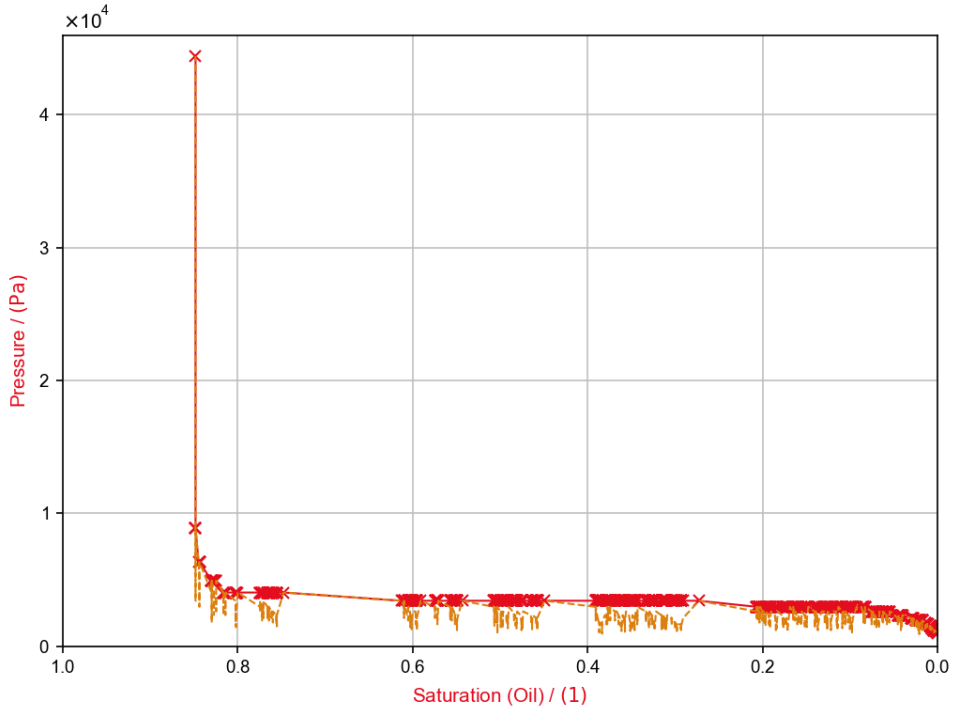
However, certain physical phenomena, e.g., formation of water droplets above a fiber structure with large pore space at the top, cannot be modelled with this method. This requires that the capillary pressure can have a non-monotonic behavior.

Dynamic Pore-Morphology Method with non-monotonic capillary pressure

For drainage simulations, the capillary pressure is non-monotonically increasing. At each simulation step, the capillary pressure may be decreased or it stays the same, if possible, otherwise the pressure is increased.

For imbibition simulations, the capillary pressure is non-monotonically decreasing. At each simulation step, the capillary pressure may be increased or it stays the same if possible, otherwise the pressure is decreased.

If this method is selected, it provides two capillary pressure curves in the result file. One for the monotonic and one for the non-monotonic behavior, shown below for the example.



The non-monotonic method avoids large saturation jumps as well, but can predict many more intermediate saturation steps. It allows to model more complex physical phenomena, e.g. the formation of water droplets above a fiber strcture with large pore space at the top. The method is more precise than the other two methods, but also the runtime is higher. The interface step size is used in the same way as for the monotonic method, described above

Model Fits

Thomeer Model

In GeoDict 2023, for drainage simulations without residual of the replaced fluid, a Thomeer model [5] can be fitted to the capillary pressure curve.

The Thomeer Model is designed for Mercury Intrusion Capillary Pressure (MICP) experiments and predicts the unresolved porosity, a G-shape factor, and the displacement pressure.

The saturation of the non-wetting phase is described by the exponential function

$$S_{NWP} = S_d * \exp\left(-\frac{G}{\log\left(\frac{P_c}{P_d}\right)}\right). \tag{2}$$

The parameters G (Pore Geometric Shape Factor), P_d (Displacement Pressure) and S_d (Displacement Saturation) are fitted from the simulated capillary pressure curve.

This feature requires a special license. Please contact our support at support@math2market.de for more information.

Thin Film Model

When computing the Relative Electrical Conductivity in the Resistivity Index command the usage of the **Thin Film Model** can be enabled. This is recommended when the solid is strongly wetting for the replaced fluid (e.g. Water (Brine)) and therefore the replaced fluid would leave a thin film on the solid surface. Another condition would be that the thin film still have a significant non-zero conductivity and the invading fluid has a very low conductivity. Without modelled thin film, the electrical conductivity would suddenly drop to zero when the voxel connectivity is lost.

With this feature, a thin film of replaced fluid, which is conductive, is added between the solid and the invading fluid. This film has a thickness which is much smaller than the voxel length. Thus, the thin film is modelled as mixed (porous) voxel of replaced fluid / invading fluid and replace fluid / solid. The thin film allows to maintain previously existent non-zero conductivity.

The new conductivities K_{ws} and K_{wo} of the thin film porous voxels at the solid boundary and invading fluid is determined by the following formula:

$$K_{ws} = \frac{t \cdot 0.5}{h} K_w + \frac{h - t \cdot 0.5}{h} K_s, \qquad K_{wo} = \frac{t \cdot 0.5}{h} K_w + \frac{h - t \cdot 0.5}{h} K_o \tag{3}$$

where K_w is the conductivity of the replaced fluid (e.g., 5 S/m), K_s is the conductivity of the solid, K_o is the conductivity of the invading fluid (e.g., 0 S/m), h is the voxel length and t is the thickness of the thin film (e.g., 5 nm).

This feature requires a special license. Please contact our support at support@math2market.de for more information.

SATUDICT COMPUTATIONS

Saturation alters the values of material properties of the porous media, such as flow permeability, diffusivity, and thermal or electrical conductivity. These material properties (constant for one-phase systems) come to depend on its saturation.

In the SatuDict GUI, these saturation-dependent properties are named as *relative* (Relative Permeability, Relative Gas Diffusivity, and Relative Thermal Conductivity and Relative Electrical Conductivity (Resistivity Index)).

Regarding the permeability, the values computed with SatuDict 2023 and displayed in the GDR result file include the relative permeability and the saturation-dependent permeability (shown as Effective Permeability under the Results-Report tab). See the GDR result file in detail below on page 46.

The absolute permeability is given as the permeability of the completely saturated medium (K_s, $s = 1$), whereas the **saturation-dependent or effective permeability** is the permeability of the medium at given saturation levels (K_s, $s \in [0,1]$). The permeability is 0 at saturation 0 ($K_s = 0$, $s = 0$).

The **relative permeability** is a dimensionless measure, defined as the ratio of the saturation-dependent permeability to the **absolute permeability**. The relative permeability must be between zero and one:

$$\frac{K_s}{K_1} \in [0,1] \tag{4}$$

where K_s is the saturation-dependent permeability and K_1 is the absolute permeability.

SatuDict can be used to:

- **Determine the capillary pressure curve** using the pore morphology method or the dynamic pore morphology method to evaluate the distribution of non-wetting and wetting phases for a given (quasi-stationary) capillary pressure $\boldsymbol{P_c}$ and, in this way, determine the saturation $\boldsymbol{s}$. The capillary pressure curve, $\boldsymbol{P_c(s)}$, is determined by repeating this calculation for a variety of capillary pressures. The capillary pressure curves for drainage and imbibition are usually not identical but show a hysteresis effect.
- **Determine relative and saturation-dependent (effective) permeability** for different saturations. The pore morphology method can be used to determine the distribution of the phases (then it is assumed to be stationary) or saturation results of a previously simulated wetting process can be used.

  To calculate the permeability K_w of the wetting phase, the non-wetting phase is treated as an unmovable obstacle. The flow calculation treats it as a solid.

  To calculate the permeability K_{nw} of the non-wetting phase, the wetting phase is treated as an unmovable obstacle.

  Thus, flow only takes place in the pores filled with the corresponding fluid, whereas the other pores are ignored. Specifically, no movement of bubbles is simulated.

  The permeability values are then determined as described in the Flow permeability section of the FlowDict handbook. The resulting permeability value is now dependent on the saturation.

To determine the whole curve $K_w(s)$, it is necessary to calculate the permeability for several different saturations.

This feature requires a special license. Please contact our support at support@math2market.de for more information. Without a special license, this option is not accessible.

- **Calculate saturation-dependent (relative) gas diffusivity** using the pore morphology method or results of a previously simulated drainage or imbibition process. SatuDict calculates the saturation-dependent diffusivity as in DiffuDict (see the DiffuDict handbook). It is assumed that there is no diffusion from the gas phase into the liquid phase and no transport of the gas within the liquid phase (no-flux boundary conditions). It is also assumed that Knudsen diffusion can be neglected. The saturation-dependent gas diffusion can be calculated for successive saturations based on the gas/liquid phase distributions from the simulated drainage.

  This feature requires a special license. Please contact our support at support@math2market.de for more information. Without a special license, this option is not accessible.

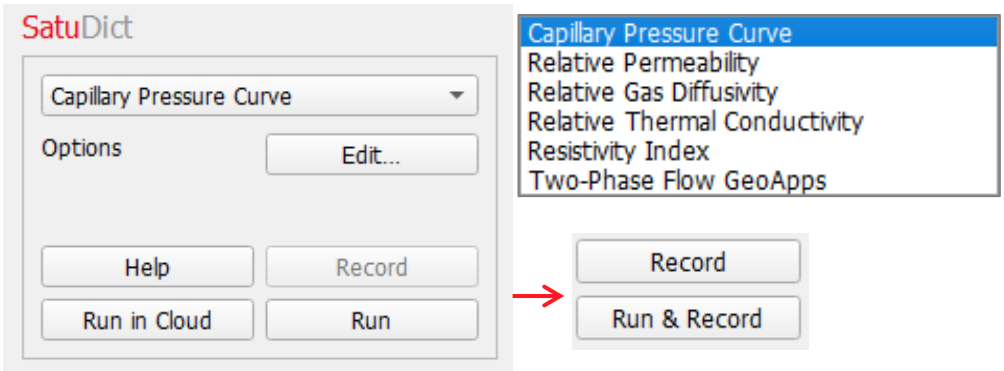
- **Determine saturation-dependent (relative) thermal conductivity, and resistivity index.** SatuDict calculates the saturation-dependent thermal conductivity and the resistivity index as in ConductoDict (see [4] and the ConductoDict handbook. The thermal conductivity or the electrical conductivity of the structure materials and of the fluid phases, and the direction(s) of conduction, are entered. For each direction of interest, equations of purely diffusive heat transport are set, and solved. Advection or radiation is not considered.

  This feature requires a special license. Please contact our support at support@math2market.de for more information. Without a special license, this option is not accessible.

The saturation process can be calculated and then visualized in various ways in the GeoDict Result Viewer from the result files saved in the project folder during the saturation simulation.

SATUDICT SECTION

SatuDict starts when selecting **Predict → SatuDict** in the menu bar. The pull-down menu in the **SatuDict section** gives access to the choice of available computations: **Capillary Pressure Curve**, **Relative Permeability**, **Relative Gas Diffusivity**, **Relative Thermal Conductivity**, **Resistivity Index** and **Two-Phase Flow GeoApps**. Note that not all commands are visible and some of them require a special license!



The **Options** for the SatuDict computations can be modified through the Options **Edit...** button.

When the parameters for the selected SatuDict computational process have been entered, clicking the **Run** button in the **SatuDict section** starts the computations.

When recording a macro, the **Record** button becomes active, and the **Run** button changes to **Run & Record**.

The parameters entered in the **Options** dialog boxes can be saved into *.gps (GeoDict Project Settings format) files and/or loaded from them. Remember to restore and reset your (or GeoDict's) default values through the icons at the bottom of the dialog box when needed and/or before every SatuDict run. Resting the mouse pointer over an icon prompts a tooltip showing the icon's function.

Capillary Pressure Curve

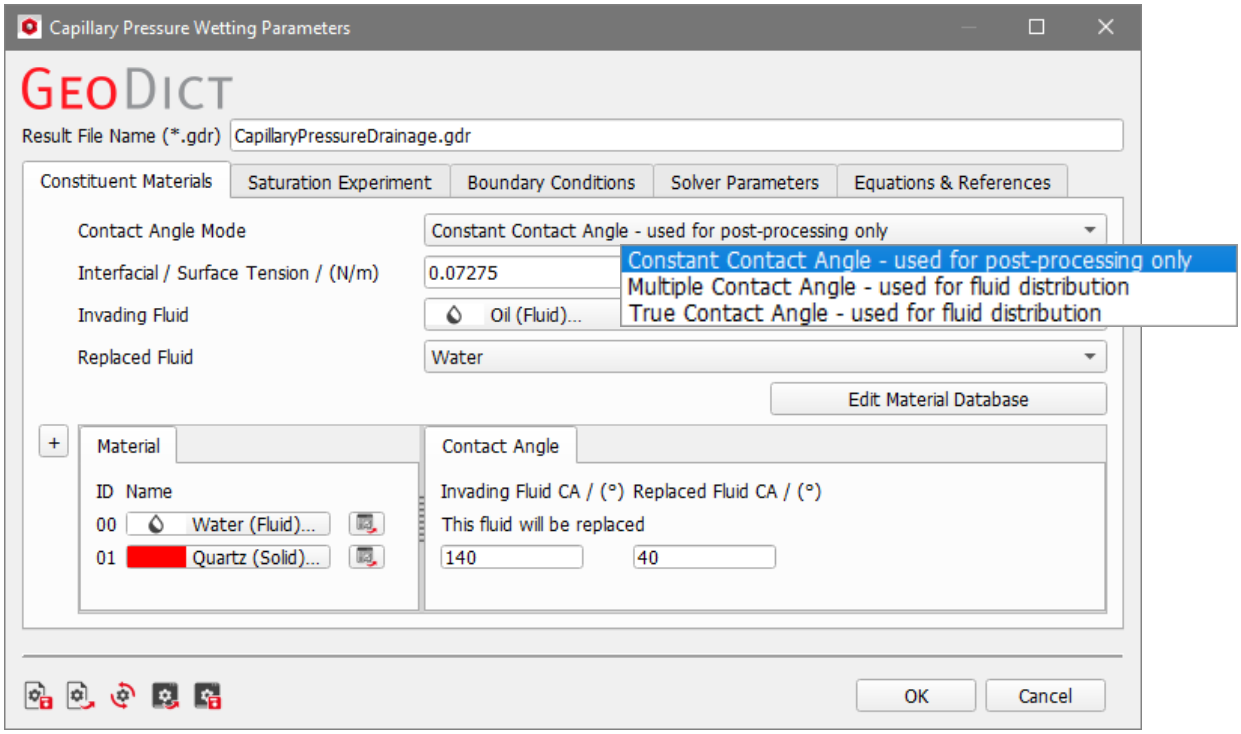
When selecting **Capillary Pressure Curve** from the pull-down menu, the **Wetting Parameters** needed for running this process can be entered (or modified) through the **Edit...** button.

The name for the result file is entered in the **Result File Name** box. Keep the default name or rename it according to your current project, to differentiate the results of sets of SatuDict computations. The resulting GDR result file is placed inside the chosen project folder.

The wetting parameters are grouped under four tabs: **Constituent Materials**, **Saturation Experiment**, **Boundary Conditions**, and **Solver Parameters**. The last tab **Equations & References** provides further information about the equations used in this calculation.

Constituent Materials

All material properties of invading and replaced fluid can be defined on the **Constituent Materials** tab.



Contact Angle Mode

Depending on the number and type of solid phases, the **Contact Angle Mode** can be selected as:

1. **Constant Contact Angle**. In this default setting, for the Pore Morphology method, a single (constant) contact angle is assumed between all solid materials and the invading fluid, and another constant contact angle between all solid materials and the replaced fluid. The given contact angle is considered for the computation of the capillary pressure, but a contact angle of 0° is used for the distribution of the fluids!

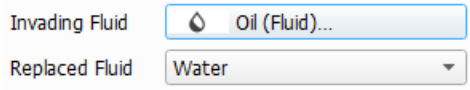
2. **Multiple Contact Angle**. For a more general Pore Morphology method, different (multiple) contact angles are specified for every solid material with the invading fluid and the replaced fluid. The contact angles of every material can be entered under the **Contact Angle** tab on the right-hand side below. The different contact angles are considered for the computation of the capillary pressure and for the distribution of the fluids. Surfaces of solid materials are assumed to be planar for this approach.
3. **True Contact Angle**. In the same way as for **Multiple Contact Angle**, contact angles for every solid material with the invading and the replaced fluid can be defined. To inscribe fluids with a more accurate contact angle, the curvature of the surface of solid materials is considered. For contact angles near 90°, the artefacts occurring for the Multiple Contact Angle method are avoided.

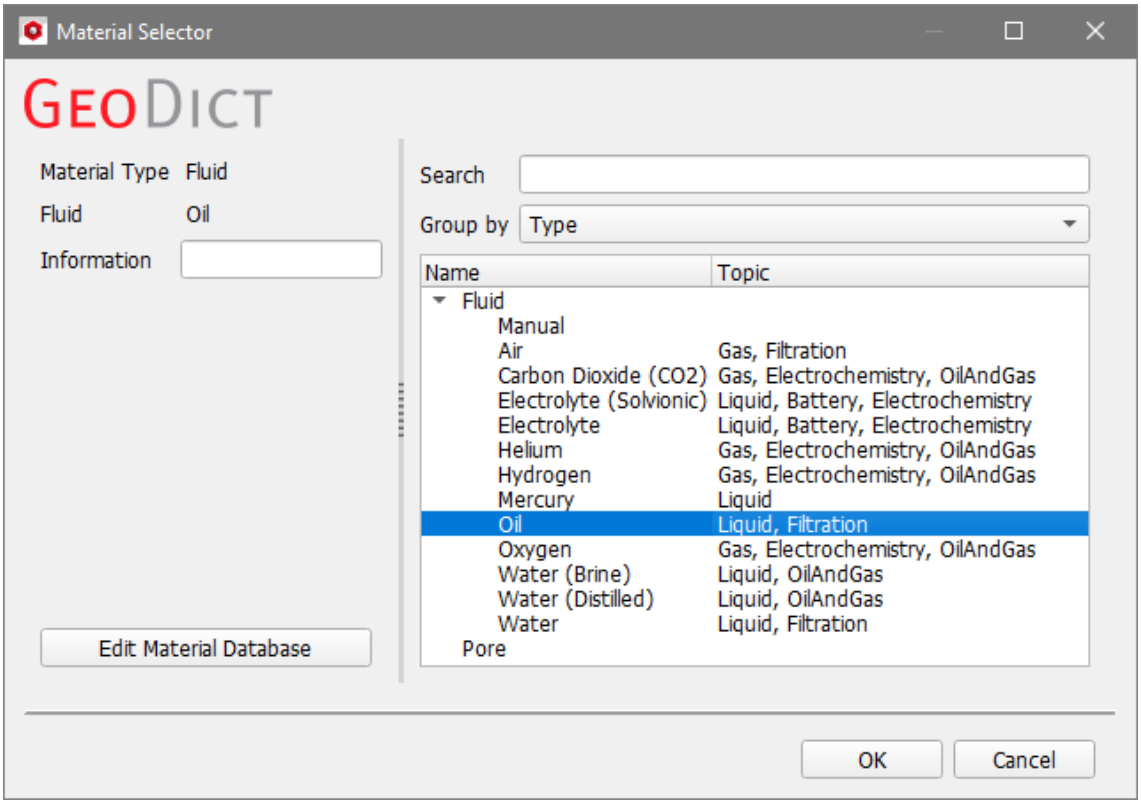
Interfacial / Surface Tension

Enter the **Interfacial / Surface Tension** between the invading and replaced fluid or use the default value corresponding to the surface tension between water and air.

Invading Fluid and Replaced Fluid

The **Invading Fluid** invades the current structure and displaces the **Replaced Fluid**. The invading fluid can be selected through the **Material Selector** dialog box, by clicking on the button for the material.



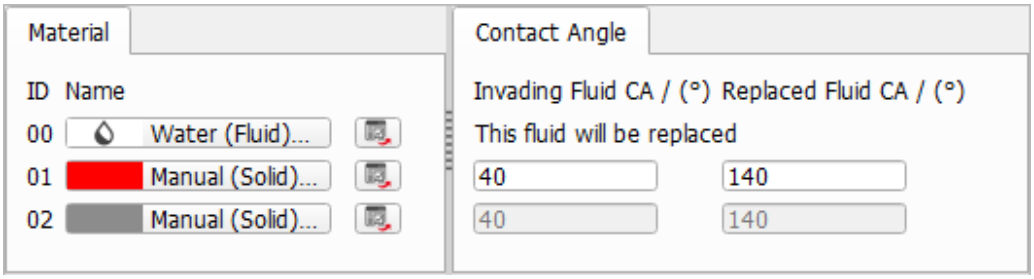


The **Replaced Fluid** must already be present in the model of the structure currently in memory. Choose the replaced fluid from the pull-down menu.

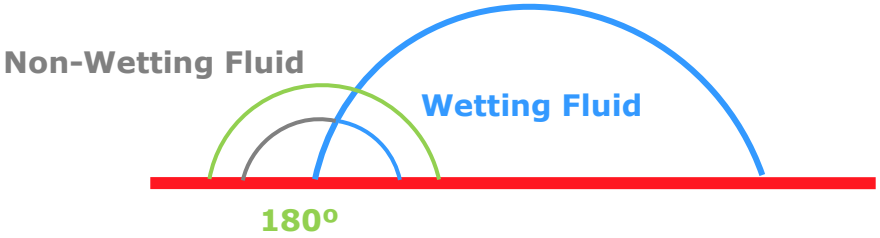
Material and Contact Angle

The **Contact Angle** can be entered for all solid materials (after choosing Constant Contact Angle as **Contact Angle Mode**) or for each solid material separately (after choosing Multiple Contact Angle or True Contact Angle as **Contact Angle Mode**).

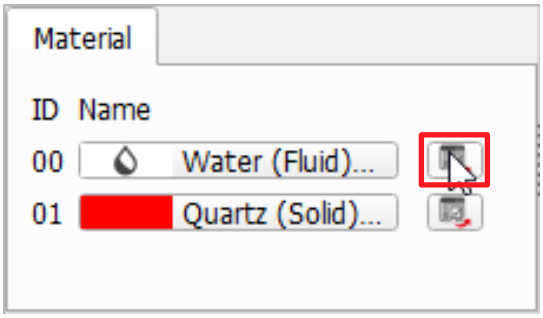
In the **Material** tab, the material of each material ID can be selected. The **Contact Angle** tab shows which fluid will be replaced (here, Water will be replaced).

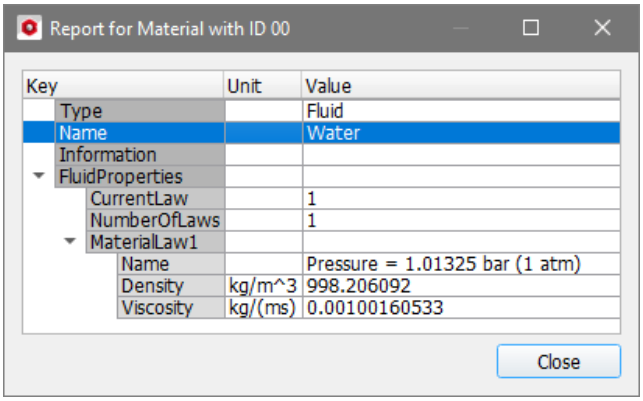


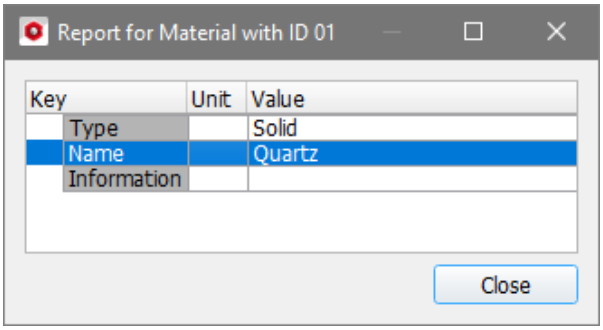
The **Invading Fluid CA** (Contact Angle) and the **Replaced Fluid CA** values add up to 180° and they are adjusted automatically when changing one of the two values. For a given solid material phase, the fluid with a contact angle smaller than 90° is **wetting** and the other fluid (with contact angle larger than 90°) is **non-wetting**.



Click the Material Report button to see the relevant parameters for the material with a selected ID.

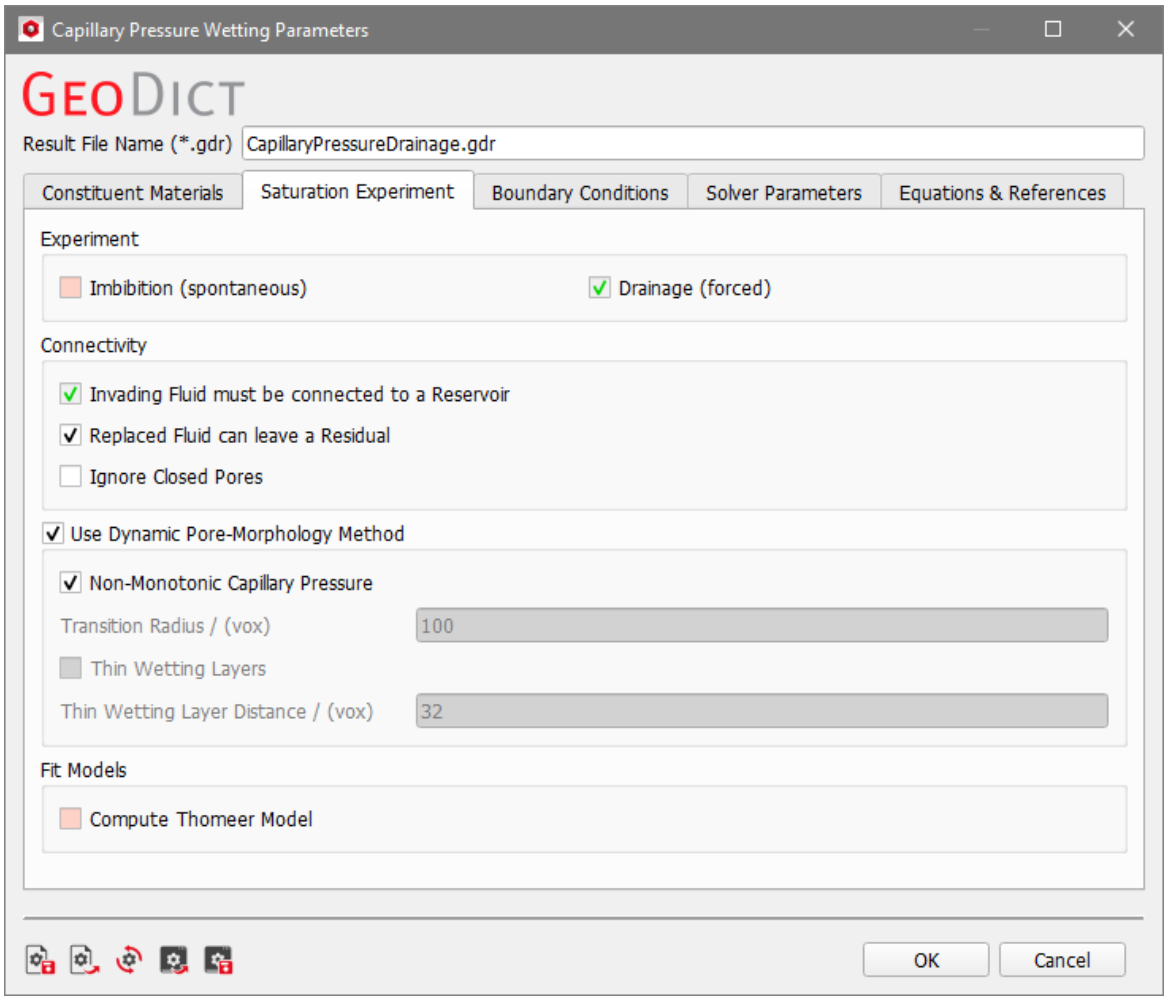






Saturation Experiment

The **Saturation Experiment** tab is divided into four groups: **Experiment**, **Connectivity**, **Use Dynamic Pore-Morphology Method** and **Fit Models**. Depending on the choices made before, some options may not be editable.



Experiment

It is shown here which kind of experiment is performed. This depends on the choice of the contact angles made in the **Constituent Materials** tab.

In some cases, both **Imbibition** and **Drainage** are conducted and the user can decide to execute only one of them.

If all contact angles of the invading fluid are above 90° then a **Drainage** experiment will be performed. If all contact angles of the replaced fluid are below 90° then a **Imbibition** experiment is performed. In mixed-wet cases where the contact angles of the invading fluid are above and below 90° then both options can be enabled.

Connectivity

The pore size and the pore connectivity to the wetting phase (WP) reservoir or non-wetting phase (NWP) reservoir determine the final distribution of the phases.

Check **Invading Fluid must be connected to a Reservoir** to connect the invading fluid continuously to a phase reservoir at a given spatial location outside of the domain (defined in the **Boundary Conditions** tab, see page 15). If this is

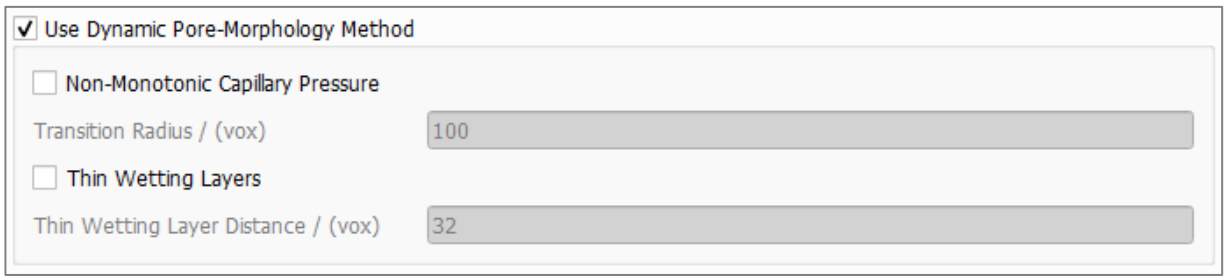
unchecked, it models the sudden appearance of the wetting phase as condensation on the surface of the material in the structure. If a Drainage simulation is performed **Invading Fluid must be connected to a Reservoir** cannot be unchecked.

Check **Replaced Fluid can leave a Residual** if the replaced fluid is allowed to leave a residual in pores that are separated from the replaced fluid reservoir, e.g., by the invading fluid. In this case, the replaced fluid needs to be connected to a reservoir, also defined in the **Boundary Conditions** tab, see page 15. The residual of the replaced fluid is assigned a new material ID. If this option is not checked, pores that have no connection to the replaced fluid reservoir and contain the replaced fluid are ignored and have after the simulation the same material ID as before.

Check **Ignore Closed Pores** to fill only the open pores with the invading fluid. Open pores are connected to the inflow and outflow region. All pores not connected to the domain boundary (closed pores) are pores without fluid at the beginning of the simulation. These closed pores are ignored and considered as solid regions during the simulation. After the simulation they are assigned to a separate material ID.

Dynamic Pore-Morphology Method

Check **Use Dynamic Pore-Morphology Method** to use this method for dynamic simulation of the drainage and imbibition processes.



Select **Non-Monotonic Capillary Pressure** to allow that the capillary pressure can drop down during a drainage simulation when the invading fluid passes a pore-throat. During an imbibition simulation, the capillary pressure can rise again, when the invading fluid passes a big pore.

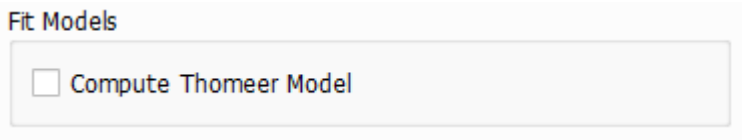
The option to define a **Transition Radius** is only available for mixed wet cases, where there is a transition from imbibition to drainage algorithm. With the **Non-Monotonic Capillary Pressure** option, it is possible to dynamically switch between both algorithms multiple times (automatically done during calculations). In this case the **Transition Radius** determines at which interface curvature radius (in voxel) corresponding to the fluid-fluid interface the switch happens.

To consider a modified connectivity check for thin wetting layers, check **Thin Wetting Layers** and define a **Thin Wetting Layer Distance** in voxels. Like this, wetting residuals not more than the defined distance away from the invading wetting phase front are always treated as connected. In addition, new wetting residual layers may emerge in small pores near the invading wetting front. This option is only available for imbibition processes.

Fit Models

For drainage simulation without the option **Replaced Fluid can leave a Residual**, the option **Compute Thomeer Model** can be selected.

This option computes the Thomeer Model based on the computed capillary pressure curves, see page 6.

