SatuDict

User Guide

GeoDict release 2022

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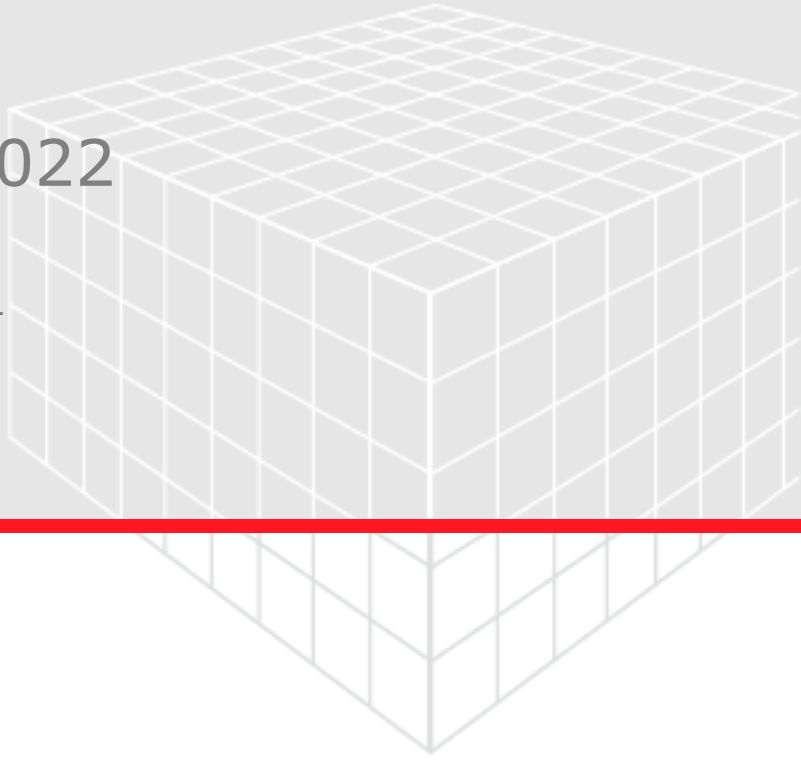


GeoDict

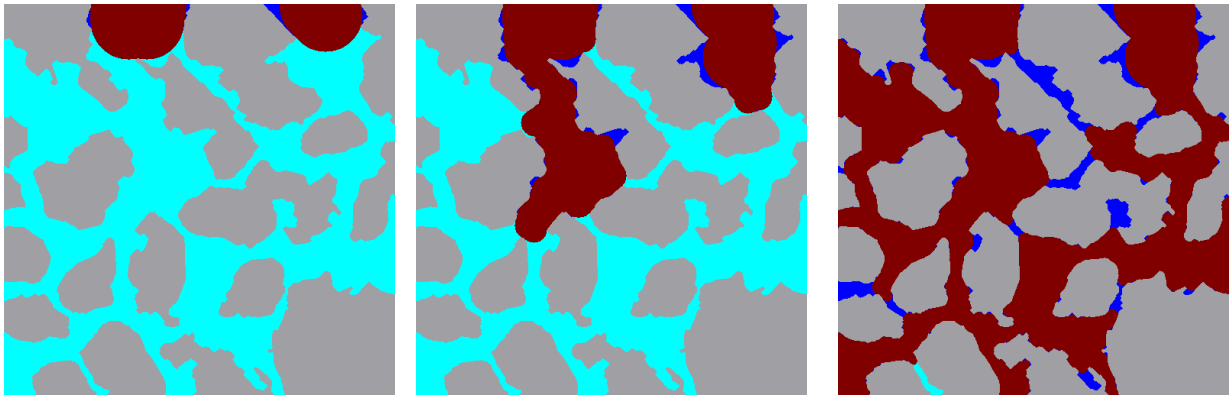
https://doi.org/10.30423/userguide.geodict2022-satudict

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.

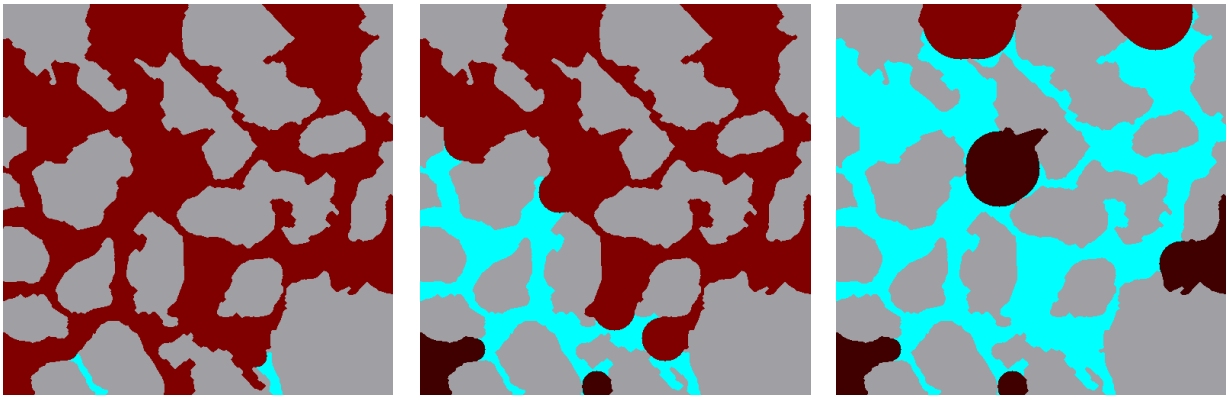
A **Drainage** displacement occurs where a **non-wetting** invading fluid enters the porous media and displaces a **wetting** fluid, which was saturating it.



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

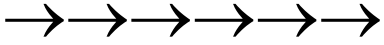
Drainage process

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,

$$r = \frac{2\sigma}{p_c} cos\,\alpha$$

The contact angle α can be different at each solid phase inside the porous medium [3] 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.

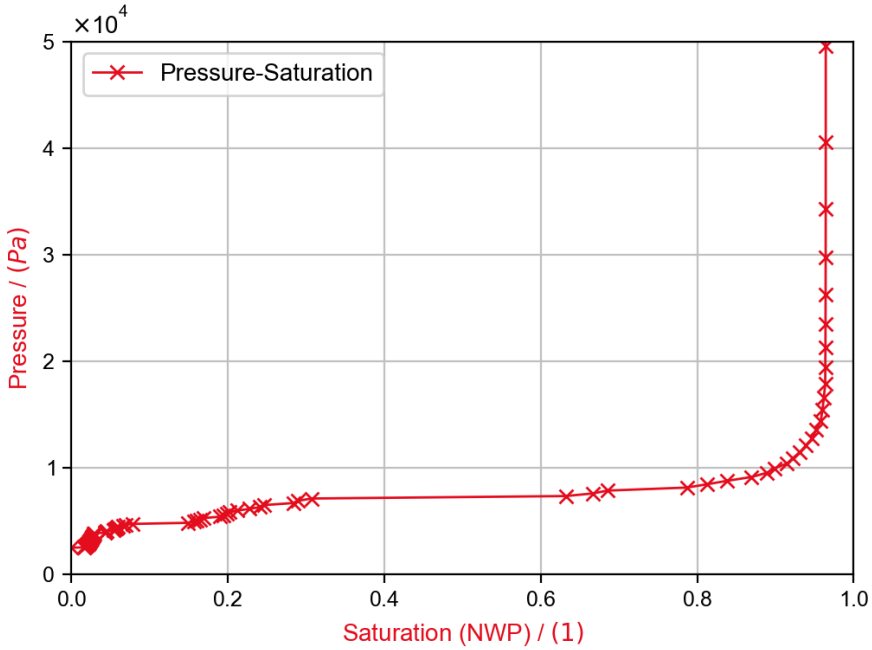
In the following, an example of the resulting capillary pressure curve of a drainage simulation with all three methods is shown below.

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 25% and 75%. In the example shown above, no saturation point is computed between a saturation of 40% and 60%.

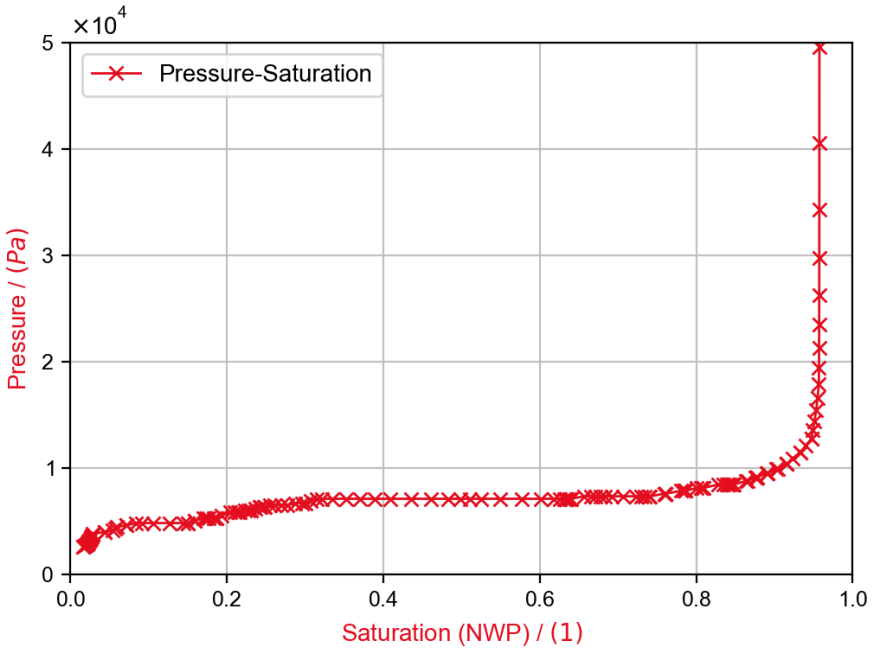


This method is useful for the prediction at which capillary pressure the breakthrough occurs and provides detailed information about fluid distributions for high and low saturated structures. If the detailed fluid distribution at a broad range of saturations is of interest, this method should not be 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 40% and 60% 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.