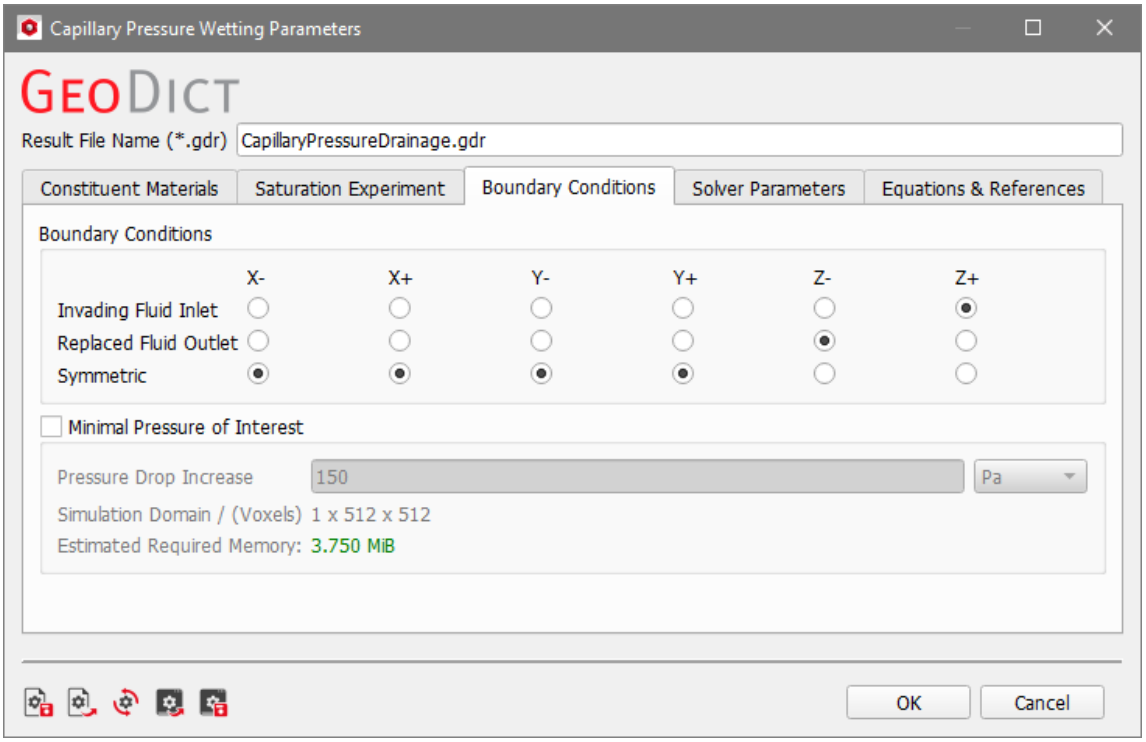


Boundary Conditions

The **Boundary Conditions** define if a side of the sample (X-, X+, Y-, Y+, Z-, and Z+) is connected to the **Invading Fluid Inlet** or the **Replaced Fluid Outlet**.

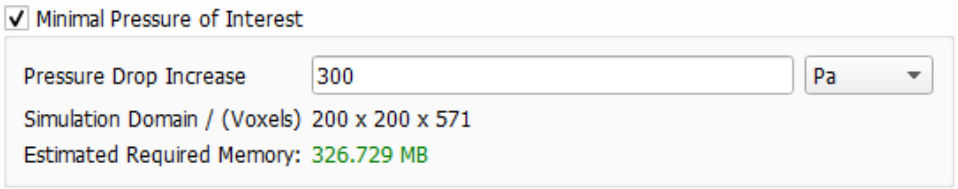
If a side is not connected to a reservoir, e.g. if the porous medium continues in that direction, SatuDict determines pore sizes and checks connectivity using symmetric boundary conditions in these directions, i.e. the pore structure is mirrored at this side.

The boundary conditions are greyed out and cannot be edited, if there is no invading fluid reservoir. Then, symmetric boundary conditions are used.



By checking **Minimal Pressure of Interest**, the size of the original simulation domain (voxels) is artificially increased in the direction(s) of the flow (here Z). The effect is to improve the capillary pressure results at least down to the desired value, by increasing the structure size such that a sphere, corresponding to the minimal pressure, fits into the whole structure. The cost for this increased accuracy is that it is increasing the memory requirements for the calculations as well.

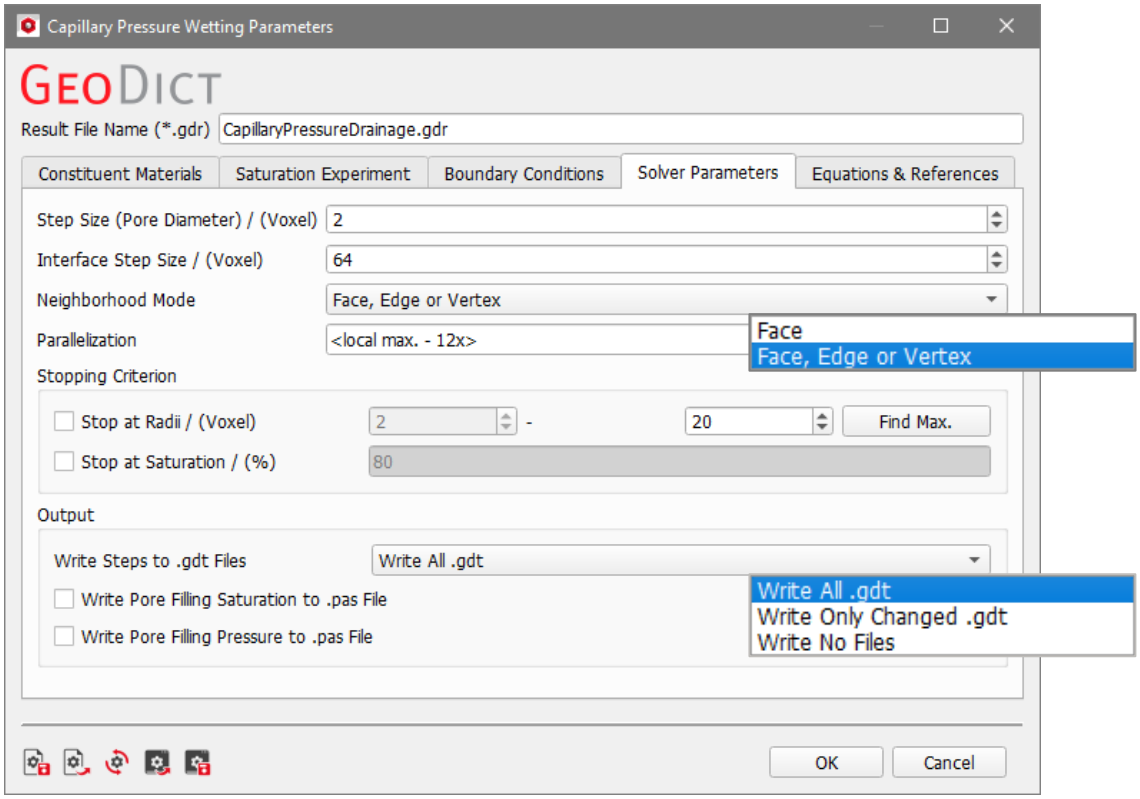
The size of the increased **Simulation Domain** (in voxels) and the **Estimated Required Memory** for this are shown.



Solver Parameters

The **Solver Parameters** define the settings for the solver run, and also the format of the output files is entered here.

Step Size (Pore Diameter)



The pore diameter, together with the connectivity rule based on the Neighborhood Mode and the defined contact angles, determine the distribution of the wetting and non-wetting phases.

The pore sizes to be considered for the calculations can be defined by entering the **Step Size**. The algorithm increases or decreases the pore diameter (and thus changes the capillary pressure) from step to step by this amount. Small values increase the accuracy of the result but lead to longer calculation times.

Interface Step Size

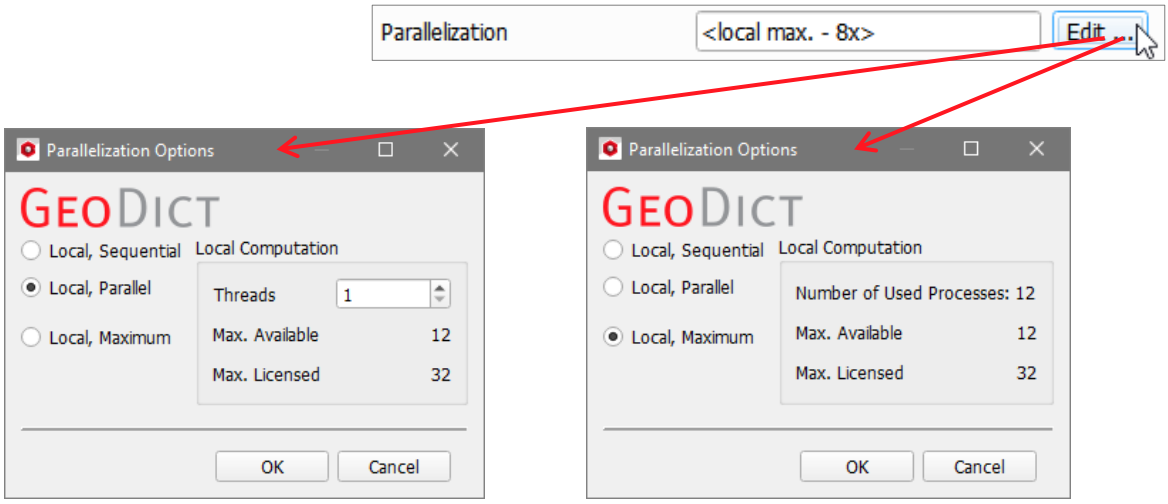
This feature is only available if the Dynamic Pore Morphology Method is used. It specifies how far the interface between the phases is allowed to move within one simulation step and like this influences the accuracy of the simulated capillary pressure curve. The Dynamic Pore Morphology Method tries to approximate the specified interface distance, but in some cases smaller interface distances are realized. If the Interface Step Size is small, then the accuracy and thus the number of simulation steps is increased but it also increases the overall runtime.

Neighborhood Mode

The **Neighborhood Mode** determines how the voxels of the material occupying the pore space in the porous media are perceived as belonging to a connected group. Checking **Face** is more restrictive than choosing **Face, Edge, or Vertex**. See more details on the neighborhood mode in the MatDict handbook (Connected Components) and the ProcessGeo handbook (Cleanse command) of this User Guide.

PARALLELIZATION

Calculations can be parallelized if the user's license and hardware allow it. The **Parallelization Options** dialog opens when clicking the **Edit...** button, to choose between **Local, Sequential**, **Local, Parallel** or **Local, Maximum**.



For **Local, Sequential** only one Process is used for the computation.

When **Local, Parallel** is selected, the **Number of Processes** can be entered. Then the maximum number of available processors and the maximum number of licensed parallel processes is shown in the dialog.

STOPPING CRITERION

If the check box **Stop at Radii / (Voxel)** is enabled, the simulation stops if either the minimal pore radius is reached (for a Drainage) or the maximal pore radius is reached (for an Imbibition).

Click **Find Max** to find the maximum pore radius present in the structure. The value found by **Find Max** is inserted automatically in the right box.

For a **Drainage** simulation, only the minimum radius can be set. If an **Imbibition** is computed, only the maximum radius can be set.

When **Stop at Saturation / (%)** is checked, the simulation stops if the invading fluid has reached this saturation value.

OUTPUT

Under the Output group it can be defined which information should be written as output files. If **Write All .gdt** is selected, the computed phase distributions are also saved as GDT files that can be imported for visualization.

The material IDs and colors of the Invading Fluid, the Residual Invading Fluid, the Replaced Fluid, and the Residual Replaced Fluid are chosen automatically from the set of free material IDs.

Depending on inlet and step size, different steps might lead to the same .gdt file. With **Write Only Changed .gdt** selected, only .gdt files that differ from previous ones are written to the hard drive. This leads to a reduced hard drive memory consumption and a slightly reduced runtime.

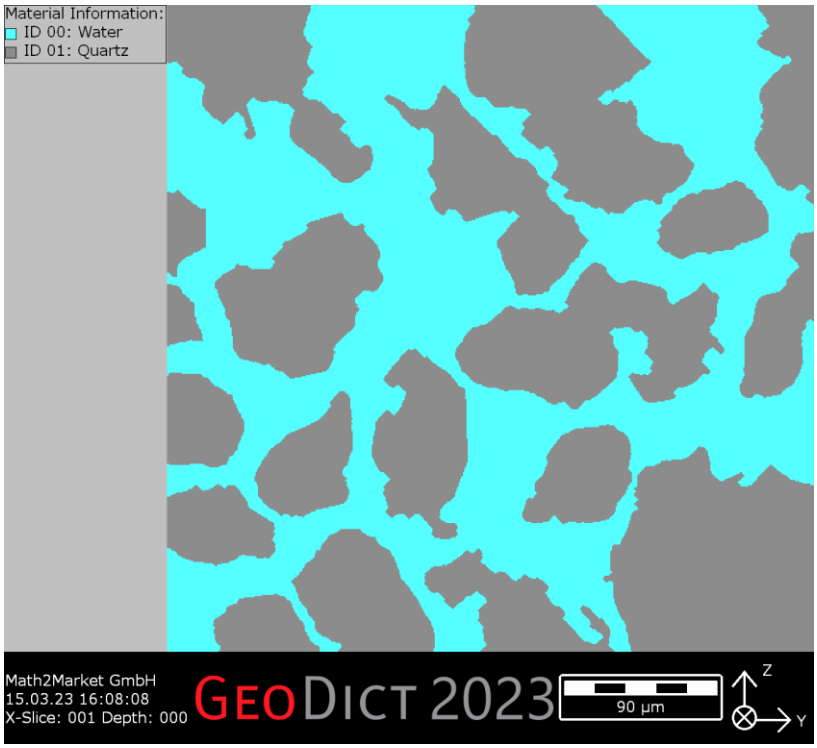
Select **Write No Files** if no intermediate .gdt files should be saved.

If one of the options **Write Pore Filling Saturation to .pas File** and **Write Pore Filling Pressure to .pas File** is checked a .pas (**p**ressure **a**nd **s**aturation) file is written and saved in the result folder. This is a volume file and can be loaded in the result viewer (see page 26). Depending on the checked options, either the Saturation of the invading fluid, the pressure at which a pore is filled or both are written in the .pas file.

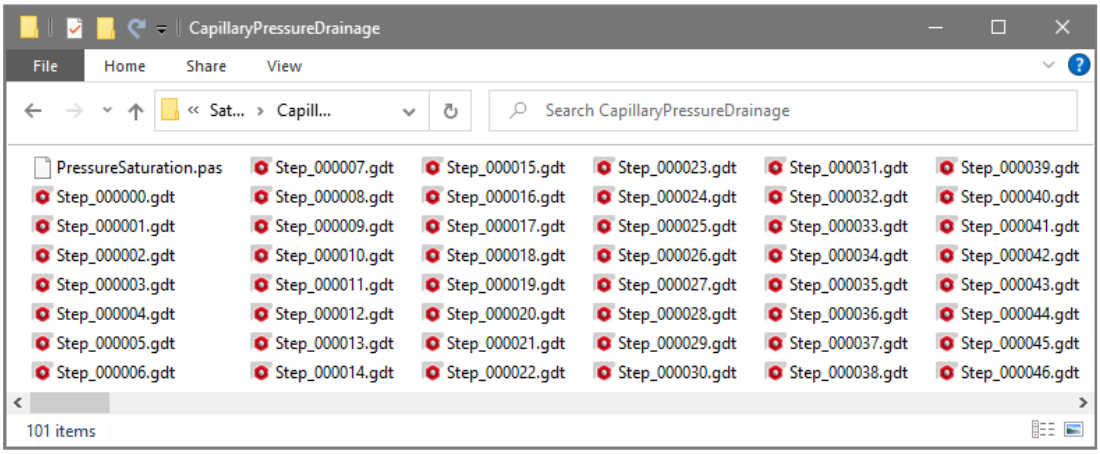
CAPILLARY PRESSURE CURVE RESULT FILE

General details on the result viewer are found in the Result Viewer handbook of this User Guide. Here, only the special features for SatuDict Capillary Pressure are shown.

In the example, the calculations of Capillary Pressure Curve are run on a porous structure with 54% SVF, originated from Berea sandstone. A 2D cross-section view of the structure is shown below. The invading fluid oil is non-wetting and displaces the wetting fluid water during a drainage simulation.

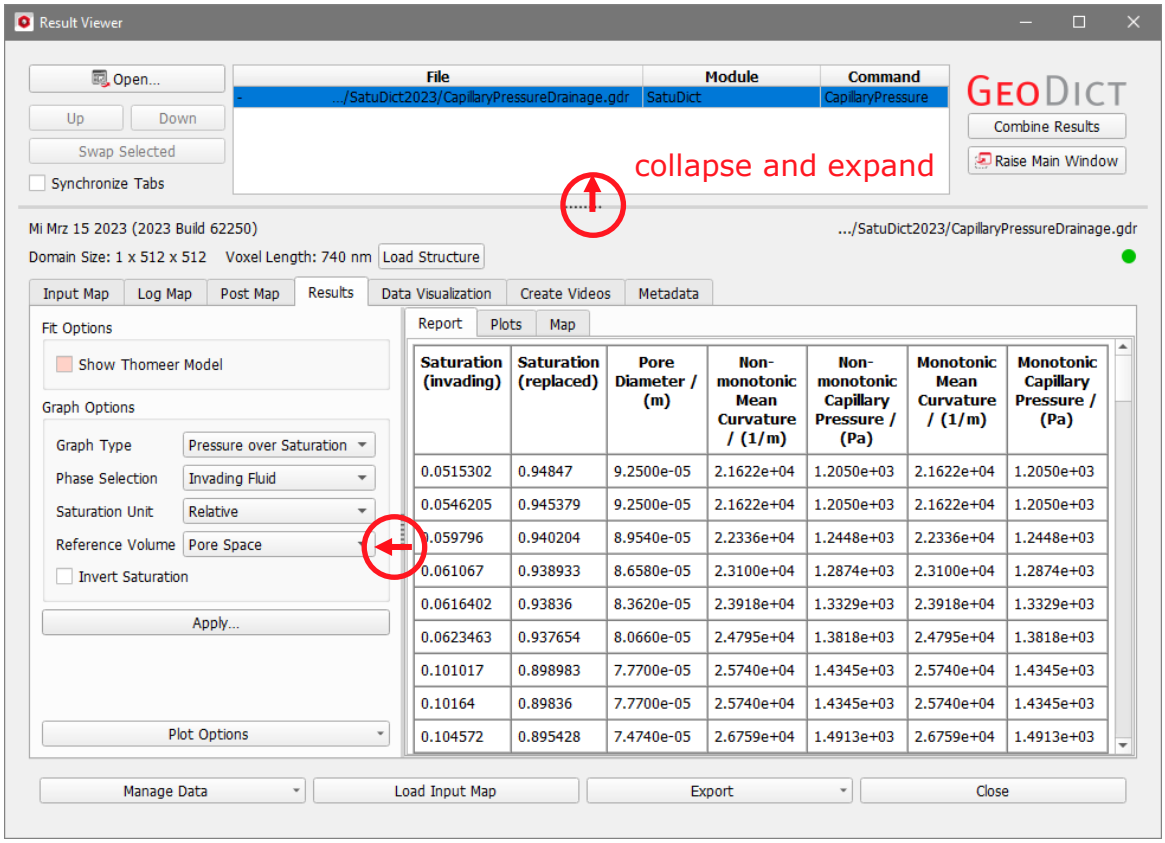


The GDT files corresponding to the computational steps (Step_000000.gdt, etc.) are stored in the automatically created result folder with the name of the result file name in the project folder.



This is only done if **Write All .gdt** or **Write Only Changed .gdt** was selected in the Solver Parameters tab, see page 17). This folder also contains the **PressureSaturation.pas** file and the Structure.gdt file, with the original structure, before the drainage simulation is started.

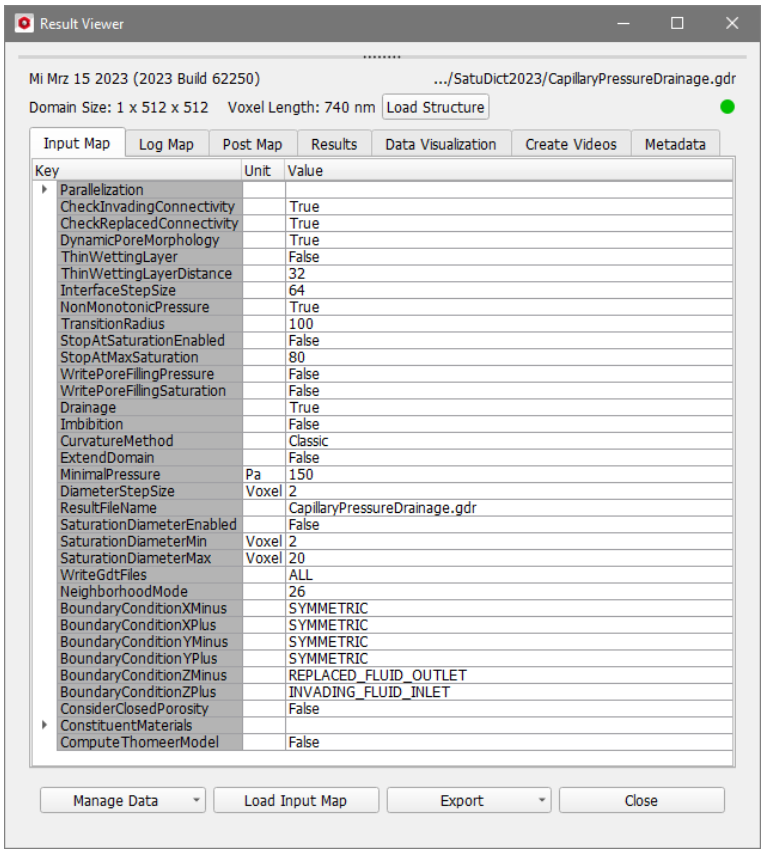
After the solver has finished, the Result Viewer opens immediately.



The computational results are accessed through the tabs **Input Map**, **Log Map**, **Post Map**, **Results**, **Data Visualization**, **Create Videos** and **Metadata**.

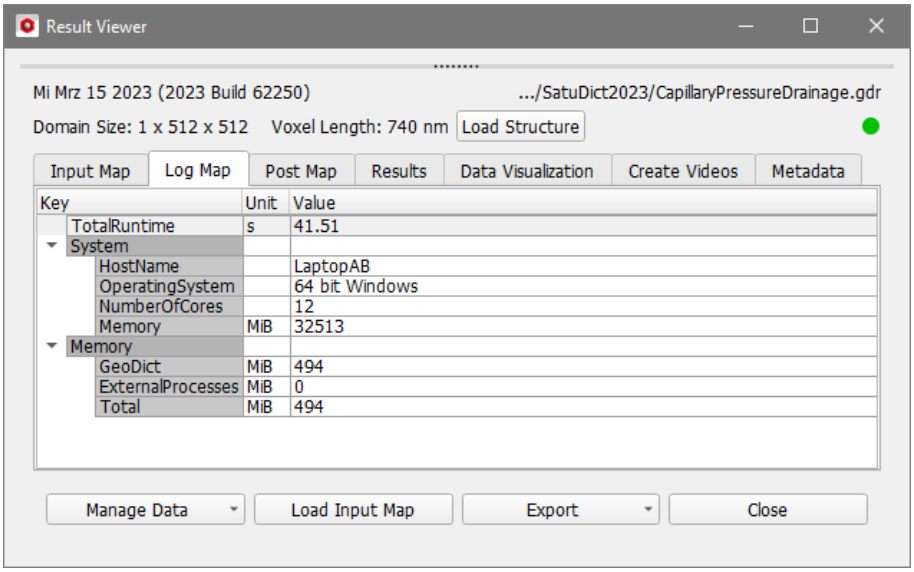
INPUT MAP

The **Input Map** provides a simplified overview of all data entered in the Wetting Parameters dialog.



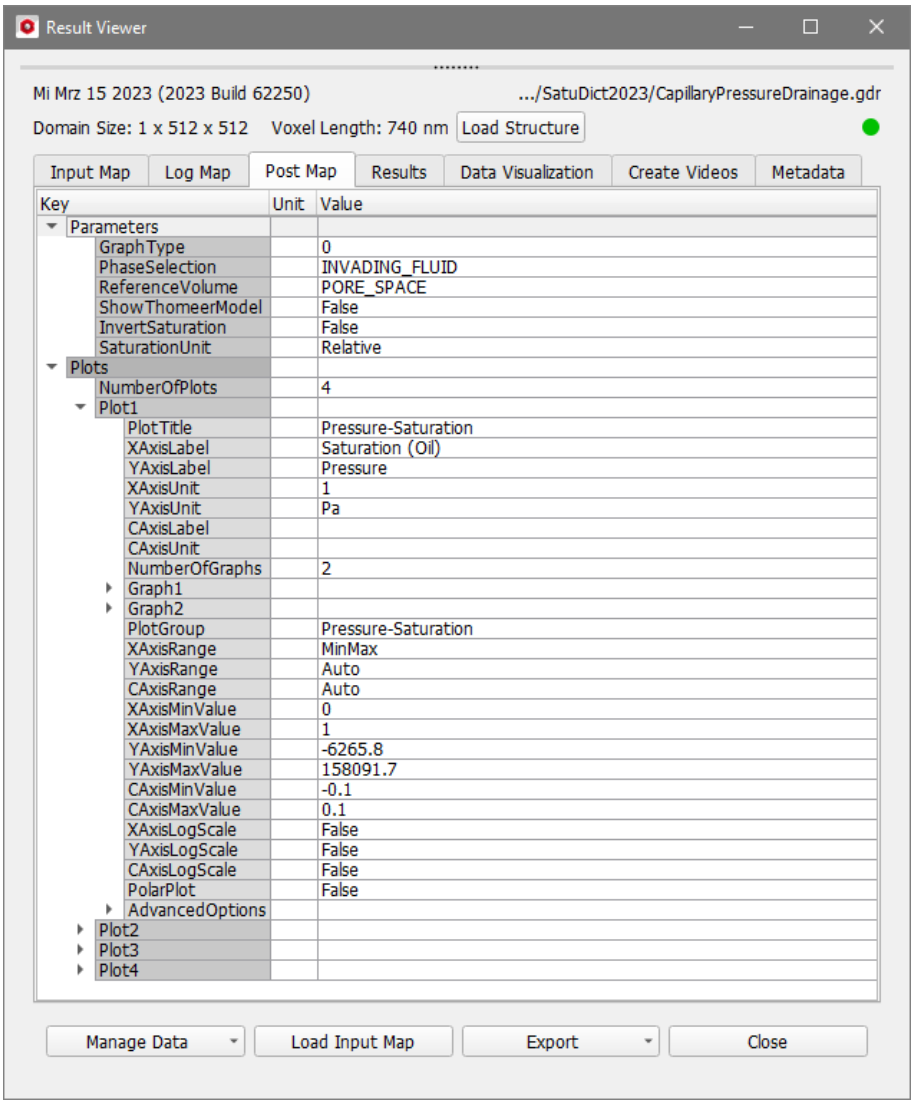
Log Map

The **Log Map** provides information about the solver runtime, the memory usage and the hardware.



Post Map

The **Post Map** provides information about the plots shown under the **Results** tab.



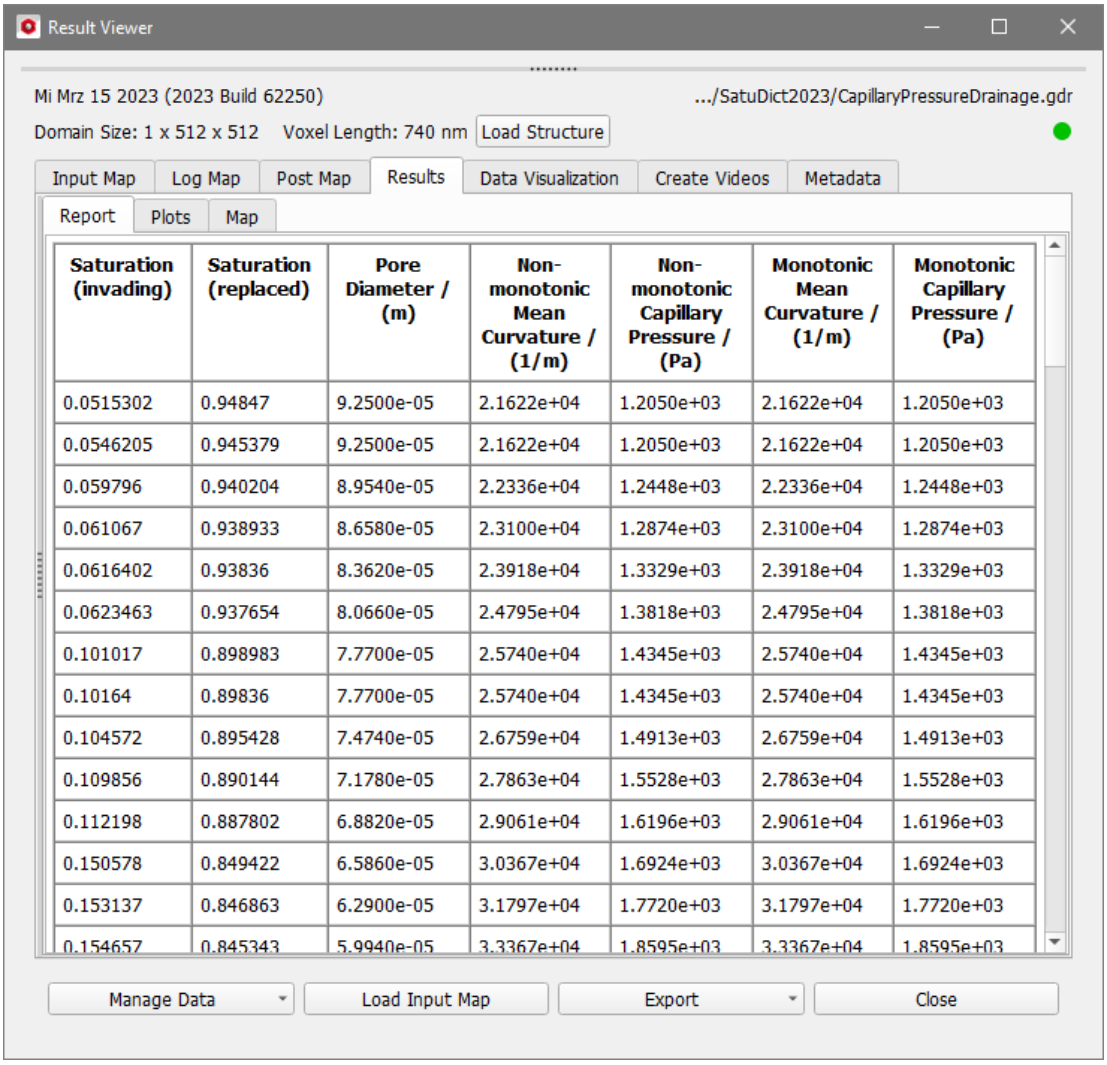
RESULTS

The **Results** tab has the three subtabs **Report**, **Plots**, and **Map**.

Report

When clicking the **Results - Report** subtab, a detailed table with the calculated values is shown.

For a typical capillary pressure result file, the table shows the Saturation of the invading fluid, the Saturation of the replaced fluid, as well as the Pore Diameter, the Mean Curvature and the calculated corresponding Capillary Pressure for every step (pore size). If the Dynamic Pore-Morphology Method with the option Non-Monotonic Capillary Pressure was used for the computation, Mean Curvature and Capillary Pressure are shown both for the monotonic and non-monotonic capillary pressure curve.



Saturation (invading)	Saturation (replaced)	Pore Diameter / (m)	Non-monotonic Mean Curvature / (1/m)	Non-monotonic Capillary Pressure / (Pa)	Monotonic Mean Curvature / (1/m)	Monotonic Capillary Pressure / (Pa)
0.0515302	0.94847	9.2500e-05	2.1622e+04	1.2050e+03	2.1622e+04	1.2050e+03
0.0546205	0.945379	9.2500e-05	2.1622e+04	1.2050e+03	2.1622e+04	1.2050e+03
0.059796	0.940204	8.9540e-05	2.2336e+04	1.2448e+03	2.2336e+04	1.2448e+03
0.061067	0.938933	8.6580e-05	2.3100e+04	1.2874e+03	2.3100e+04	1.2874e+03
0.0616402	0.93836	8.3620e-05	2.3918e+04	1.3329e+03	2.3918e+04	1.3329e+03
0.0623463	0.937654	8.0660e-05	2.4795e+04	1.3818e+03	2.4795e+04	1.3818e+03
0.101017	0.898983	7.7700e-05	2.5740e+04	1.4345e+03	2.5740e+04	1.4345e+03
0.10164	0.89836	7.7700e-05	2.5740e+04	1.4345e+03	2.5740e+04	1.4345e+03
0.104572	0.895428	7.4740e-05	2.6759e+04	1.4913e+03	2.6759e+04	1.4913e+03
0.109856	0.890144	7.1780e-05	2.7863e+04	1.5528e+03	2.7863e+04	1.5528e+03
0.112198	0.887802	6.8820e-05	2.9061e+04	1.6196e+03	2.9061e+04	1.6196e+03
0.150578	0.849422	6.5860e-05	3.0367e+04	1.6924e+03	3.0367e+04	1.6924e+03
0.153137	0.846863	6.2900e-05	3.1797e+04	1.7720e+03	3.1797e+04	1.7720e+03
0.154657	0.845343	5.9940e-05	3.3367e+04	1.8595e+03	3.3367e+04	1.8595e+03

Warnings in the Result File:

If the Contact Angle Method **Multiple Contact Angle** was used for the computation of the saturation pressure curve (see page 11), a warning may appear in the result file created.

Warning: The multiple contact angle method requires that the *ratio between pore diameter and structure diameter (e.g. fiber or grain diameter)* does not become too large.
In detail, (Pore Diameter)/(Structure Diameter) should always be smaller than 2*cos(theta)/(1-cos(theta)), where theta is the wetting phase contact angle.
For the current geometry, this requirement is not met and the solution may contain numerical artifacts!
Recommendation: Use smaller contact angles or use the true contact angle method so resolve that issue.