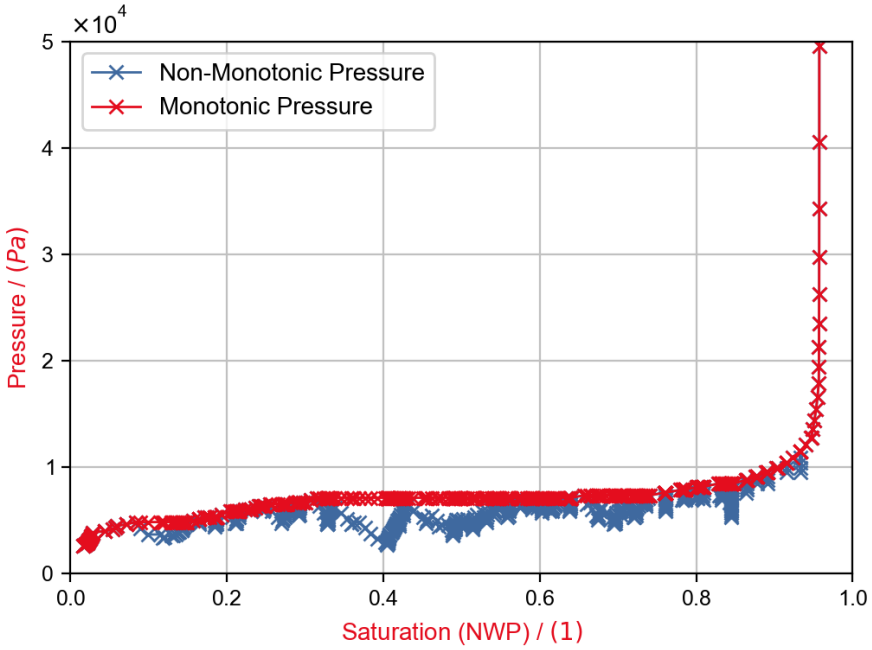
However, certain physical phenomena, e.g., formation of water droplets above a fiber structure with large pore space at the top, cannot be modelled with this method. This requires that the capillary pressure can have a non-monotonic behavior.

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 increasing. At each simulation step, the capillary pressure may be decreased of it stays the same if possible, otherwise the pressure is increased.

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 above 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

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 or Electrical Conductivity).

Regarding the permeability, the values computed with SatuDict 2022 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 in page 47.

The absolute permeability is given as the permeability of the completely saturated medium (K_1, $s = 1$), 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_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.

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

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 P_c and, in this way, determine the saturation s. The capillary pressure curve, $P_c(s)$, 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 FlowDict 2022 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.

To calculate the relative permeability, the module FlowDict is necessary. Without a licensed FlowDict module, 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 2022 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.

  To calculate the relative gas diffusivity the module DiffuDict is necessary. Without a licensed DiffuDict module, 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 2022 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.

  To calculate the relative thermal conductivity and the resistivity index, the module ConductoDict is necessary. Without a licensed ConductoDict module, these options are 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.

References

[1] M. Hilpert, and C. Miller: Pore-morphology-based simulation of drainage in totally wetting porous media. *Adv. Water Resources*, **24** (2001), pp. 243 – 255.

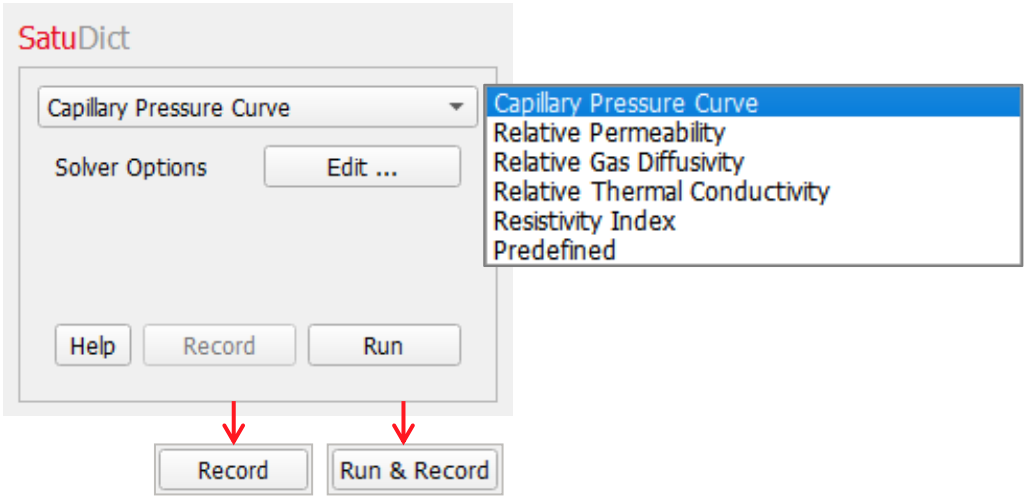
[2] J. Becker, V.P.Schulz, A. Wiegmann: Numerical determination of two-phase material parameters of a gas diffusion layer using tomography images. J. Fuel Cell Sci. Tech. 5 (2008).

[3] V.P. Schulz, E. A. Wargo, and E. Kumbur: Pore-Morphology-Based Simulation of Drainage in Porous Media Featuring a Locally Variable Contact Angle. *Transport in Porous Media*, **107** (2015), pp. 13 – 25.

[4] A. Pfrang, D. Veyret, F. Sieker and G. Tsotridis. X-ray computed tomography of gas diffusion layers of PEM fuel cells: Calculation of thermal conductivity. International Journal of Hydrogen Energy, 35, No. 8, pp 3751 – 3757 (2010).

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 **Predefined**.



The **Wetting Parameters** or **Options** for the SatuDict computations can be modified through the Solver Options' **Edit...** buttons.

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 **Wetting Parameters** or **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.

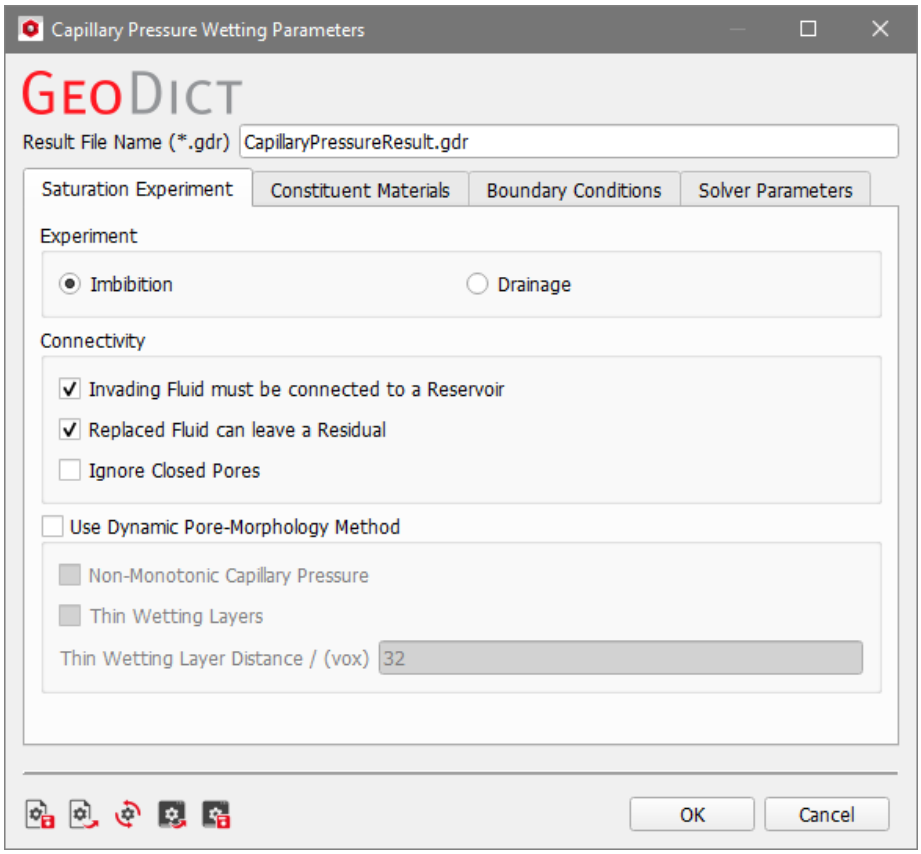
The wetting parameters are grouped under four tabs: **Saturation Experiment**, **Constituent Materials**, **Boundary Conditions**, and **Solver Parameters**.

Saturation Experiment

Under the **Saturation Experiment** tab, the parameters **Experiment** and **Connectivity** are included. Additionally, it can be selected to use the **Dynamic Pore-Morphology Method** and parameters for it can be set.

Experiment

During two-phase flow in a porous media, one fluid is displaced by another fluid. **Imbibition** occurs when a wetting fluid displaces a non-wetting fluid. **Drainage** occurs when a non-wetting fluid displaces a wetting fluid. The two processes are governed by different mechanisms and should not be confused.



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.

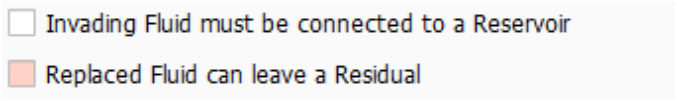
Check **Invading Fluid must be connected to a Reservoir** to connect the invading phase continuously to a phase reservoir at a given spatial location (defined on the **Boundary Conditions** tab, see page 15).

Check **Replaced Fluid can leave a Residual** if the replaced phase will leave a residual if not connected to a reservoir.

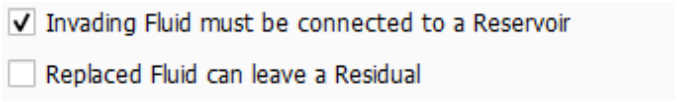
Check **Ignore Closed Pores** to fill only the open pores with the invading phase. Open pores are connected to the inflow and outflow region. All pores not connected to the domain boundary (closed pores) are pores without fluid at the beginning of the simulation. These closed pores are ignored and considered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

For **Imbibition**:

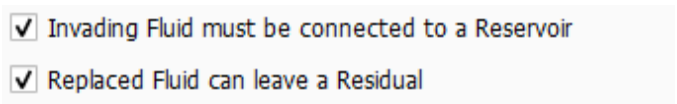
- Uncheck **Invading Fluid must be connected to a Reservoir** to model the sudden appearance of the wetting phase as condensation on the surface of the material in the structure. The wetting phase spreads out and, thus, the non-wetting phase is displaced from the material surface and disappears from the structure. This corresponds to **Imbibition I** in previous GeoDict versions. **Replaced Fluid can leave a Residual** cannot be checked in this case.



- Check **Invading Fluid must be connected to a Reservoir** and uncheck **Replaced Fluid can leave a Residual** to model an imbibition process considering the displacing wetting phase continuously connected to a wetting phase reservoir at a given spatial location. The replaced non-wetting phase will leave no residual (**Imbibition II** in previous GeoDict versions).



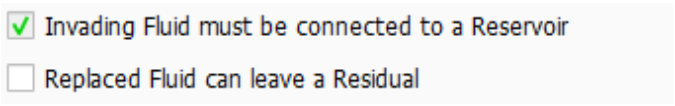
- Check **Invading Fluid must be connected to a Reservoir** and check **Replaced Fluid can leave a Residual** to model an imbibition process considering the displacing wetting phase continuously connected to a wetting phase reservoir and a residual non-wetting phase remaining trapped in the porous media during advancing of the wetting phase. This corresponds to **Imbibition III** in previous GeoDict versions.



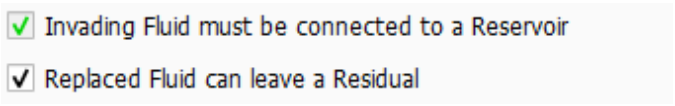
For **Drainage**:

- **Invading Fluid must be connected to a Reservoir** cannot be unchecked for drainage simulations. The invading non-wetting phase is always connected to a reservoir.

- Uncheck **Replaced Fluid can leave a Residual** to model the drainage without residual wetting phase remaining in the porous media. This corresponds to **Drainage I** in previous GeoDict versions.

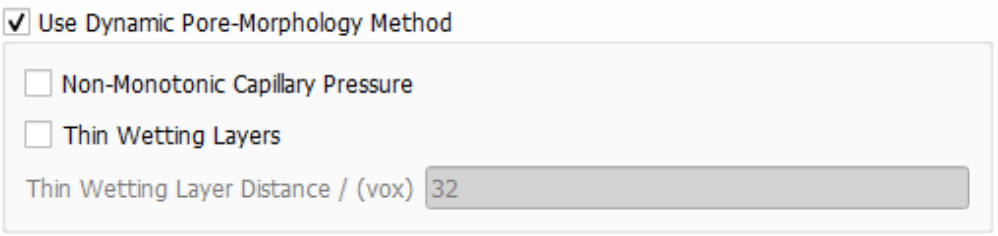


- Check **Replaced Fluid can leave a Residual** to consider a residual wetting phase remaining trapped in the porous media, as the non-wetting phase invades the structure and displaces the wetting phase. This is **Imbibition II** of previous GeoDict versions.



Dynamic Pore-Morphology Method

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

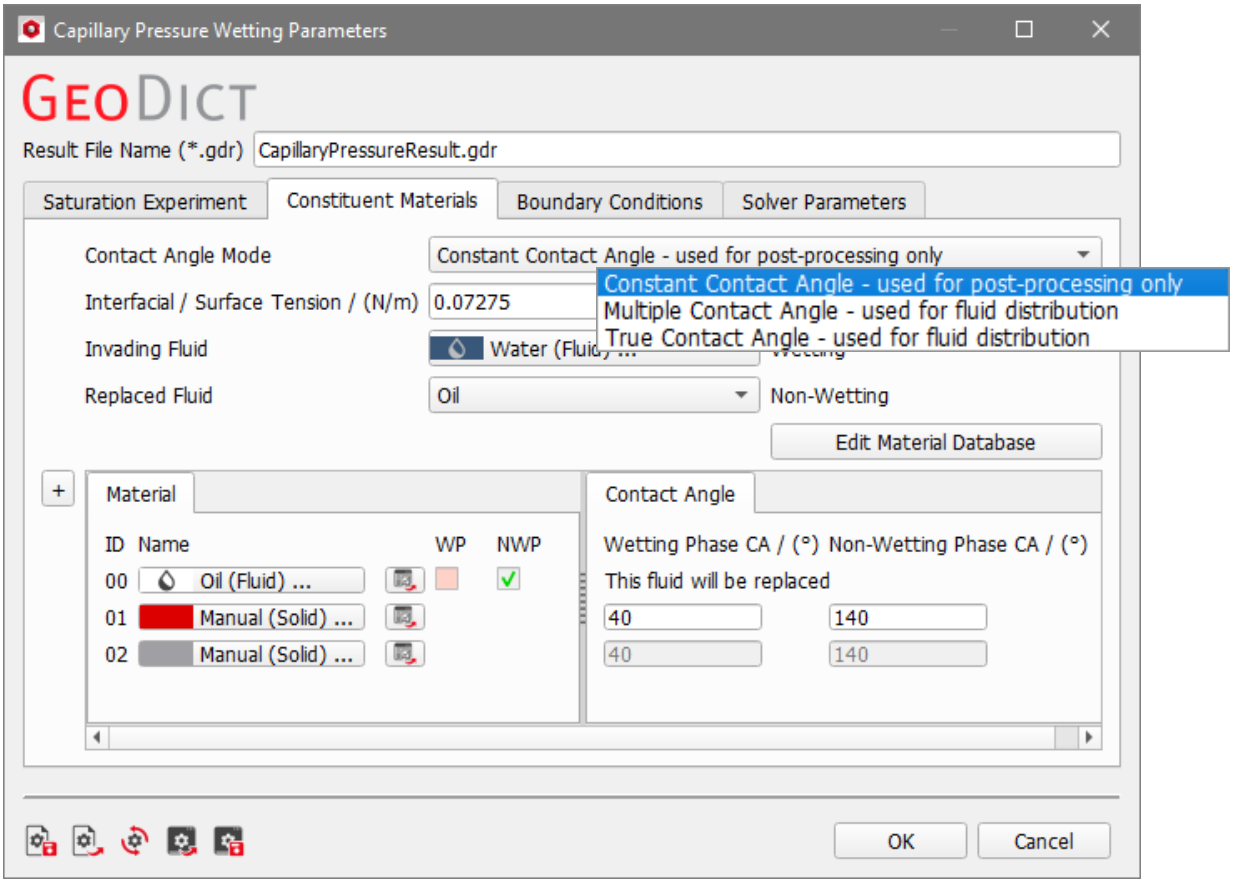


Select **Non-Monotonic Capillary Pressure** to allow that the capillary pressure can drop down during a drainage simulation when the non-wetting phase passes a pore-throat. During an imbibition simulation, the capillary pressure can rise again, when the wetting phase passes a big pore.

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.

Constituent Materials

All material properties of wetting and non-wetting phase can be defined on the **Constituent Material** tab.



Contact Angle Mode

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

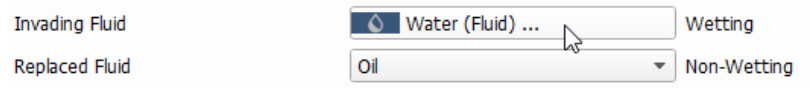
1. **Constant Contact Angle**. In this default setting, for the Pore Morphology method, a single (constant) contact angle is assumed between all solid materials and the wetting phase, and another constant contact angle between all solid materials and the non-wetting phase. The given contact angle is 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 wetting phase and with the non-wetting phase. 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 wetting and the non-wetting phase 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.

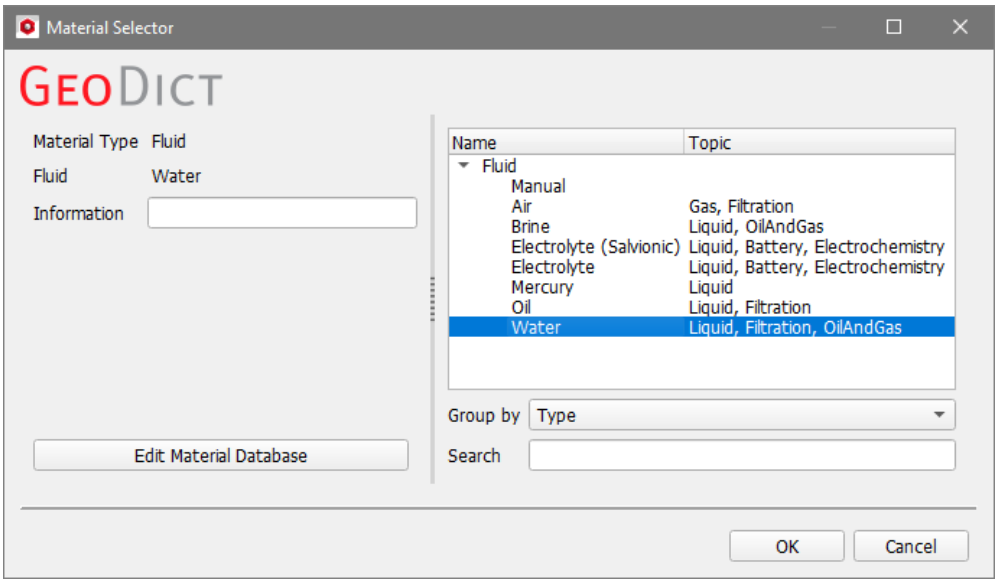
Interfacial / Surface Tension

Enter the **Interfacial/Surface Tension** between the wetting and the non-wetting phase 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.





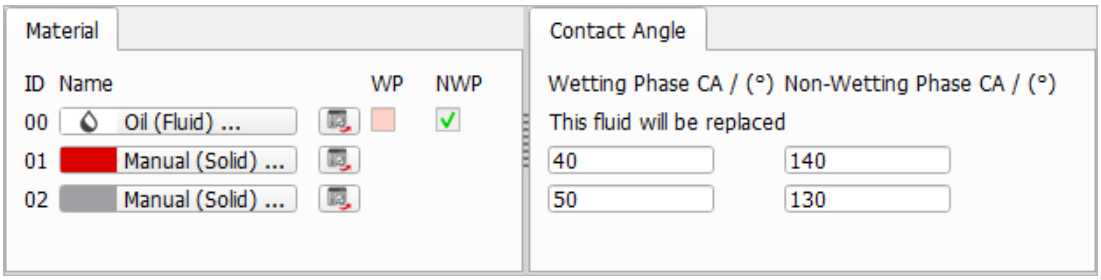
The fluid displaced by the **Invading Fluid** is called **Replaced Fluid** and must be already present in the model of the structure currently in memory. Choose the replaced fluid from the pull-down menu.