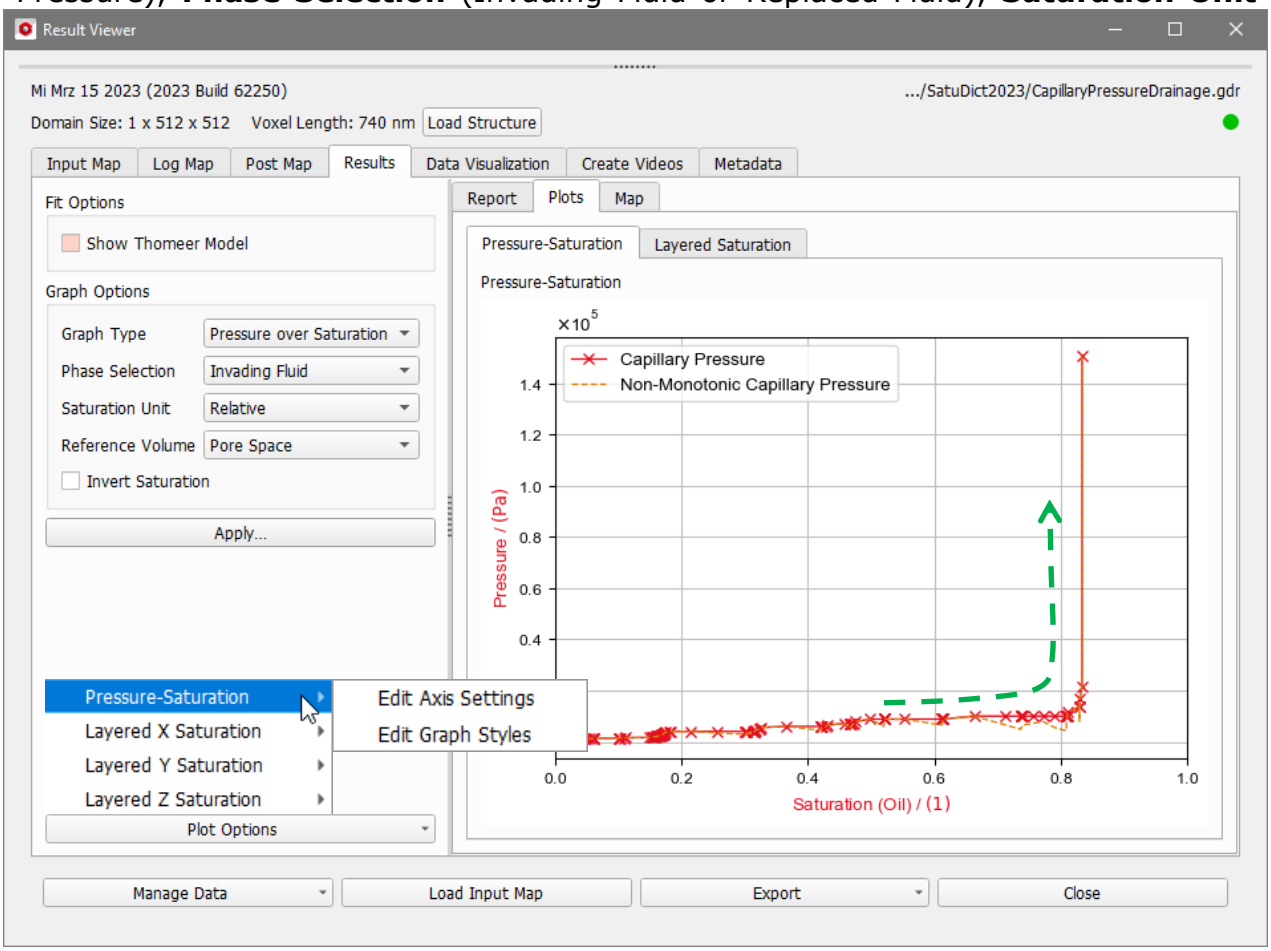
The reason is that the defined contact angle for the invading fluid is close to 90° and the diameter of pores in the structure is high compared to the diameter of components of the structure.

Two main ingredients of the multiple contact angle method are a dilation and an erosion process. For high contact angles, the dilation radius can get much higher than the erosion radius. For solid objects in the structure with diameter much smaller than the maximum pore diameter, this can lead to artefacts in the fluid distribution, like contact angles higher than desired, larger saturation steps and fewer saturation steps. This happens if the ratio between pore diameter and diameter is larger than $2 * \frac{\cos(\theta)}{1-\cos(\theta)}$. With the new **True Contact Angle** method, this problem can be avoided.

Plots

Click the **Results** - **Plots** subtab to observe the tabular results of the Report subtab as a diagram in the **Pressure- Saturation** subtab.

At the left side of the Result Viewer, the user can modify the way the graph is displayed by selecting **Graph Type** (Pressure over Saturation or Saturation over Pressure), **Phase Selection** (Invading Fluid or Replaced Fluid), **Saturation Unit**



(Relative or Absolute) and Reference Volume (Pore Space, Pore Space (Thomeer), or Total Sample Volume). The option Pore Space (Thomeer) is only available after a Drainage simulation without residual of the replaced fluid was performed.

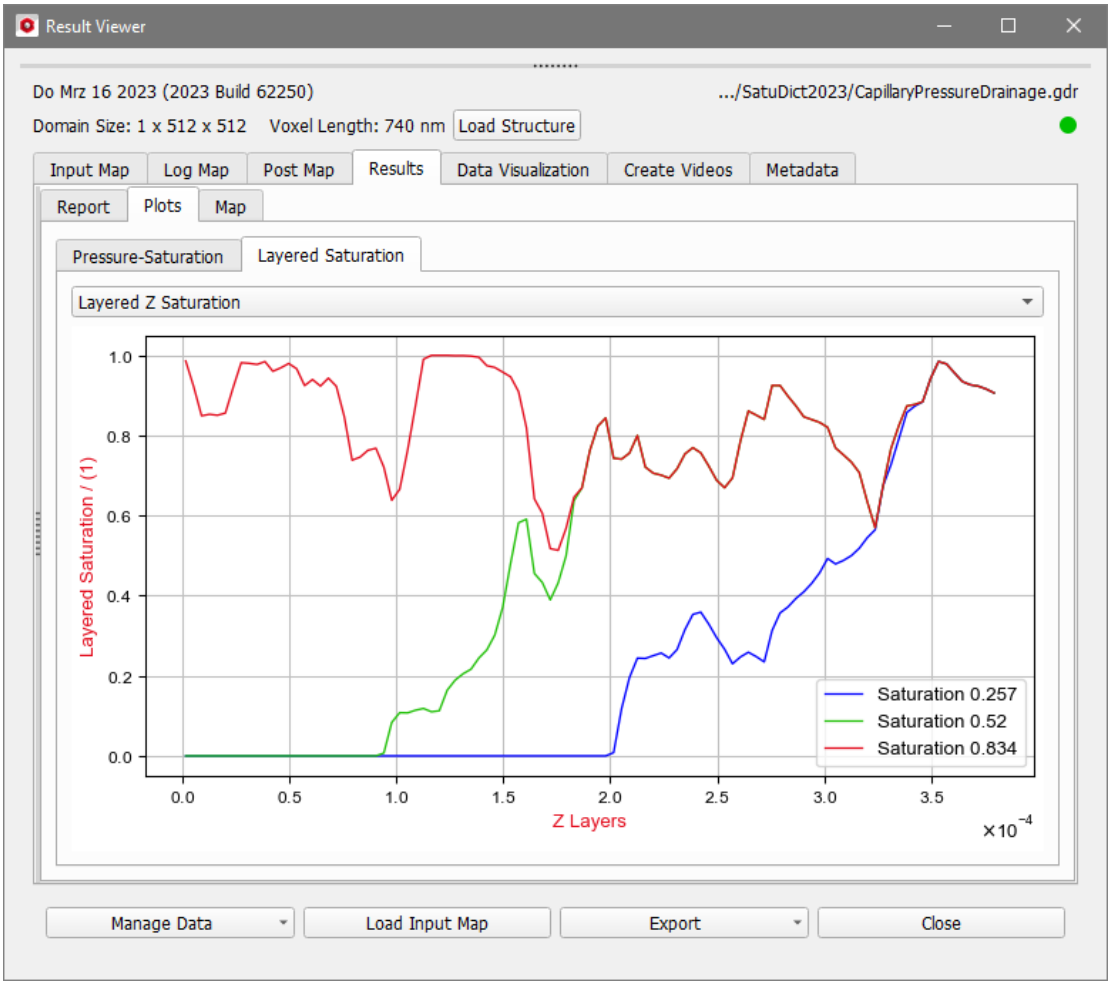
If a Thomeer Model is fitted, see page 6, this model can be shown by checking **Show Thomeer Model** under **Fit Options**.

Check **Invert Saturation** to show the values of the saturation in decreasing instead of increasing order.

As usual, right clicking on the plot opens a small dialog box with the possibility to modify the axis settings, the graph styles or to save the graph in different ways. With **Edit Axis Settings**, e.g., the scale of the X- and Y-axis can be changed to compare plotted results from different capillary pressure curve calculations side by side. From GeoDict 2022 on, the options **Edit Axis Settings** and **Edit Graph Styles**, can be accessed also by choosing **Plot Options→Pressure-Saturation** at the bottom of the left panel.

In the example, at the beginning of the drainage process, the porous structure is saturated (100%) by the Water. As the pressure increases, the Oil starts invading the structure and forces the Water out of it. Thus, the saturation of the Oil is increasing. By the end of the drainage process, where the pressure is at its highest level, the structure is 83% saturated with Oil and 17% saturated with Water (Residual). The non-monotonic increase of the pressure value for the simulation with the Dynamic Pore-Morphology Method is visible, especially for saturation values between 70% and 80%.

In the subtab **Layered Saturation**, the saturation along each of the three axes (X-, Y-, and Z-axis) is shown.

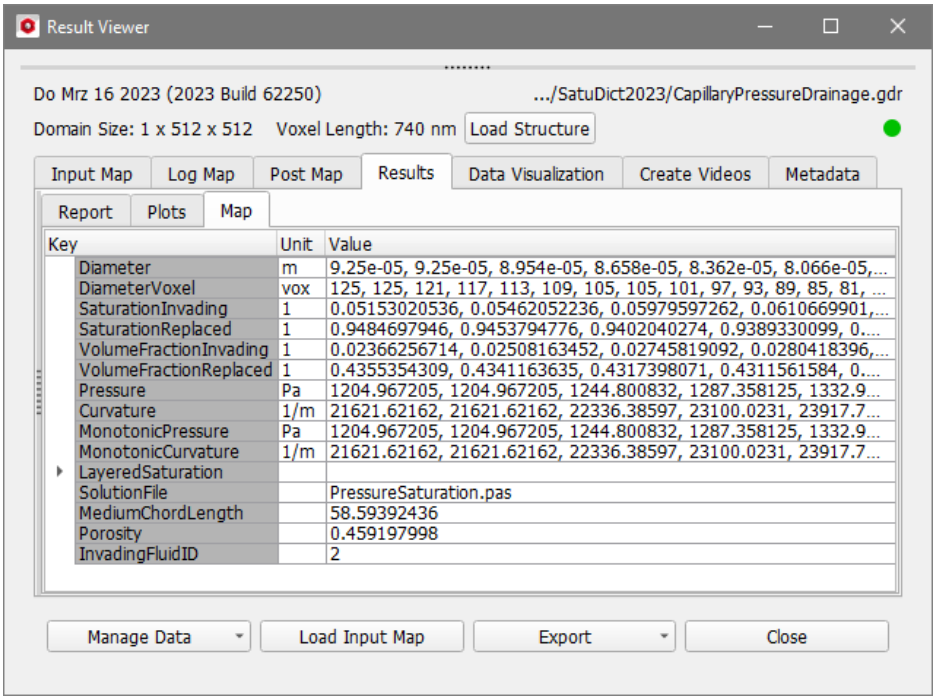


From the drop-down menu choose the direction to observe. For each layer, the occupied space of the invading fluid relative to the pore volume of this layer is plotted. This can be done for several steps of the calculation, which corresponds to different saturations of the whole structure. By right-clicking into the plot area, the curves of different simulations steps can be selected.

Map

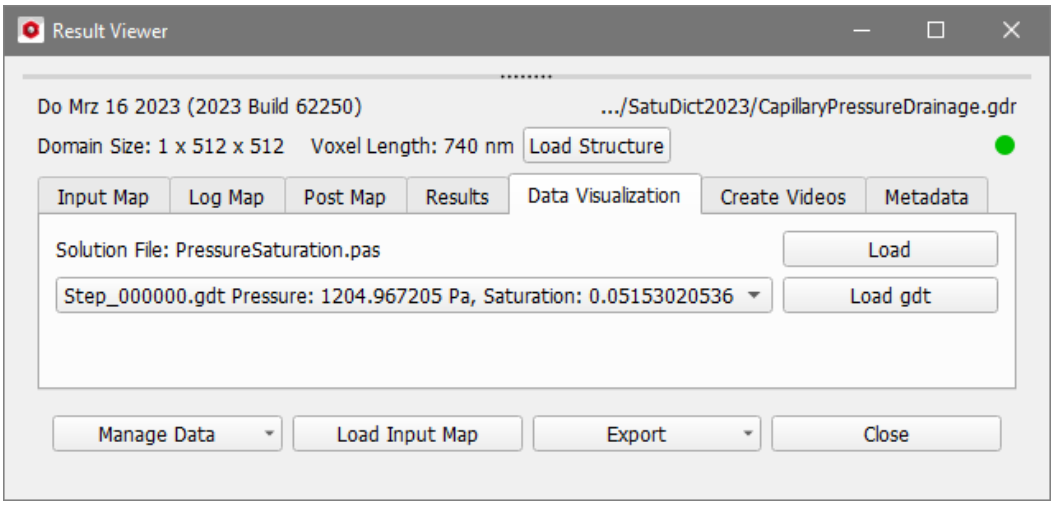
The **Results - Map** subtab gives access to the computed values. It contains also the values from the Report and Plots subtabs.

For the capillary pressure curve, it lists e.g. the calculated Pressure, Diameter, and Saturation values. The name of the *.pas file for the visualization of results is also given. The Invading Phase ID (here, 2 is Oil) shows the assigned Material ID of the invading fluid.



Data Visualization

In the **Data Visualization** tab the *.pas file and the step-by-step images of the computed process can be loaded.



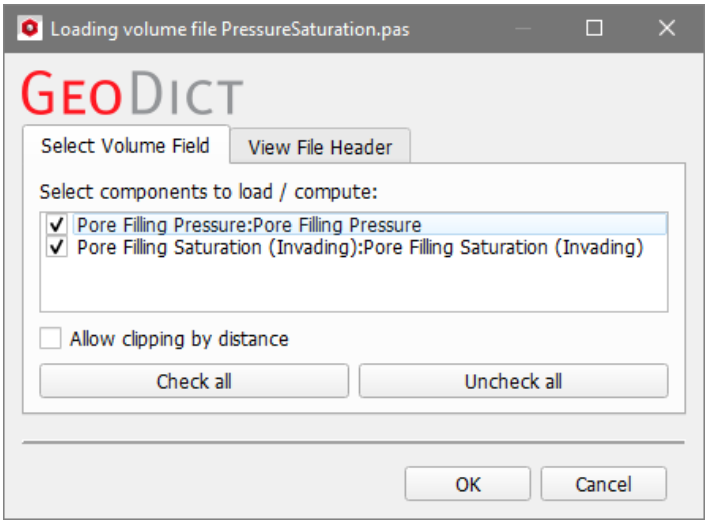
Under the **Data Visualization** tab, click **Load** to access the pressure and saturation field data saved in the **PressureSaturation.pas** file. Depending on the choice made in the Solver Parameters tab under the output options (see page 17) the **Pore Filling Pressure** and the **Pore Filling Saturation (Invading)** can be selected for the visualization.

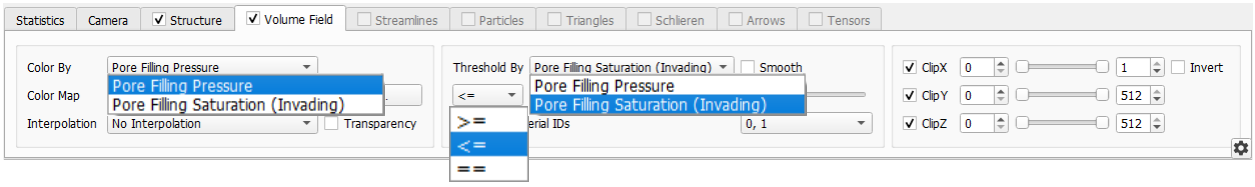
The initial visualization, in 2D view or 3D rendering, is done using default settings that the user can modify to visualize the imbibition and drainage results obtained with SatuDict. These parameters can be found under the **Volume Field** tab in the **Visualization Panel**, above the Visualization Area. For more information on a particular visualization setting, see the Visualization handbook of this User Guide.

A color bar or color scale appears in the Visualization area near the structure during the visualization of the results, indicating the gradation of pressure or saturation.

Switch between the two components of the results (Pore Filling Pressure, Pore Filling Saturation (Invading)) through the **Color By** pull-down menu.

While in 3D rendering, the progress of the drainage or imbibition process can be followed by selecting Pore Filling Pressure from the **Color By** and Pore Filling Saturation (Invading) from the **Threshold By** pull down menus.





With these settings, the visualization is twofold because, for a given invading fluid saturation level (threshold value), the capillary pressure at particular locations in the structure is shown together with the distribution of the two phases. While the color gradation refers to the capillary pressure values as displayed in the color bar, the distribution of the phases is given by the presence or absence of colored voxels in the pore space, without relation to the color bar scale.

For this dual visualization of capillary pressure level and distribution of phases, the interplay of **Threshold Slider** and **Clip Mode** selection are essential:

- **Threshold Slider / Box**

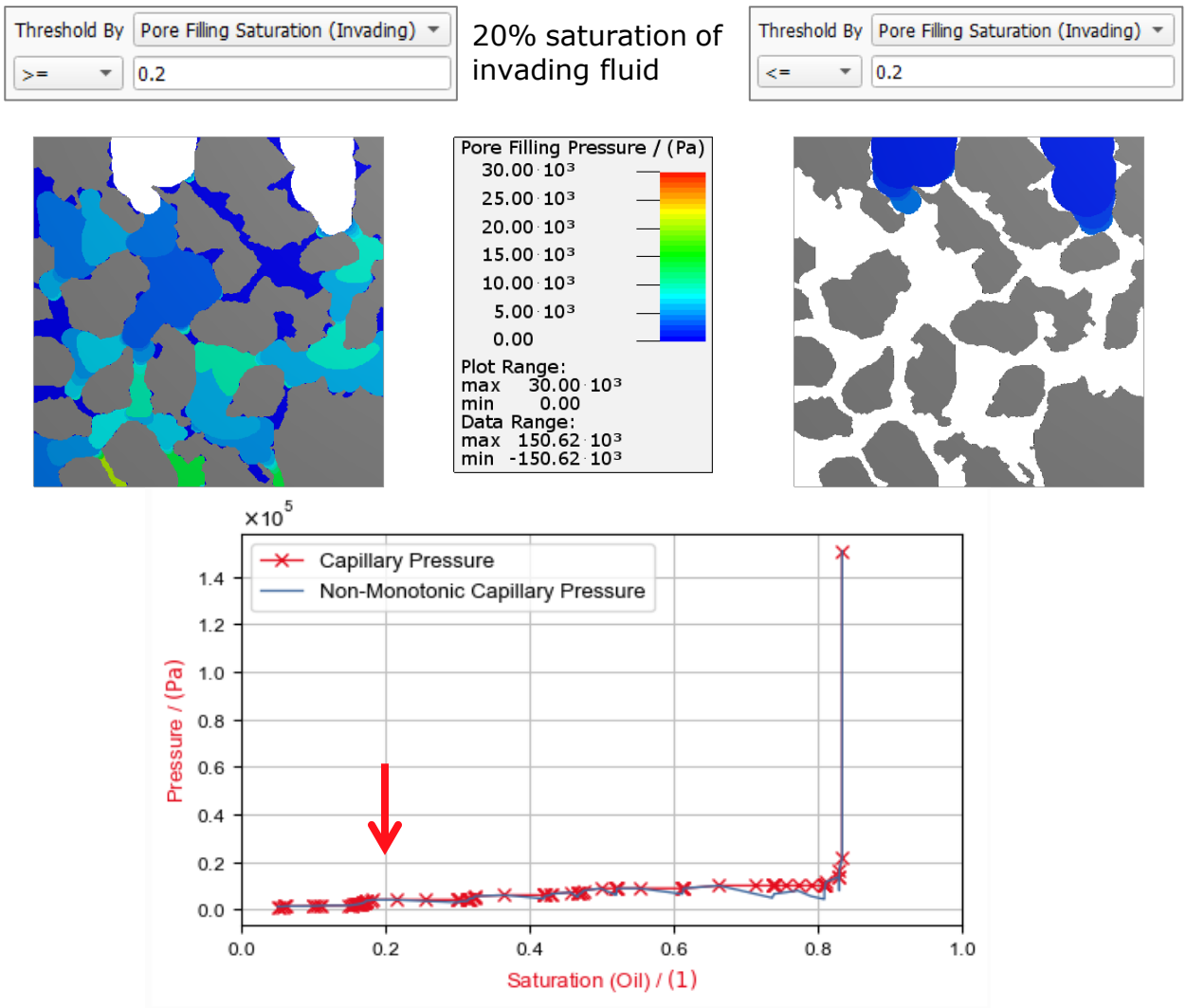
  The intrusion process is observed when moving the threshold slider from left to right or entering increasing values from 0 to 1 in the clip box. This parallels the increasing saturation of the invading fluid (from 0% to 100%) in the porous structure.

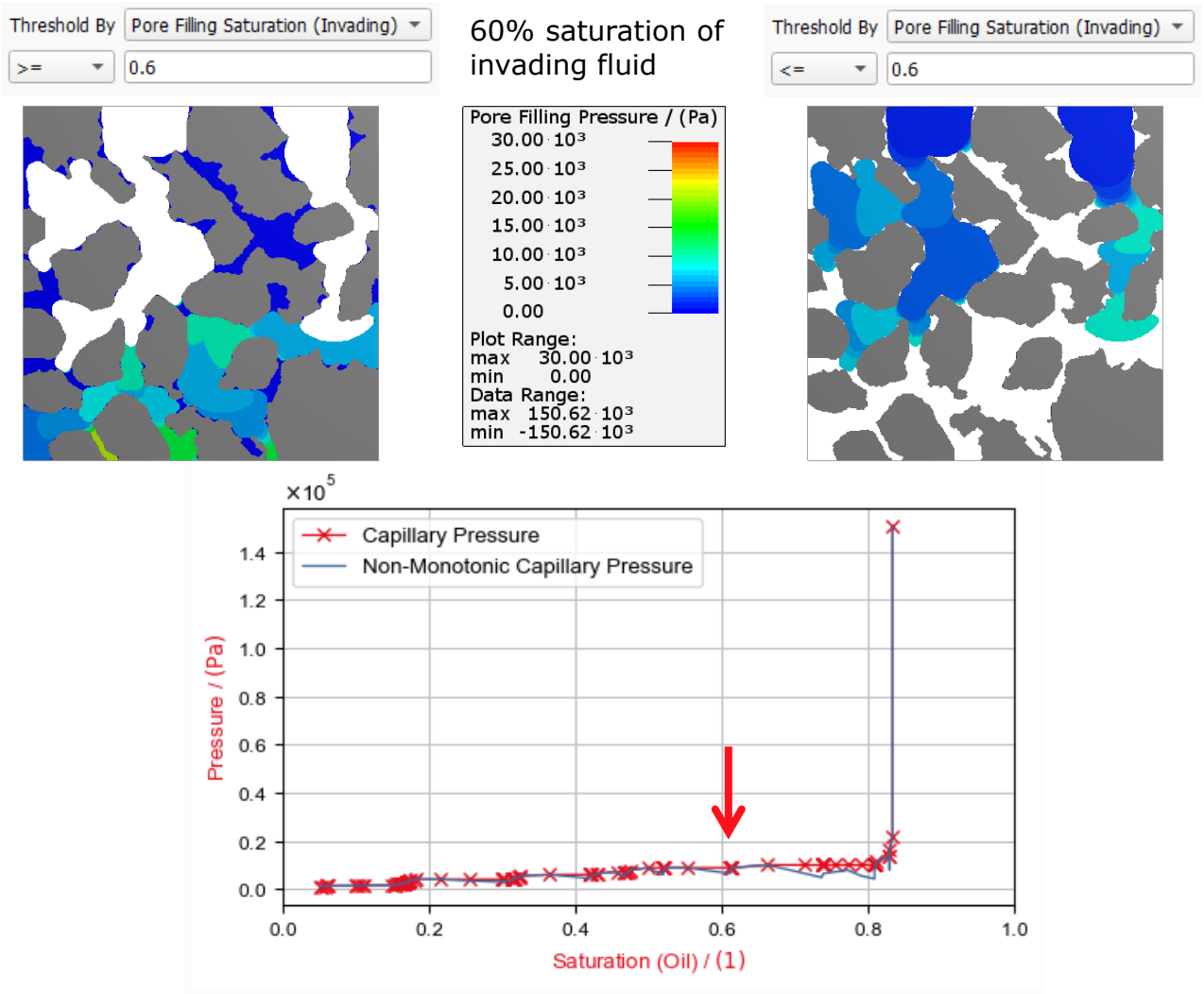
The **beginning** of the process is observed with the slider all the way to the left. By moving it to the right or by entering increasing values in the threshold slider box, the intrusion process is visualized forward and at the **end** the clip slider is all the way to the right.

Observe, that in the example shown here, the solution was computed till a saturation of 83%.

- **Clip Mode**: makes the dual visualization of pressure values and distribution of phases possible because it links them based on the capillary pressure saturation curve (see page 23).
  - By selecting >=, color is shown in the pore space where the invading fluid occupies the structure only at a higher saturation than the Pore Filling Saturation (Invading) set in the threshold slider. This shows the locations where the replaced fluid is still in the structure at this saturation or below.
  - By selecting <=, color is shown in the pore space where the invading fluid is already present for a saturation below the value for Pore Filling Saturation (Invading) set in the threshold slider. This shows the locations where the invading fluid has already entered the structure and replaced the replaced fluid.

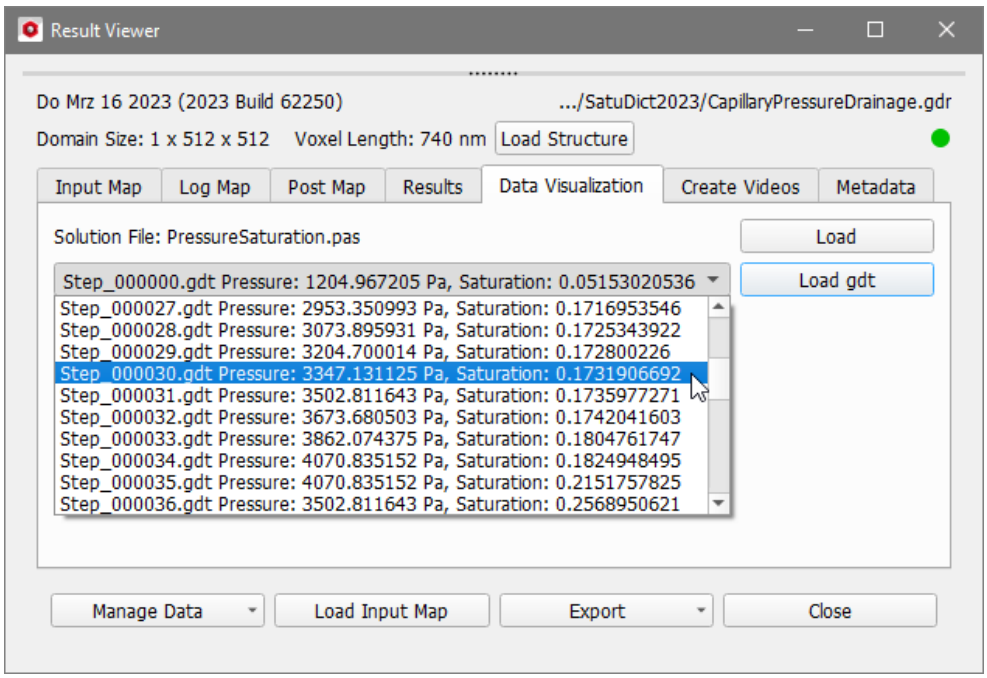
The following are two examples of the effect of setting the **Threshold** slider/box and **Clip Mode**. Visualization of freeze-frame shots of displacement





Finally, the computed process can be visualized step-by-step with GDT files saved during the capillary pressure curve calculation.

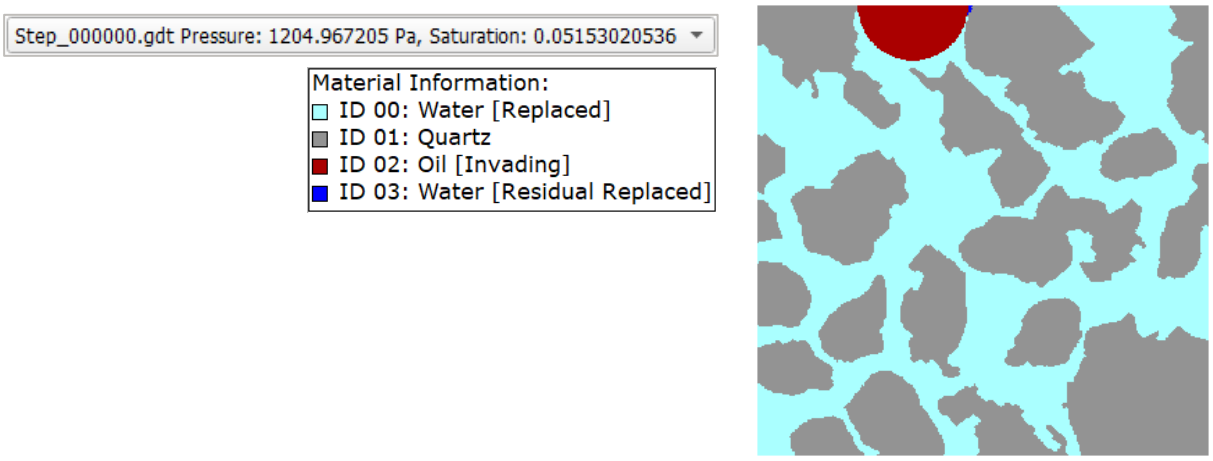
To analyze these images, make sure that the visualization of the Structure is switched on (**View** → **Structure**, in the menu bar).



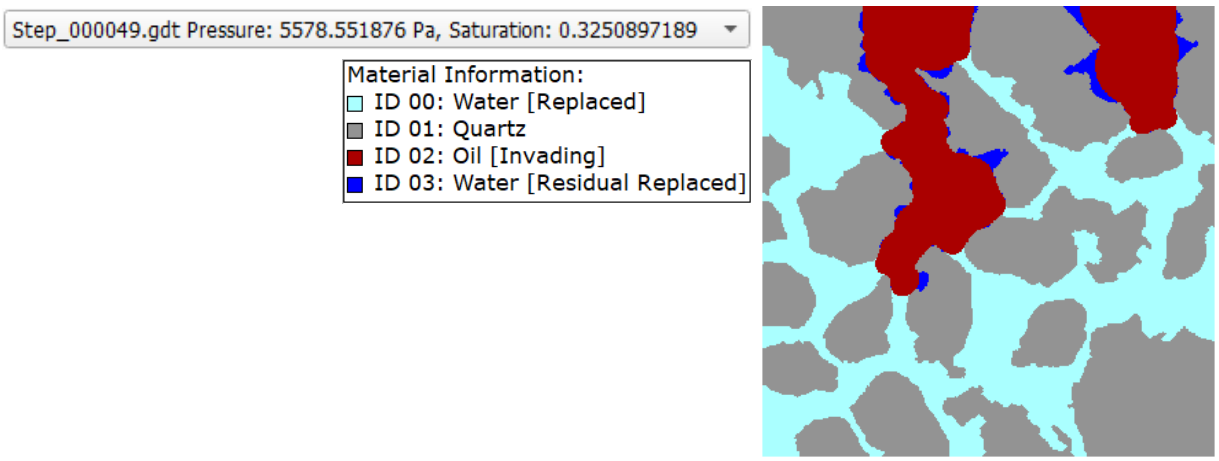
Select one of the GDT files , where the file names correspond to the simulation step in which the GDT file was saved. Also, the pressure und saturation of the invading fluid in this step are shown, which is the same as in the corresponding row of the table in the Results-Report tab.

Click **Load gdt** to open the desired file and the image from that step is displayed in the visualization area.

The GDT file Step_000000.gdt (Pressure: 1205 Pa, Saturation: 0.0515) corresponds to the beginning of the intrusion process. The structure appears (almost fully) saturated by the replaced fluid.



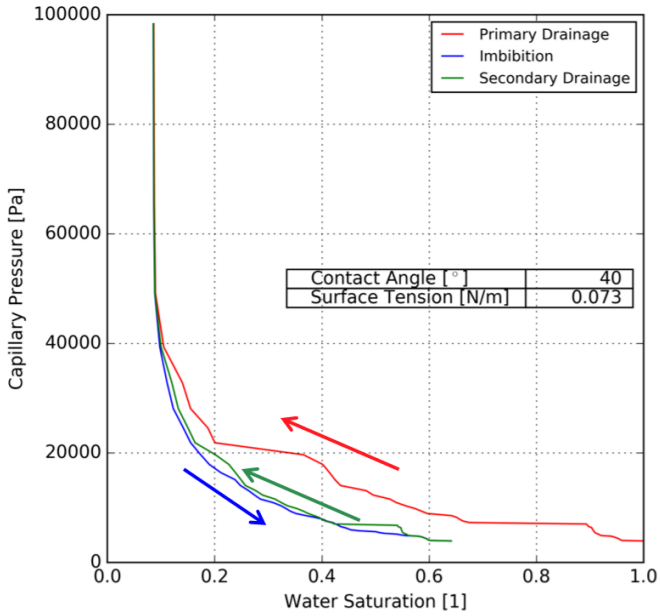
The GDT file Step_000049.gdt (Pressure: 5578.5 Pa, Saturation: 0.325) corresponds to an intermediate part of the intrusion process. The structure appears partly saturated by the invading fluid and the replaced fluid.