The **Wettability** is already assigned to the invading and the replaced fluid, dependent on the Experiment selected on the Saturation Experiment tab, see page 9. For Imbibition, the invading fluid is the wetting phase, and the replaced fluid the non-wetting phase. For Drainage, the invading fluid is the non-wetting phase.

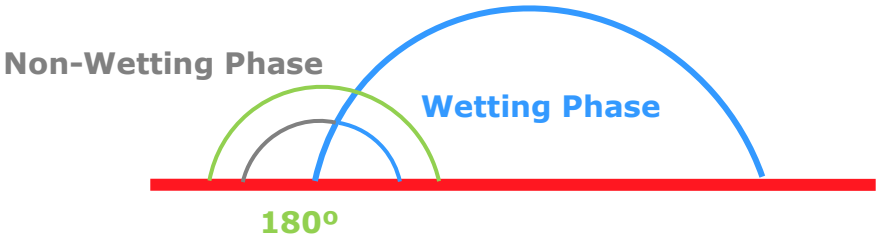
Material and Contact Angle

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**).

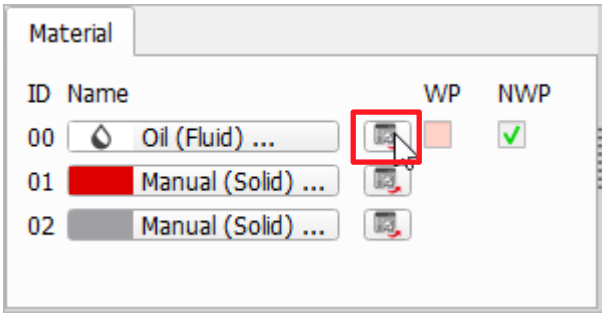
On the **Material** tab, the material of each material ID can be selected, and the wettability for each fluid is shown. The **Contact Angle** tab shows which fluid will be replaced (here, Oil will be replaced).

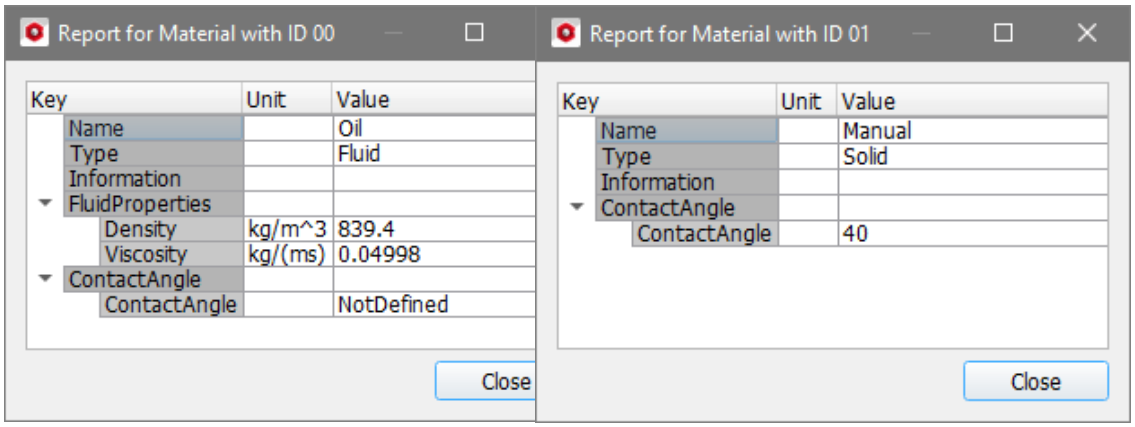


The **Wetting Phase CA** (Contact Angle) and the **Non-Wetting Phase CA** values add up to 180° and they are adjusted automatically when changing one of the two values. The **Wetting Phase CA** must be less than 90°.



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



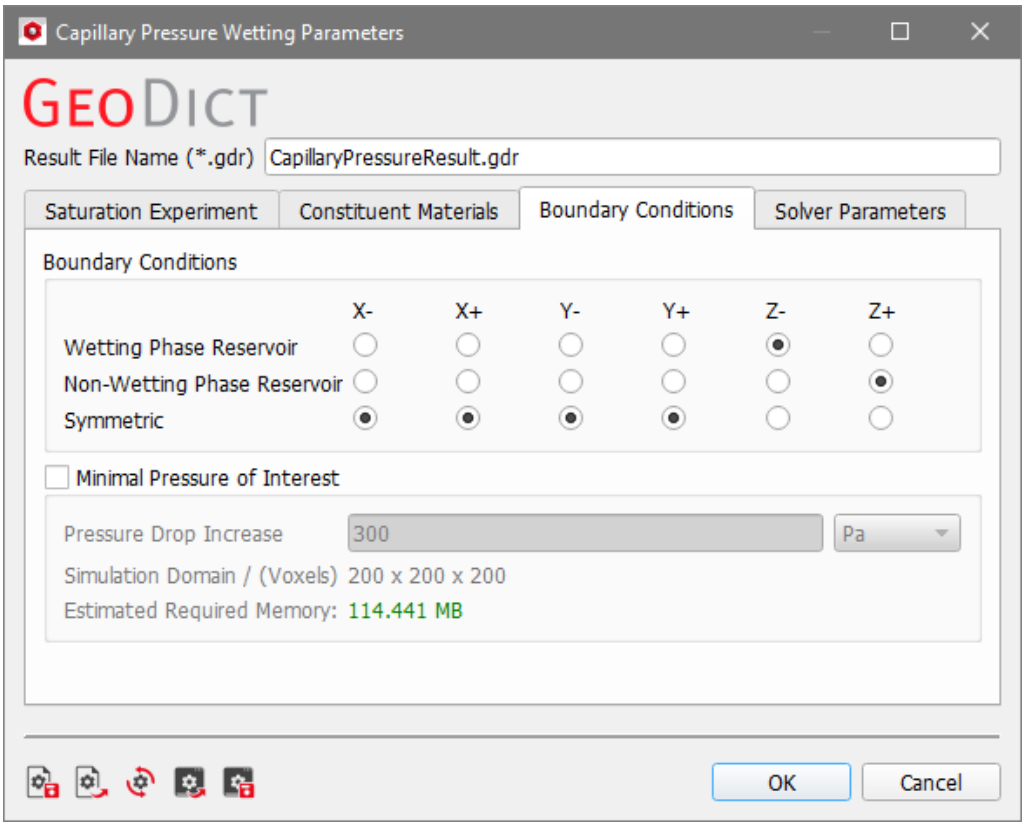


Boundary Conditions

The **Boundary Conditions** define if a side of the sample (X-, X+, Y-, Y+, Z-, and Z+) is connected to a wetting phase reservoir or a non-wetting phase reservoir.

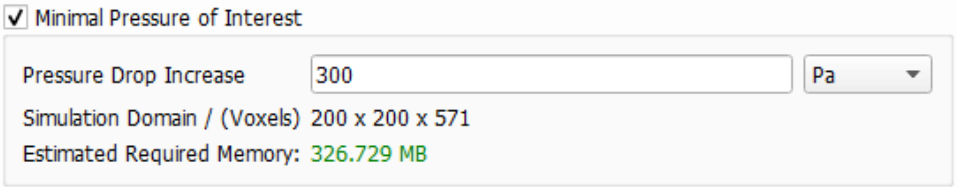
If a side is not connected to a reservoir, e.g. if the porous medium continues in that direction, SatuDict determines pore sizes and checks connectivity using symmetric boundary conditions in these directions, i.e. the pore structure is mirrored at this side.

Boundary conditions can only be entered if the chosen wetting model is not **Equilibrium State** (Imbibition I, i.e. Imbibition with invading fluid not connected to a reservoir).



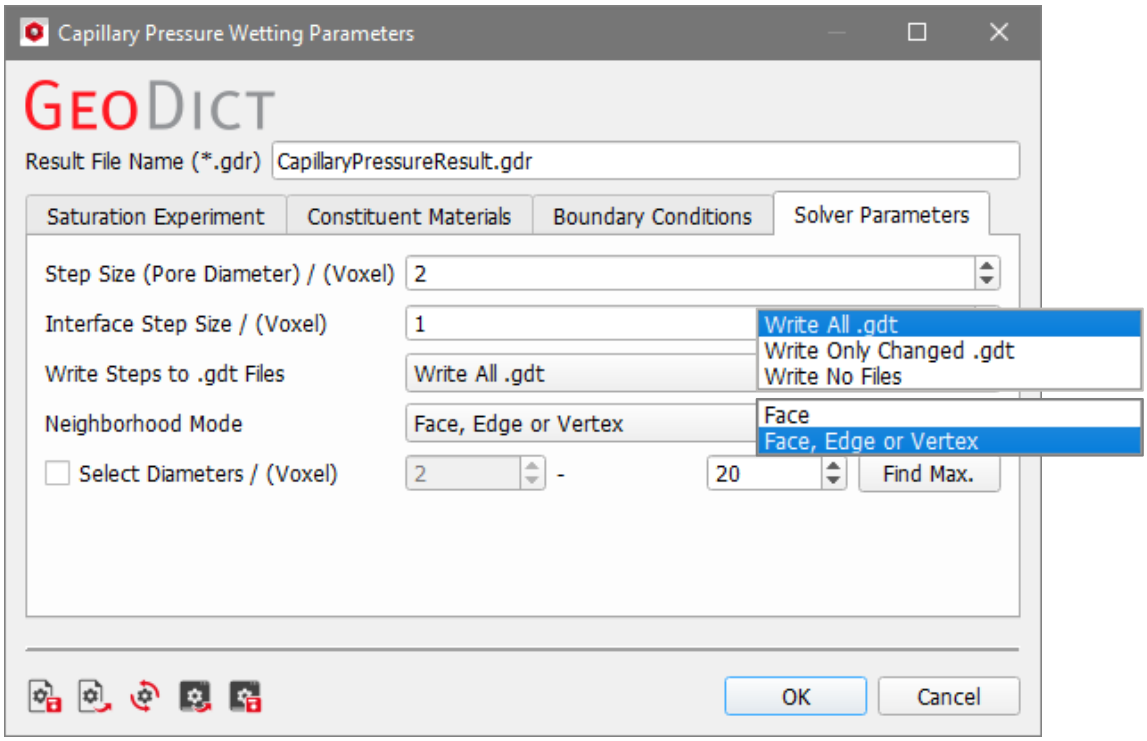
By checking **Minimal Pressure of Interest**, the size of the original simulation domain (voxels) is artificially increased in the direction(s) of the flow (here Z). The effect is to improve the capillary pressure results at least down to the desired value, by increasing the structure size such that 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 it are shown.



Solver Parameters

The **Solver Parameters** are **Step Size**, **Interface Step Size**, **Write Steps to .gdt Files**, **Neighborhood Mode** and **Select Diameters**. These parameters control the number of pressure steps computed, the format of the output files, and the connectivity rule, respectively.



Step Size (Pore Diameter)

The pore size (together with the connectivity rule based on the Neighborhood Mode and the defined contact angles) determines 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 radius (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.

Write Steps to .gdt Files

If **Write All .gdt** is selected, the computed phase distributions are also saved as GDT files that can be imported at any time for visualization. The file names saved as

GDT contain the name of the experiment and the corresponding pore size, defined by the entered **Step Size** (e.g. Imbibition_000000_d00001.00.gdt).

The colors in which the Wetting Phase, the Residual Wetting Phase, the Non-Wetting Phase, and the Residual Non-Wetting Phase are displayed in the visualization 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.

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 GeoDict 2022 Base Reference and the ProcessGeo 2022 (Cleanse command) handbooks of this User Guide.

Select Diameters and Find Max.

The range of pore diameters that should be considered in the calculations is defined by the **Select Diameters** parameter. If the check box is enabled, then the minimum and maximum pore diameter can be entered.

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

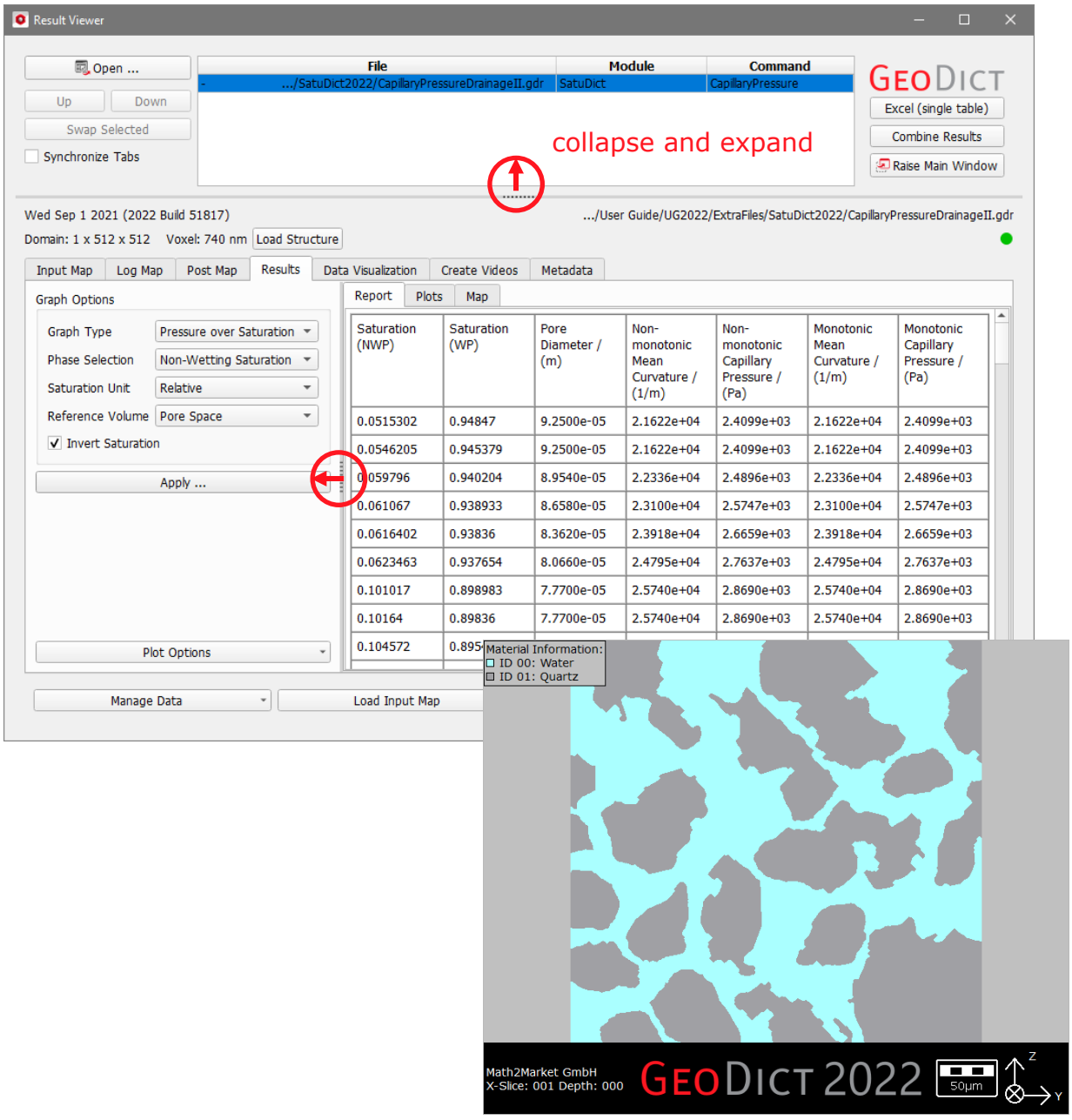
For **Drainage** selected as Experiment, only the minimum diameter can be set. If **Imbibition** is selected as Experiment, only the maximum diameter can be set.

CAPILLARY PRESSURE CURVE RESULT FILE

Here, the case in which a wetting fluid (water) is displaced by a non-wetting fluid (oil) during Drainage (Drainage Process with WP-Residual and NWP-Reservoir) is shown. The calculations of capillary pressure curve are run on a porous structure (54% SVF, originated from Berea sandstone).

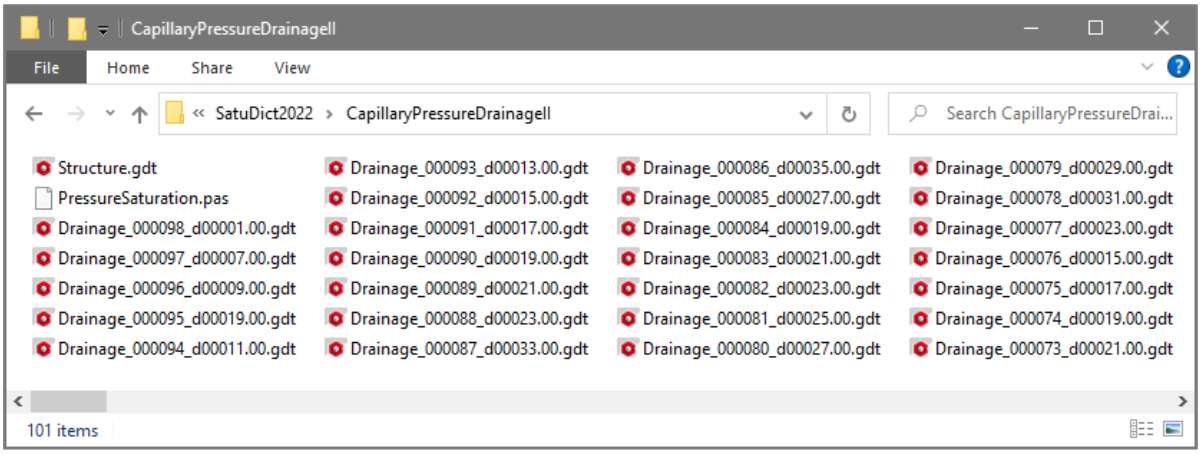
After the solver has finished, the calculation results are immediately displayed in the Result Viewer and saved into a GDR (GeoDict Result) file in the chosen project folder (**File → Choose Project Folder...**). The entered **Result File Name** (here, CapillaryPressureDrainageII.gdr) appears at the top. The GDR file can be opened at any time by selecting **File → Open *.gdr File...**in the menu bar.

The green dot in the right corner of the Result Viewer indicates that it contains the results computed for the structure currently in memory and showing in the **Visualization** area (here in 2D cross-section view).

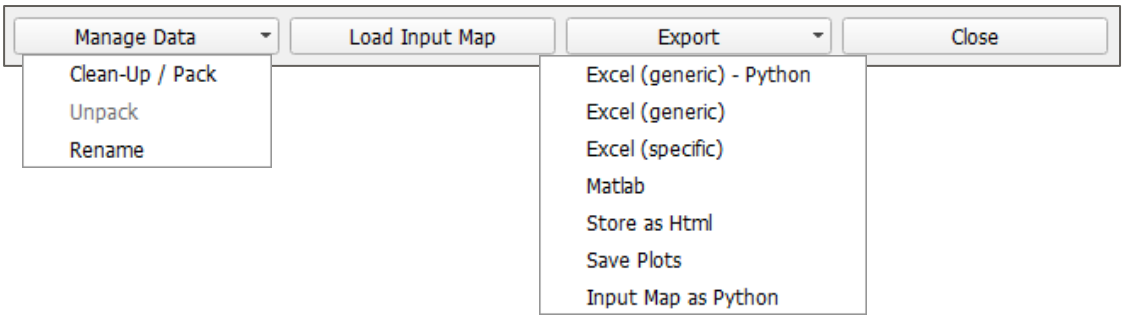


The GDT files corresponding to the computation steps for the chosen wetting model (Drainage_000000_d00125.00.gdt, etc.) are stored in the automatically created

folder **CapillaryPressureDrainageII** in the project folder (if **Write All.gdt** was selected on the Solver Parameters tab, see page 16). This folder also contains the **PressureSaturation.pas** file, necessary for the visualization, and the Structure.gdt file, with the original structure, before the drainage simulation is started.