Capillary Pressure with Hysteresis Effect

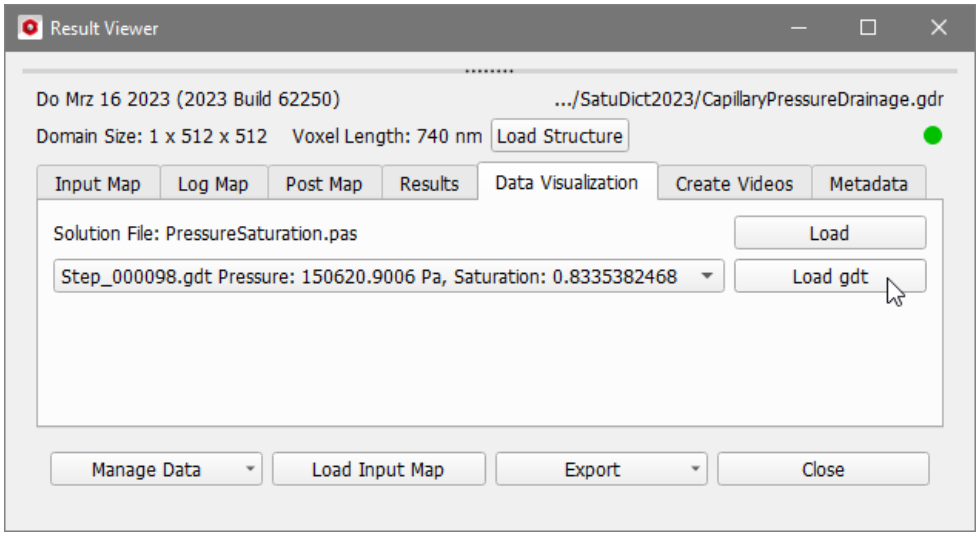
A generalization of the pore morphology method allows considering structures in which the invading fluid is already present in the structure. This makes the simulation of primary and secondary drainage experiments possible, as well as primary and secondary imbibition experiments.

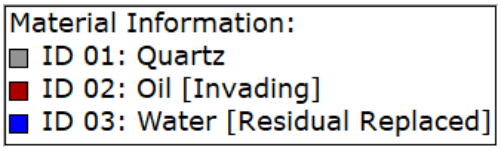
The following figure shows a typical graph for primary drainage, imbibition, and secondary drainage.

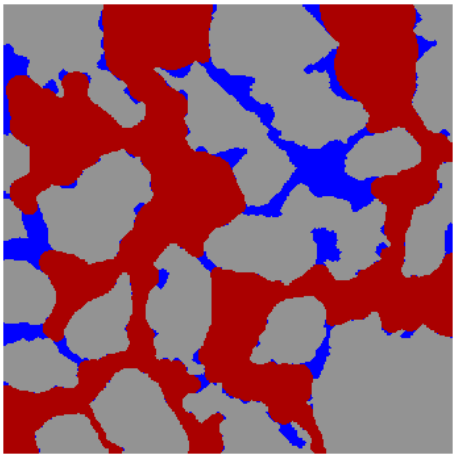


After the primary drainage simulation shown in pages 19 ff. with the result file obtained, perform a follow-up imbibition simulation where the WP displaces the NWP.

First, the final state of the previous drainage simulation (Step_000098.gdt with 150621 Pa) is loaded.



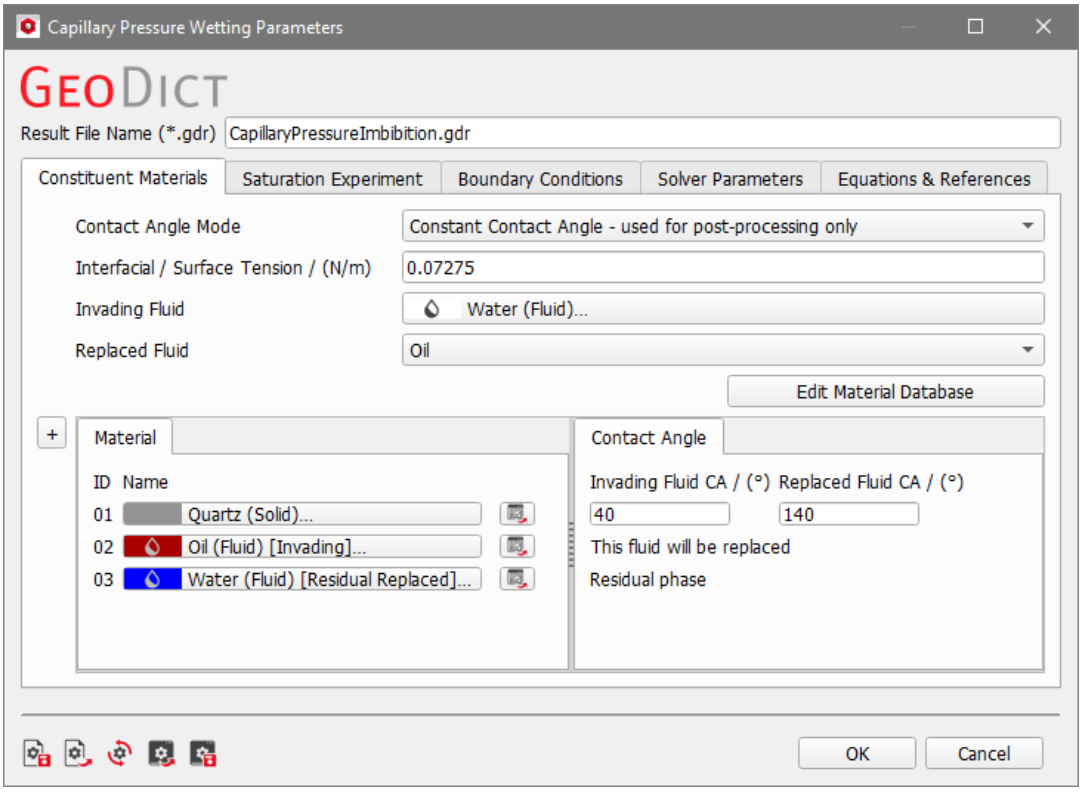




Then, return to the main GeoDict GUI and click the **Solver Options' Edit...** button in the **SatuDict** section to select the wetting parameters for the capillary pressure curve simulation.

Change the name for the result file from **CapillaryPressureDrainage.gdr** to **CapillaryPressureImbibition.gdr**.

In the **Constituent Materials** tab, select the **Invading Fluid** to be Water and the **Replaced Fluid** to be Oil. Set the **Invading Fluid CA** to 40°, the contact angle for the replaced fluid will automatically be changed.



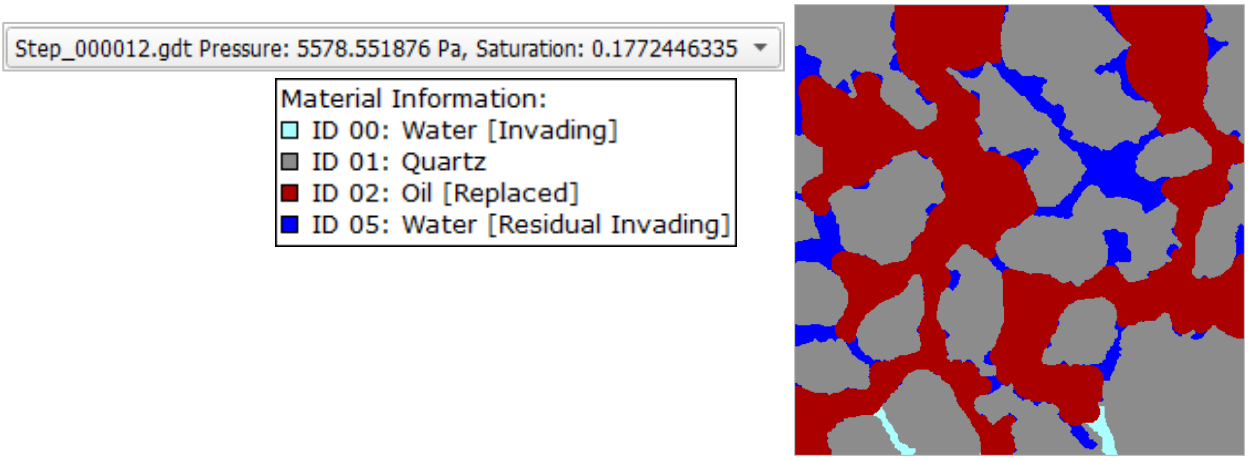
Under the **Saturation Experiment** tab, the Experiment has automatically changed to **Imbibition**. Check that **Invading Fluid must be connected to a reservoir** as well as **Replaced fluid can leave a residual** are selected.

In the **Boundary Conditions** tab, switch the reservoirs boundary conditions of invading and replaced fluid.

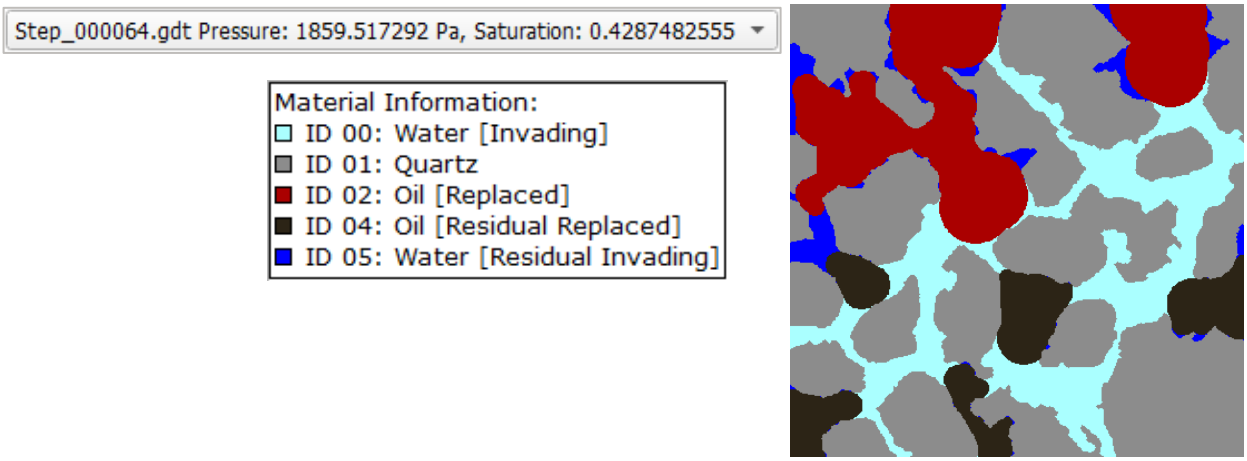
Click **Run** in the SatuDict section to start the simulation.

The Result Viewer of the result file opens at the end of the computations. Load the GDT files as explained in pages 29 ff. to visualize the imbibition process.

Observe that, step-by-step, the oil is replaced by invading water, which reconnects with the water previously trapped in the structure (purple Residual Invading Phase) from the earlier drainage simulation.



As previously for the Drainage simulation also during the Imbibition simulation parts of the replaced fluid (here Oil) get trapped in the structure.



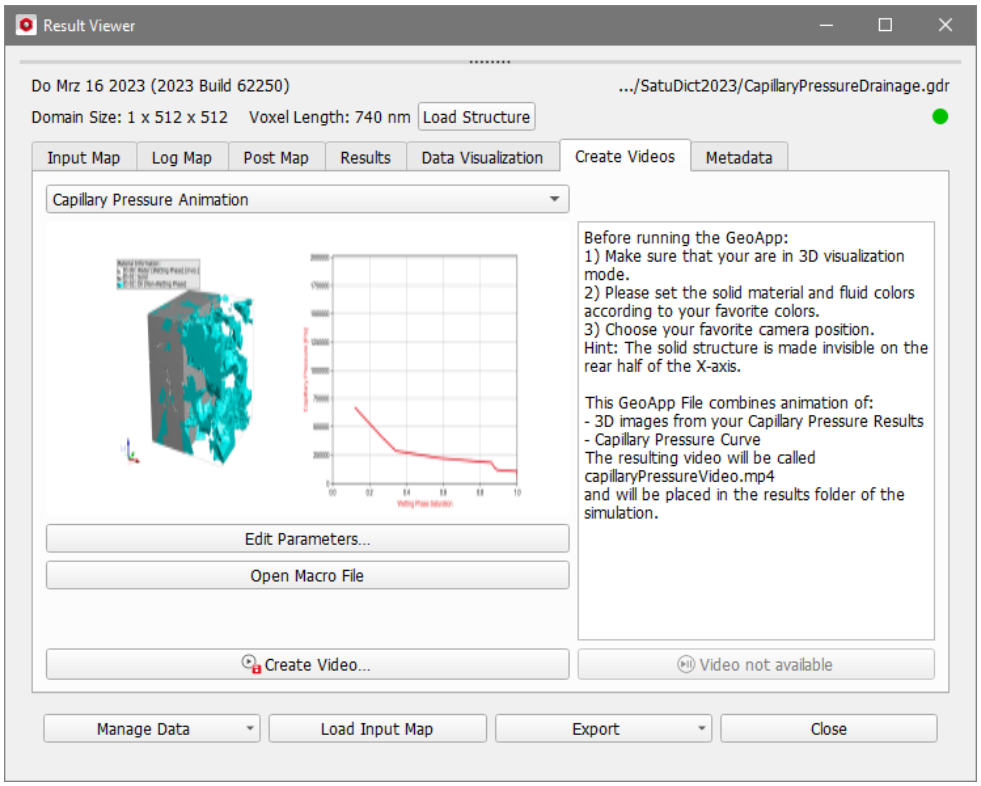
CREATE VIDEOS

In the **Create Videos** tab, a *.mp4 file with an animation of the drainage or imbibition process can be created. Follow the steps listed on the right panel:

1. Make sure that you are in 3D mode,
2. Set the colors of solid and fluid materials to your preferred ones,
3. Choose your favorite camera position.

Select **Edit Parameters** to change the capillary pressure result file as input for the video creation.

Click **Create Video**, to create the video capillaryPressureVideo.mp4 in the result file folder.

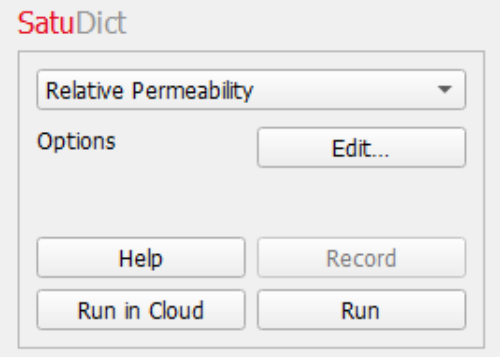


The video shows the capillary pressure curve on the right, and the changing distribution of wetting and non-wetting phase during the saturation simulation on the left. For a better visualization, only part of the structure is shown.

If the video was created successfully, the grayed-out **Video not available** button, is enabled and changes to a **Play Video** button. With **Open Macro File** it is possible to open a text editor with the python file used for the video creation.

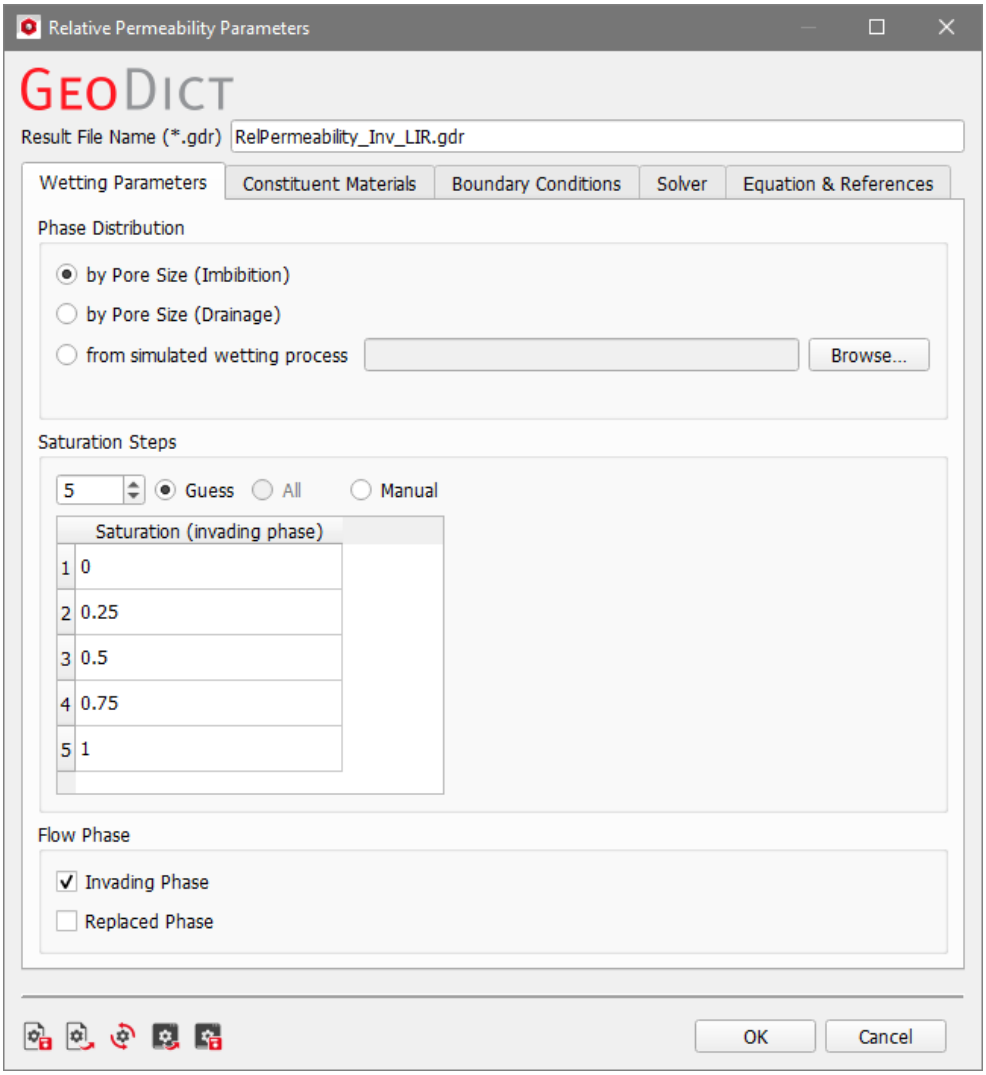
Relative Permeability

When selecting **Relative Permeability** from the pull-down menu in the **SatuDict** section, the **Solver Options** needed for running this computation can be entered (or modified) through the **Edit...** button.



In the **Relative Permeability Parameters** dialog, the name for the result file is entered in the **Result File Name (*.gdr)** box. Keep the default name or rename it according to your current project to differentiate the results of SatuDict computations. The resulting GDR file is placed inside the chosen project folder (**File** → **Choose Project Folder**, in the Menu bar).

The **Relative Permeability Parameters** are grouped under the **Wetting Parameters**, **Constituent Materials**, **Boundary Conditions**, and **Solver** tabs. The last tab **Equations & References** provides further information about the equations used in this calculation. The settings in the tabs **Constituent Materials, Boundary Conditions** and **Solver** are very similar to the solver options in FlowDict. Explanations to these settings can also be found in the FlowDict handbook of this User Guide.

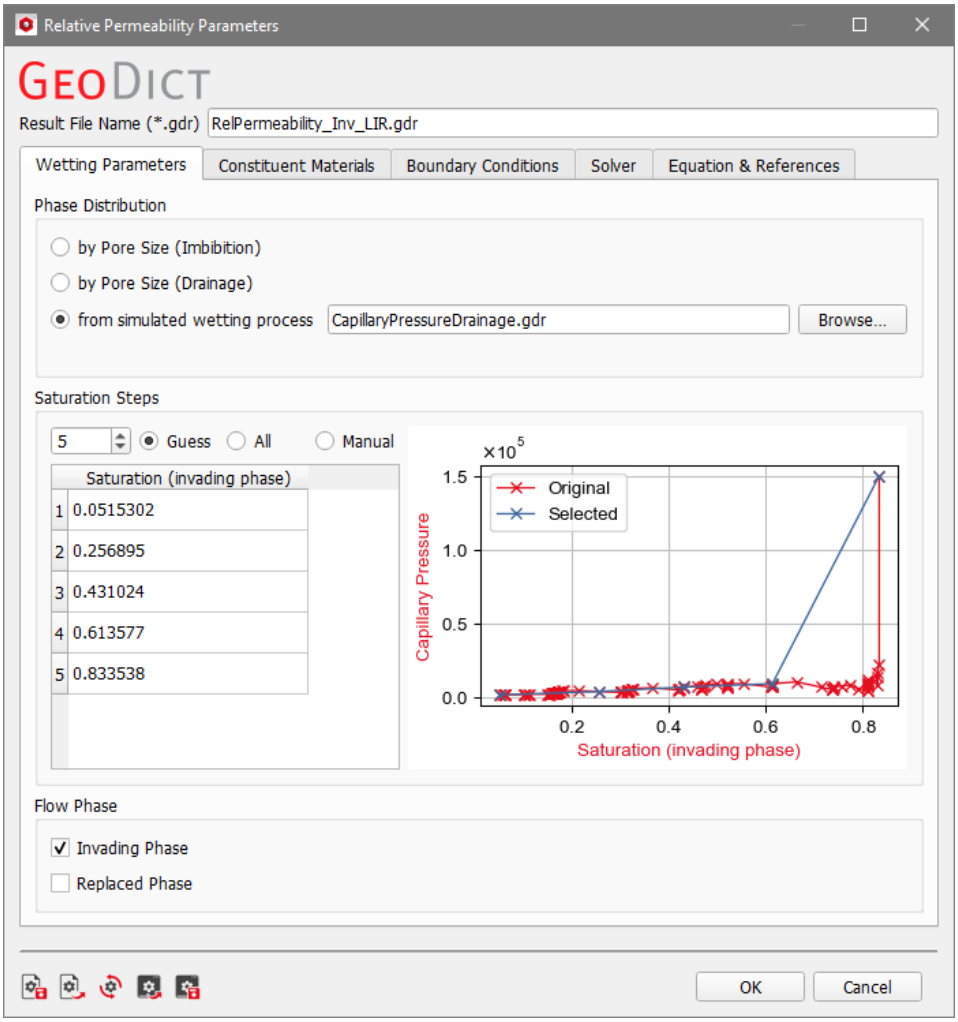


Wetting Parameters

Phase Distribution

The calculation of phase distribution can be based on the pore size alone (**by Pore Size (Imbibition)** or **by Pore Size (Drainage)**), corresponding to a saturation experiment with **Invading Fluid must be connected to a Reservoir** unchecked. The same calculation as for the capillary pressure command is performed, but without a connectivity check. Only the pore sizes are considered. For the Imbibition a contact angle of 0° for the invading fluid is assumed. When choosing **by Pore Size (Drainage)**, the invading fluid contact angle is assumed to be 180°.

However, the phase or fluid distribution at different saturation points can be taken from a previously simulated imbibition or drainage process by checking **from simulated wetting process** and clicking **Browse...** to choose a result file (GDR file) in your project folder.



Saturation Steps

The saturation steps of the non-wetting phase in the porous media, for which the permeability is to be calculated, can be set in the **Saturation (invading phase)** table.

There are three different modes to select the saturations:

- **Guess**: The number of guessed saturation points is specified in the box to the left.

- If the **Phase Distribution** is set to **by Pore Size**, the saturation steps are chosen uniformly.
- If the **Phase Distribution** is set to **from simulated wetting process**, the saturation steps are chosen from the provided GDR file. An internal selection process tries to find representative saturation steps based on the saturation and capillary pressure. A plot shows the original saturation points and the selected saturation points. This way the user can control if the guessed saturation points are indeed representative.

- **All** is only available when the **Phase Distribution** is set to **from simulated wetting process**. Then all saturation steps provided in the GDR file are used.
- **Manual**: In manual mode, the table can be modified at will, and the desired saturation steps can be entered.

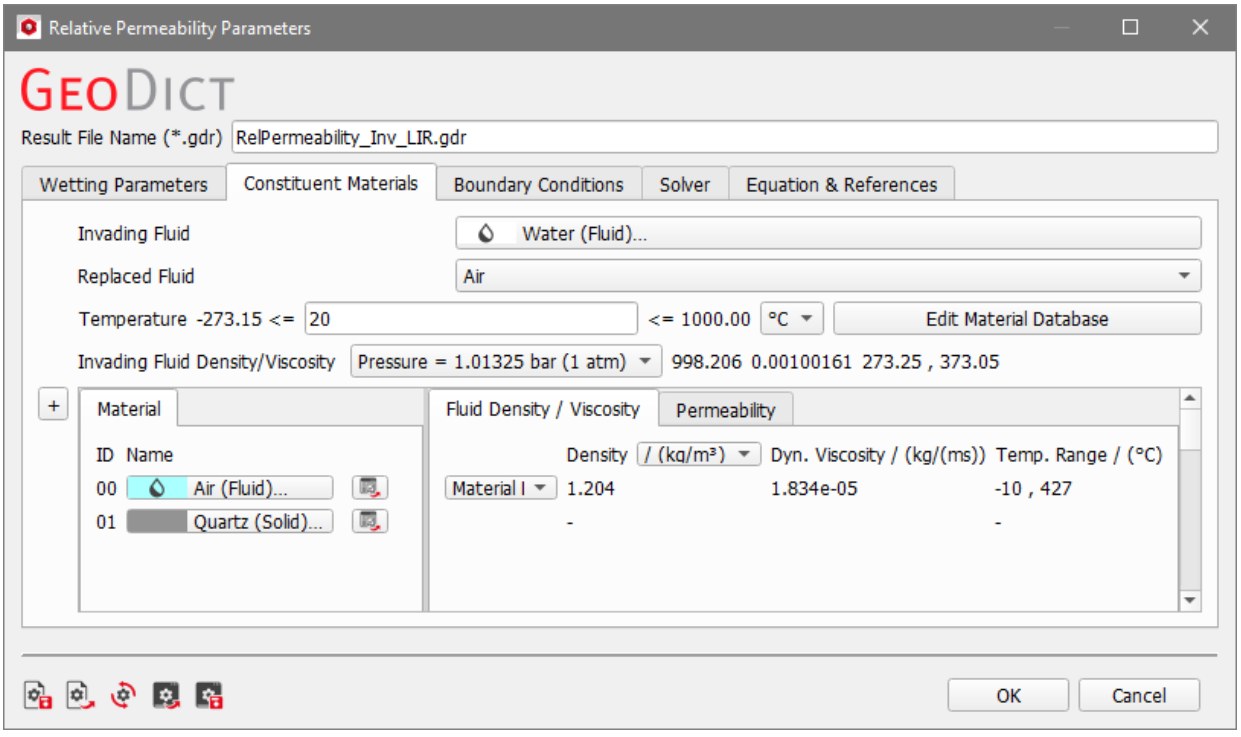
Flow Phase

In the **Flow Phase** panel, choose the phase (Invading Phase and/or Replaced Phase) for which the Relative Permeability is to be calculated.

Constituent Materials

Under the **Constituent Materials** tab, the **Invading Fluid** and **Replaced Fluid** can be entered. The tab is very similar to the one for capillary pressure (see page 10) but some properties cannot be entered (e.g. surface tension).

If the phase distribution under the Wetting Parameters tab is chosen **by Pore Size**, the replaced fluid must be present in the structure. If it is taken **from simulated wetting process**, then both fluids can be changed and do not have to be already present in the current structure.



Boundary Conditions

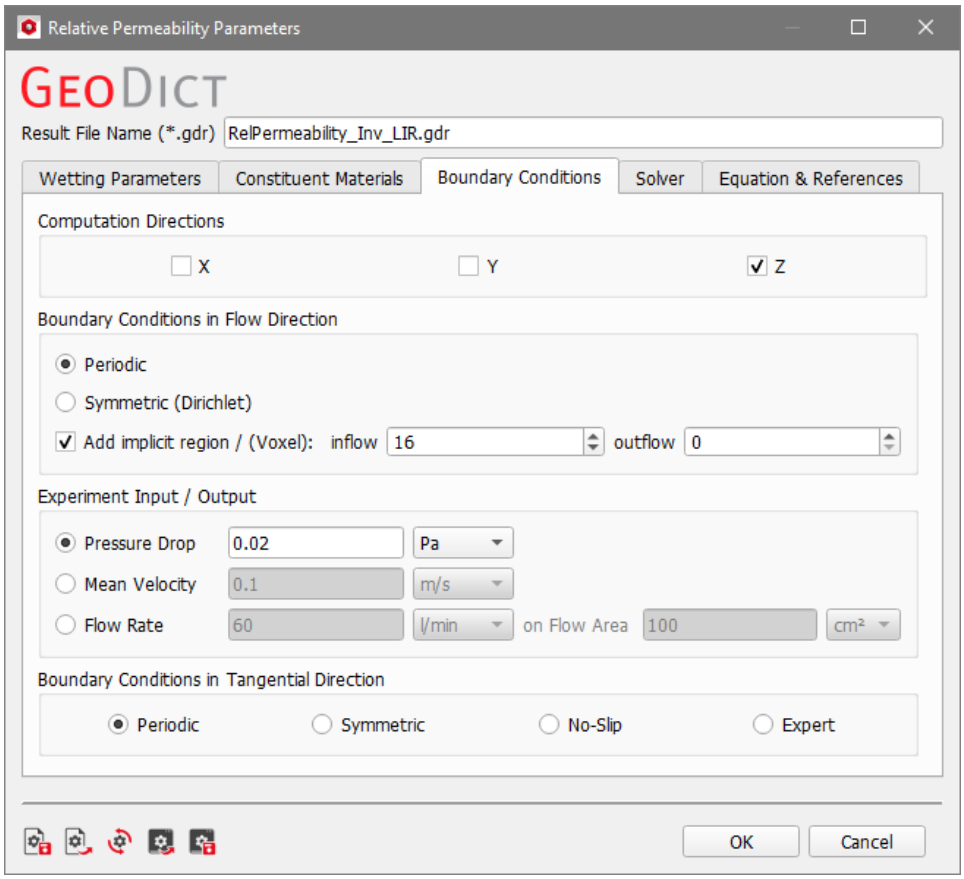
Computation Directions

For the **Computation Directions** choose the direction of the calculated flow. To obtain the whole 3x3 permeability matrix in the result file, it is necessary to choose all three directions.

Boundary Conditions in Flow Direction

The **Boundary Conditions in Flow Direction** can be checked to be **Periodic** or **Symmetric**. Periodic boundary conditions are recommended for periodically generated structure models and for non-periodic structures with high porosity.

After checking **Periodic** boundary conditions in flow direction an implicit inflow region (also called inlet) and outflow region (also called outlet) can be automatically added by checking **Add implicit region** and entering its size in voxels. The default added implicit inflow is 10 voxels and implicit outflow is 10 voxels. The inlet and outlet are essential to avoid the possibility of closing the flow channels when the structure is periodically repeated.



Experiment Input / Output

In fluid dynamics, three experiments are typical:

- Measure the mean velocity for the applied pressure drop.
- Measure the pressure drop for a given mean velocity.
- Measure the pressure drop for a given mass flow rate.

Input a prescribed **Pressure Drop** value and obtain the calculated **Mean Velocity** in the result file as output. Alternatively, the input of the mean velocity results in the output of pressure drop.

The **Flow Rate on Flow Area** in l/min per cm^2 (default) or in other units, can be inputted to obtain the pressure drop at a given mean velocity. The volumetric flow rate per flow area is the volume of fluid which passes per unit time through a given area. For each property, the desired unit can be selected from the pull-down menu.

Boundary Conditions in Tangential Direction

The Boundary Conditions in Tangential Directions can be checked to be **Periodic**, **Symmetric**, **No-Slip**, or **Expert**. With the default **Periodic** selected, the process of periodic continuation is internally done during the run of the solver, repeatedly adding the volume structure in the directions tangential to the flow direction. For **Symmetric**, the volume structure is mirrored in the tangential directions. When **No-Slip** is used, the solver internally adds a one-voxel layer in the required direction and solves with periodic boundary conditions. That effectively is equivalent to solve the structure with casing in two ends in the direction of interest.

The boundary conditions in the two directions tangential to the flow can also be set to be different by checking **Expert** boundary conditions. For example, when the fluid is chosen to flow in the Z-direction, the boundary conditions could be chosen to be **Periodic** in X-direction and **Symmetric** in the Y-direction.

Solver

Internally SatuDict solves several equations for values of permeability at each voxel by using an iterative solver. The basic idea of an iterative method is to:

1. Start with some initial guess for the unknown values.
2. Improve the current values in each iterative step. The improvement can be fast or extremely slow depending on problem parameters,
3. Repeat the iterative process until one of the stopping criteria occurs.

For **Relative Permeability**, the three flow solvers **EJ**, **SimpleFFT**, and **LIR** are available and can be chosen from the pull-down menu. For structures with low porosity, the **SimpleFFT** or **LIR** flow solver should be used for best performance, i.e., low runtimes.

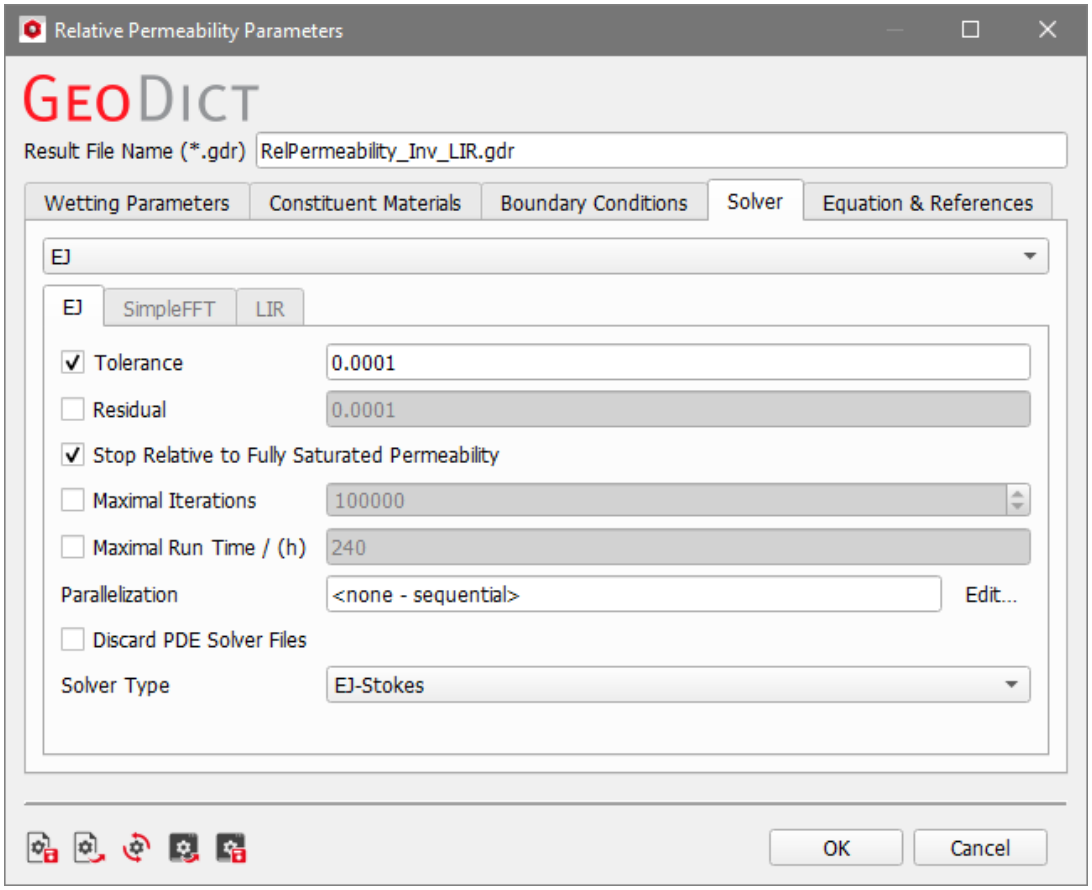
EJ

The EJ solver is assigned to compute the flow fields and relative permeability after selecting **EJ** from the pull-down menu.