At the bottom of the result file window, several buttons are available:



- **Manage Data:**
  - **Clean-Up/Pack:** Zip the information contained in the result folder or clean-up the result folder.
  - **Rename:** Change the name of result file and result folder.
- Click **Load Input Map** to re-enter (in the SatuDict GUI) the options and parameters that were used for the calculation results displayed in the result file.
- **Export:** Export the results for postprocessing with another tool
  - **Excel (generic)**: Export the information of the section Result Map of the GeoDict result file to Microsoft Excel®. You can analyze computation results in Microsoft Excel® using GeoDexcel provided with GeoDict. See the GeoDexcel handbook for more information.
  - **Excel (generic) – Python**: Export the information to an .xlsx Excel file in the same way as with **Excel (generic)**, but using a Python script. This export does not need an Excel installation and can therefore also be used on Linux systems.
  - **Excel (specific):** Export the information of the result file to Microsoft Excel® to use the predefined chart and analysis options for SatuDict results. See page 26 and the GeoDexcel handbook for more information.

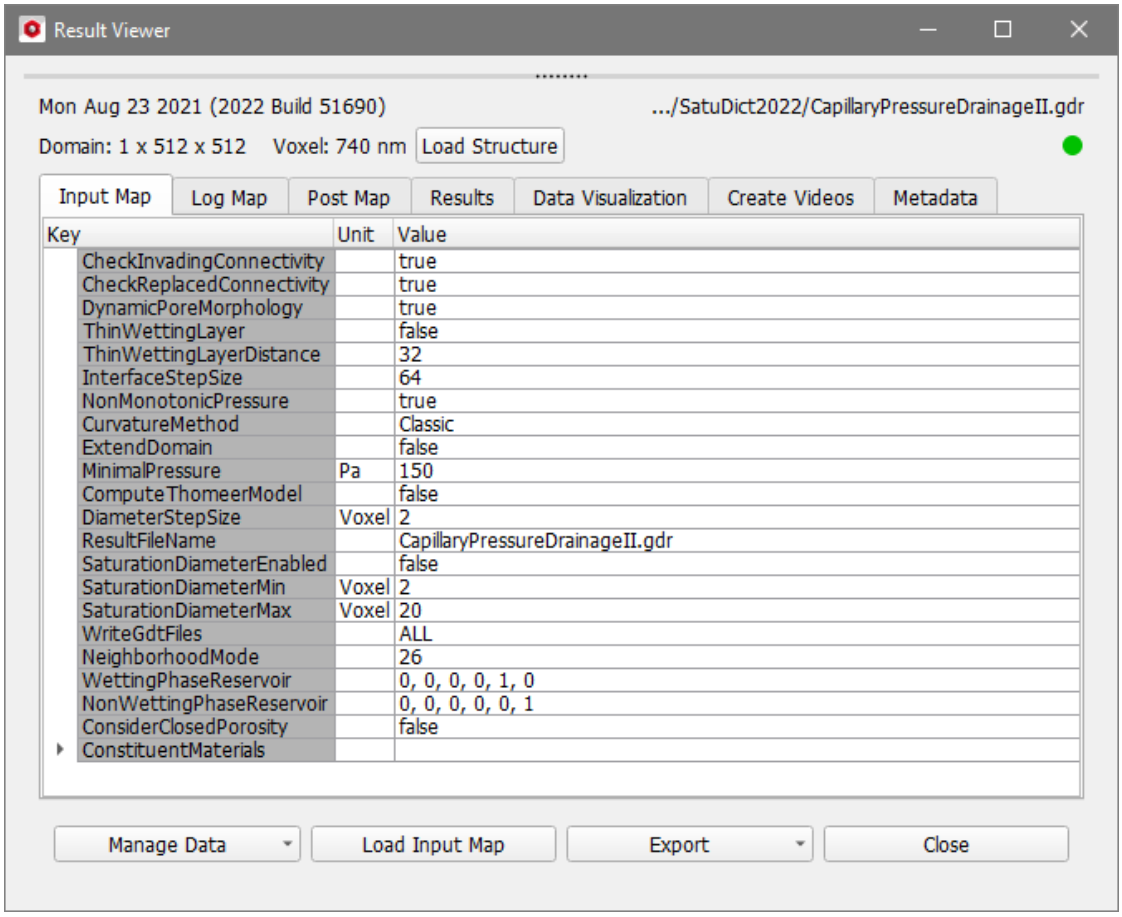
- **Matlab**: Open Matlab® if an installation and license is available, change to the project folder, and load the result file with GeoLab. See the GeoLab handbook for more information.
- **Store As Html**: Export the information shown in the **Results** tab to a html file.
- **Save Plots**: Export all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

■ Close the Result Viewer by clicking **Close**.

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

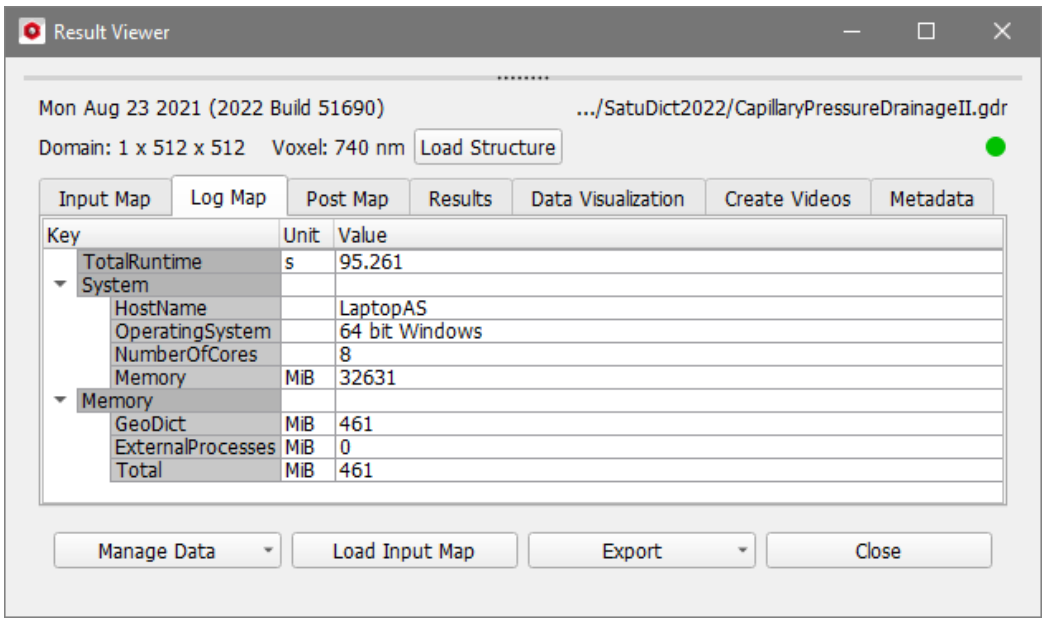
INPUT MAP

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



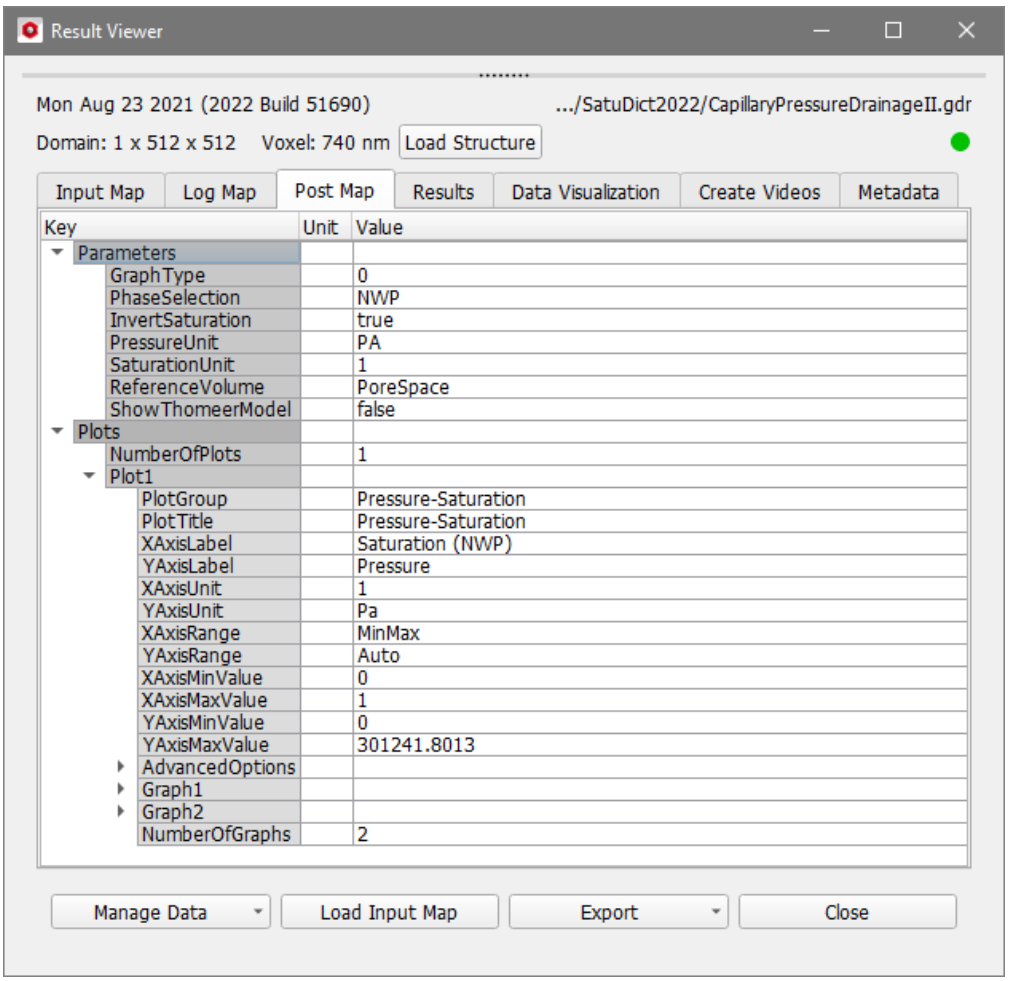
Log Map

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.