The iterative process is controlled by setting the values and activation for **Tolerance**, **Residual**, **Maximal Iterations**, **Maximal Run Time (h)**. The stopping criterions can be enabled and disabled by the check boxes.

The default and recommended stopping criterion is **Tolerance** for the EJ solver. The **Tolerance** stopping criterion looks for stagnation of the method when the process becomes stationary. This occurs when from iteration to iteration the improvement in the permeability value becomes extremely small.

By setting the stopping criterion to **Residual**, the computations terminate as soon as the relative norm drops below the selected residual threshold. This stopping criterion is only available for **SimpleFFT** and **EJ**.



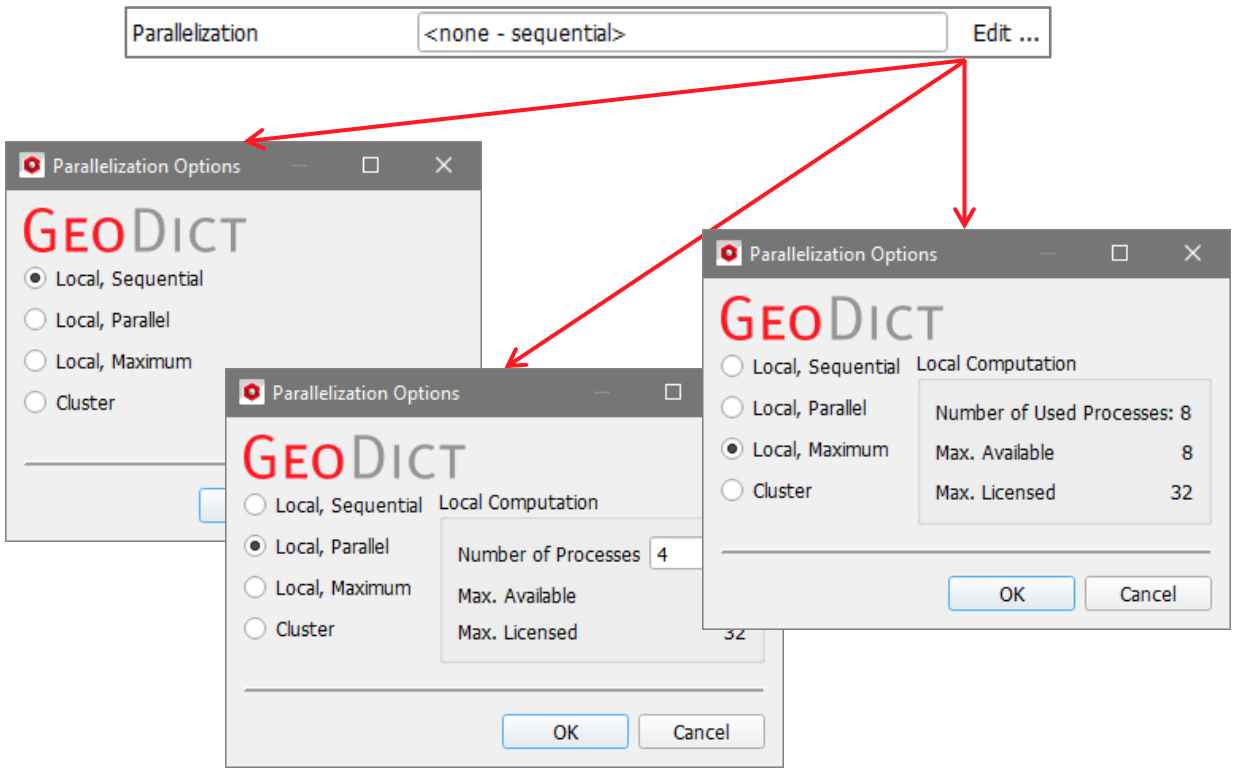
The option to **Stop Relative to Fully Saturated Permeability** alters the chosen stopping criterion such that for low saturated states the solver stops relative to the result of the computation where the structure was fully saturated. The fully saturated structure has the highest permeability and decreases when lowering the saturation. For low saturation states the permeability is almost zero and the computation is much more expensive. This option significantly speeds-up the overall runtime and stops the solver earlier for low saturation states while keeping the overall quality of the result relative to the highest permeability.

The Relative Permeability solver allows setting the maximal number of steps (**Maximal Iterations**, default value is 100000) or the maximum run time (**Maximal Run Time**, default 240 h). However, when the solver stops because the **Maximal Iterations** value or the **Maximal Run Time / (h)** has been reached, no guarantee on the quality of solution can be given.

Parallelization

Calculations can be parallelized if the user's license and hardware allow it. The threads of the program can be executed concurrently. The **Parallelization Options** dialog box opens when clicking the **Edit...** button, to choose between **Local, Sequential**, **Local, Parallel** or **Local, Maximum**. When **Local, Parallel** is chosen, the number of **Processes** to run can be entered. **Local, Maximum** sets the number of used processes to the maximum possible number, restricted by the hardware and number of licensed processes.

The choice of **Cluster** is for Linux users with floating licenses only. See the High Performance Computing handbook for information on how to setup GeoDict such that these options can be used.



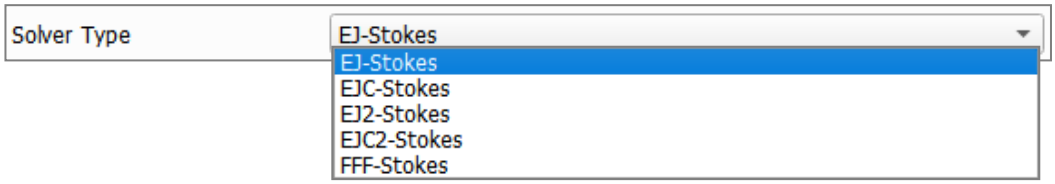
Discard PDE Solver Files

The files with results (*.gdr) of the permeability computations are saved in the chosen project folder (**File → Choose Project Folder**, in the Menu bar). An additional directory with the same name is created to keep the intermediate computation files (PDE solver files).

Checking the **Discard PDE Solver Files** box causes the erasing of all intermediate computation files, log-files, flow fields etc. stored in this folder. While having the benefit of saving storage place, discarding these files has also the effect of disabling the 3D visualization of the results. Only the result file *.gdr is saved.

Solver Type

For the flow computation with EJ solver, five different ways to implement no-slip boundary conditions of the flow solver are available: **EJ-Stokes**, **EJC-Stokes**, **EJ2-Stokes**, **EJC2-Stokes**, and **FFF-Stokes**.



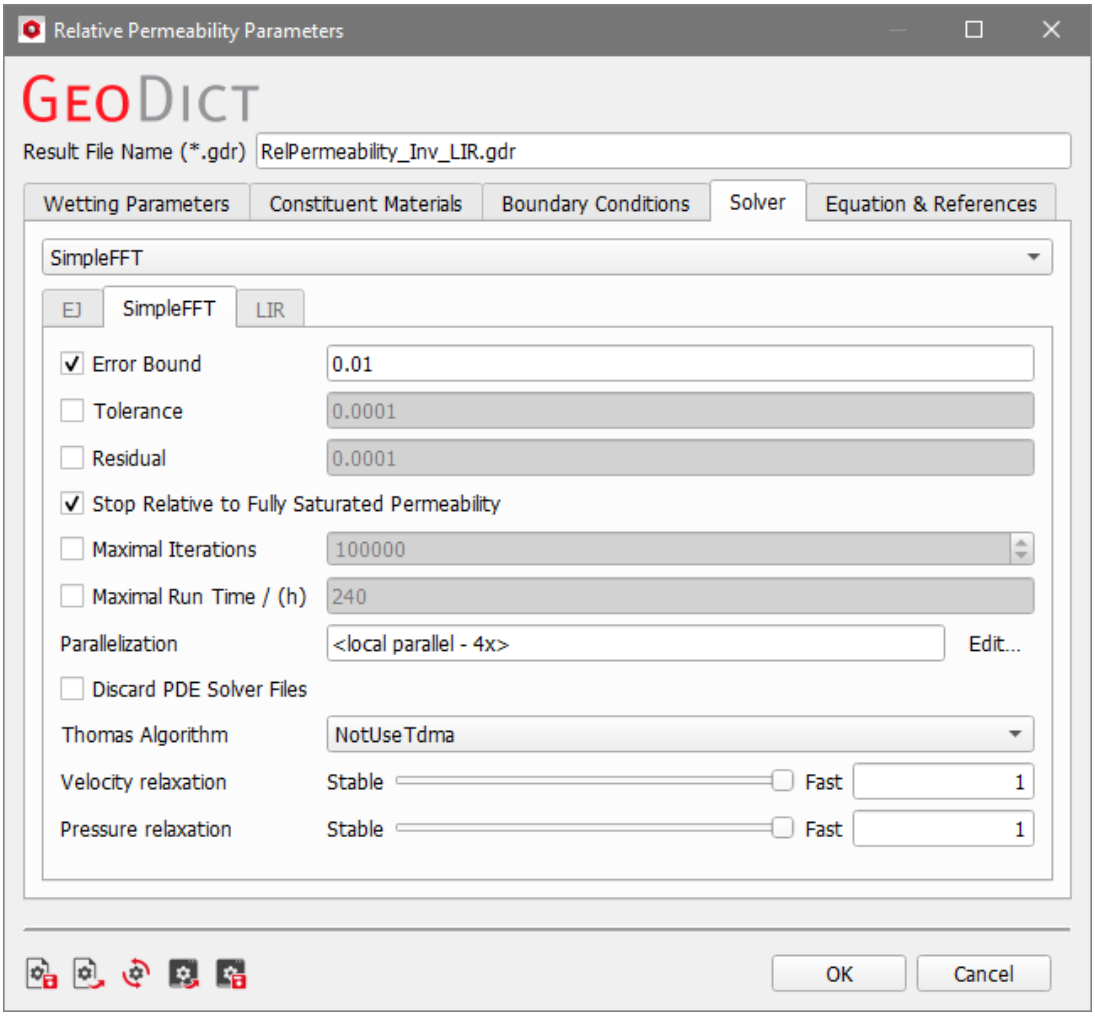
The implementations describe how the no-slip boundary conditions are discretized, i.e., at which discrete point the tangential velocity reaches zero.

The default **EJ-Stokes** (Explicit Jump-Stokes solver) sets the tangential velocity to zero at the center of the voxel surfaces. It is a newer implementation of the Finite Volume solver that solves moderately slower, but it is noticeably more accurate for low porosity structures.
EJC-Stokes sets the tangential velocity to zero at the voxel corners.

EJ2-Stokes sets the tangential velocity to zero at the center of the voxel surfaces and uses a 2nd order approximation of the velocity field.
EJ2C-Stokes sets the tangential velocity to zero at the voxel corners and uses a 2nd order approximation of the velocity field.
FFF-Stokes sets the tangential velocity to zero at the voxel centers.

SIMPLEFFT

The SimpleFFT solver is assigned to compute the flow field after selecting **SimpleFFT** from the pull-down menu.



The explanations given in pages 38 ff. for the EJ solver, regarding **Stopping Criterion**, **Stop Relative to Fully Saturated Permeability**, **Parallelization**, and **Discard PDE Solver Files** apply also here for the SimpleFFT solver.

The recommended stopping criterion is **Error Bound** for the SimpleFFT and the LIR solver. The **Error Bound** stopping criterion uses the result of previous iterations and predicts the final solution. The solver stops if the relative difference with respect to the prediction is smaller than the specified error bound.

Thomas Algorithm

The tridiagonal matrix algorithm (Tdma), also known as the **Thomas Algorithm**, can help to improve the convergence for structures with high porosity and therefore speedup the computation with SimpleFFT. Here, **Automatic**, **NotUseTdma** or **UseTdma** can be selected. With **UseTdma** / **NotUseTdma** it can be switched on or

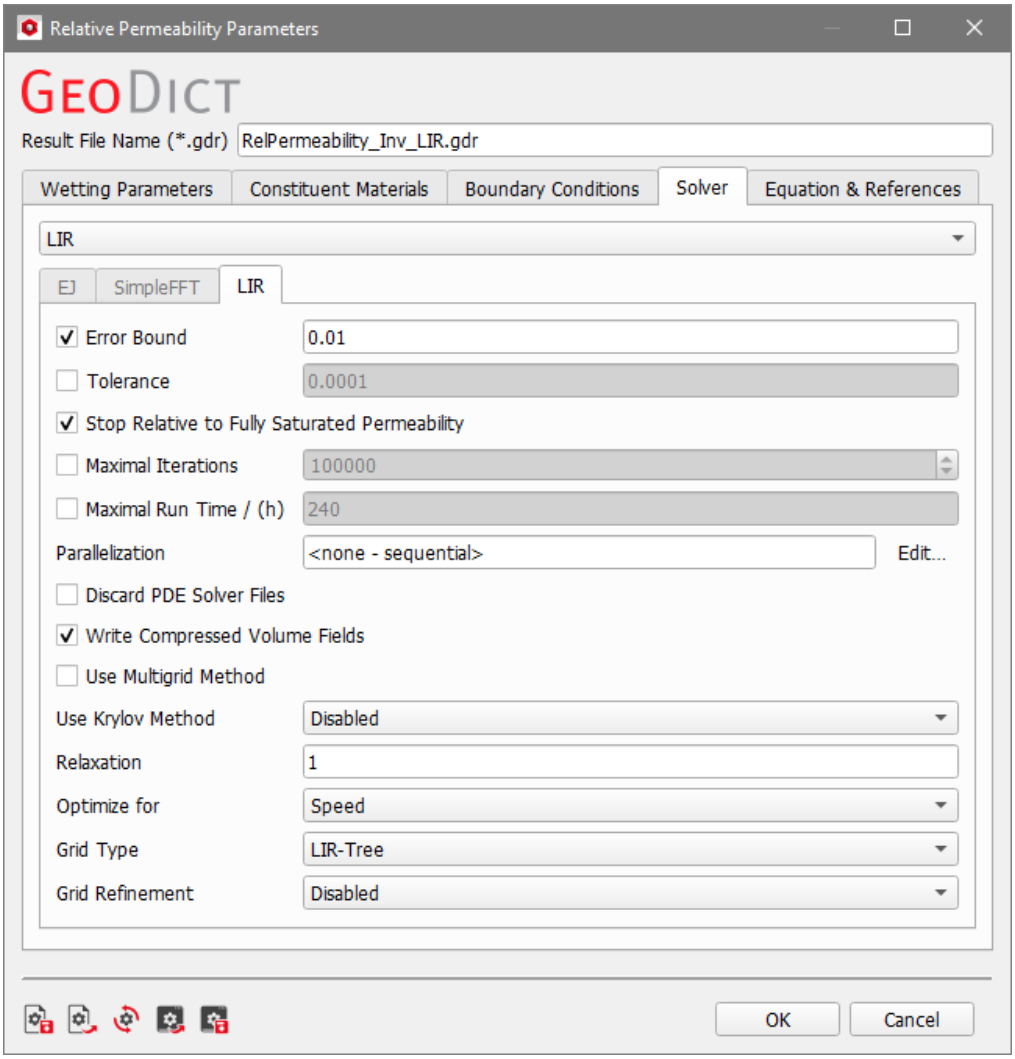
off. Choosing **Automatic** makes the selection based on the porosity of the structure and on the partial differential equation for the flow solver. For Stokes equation, which is always solved in the **Relative Permeability** computations in SatuDict, Tdma is always switched off for **Automatic** selected.

Velocity and Pressure Relaxation

The balance between stability and speed of the simulation can be specified by the **Velocity relaxation** and **Pressure relaxation: Stable ↔ Fast** slide bars. The parameter has to be greater than 0.0 and less or equal to 1.0. Setting the balance of **Stable** versus **Fast** is a trial-and-error process. There is no general rule to optimize it but in most cases a value of 1 for both relaxation parameters is optimal.

LIR

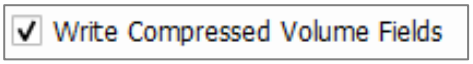
The explanations given in pages 38 ff. for the EJ solver, regarding **Stopping Criterion**, **Stop Relative to Fully Saturated Permeability**, **Parallelization**, and **Discard PDE Solver Files** apply also here for the LIR solver.



Write Compressed Volume Fields

The **LIR** solver uses a very memory efficient adaptive grid structure for flow simulations. If the option **Write Compressed Volume Fields** is checked, the

adaptive grid structure is used as compression method for writing out velocity and pressure (VAP) files to the hard drive as well.



This option allows to save 80-90% space on hard drive. The runtime for writing VAP files is also reduced significantly. But the runtime for loading and uncompressing of compressed VAP files is increased by the amount of runtime that was saved for writing out compressed VAP files.

If the option **Write Compressed Volume Fields** is not checked then the usual regular grid is used for writing out VAP files.

Use Multigrid Method

The main idea of Multigrid is the usage of multiple coarser adaptive grids to speed up convergence behavior but requires only little more memory. The **Multigrid Method** is explained in more detail in the section **Solver Options** of the FlowDict handbook of this User Guide.

Use Krylov Method

The Krylov subspace method can reduce the runtime of the LIR solver significantly. Since this is not always the case, dependent on the structure and boundary conditions, and since it needs more memory, the method can be switched on and off. Choose for **Use Krylov Method Enabled** or **Disabled** to use the method or switch it off. Select **Automatic** for an automatic selection based on the structure and the chosen boundary conditions. If **Automatic** is used, the relaxation parameter will be chosen automatically by the solver as well.

Relaxation

The **Relaxation** parameter for the LIR solver is very similar to the **Velocity relaxation** and **Pressure relaxation** for the SimpleFFT solver. The balance between stability and speed of the simulation can be specified by the **Relaxation**. The parameter must be between 0 and 2. The default value is 1 and usually provides the best balance between stability and speed.

If the relaxation value is greater than 1, the solver needs less iterations and less runtime, but this cannot be applied for all kinds of structures. If the relaxation value is smaller than 1, the solver needs more iterations and more runtime, but the simulation is more stable. To solve the Stokes equations, the **Relaxation** value never needs to be smaller than 1.

Optimize for, Grid Type, and Grid Refinement

The **Optimize for**, **Grid Type**, and **Grid Refinement** parameters are special options for the LIR solver. The defaults are already optimal for most applications.

A detailed explanation of these parameters can be found in the section **Solver Options** of the FlowDict handbook.

EQUATIONS & REFERENCES

The **Equations & References** tab shows the formulas that are used for the solver:

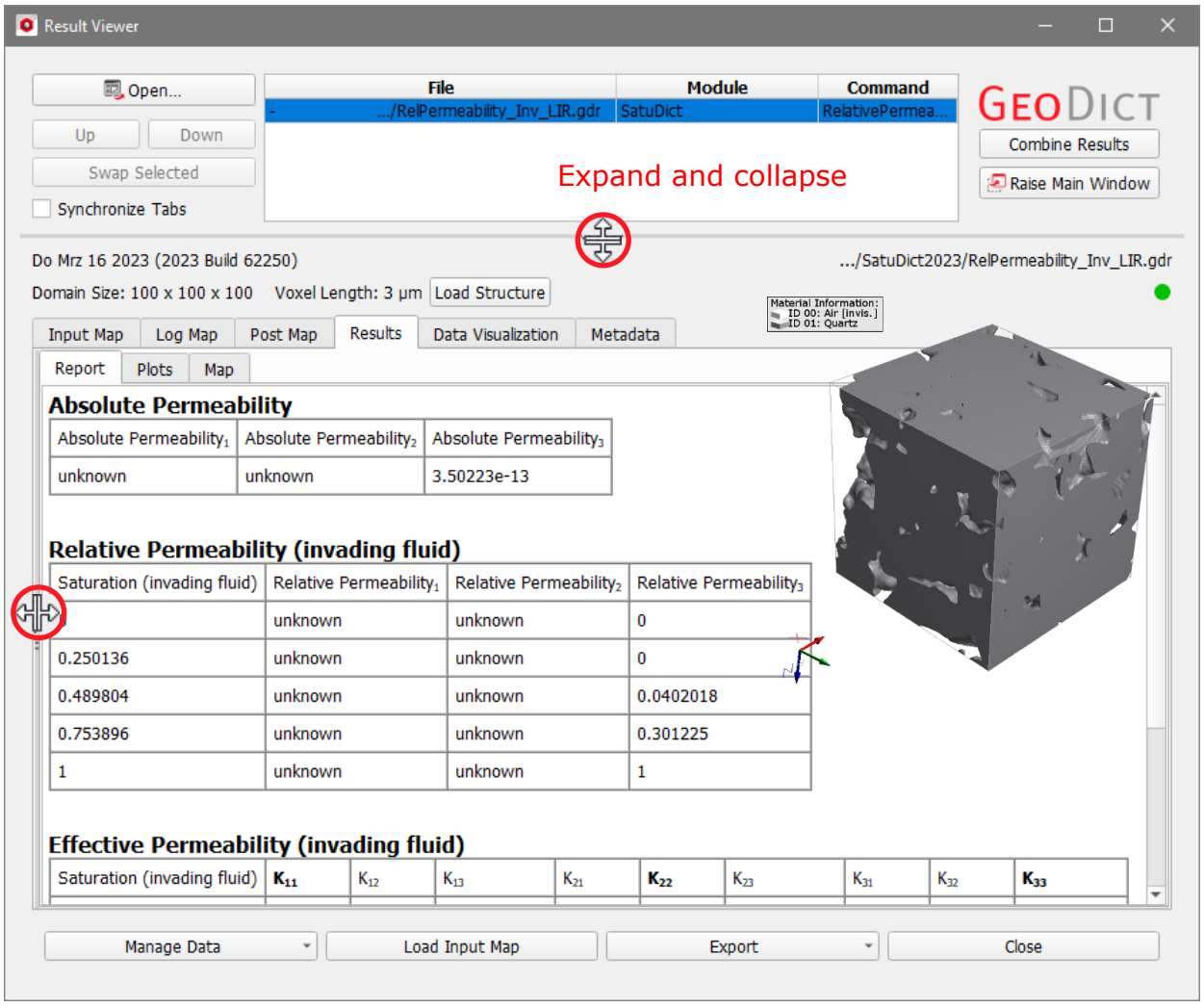
- Momentum Conservation
- Mass Conservation
- No-Slip Boundary Condition

No parameters can be edited on this tab. Also **References** relevant for this module are given.

Relative Permeability result file

Here, the results of the computation of the relative permeability of a partially saturated porous material with 17% porosity (83% SVF) are shown. The Invading Phase was selected as the flow phase (Wetting Parameters tab), and relative permeability was calculated in Z-direction (Boundary Conditions tab). Computations were run using the LIR solver.

After the solver finishes, the calculation results immediately open in the Result Viewer and are saved into a GDR file in the chosen project folder with the entered **Result File Name** (here, RelPermeability_Inv_LIR.gdr).



The results are accessed through the **Input Map**, **Log Map**, **Post Map**, **Results**, **Data Visualization**, and **Metadata** tabs.

Input Map, Log Map, and Post Map

The values under the **Input Map**, **Log Map**, and **Post Map** tabs are analog to those for the Capillary Pressure Curve result file (see pages 19 ff.).

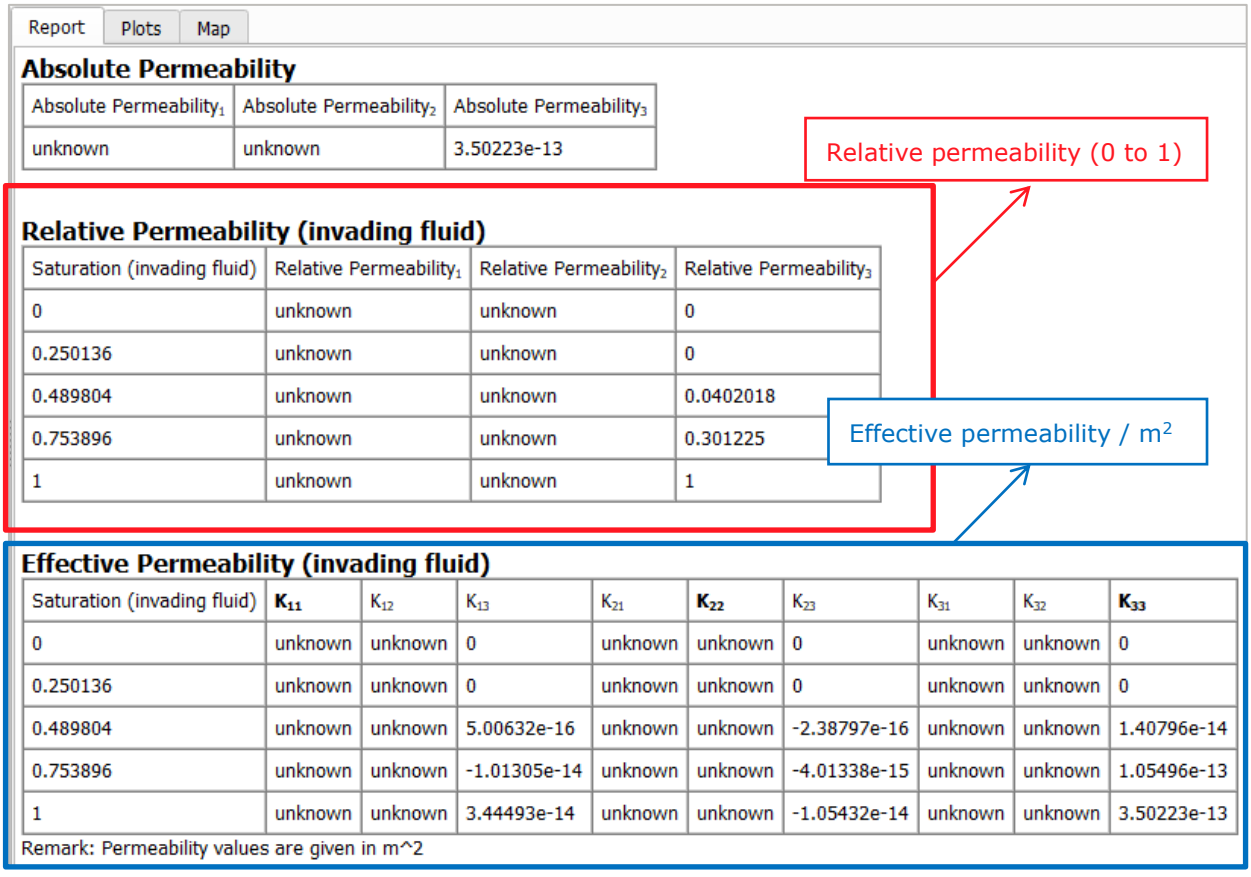
RESULTS

Report

Under the **Results-Report** subtab, the **Relative Permeability** (dimensionless relative permeability) and **Effective Permeability** (saturation-dependent permeability) tables are shown for the chosen invading fluid saturation rates (here, 0.25, 0.50, 0.75) and the start and end saturations (0.0 and 1.0) in the chosen computation directions (here, K13, K23, K33 for the computation in Z-direction). The chosen saturation rates are approximated as good as possible (here, 0.25, 0.49, 0.75).

Having selected the Invading Fluid as the flow phase under the Wetting Parameters tab, it is the permeability depending on the saturation of the invading fluid that is shown in the tables.

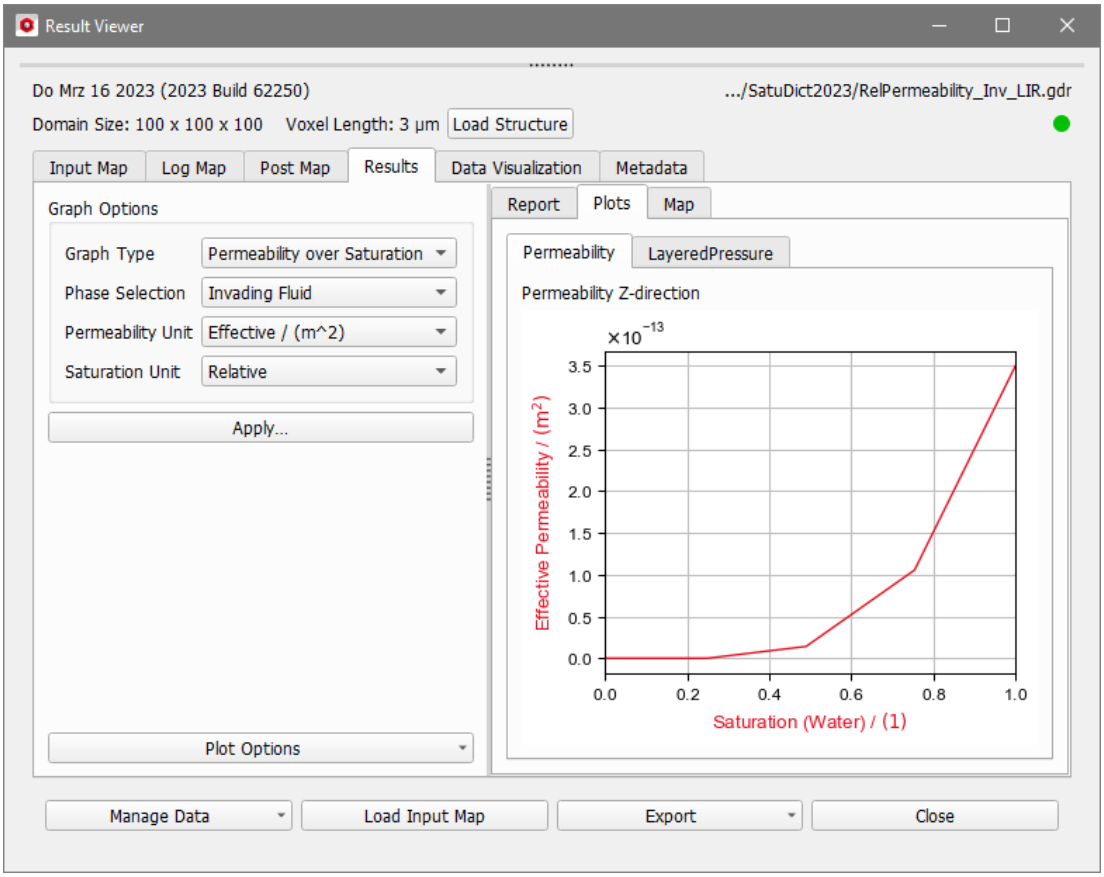
The relative permeability at 0% and 25% invading fluid saturation is zero in Z-direction, indicating that before the structure is 49% saturated with the invading fluid, there is no path for the flow. The directions for which computations have not been carried out appear as **unknown** in the permeability tables.



Plots

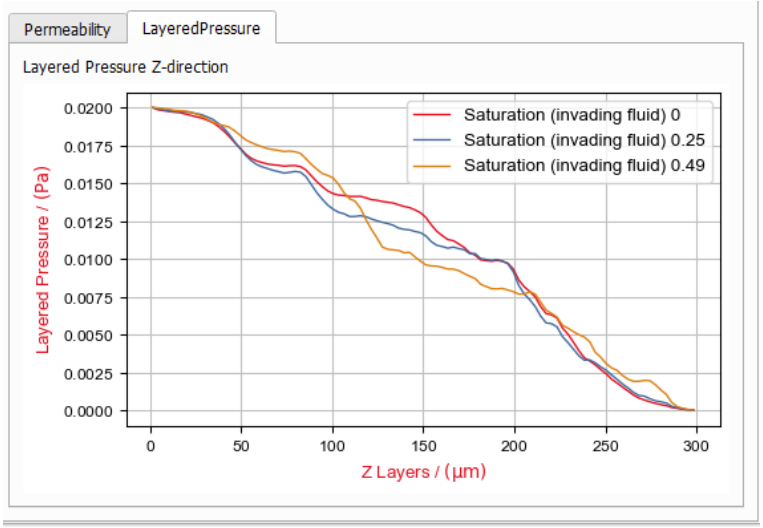
In the **Results - Plots** subtab, the values of the **Relative Permeability** or **Effective Permeability** table are shown in a graph. Also, the **Layered Pressure** in the computed directions is given.

On the left side in the expandible **Graph Options**, the user can modify the way the permeability graph is displayed by selecting the **Graph Type** (Permeability over Saturation or Saturation over Permeability), the **Phase Selection** (Invading Fluid or Replaced Fluid), the **Permeability Unit** (Effective permeability in m^2, Relative permeability between 0 and 1), and the **Saturation Unit** (Relative or Absolute). Click **Apply** to change the graph shown according to the options selected. Choose **Plot Options**, to change axis and graph settings.



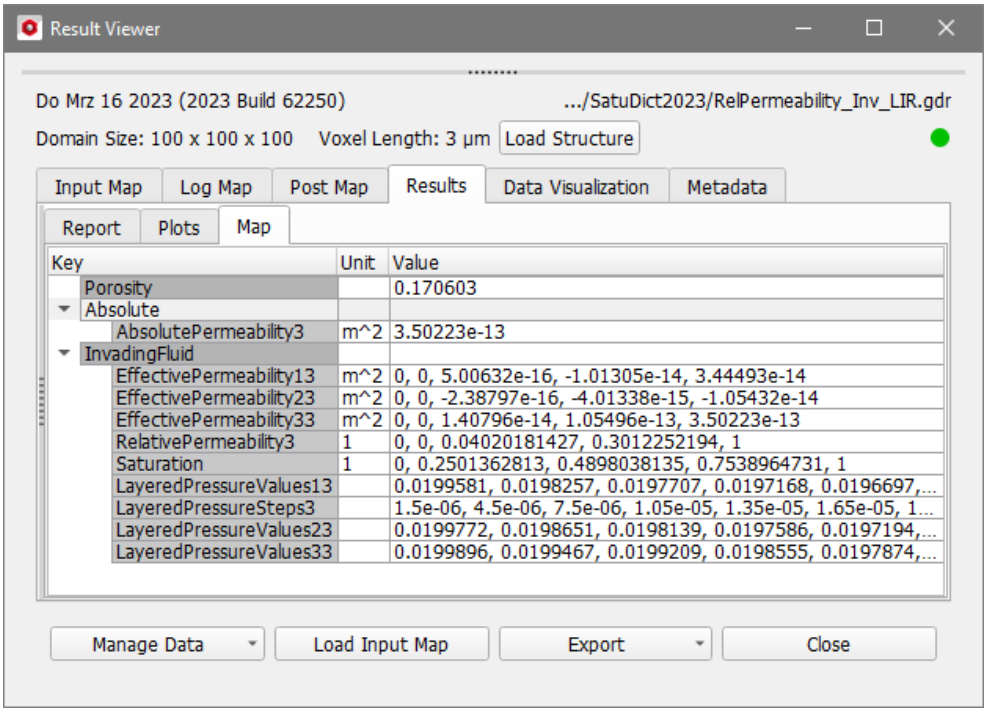
In the **Layered Pressure** tab for each computational direction the pressure in each layer is shown in a graph.

The settings made under the **Graph Options** do not apply for these plots, except for the **Saturation Unit** which changes the units inside the plot legends. But the axis settings and graph styles can be changed under **Plot Options**.



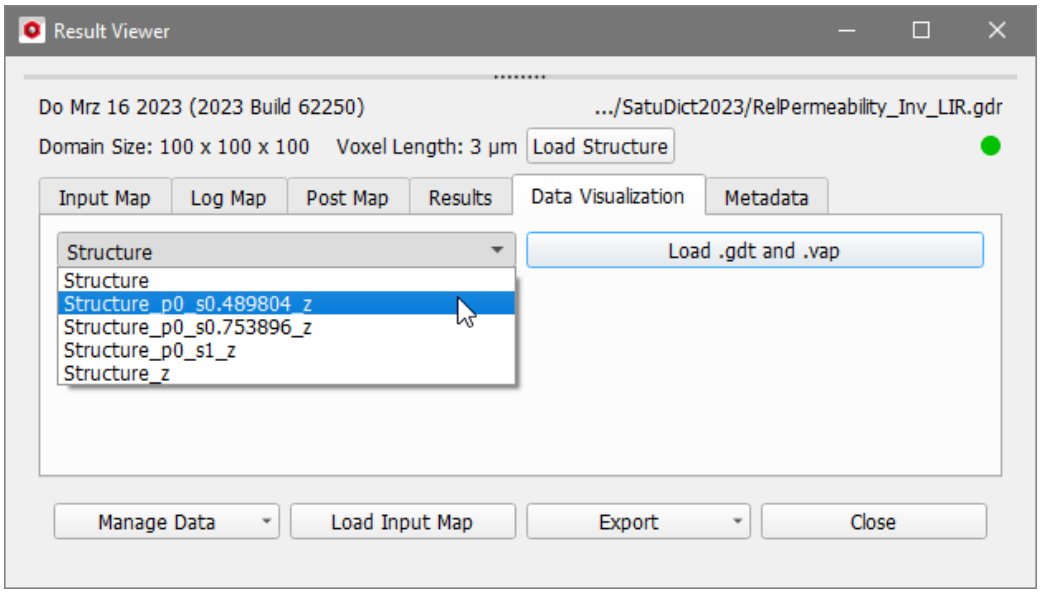
Map

Under the **Results - Map** subtab, the computed values are listed.



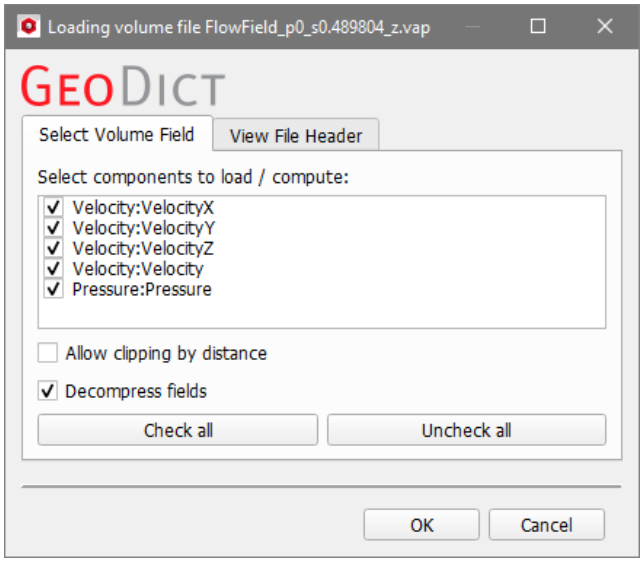
Data Visualization

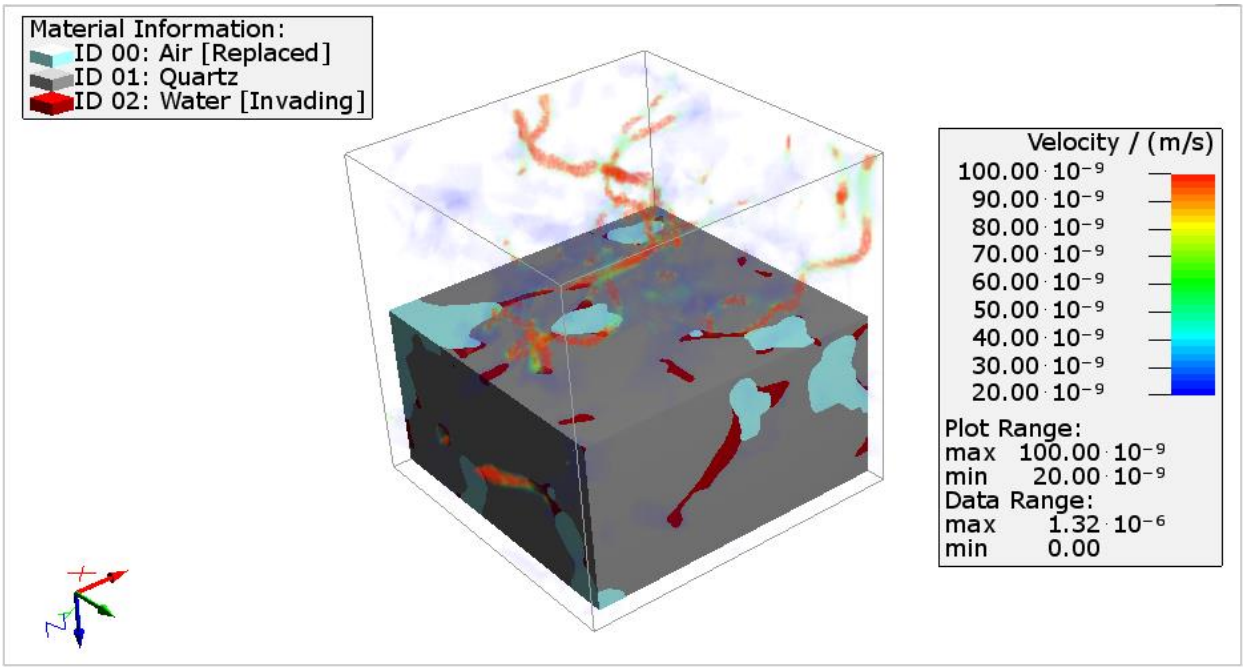
Under the **Data Visualization** tab, the .gdt and .vap files, corresponding to the saturation levels computed, can be opened, as explained above in pages 26 ff. Here shown is the GDT file for a 49% invading fluid saturation level.



The solid phase (Quartz) is shown together with the Replaced Fluid (Air) and the Invading Fluid (Water). The upper part of the image shows the velocity field of the Water with transparent effect on the clipped structure model.

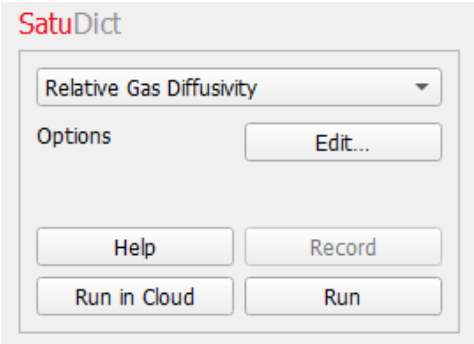
A detailed explanation of the procedure to obtain this kind of visualization can be found in the Visualization handbook.


Loading volume file FlowField_p0_s0.489804_z.vap
GeoDict
Select Volume Field
View File Header
Select components to load / compute:
Velocity:VelocityX
Velocity:VelocityY
Velocity:VelocityZ
Velocity:Velocity
Pressure:Pressure
Allow clipping by distance
Decompress fields
Check all
Uncheck all
OK
Cancel


Material Information:
ID 00: Air [Replaced]
ID 01: Quartz
ID 02: Water [Invading]
Velocity / (m/s)
100.00 · 10⁻⁹
90.00 · 10⁻⁹
80.00 · 10⁻⁹
70.00 · 10⁻⁹
60.00 · 10⁻⁹
50.00 · 10⁻⁹
40.00 · 10⁻⁹
30.00 · 10⁻⁹
20.00 · 10⁻⁹
Plot Range:
max 100.00 · 10⁻⁹
min 20.00 · 10⁻⁹
Data Range:
max 1.32 · 10⁻⁶
min 0.00

Relative Gas Diffusivity

When selecting **Relative Gas Diffusivity** from the pull-down menu in the **SatuDict** section, the **Options** needed for running this process can be entered (or modified) through the **Edit...** button.



The name for the result file is entered in the **Result File Name** box. Keep the default name (RelDiffusivity.gdr) or rename it according to the current project.

Clicking the **Wetting Parameters**, **Constituent Materials**, **Boundary Conditions**, and **Solver** tabs, the parameters necessary to run the Relative Gas Diffusivity calculations can be entered. The last tab **Equations & References** provides further information about the equations used in this calculation.

Wetting Parameters

The wetting parameters for the calculation of the Relative Diffusivity are the same as seen above (pages 35 f.) for the Relative Permeability.

Only one of the phases can be set as the phase for that the diffusivity is computed (Flow Phase).

Constituent Materials

In the **Constituent Materials** tab the **Invading Fluid** and the **Replaced Fluid** can be entered. No more settings need to be done as the conductivity is always set to 1.

Boundary Conditions

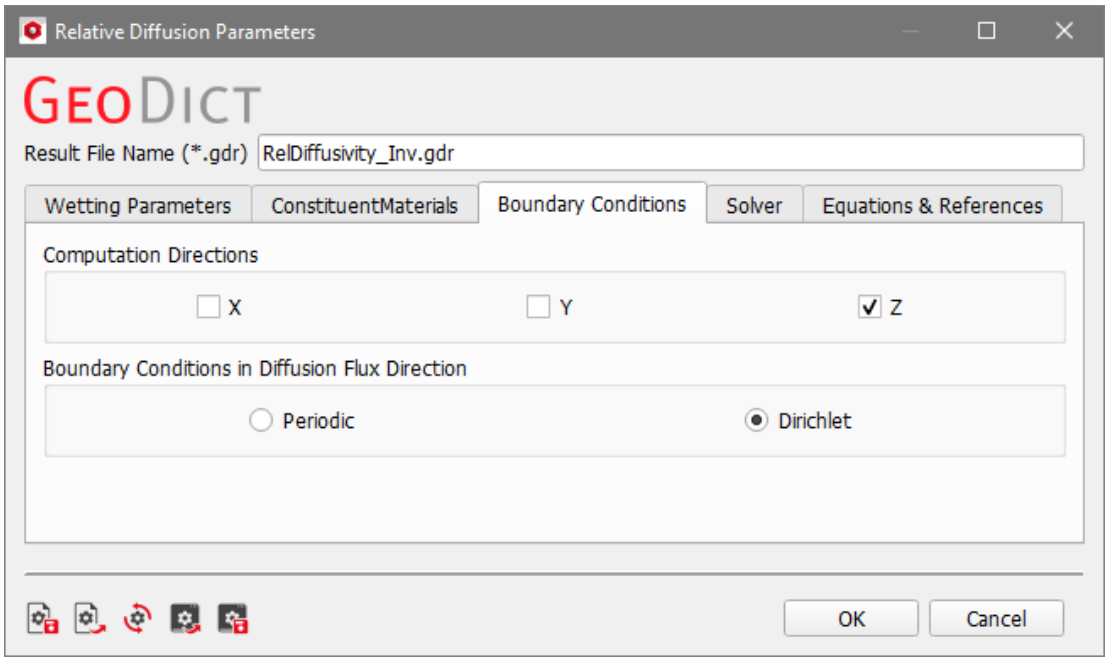
For the **Computation Directions**, choose the direction of the calculated flow. To obtain the whole diffusivity matrix in the result file, it is necessary to choose all three directions.

When computing the relative gas diffusivity, **Boundary Conditions** must be entered for the computations of the diffusion solver.

If **Periodic** is checked, the solution is computed assuming that the structure is periodically repeated in the diffusion direction(s).

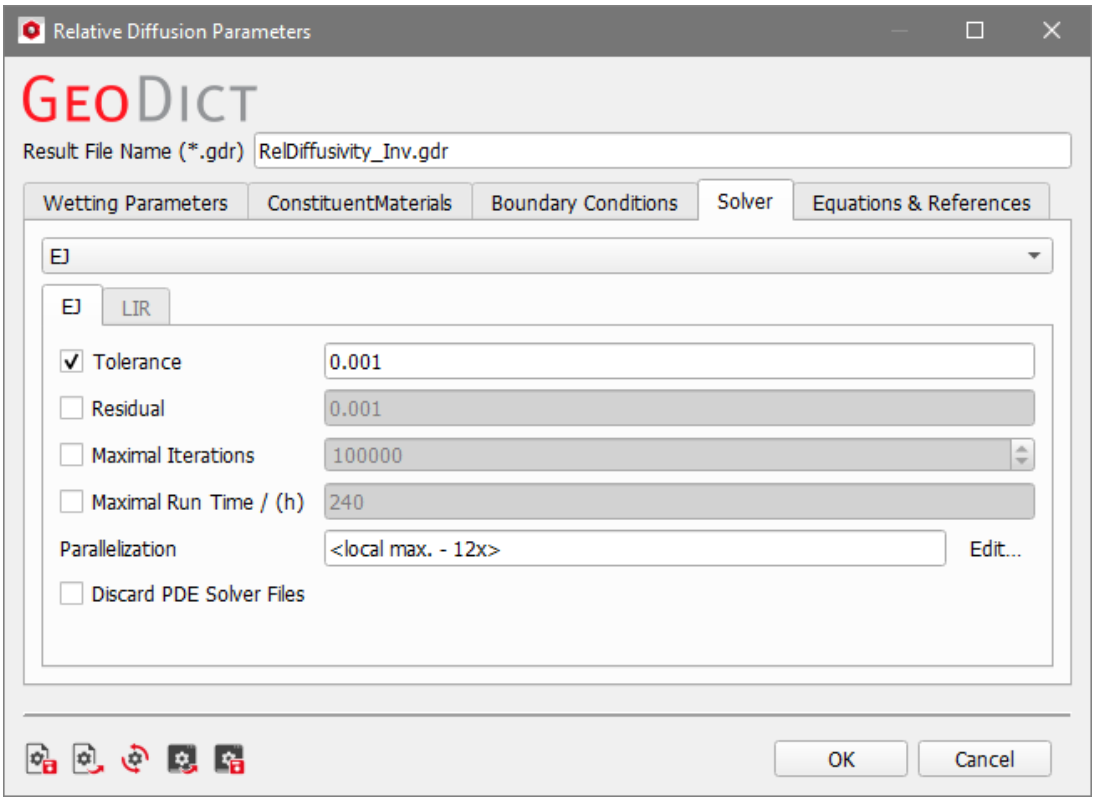
If **Dirichlet** is checked, a constant concentration is ensured along both border planes in the diffusion direction. The use of Dirichlet boundary conditions approximately doubles the computational costs for the EJ solver.

In most cases, the difference between these two settings is not significant and can be compared with a computational error. In general, we suggest using periodic boundary conditions, as the computation time is longer. In few situations, due to the structure's geometry, using Dirichlet boundary conditions is unavoidable.



Solver

For **Relative Gas Diffusivity**, the two flow solvers **EJ** and **LIR** are available and can be chosen from the pull-down menu. The parameters for the **EJ** solver and the **LIR** solver are the same as for the computations of the Relative Permeability (see pages 38 ff.). The options **Stop Relative to Fully Saturated Permeability** and **Solver Type** (for EJ) are not available for the diffusivity computations.



Equations & References

The **Equations & References** tab shows the formulas that are used for the solver:

- Fick's First Law
- Laplace Equation
- Tortuosity Definition

No parameters can be edited on this tab. Also **References** relevant for this module are given.

RELATIVE GAS DIFFUSIVITY RESULT FILE

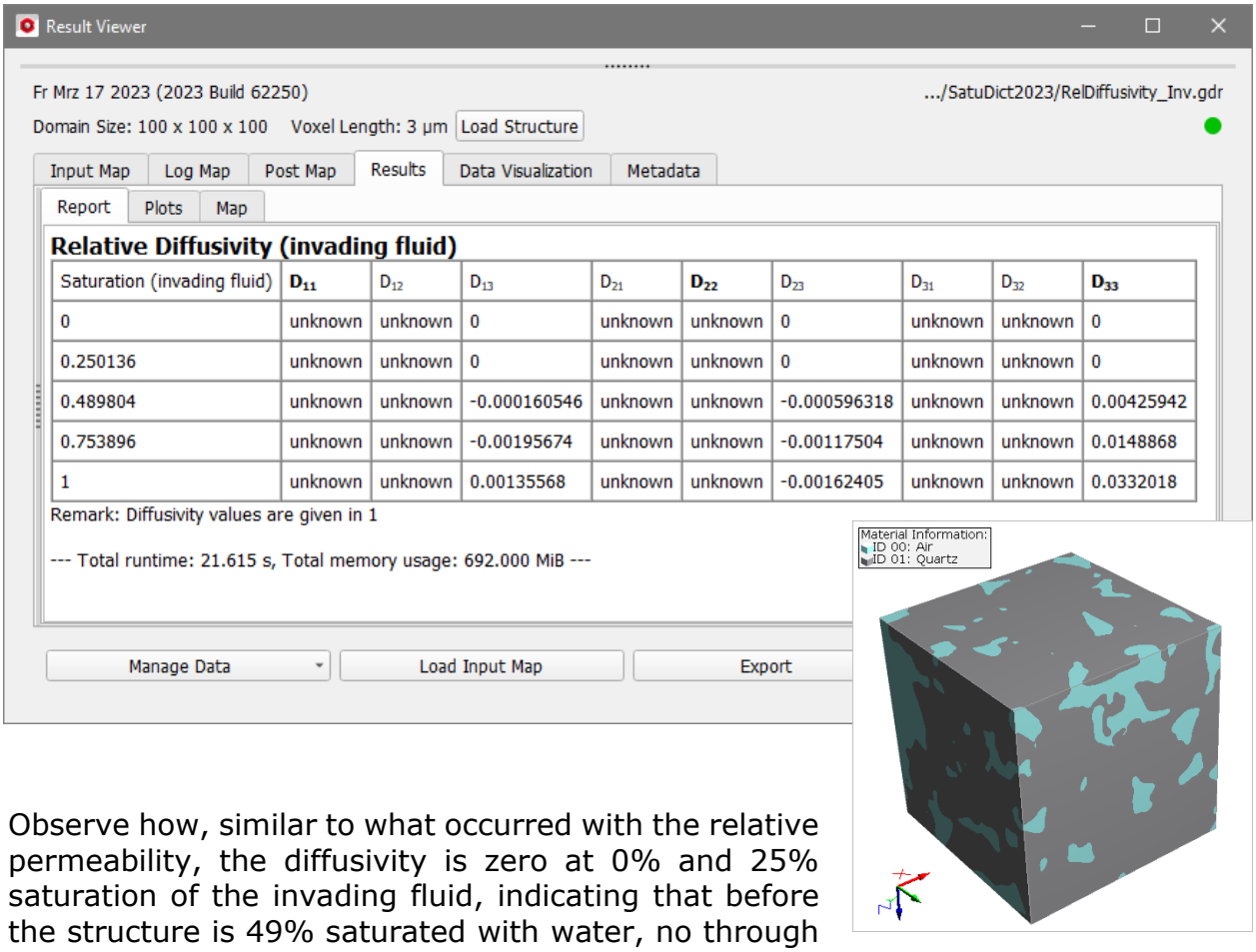
Here, the results of the computation of the relative diffusivity of a partially saturated porous media with 17% porosity (83% SVF) are explained.

The Invading Fluid Water was selected as the flow phase (Wetting Parameters tab), and the relative diffusivity was calculated in Z-direction with Dirichlet boundary conditions (Boundary Conditions tab).

After the solver has finished, the calculation results are immediately displayed in the Result Viewer and saved into a GDR file in the chosen project folder (**File → Choose Project Folder...**). The entered **Result File Name** (here, RelDiffusivity_Inv.gdr) appears at the top.

In the result files for the **Relative Gas Diffusivity**, the computational results are organized into and are accessed through the **Input Map**, **Log Map, Post Map**, **Results**, **Data Visualization** and **Metadata** tabs. The values under these tabs are analog to those for the Capillary Pressure Curve result file (see pages 19 ff.).

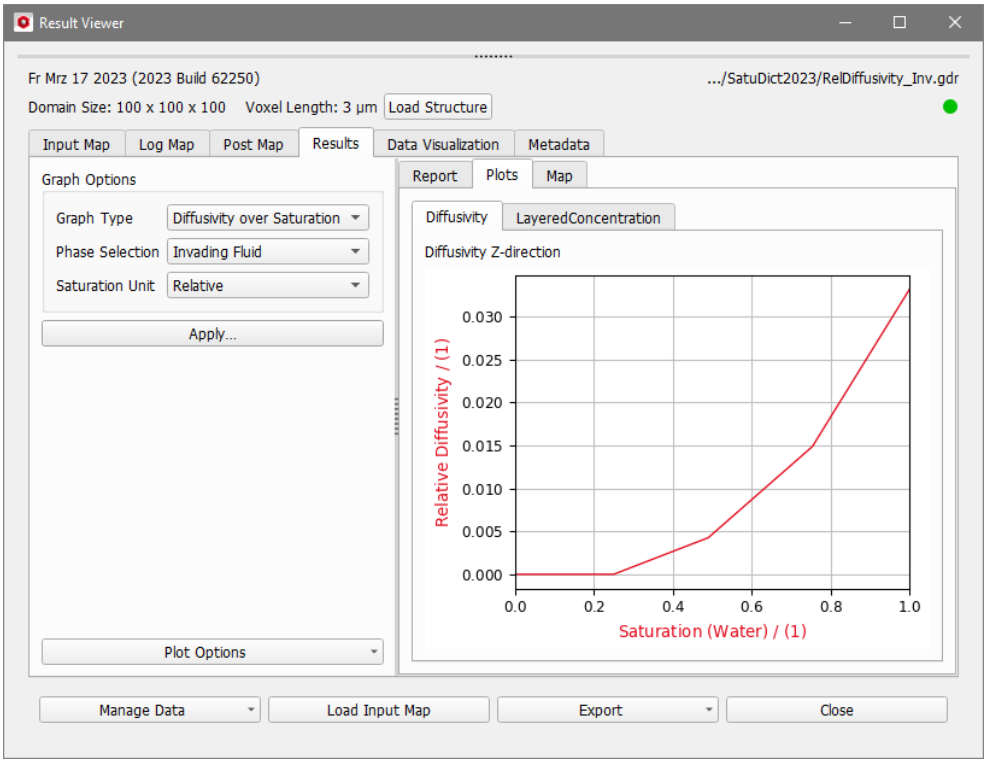
Under the **Results-Report** subtab, the **Relative Diffusivity** table (saturation-dependent diffusivity) is shown for the chosen saturation rates (0.00, 0.25, 0.5, 0.75, 1.00) in the chosen directions (here, D13, D23, D33 for the diffusion in Z-direction). The chosen saturation rates are approximated as good as possible. As the Invading Fluid was selected as the flow phase, it is the diffusivity depending on the saturation of the invading fluid that is shown in the **Relative Diffusivity** table. The directions for which computations have not been carried out appear as **unknown** in the diffusivity table.



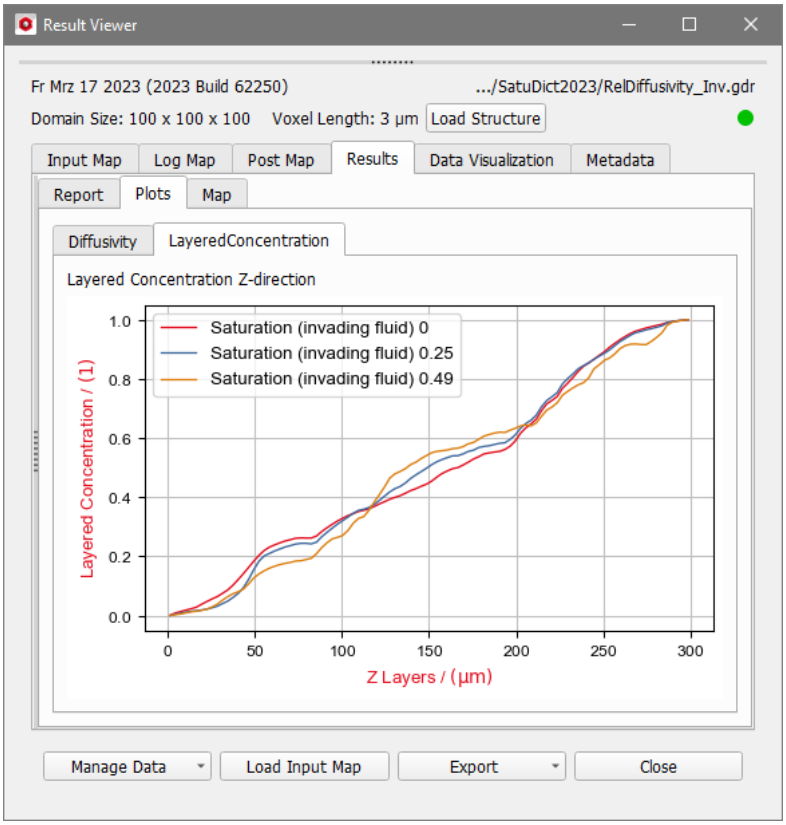
Observe how, similar to what occurred with the relative permeability, the diffusivity is zero at 0% and 25% saturation of the invading fluid, indicating that before the structure is 49% saturated with water, no through path of this fluid is available.

In the **Results**-**Plots** subtab, the values in the **Relative Diffusivity** table of the **Report** tab are shown in a graph. Also, the **Layered Concentration** in the computed directions is given.

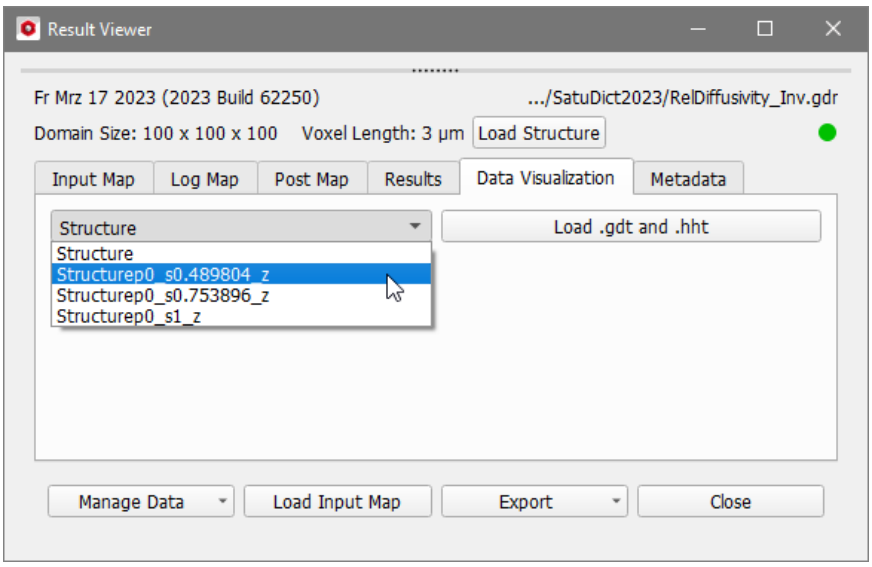
On the left panel in the expandible **Graph Options**, the user can modify the way the graph is displayed by selecting **Graph Type** (Diffusivity over Saturation or Saturation over Diffusivity), **Phase Selection** (Invading Fluid or Replaced Fluid), and **Saturation Unit** (Relative or Absolute). Click **Apply** to change the graph shown according to the options selected. Choose **Plot Options**, to change axis and graph settings.



For each computational direction the concentration in each layer is shown in a graph in the **Layered Concentration** tab. The settings made under the **Graph Options** do not apply for these plots, except for the **Saturation Unit** which changes the units inside the plot legends. But the axis settings and graph styles can be changed under **Plot Options**.

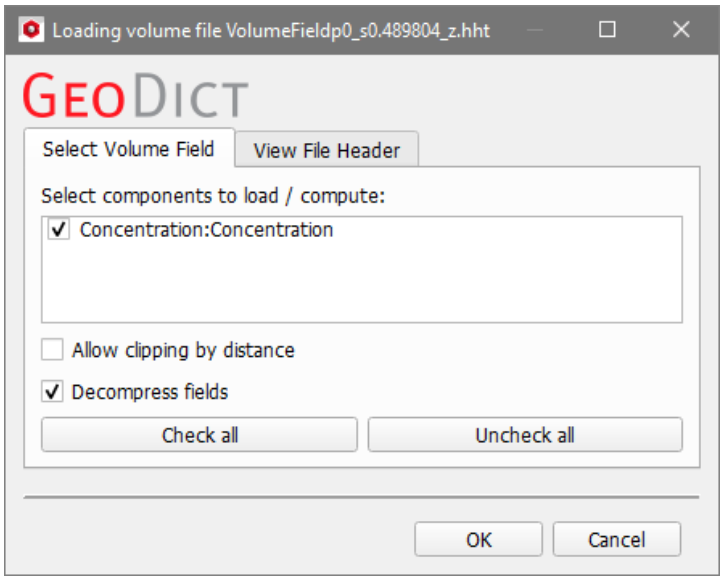


The **RelDiffusivity_Inv.gdr** result file that opens at the end of the computation is saved in the project folder, together with the **RelDiffusivity_Inv** result folder. If **Discard PDE Solver Files** was unchecked, the result folder contains various files for the saturation levels entered in the wetting parameters dialog box.



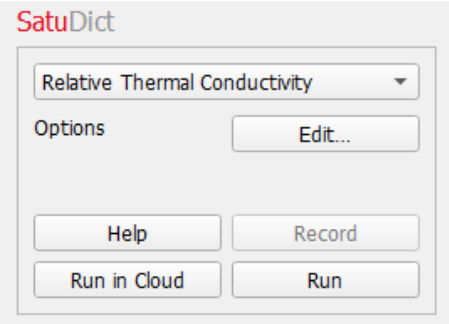
Among these files, the GDT and HHT (homogenized heat file; containing the concentration values) files can be opened on the **Data Visualization** tab.

Click **Load .gdt and .hht** to load the structure for a certain saturation of the invading fluid and the corresponding concentration field in the same way as explained in pages 48 ff. for the relative permeability results.