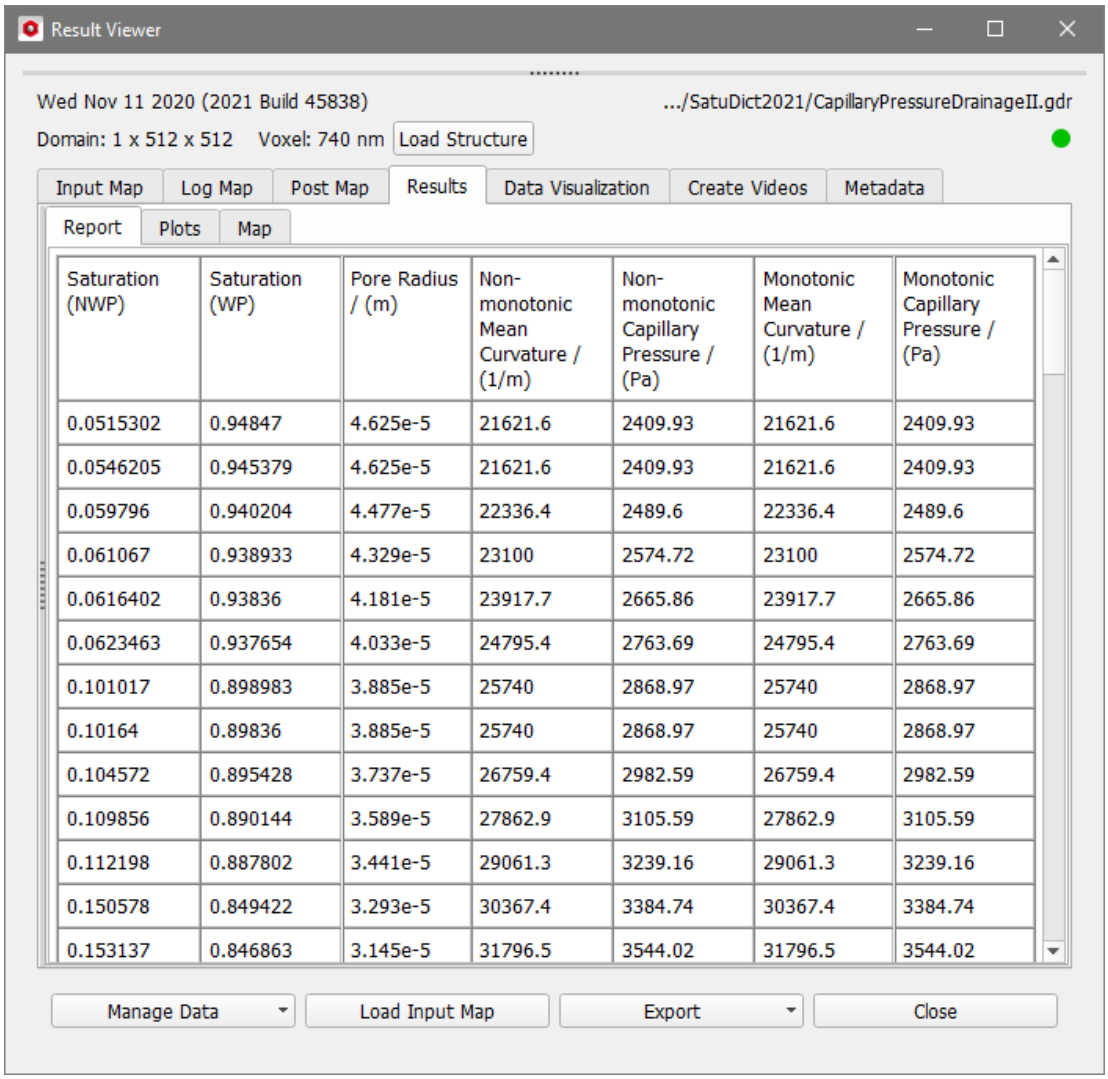


RESULTS

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 non-wetting phase (NWP), the Saturation of the wetting phase (WP), 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 (NWP)	Saturation (WP)	Pore Radius / (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	4.625e-5	21621.6	2409.93	21621.6	2409.93
0.0546205	0.945379	4.625e-5	21621.6	2409.93	21621.6	2409.93
0.059796	0.940204	4.477e-5	22336.4	2489.6	22336.4	2489.6
0.061067	0.938933	4.329e-5	23100	2574.72	23100	2574.72
0.0616402	0.93836	4.181e-5	23917.7	2665.86	23917.7	2665.86
0.0623463	0.937654	4.033e-5	24795.4	2763.69	24795.4	2763.69
0.101017	0.898983	3.885e-5	25740	2868.97	25740	2868.97
0.10164	0.89836	3.885e-5	25740	2868.97	25740	2868.97
0.104572	0.895428	3.737e-5	26759.4	2982.59	26759.4	2982.59
0.109856	0.890144	3.589e-5	27862.9	3105.59	27862.9	3105.59
0.112198	0.887802	3.441e-5	29061.3	3239.16	29061.3	3239.16
0.150578	0.849422	3.293e-5	30367.4	3384.74	30367.4	3384.74
0.153137	0.846863	3.145e-5	31796.5	3544.02	31796.5	3544.02

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 12), 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 wetting phase is high 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 erosion radius can get much higher than the dilation 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 chart showing **Saturation** and **Pressure** values.

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, Saturation over Pressure), **Phase Selection** (Non-Wetting Saturation, Wetting Saturation), **Saturation Unit** (1, %, mL) and Reference Volume (Pore Space, Total Sample Volume).

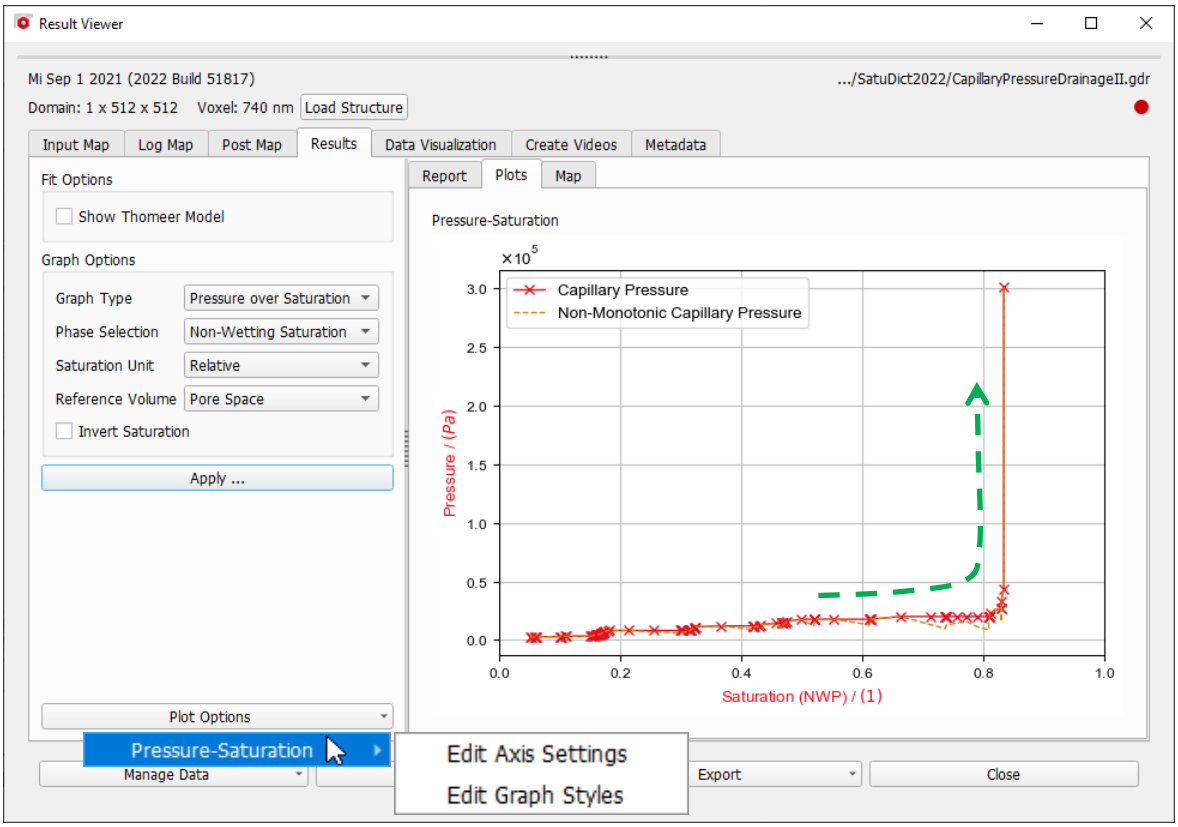
As usual, right clicking on the plot opens a small dialog box with the possibility to modify the axis settings, the graph styles or to save the graph in different ways. With **Edit Axis Settings**, e.g., the scale of the X- and Y-axis can be changed to compare plotted results from different capillary 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.

At the beginning of the drainage process, the porous structure is saturated (100%) by the WP when the initial pressure is low. As the pressure increases, the Oil as NWP starts invading the structure and forces the water as WP out of it.

By the end of the drainage process, the structure is saturated with Oil as NWP (17% Water as residual WP vs. 83% Oil as NWP) and the pressure is at its highest level.

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%.