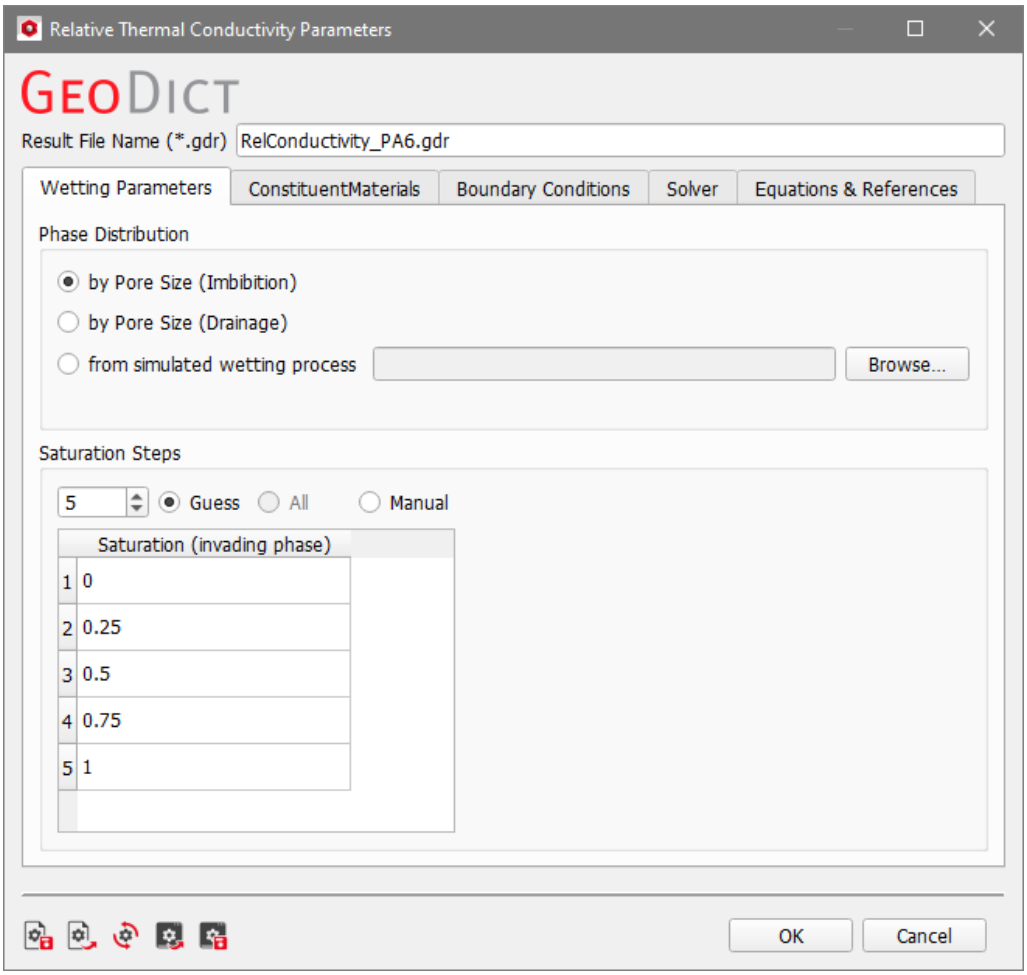


Relative Thermal Conductivity

When selecting **Relative Thermal Conductivity** from the pull-down menu, the **Options** needed for running this process can be entered (or modified) through the **Edit...** button.



The name for the result file is entered in the **Result File Name** box. Keep the default name (RelConductivity.gdr) or rename it according to your current project.



Clicking the **Wetting Parameters**, **Constituent Materials**, **Boundary Conditions**, and **Solver** tabs, the parameters necessary to run the Relative Thermal Conductivity calculations can be entered. The last tab **Equations & References** provides further information about the equations used in this calculation.

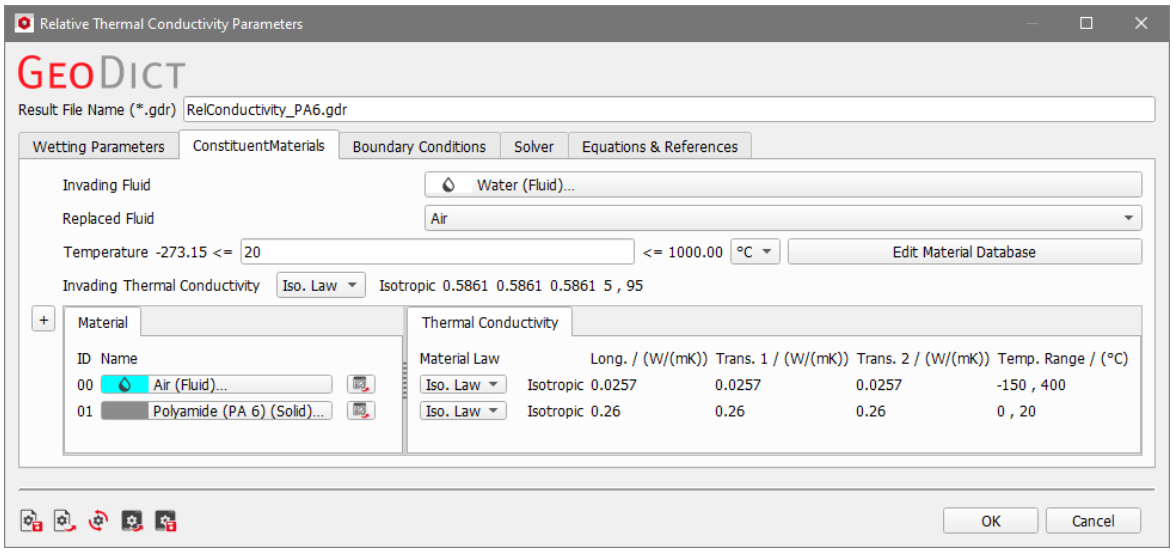
Wetting Parameters

The wetting parameters for the calculation of the Relative Thermal Conductivity are the same as seen above (pages 35 ff.) for the Relative Permeability. No Flow Phase needs to be selected for thermal conductivity computations.

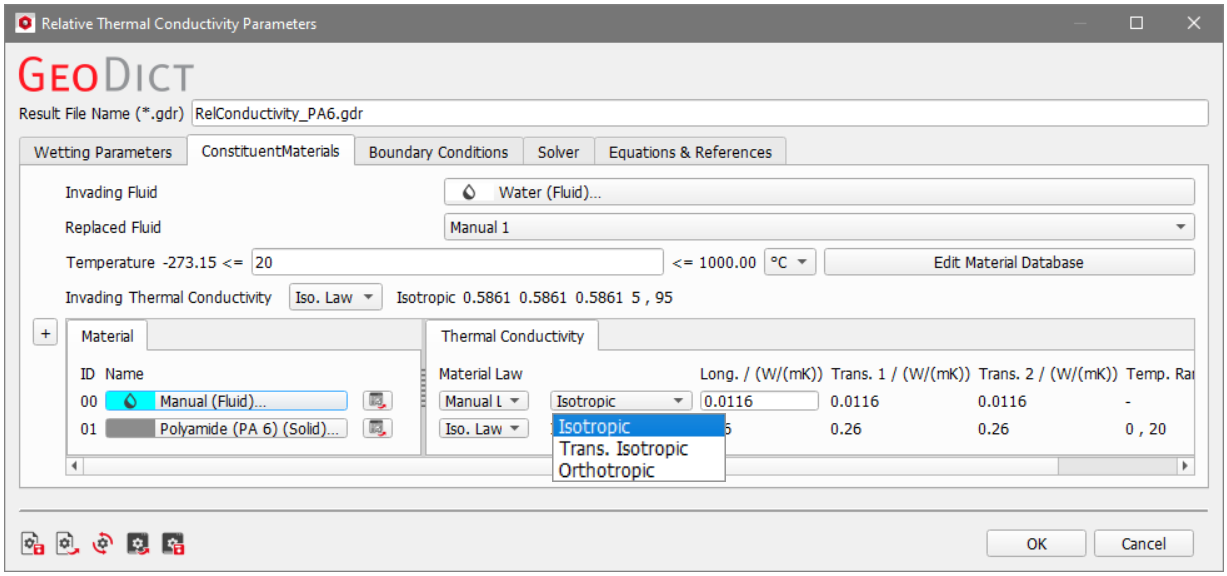
Constituent Materials

Under the **Constituent Materials** tab, the Invading Fluid (in the Pore space), all constituent materials of the structure, and the Replaced Fluid can be selected and their thermal conductivity (W/(mK)) can be defined. The properties of the invading fluid appear above the thermal conductivity tab. The replaced fluid must be present in the current structure or set to manual.

Many materials, together with their thermal conductivity values, are available in the GeoDict Material Database. Other materials or fluids can be added to the material database and saved together with their user-defined thermal conductivity.



For materials defined as Manual, thermal conductivities can be defined directly on the Constituent Materials tab. **Isotropic**, **Transverse Isotropic** or **Orthotropic** thermal conductivities can be defined.

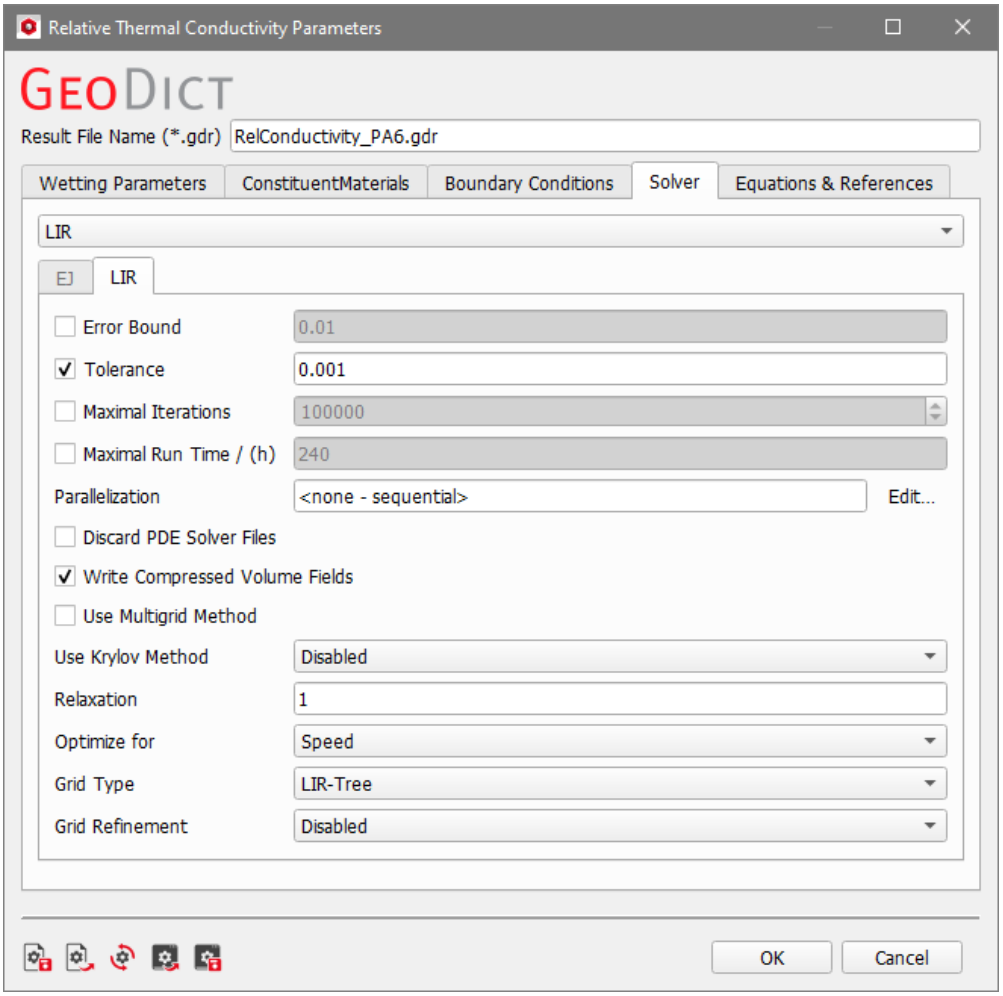


Boundary Conditions

The choice of **Boundary Conditions** and the selection of **Computation Directions** for the calculation of the Relative Thermal Conductivity are the same as seen above (pages 51) for the Relative Diffusivity.

Solver

For **Relative Thermal Conductivity**, the two flow solvers **EJ** and **LIR** are available and can be chosen from the pull-down menu. The parameters for the **EJ** solver and the **LIR** solver are the same as for the computations of the Relative Permeability (see pages 38 ff.). The options **Stop Relative to Fully Saturated Permeability** and **Solver Type** (for EJ) are not available for the diffusivity computations.



Equations & References

The **Equations & References** tab shows the formulas that are used for the solver:

- Fourier's Law
- Poisson Equation

No parameters can be edited on this tab. Also **References** relevant for this module are given.

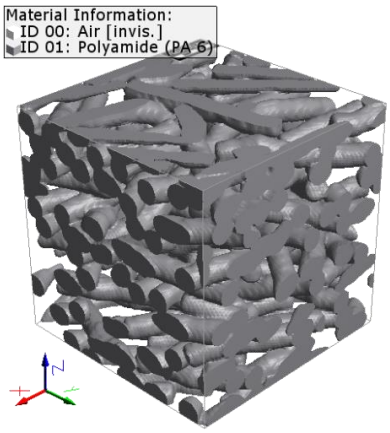
Relative Thermal Conductivity result file

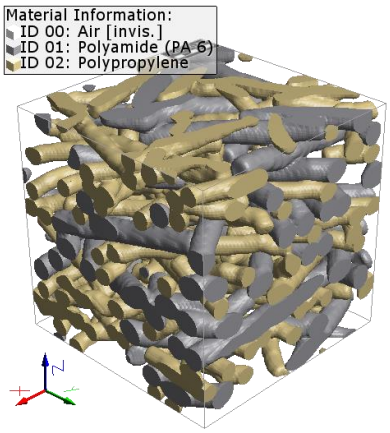
The Result File for the Relative Thermal Conductivity is very similar to the Result File of the Relative Gas Diffusivity. The settings described on pages 53 ff. apply also here, but with Conductivity instead of Diffusivity. In the Plots subtab, the **Layered Temperature** is shown.

Additionally, we show here how to set-up and compare two result files, where the saturation-dependent relative thermal conductivity is computed at various invading fluid saturation levels (0%, 25%, 50%, 75%, and 100%) for two structures, both with 70% porosity, but different constituent materials. The invading fluid is water, and the replaced fluid is air. The relative thermal conductivity is calculated in Z-direction.

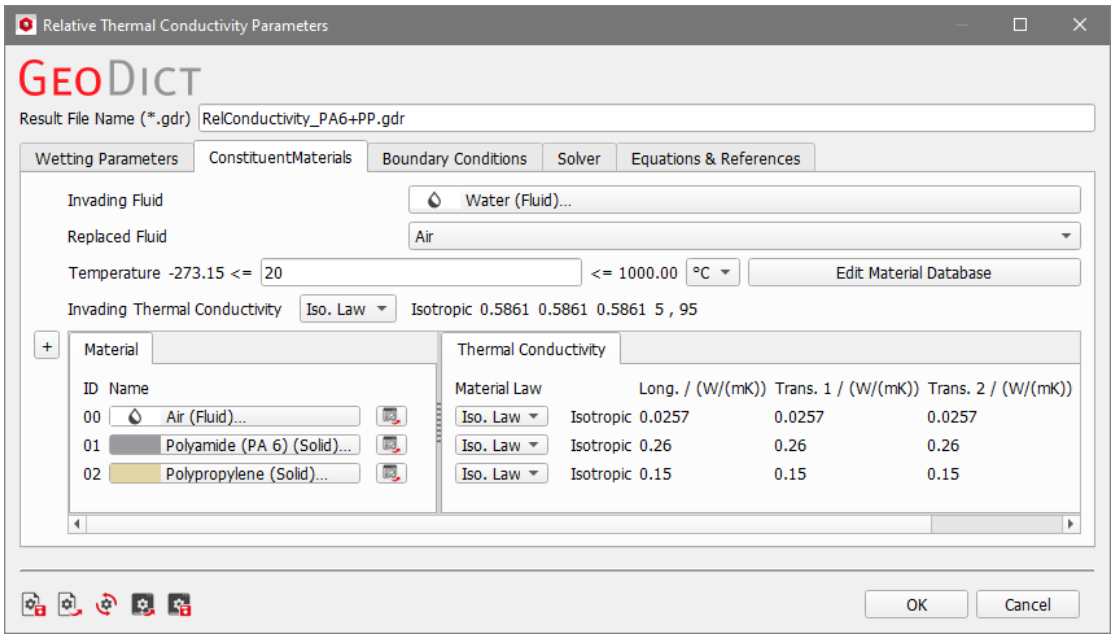
In the **first experiment**, the only fiber material in the structure is 100% polyamide PA6 (Material ID 01, grey).

In the **second experiment**, the structure is made of 20% polyamide (Material ID 01, grey) and 80% polypropylene PP (Material ID 02, brown) fibers. PA6 and PP have different thermal conductivities.

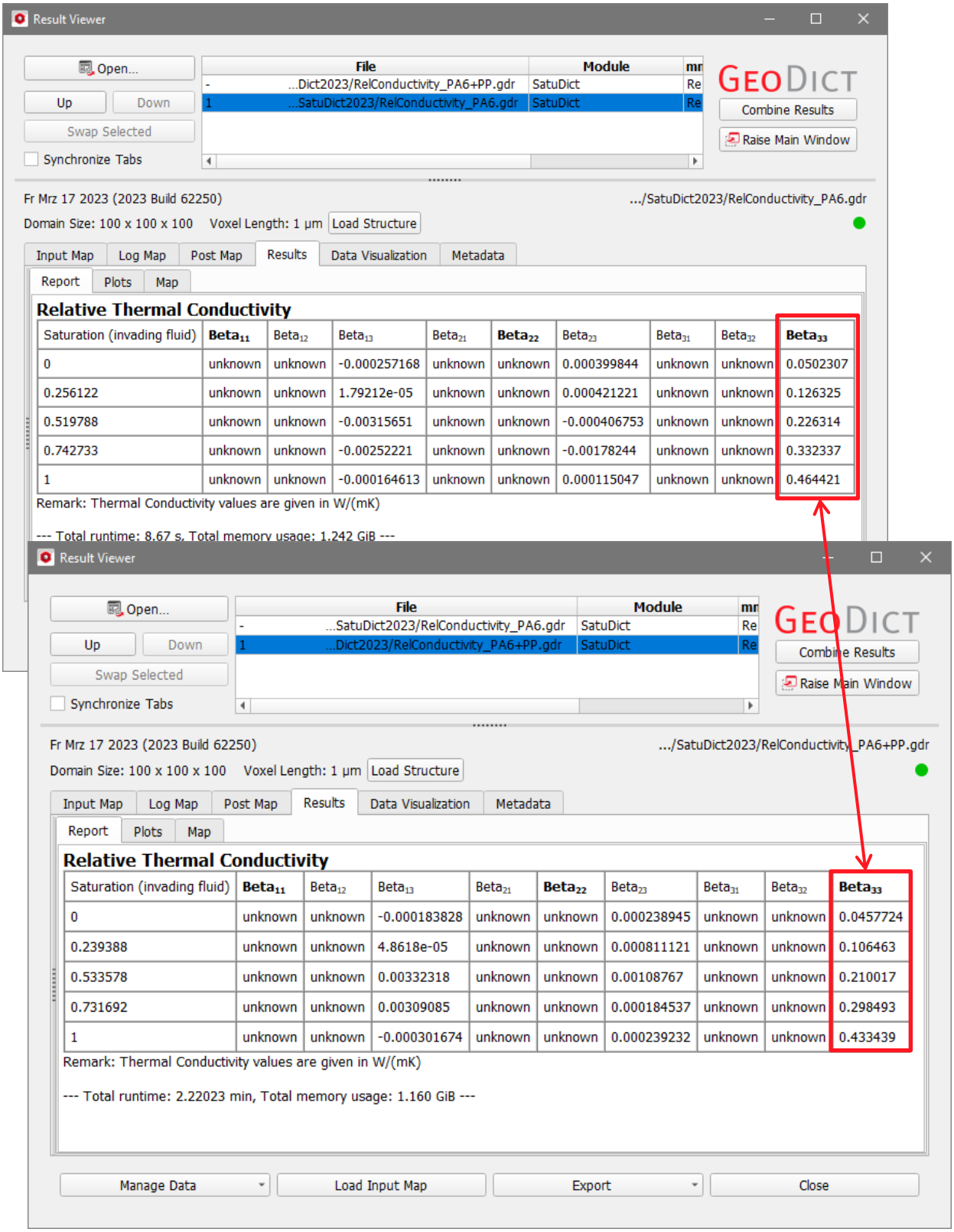




The selected materials and their thermal conductivities are entered under the **Constituent Materials** tab by selecting them from the material database (here shown for PA6+PP, above for PA6). The thermal conductivity of the materials included in the database is automatically considered.



After each computation, for the first and the second experiment, is finished, the Result Viewer opens. The result data contained in the result file is visible below when the file names are highlighted in the Header section box.



Both result files, from the first experiment and the second experiment, can be selected and highlighted by using **Shift-click** on the list of file names (RelConductivity_PA6.gdr and RelConductivity_PA6+PP.gdr). Then, the results are shown side-by-side.

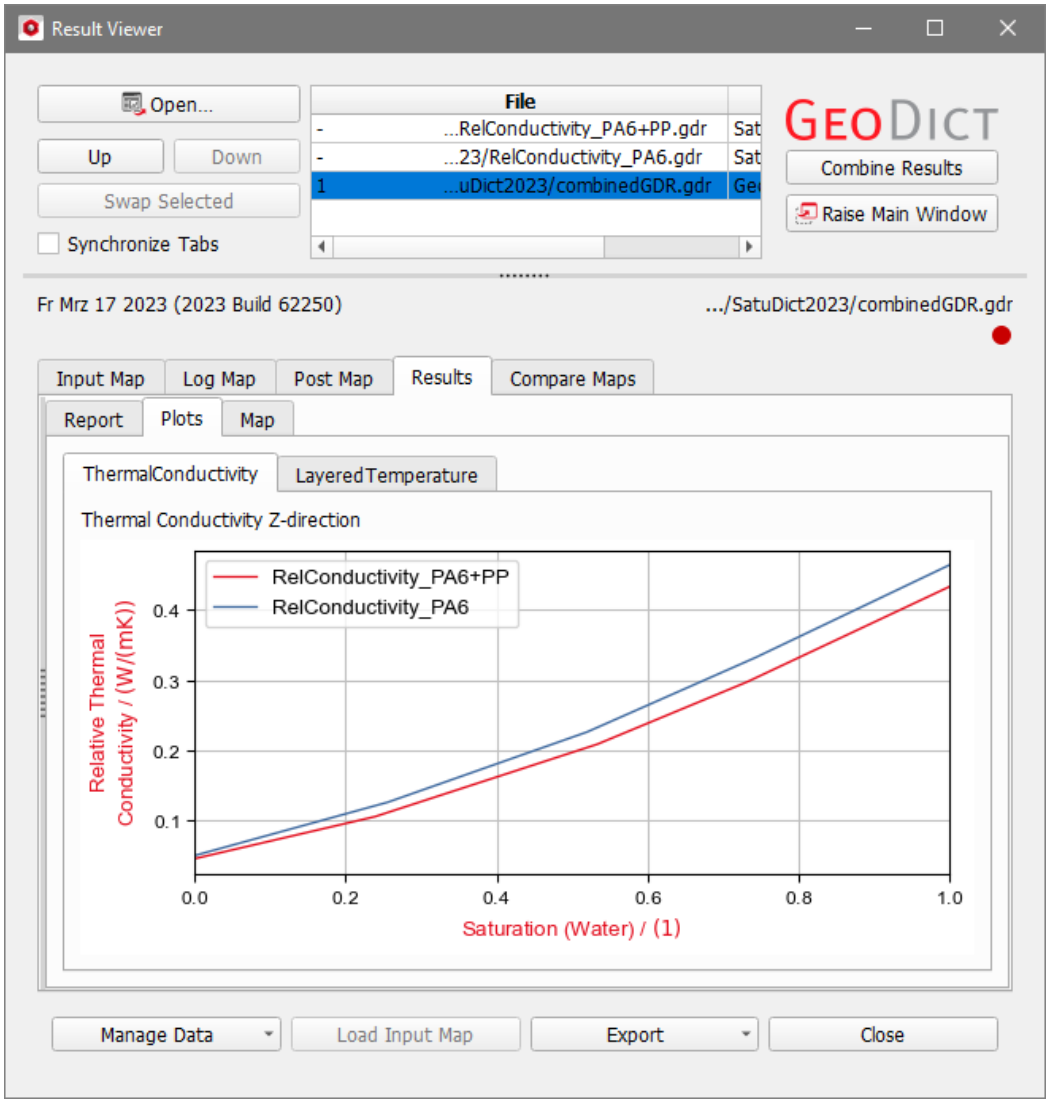
By highlighting the names of both result files and clicking the **Combine Results** button, the results of both files are combined and saved into a GDR file in the chosen project folder. The combining process enables post-processing on the combined results.

The combined result file contains the **Input Map**, **Log Map**, **Post Map**, **Results** and **Compare Maps** tabs. The **Results – Report** subtab, shows the names of the files that were used to create the combined result file (RelConductivity_PA6.gdr and RelConductivity_PA6+PP.gdr).

Plots from the original result files are merged into one plot and shown under the **Results** - **Plots** subtab. More information on combining result files and comparing their plots can be found in the Result Viewer handbook of the User Guide.

In the combined plot, the **Relative Thermal Conductivity** of the structures (Y-axis) increases with increasing saturation levels of water (Invading Fluid, X-axis). The relative thermal conductivity of the PA6+PP structure is always lower.

The parameters for the graphs can be modified (see pages 23 f.) in the Result Viewer of the original result files before combining them. The modification of the plot settings can be synchronized in both original files.

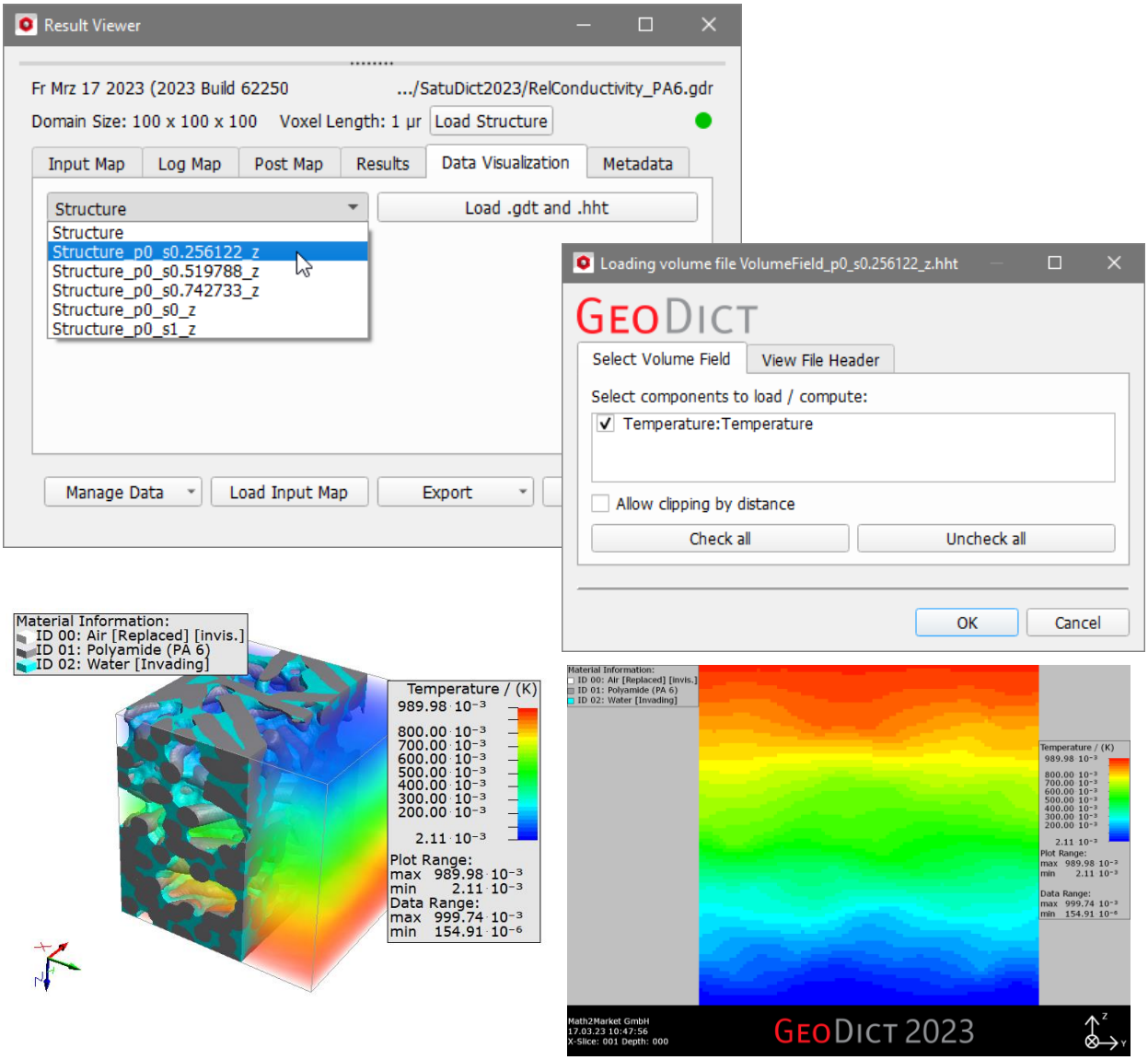


The HHT files (homogenized heat file; containing the temperature distribution) corresponding to the five saturation levels entered under the Wetting Parameters tab (0.00, 0.25, 0.50, 0.75, 1.00) are stored for each computation in the result folder, here **RelConductivity_PA6** and **RelConductivity_PA6+PP,** in the project folder.

Under the **Data Visualization** tab, click **Load .gdt and .hht**, to access the .hht files and visualize the results. This can only be done for each of the result files individually and not for the combined result file.

This is similar to opening .gdt and .vap files (see pages 48 ff.) for the visualization of the phase distribution for results of Relative Permeability directly from the result file (GDR).

For example, open the Structure_p0_s0.256122_z files that corresponds to a 25% invading fluid saturation in Z-direction from the experiment with the **100% PA6 structure**.

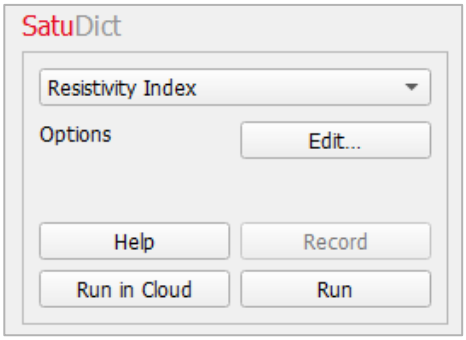


To better observe the results, clip the structure (in 3D Rendering) or switch off the visualization of the structure (in 2D cross-section, **View** → **Structure** in the menu bar), and adjust the Color Map values in the Visualization panel.

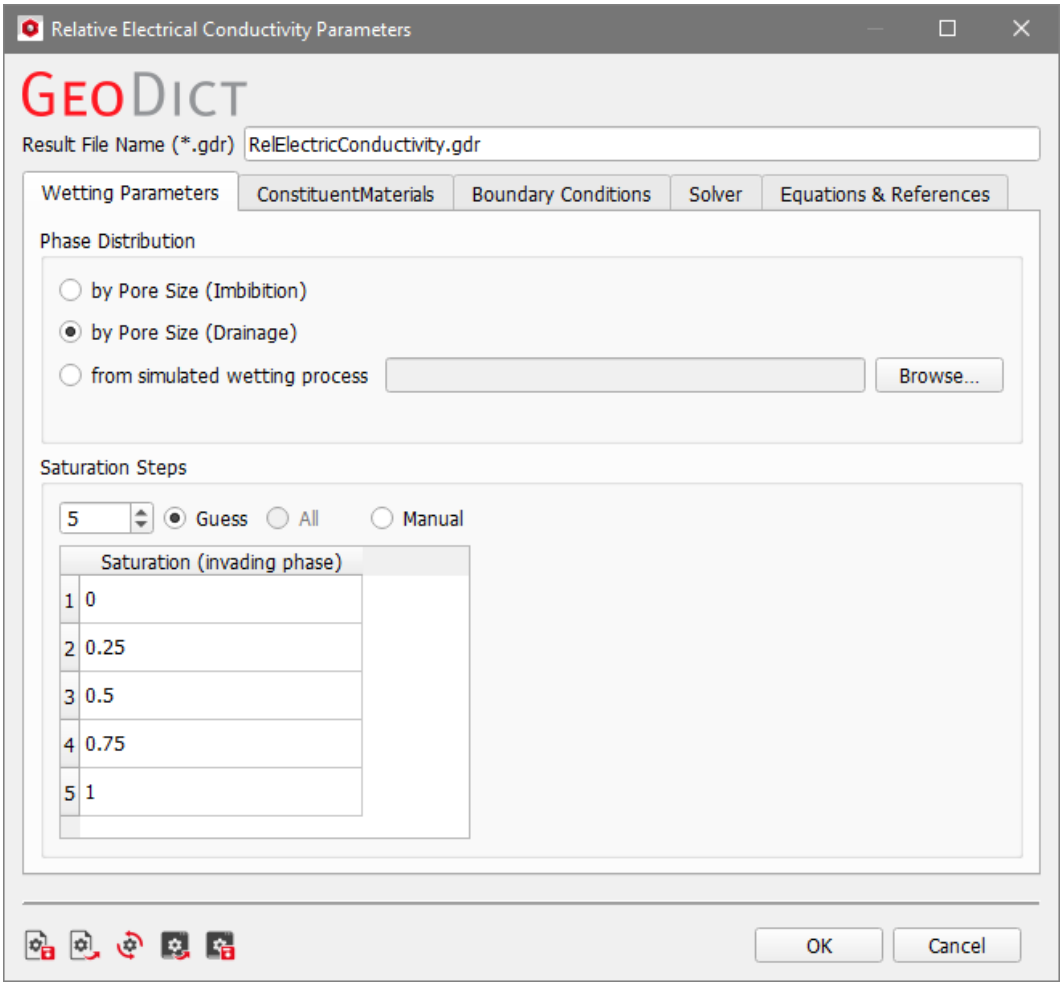
Observe how the heat is distributed in the structure.

Resistivity Index (relative electrical conductivity)

When selecting **Resistivity Index** from the pull-down menu, the **Options** needed for running this computation can be entered (or modified) through the **Edit...** button.



The name for the result file is entered in the **Result File Name** box. Keep the default name (RelElectricConductivity.gdr) or rename it according to your current project.



Under the **Wetting Parameters**, **Constituent Materials**, **Boundary Conditions** and **Solver** tabs, the user enters the parameters necessary to run the calculations to obtain the Saturation Exponent, Cementation Exponent, the (saturation-dependent) Resistivity Index, and Relative Electrical Conductivity. The last tab **Equations & References** provides further information about the equations used in this calculation.

All parameters are similar to those explained for the Relative Thermal Conductivity computation starting on page 57.

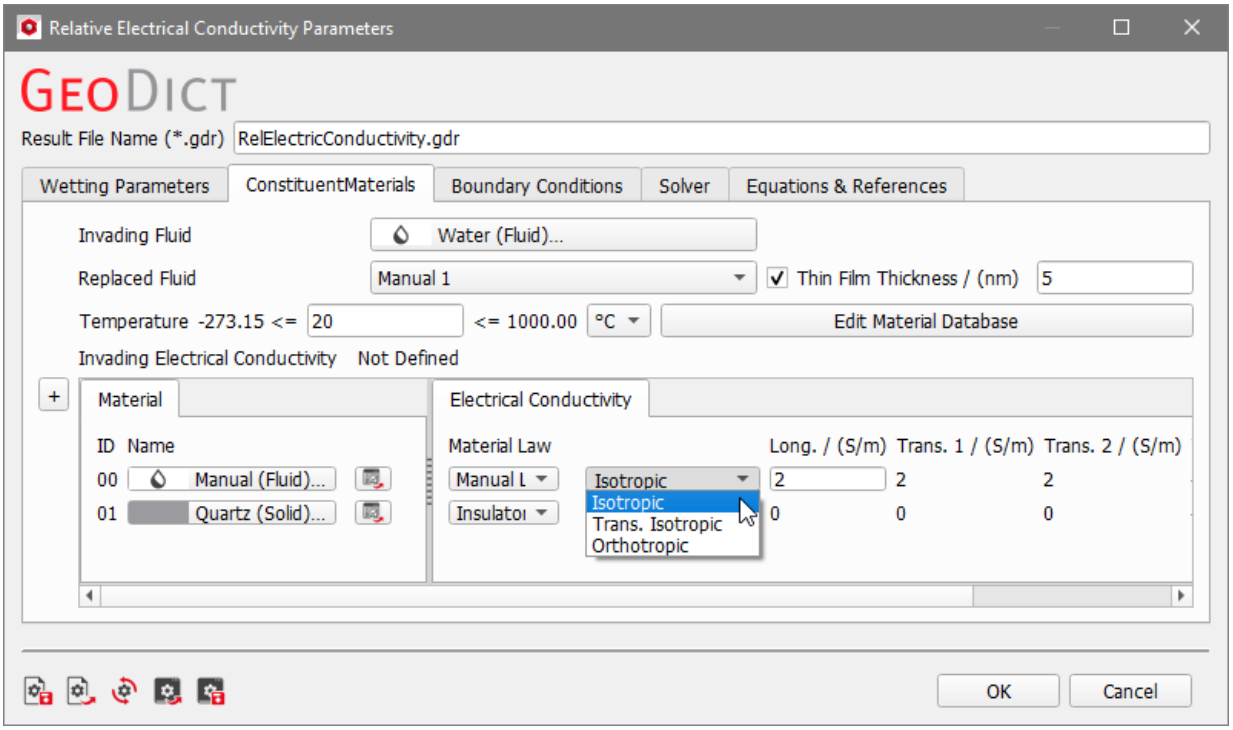
Wetting Parameters

The wetting parameters for the calculation of the Relative Electrical Conductivity (and the Resistivity Index from it) are the same as seen for the computation of the Relative Thermal Conductivity (page 57).

Constituent Materials

Under the **Constituent Materials** tab, the Invading Fluid (in the Pore space), all constituent materials of the structure, and the Replaced Fluid can be selected, and their electrical conductivity (S/m) can be defined. Many materials, together with their electrical conductivity values, are available in the GeoDict Material Database. Other materials or fluids can be added to the material database and saved together with their user-defined electrical conductivity.

Electrical conductivities can only be entered for materials present in the structure currently in memory (displayed in the Visualization area). For Manual materials, values for Isotropic, Transverse Isotropic or Orthotropic electrical conductivity can be defined directly on the Constituent Materials tab. The electrical conductivity of the invading fluid is shown on top of the other material properties and can be changed there if the material is set to Manual (Fluid).



Additionally, by checking **Thin Film Thickness**, the thin film model (see page 6) can be used. The thickness of the thin film must be smaller than the current voxel length.

Boundary Conditions

The choice of **Boundary Conditions** and the selection of **Computation Directions** for the calculation of the Relative Electrical Conductivity are the same as seen for the Relative Diffusivity (page 51) and the Relative Thermal Conductivity.

Solver Options

For **Relative Electrical Conductivity**, the two flow solvers **EJ** and **LIR** are available and can be chosen from the pull-down menu. The parameters for the **EJ** solver and the **LIR** solver are the same as for the computations of the Relative Permeability (see pages 38 ff.). The options **Stop Relative to Fully Saturated Permeability** and **Solver Type** (for EJ) are not available.

Equations & References

The **Equations & References** tab shows the formulas that are used for the solver:

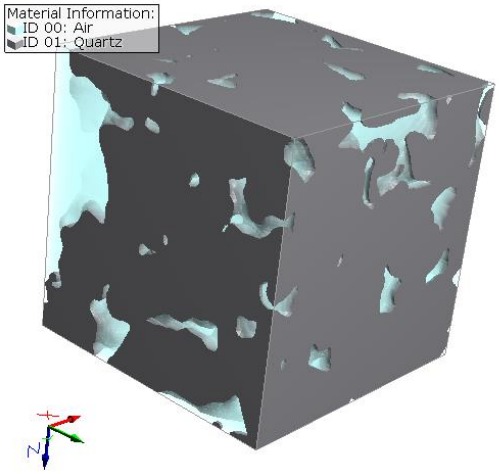
- Ohm's Law
- Poisson Equation

No parameters can be edited on this tab. Also **References** relevant for this module are given.

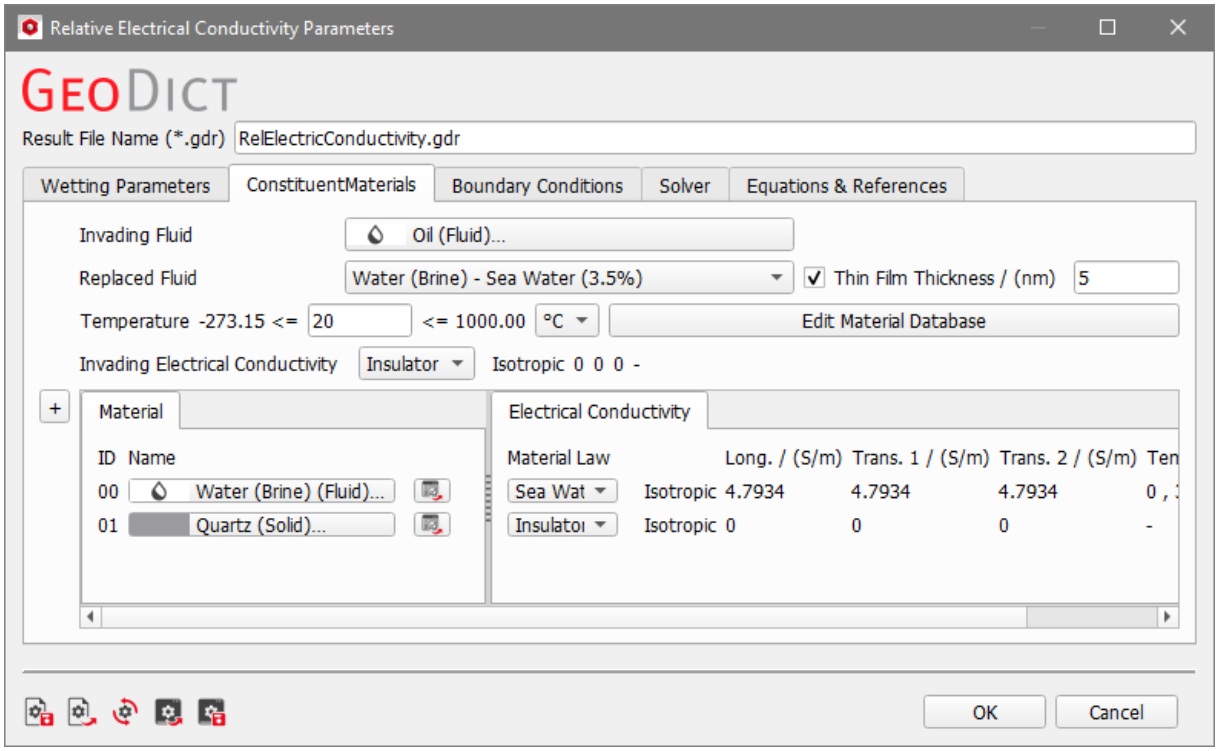
RESISTIVITY INDEX RESULT FILE

Here, the resistivity index is computed at various invading fluid saturation levels (0%, 25%, 50%, 75% and 100%) for a porous medium with 17% porosity. The invading fluid is Oil (0 S/m) and the replaced fluid is Water (Brine) (5 S/m). The relative electrical conductivity is calculated in Z-direction.

In this experiment, the only solid material in the structure is the non-conductive material Quartz (Material ID 01), with 0 S/m.



The selected materials and their electrical conductivity are entered under the **Constituent Materials** tab by selecting them from the material database. The electrical conductivity of the materials included in the database is automatically considered. For other materials, the material database has to be edited or the electrical conductivity can be entered manually.

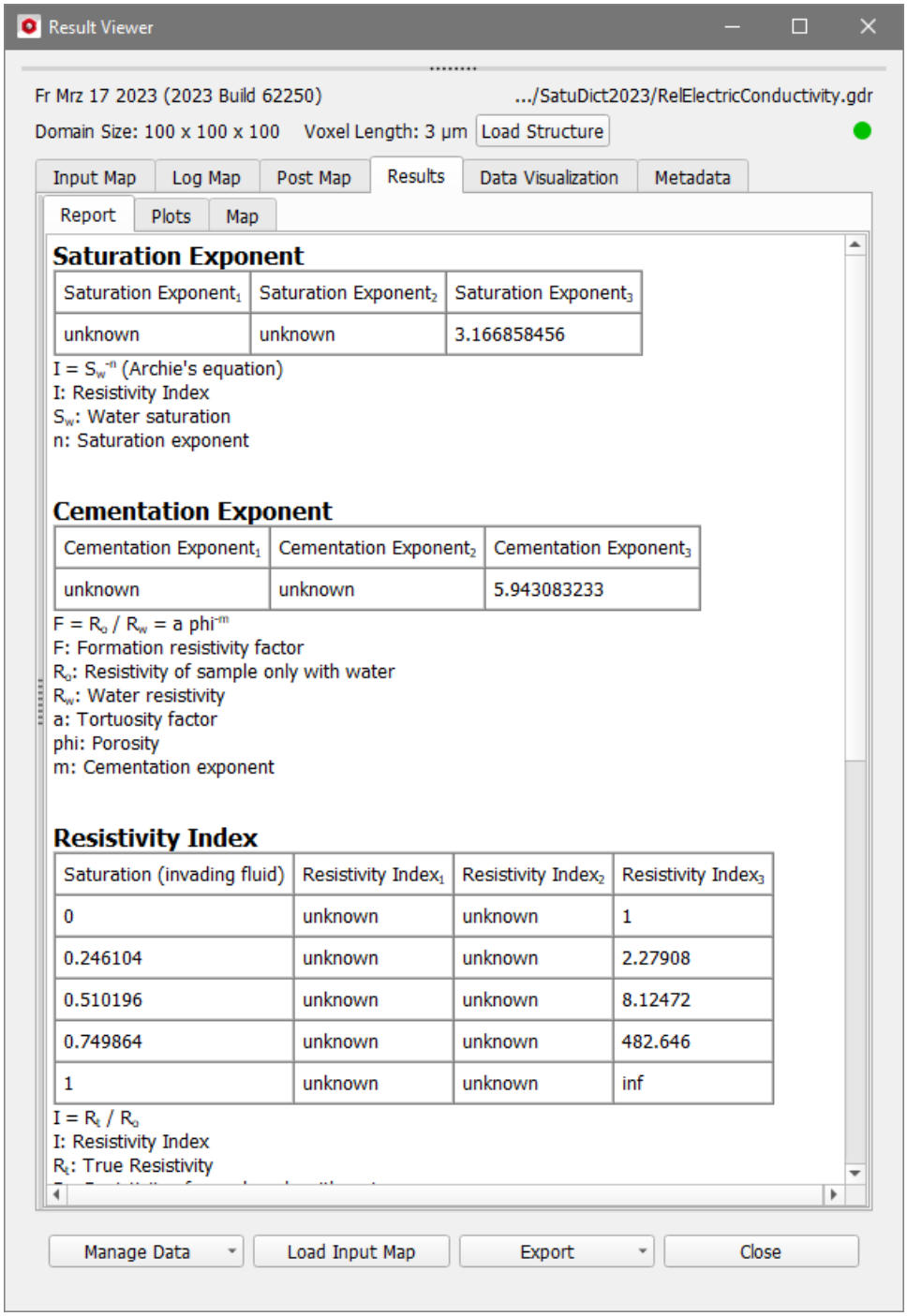


After the computations are finished, the Result Viewer of the result file opens, and the results are saved into a GDR file in the chosen project folder (**File** → **Choose**

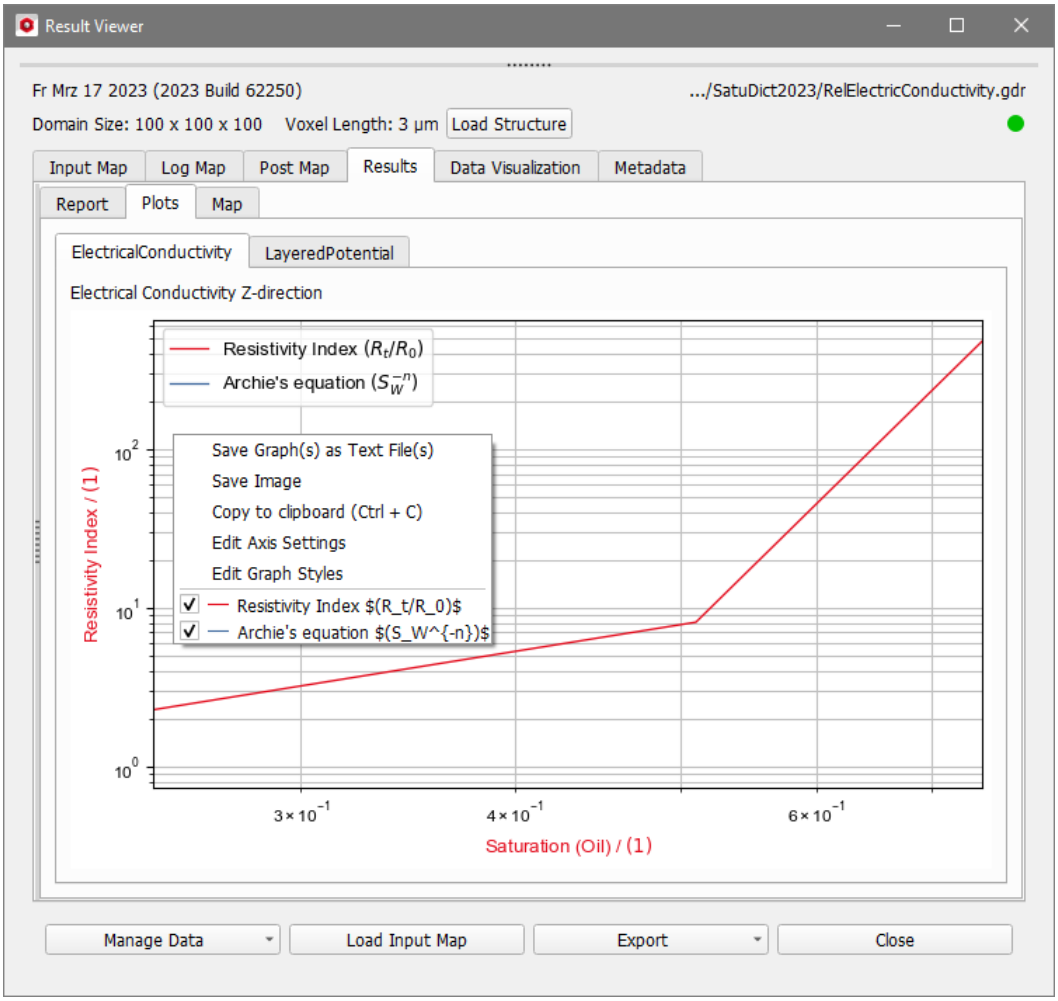
Project Folder...). In this example, the **RelElectricConductivity.gdr** result file is saved in the project folder together with the **RelElectricConductivity** result folder.

The computational results are accessed through the **Input Map**, **Log Map**, **Post Map**, **Results**, **Data Visualization**, and **Metadata** tabs (see pages 19 ff.).

Under the **Results - Report** subtab, the tables for **Saturation Exponent**, **Cementation Exponent**, **Resistivity Index**, and **Relative Electrical Conductivity** are shown for the chosen saturation rates (0.25, 0.5, 0.75) and the start and end saturations (0.0 and 1) in the directions for which results were calculated.



Under the **Results** - **Plots** subtab, these values are shown in graphs and the **Layered Potential** is shown. The parameters of the graphs can be changed as seen in pages 23 f.

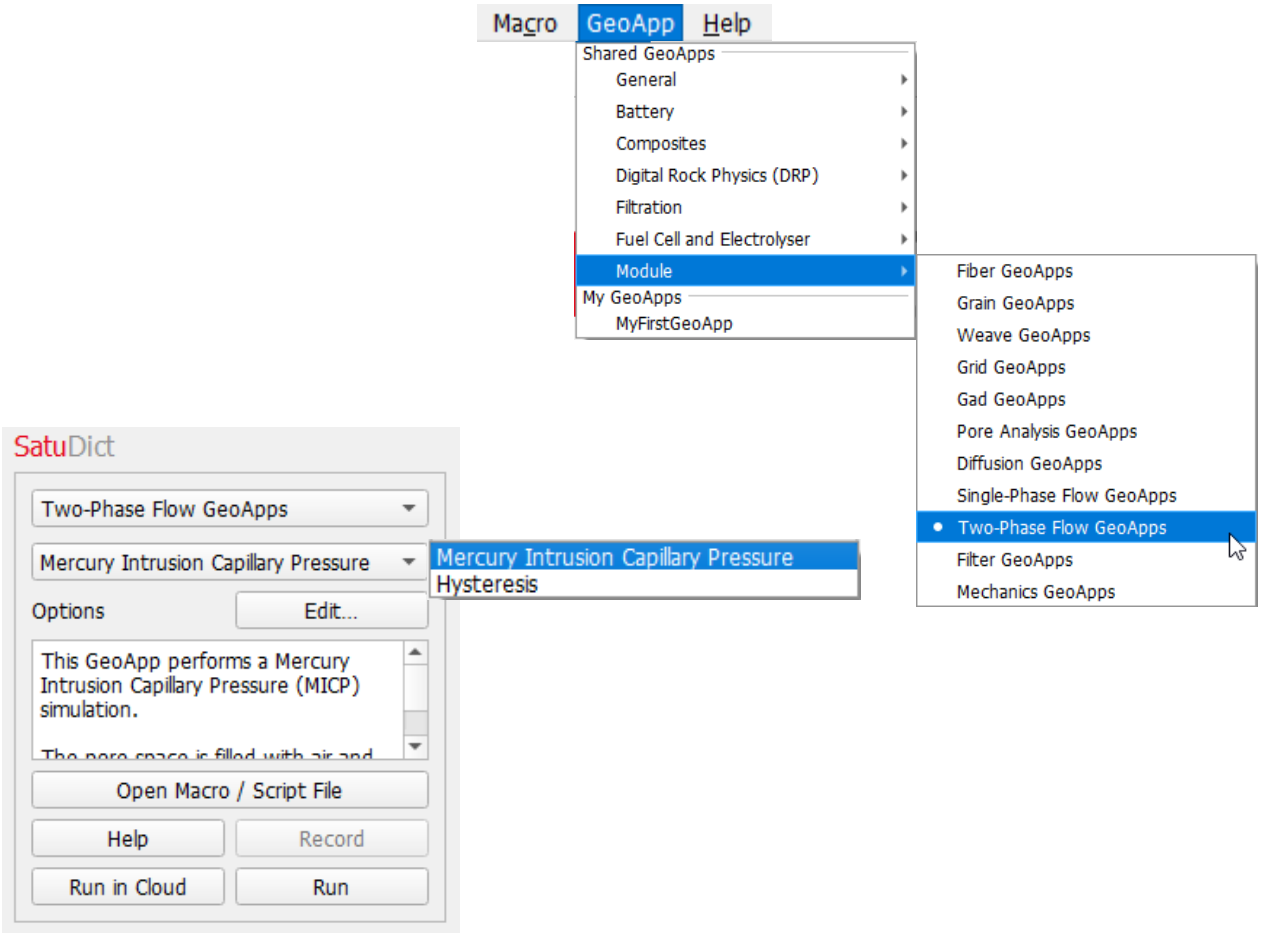


The interpretation of the result tables and the visualization of the corresponding created files are like for the results of the **Relative Thermal Conductivity,** see page 62.

Two-Phase Flow GeoApps

When **Two-Phase Flow GeoApps** is selected in the **SatuDict** section, predefined computation settings can be chosen from the pull-down menu: **Mercury Intrusion Capillary Pressure** and **Hysteresis.**

These **Predefined** SatuDict computations are also accessible directly from the menu bar as one of the **GeoApp**s.



The SatuDict **Two-Phase Flow GeoApps** are macros or scripts containing combinations of SatuDict commands with certain default parameters to mimic experiments or real observations.

Add Predefined Computations

When predefined computations are run, the corresponding GeoDict macros are called and executed. These macros can be accessed with the **Open Macro / Script File** button, alternatively they are available in the **SatuDict** folder in the GeoDict installation folder. In Windows:

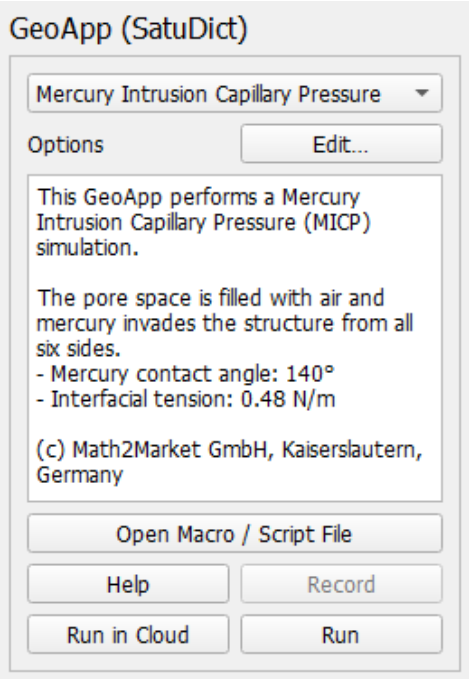
They can be opened with a text editor to check or edit the syntax of the computation steps. To add predefined computations, put the corresponding macros in this folder and restart GeoDict.

Edit and Execute Predefined Computations

By clicking the **Edit...** button, the corresponding parameter dialog box opens and the parameters defining the corresponding saturation experiments are displayed and can be modified.

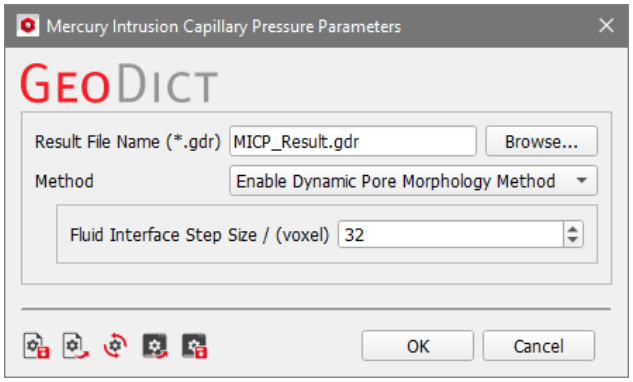
Click **OK** to close the dialog, and then **Run** to execute the computation.

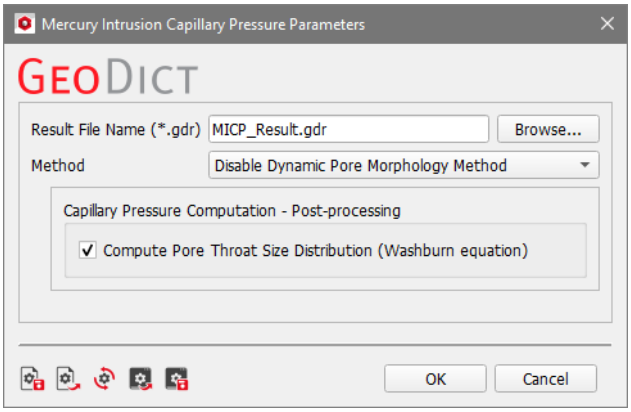
Mercury Intrusion Capillary Pressure



The **Mercury Intrusion Capillary Pressure** predefined computation sets the simulation settings for a Drainage experiment without residual of the replaced fluid from SatuDict to recreate the Mercury Intrusion Porosimetry (MIP) experiment. During the experiment, the structure's pore space is being invaded by mercury from all six sides.

After clicking **Edit...**, the Result File Name can be changed. From the drop-down menu decide which method is used, then the parameters for the chosen method can be defined.





If **Disable Dynamic Pore Morphology Method** is selected, it is possible to check **Compute Pore Throat Size Distribution** in the post-processing using the Washburn equation.

If **Enable Dynamic Pore Morphology Method** is selected, the **Fluid Interface Step Size** in voxel must be selected. This is the same parameter as the interface step size in the Capillary Pressure command (see page 16).

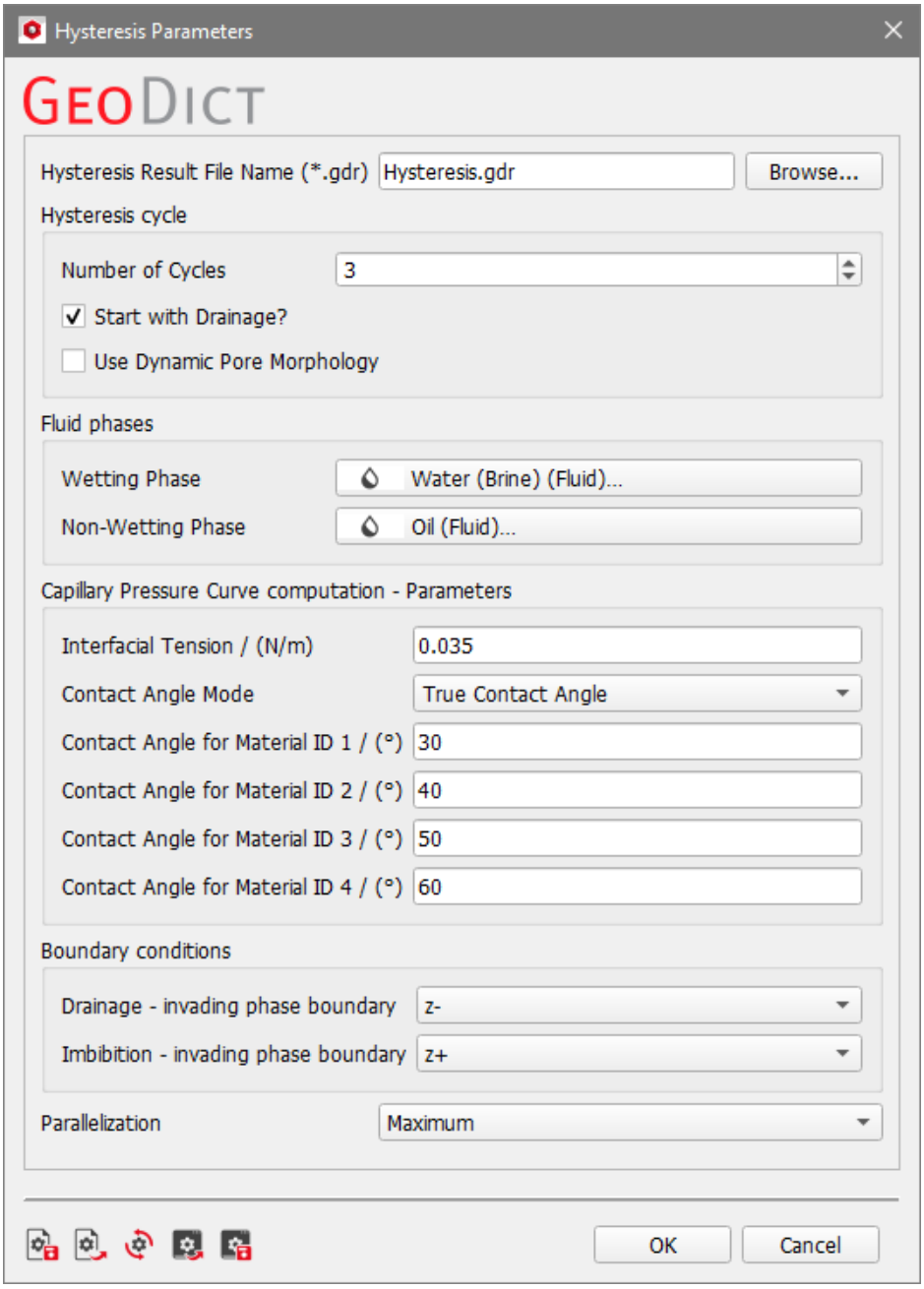
After the predefined simulation is finished, the Result Viewer opens showing the results from SatuDict Drainage simulation as seen on pages 19 ff..

The saturation table is shown in the **Results – Report** and the capillary pressure curve as well as the Layered Saturation are seen the **Results – Plots** tabs. Additionally, if chosen before, the Pore Throat Size Distribution is shown in a plot.

HYSTERESIS

The **Hysteresis** predefined computation performs a Hysteresis simulation of the SatuDict functionalities Drainage and Imbibition (both with invading fluid connected to a reservoir and the replaced fluid can leave a residual) in succession.

After clicking **Edit...**, enter the **Hysteresis Result File Name**, **Number of Cycles**, **Interfacial Tension**, and **Contact Angle**.



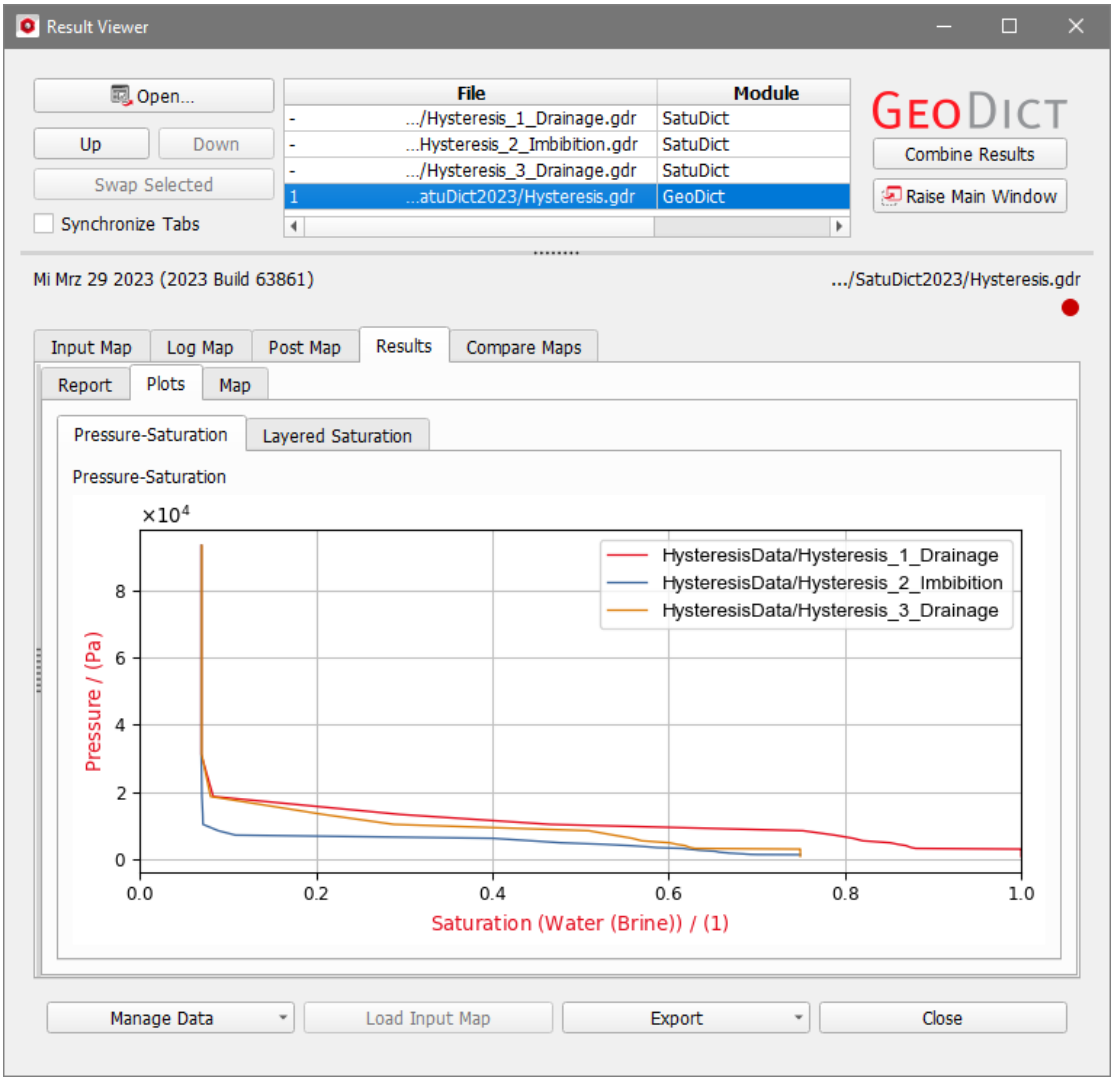
Additionally, the **Wetting Phase** and **Non-Wetting Phase** can be chosen and whether to start with Drainage or with Imbibition.

If **Use Dynamic Pore Morphology** is checked, the parameters for this method can be defined.

It is also possible to choose the **Parallelization** for computations.

Tooltips describe all those options in more detail.

After the **Predefined - Hysteresis** has finished, the Result Viewer opens. The Header section box lists all the Imbibition and Drainage result files of each cycle. The hysteresis result file is an automatically combined result file showing the Pressure-Saturation curves in a single plot.



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