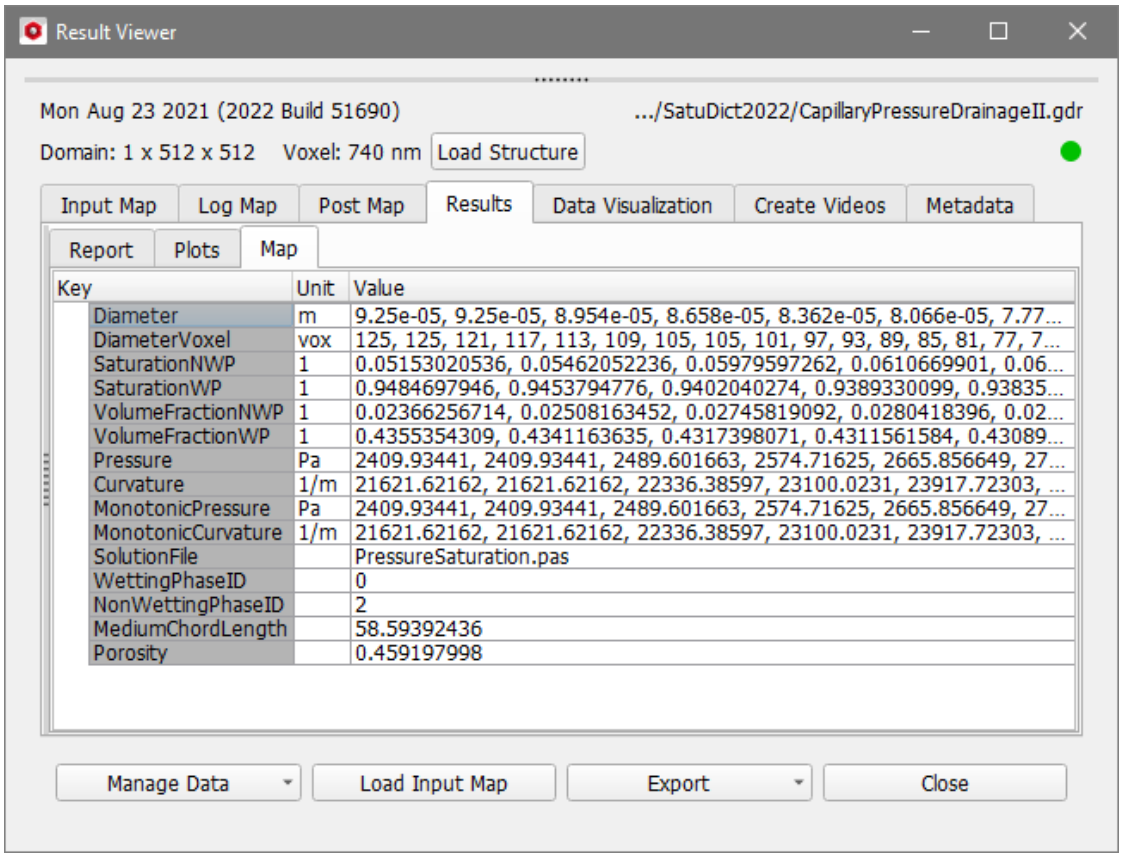


Check **Invert Saturation** in the left panel, to show the values on the X-axis in decreasing instead of increasing order.

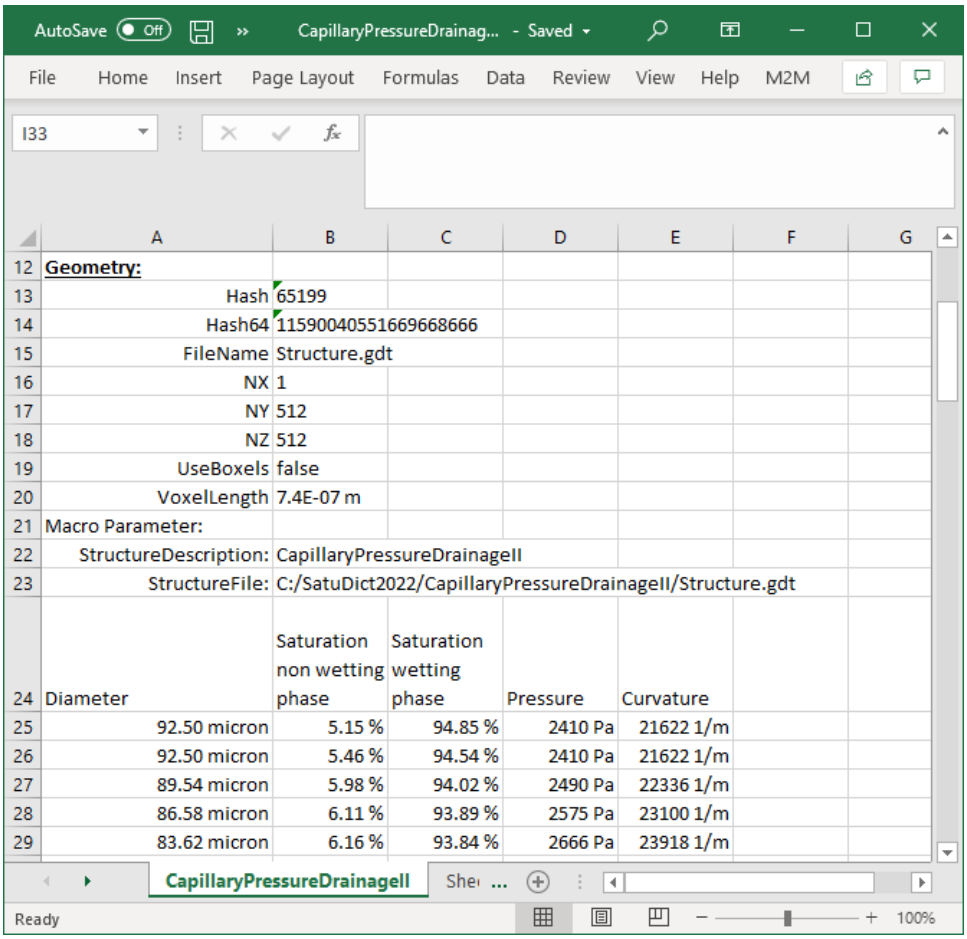
Map

The **Results - Map** subtab gives access to the computed values.

For the capillary pressure curve, it lists the calculated Pressure, Diameter, and Saturation values. The name of the *.pas (pressure and saturation fields) solution file for the visualization of results is also given. The WettingPhaseID (here, 0 is Water) and NonWettingPhaseID (here, 2 is Oil) show the assigned material IDs of the wetting fluid and non-wetting fluid, respectively.


Result Viewer
Mon Aug 23 2021 (2022 Build 51690)
.../SatuDict2022/CapillaryPressureDrainageII.gdr
Domain: 1 x 512 x 512
Voxel: 740 nm
Load Structure
Input Map
Log Map
Post Map
Results
Data Visualization
Create Videos
Metadata
Report
Plots
Map
Key
Unit
Value
Diameter
m
9.25e-05, 9.25e-05, 8.954e-05, 8.658e-05, 8.362e-05, 8.066e-05, 7.77...
DiameterVoxel
vox
125, 125, 121, 117, 113, 109, 105, 105, 101, 97, 93, 89, 85, 81, 77, 7...
SaturationNWP
1
0.05153020536, 0.05462052236, 0.05979597262, 0.0610669901, 0.06...
SaturationWP
1
0.9484697946, 0.9453794776, 0.9402040274, 0.9389330099, 0.93835...
VolumeFractionNWP
1
0.02366256714, 0.02508163452, 0.02745819092, 0.0280418396, 0.02...
VolumeFractionWP
1
0.4355354309, 0.4341163635, 0.4317398071, 0.4311561584, 0.43089...
Pressure
Pa
2409.93441, 2409.93441, 2489.601663, 2574.71625, 2665.856649, 27...
Curvature
1/m
21621.62162, 21621.62162, 22336.38597, 23100.0231, 23917.72303, ...
MonotonicPressure
Pa
2409.93441, 2409.93441, 2489.601663, 2574.71625, 2665.856649, 27...
MonotonicCurvature
1/m
21621.62162, 21621.62162, 22336.38597, 23100.0231, 23917.72303, ...
SolutionFile
PressureSaturation.pas
WettingPhaseID
0
NonWettingPhaseID
2
MediumChordLength
58.59392436
Porosity
0.459197998
Manage Data
Load Input Map
Export
Close

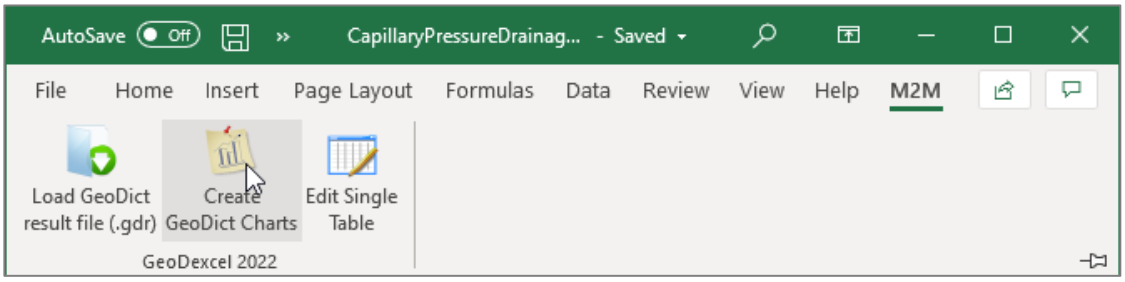
At the bottom of the Result Viewer, click **Export → Excel (specific)** to directly enter the computational results into a customized Microsoft Excel® spreadsheet.



	A	B	C	D	E	F	G
12	**Geometry:**						
13	Hash	65199					
14	Hash64	11590040551669668666					
15	FileName	Structure.gdt					
16	NX	1					
17	NY	512					
18	NZ	512					
19	UseBoxels	false					
20	VoxelLength	7.4E-07 m					
21	Macro Parameter:						
22	StructureDescription:	CapillaryPressureDrainageII					
23	StructureFile:	C:/SatuDict2022/CapillaryPressureDrainageII/Structure.gdt					
24	Diameter	Saturation non wetting phase	Saturation wetting phase	Pressure	Curvature		
25	92.50 micron	5.15 %	94.85 %	2410 Pa	21622 1/m		
26	92.50 micron	5.46 %	94.54 %	2410 Pa	21622 1/m		
27	89.54 micron	5.98 %	94.02 %	2490 Pa	22336 1/m		
28	86.58 micron	6.11 %	93.89 %	2575 Pa	23100 1/m		
29	83.62 micron	6.16 %	93.84 %	2666 Pa	23918 1/m		

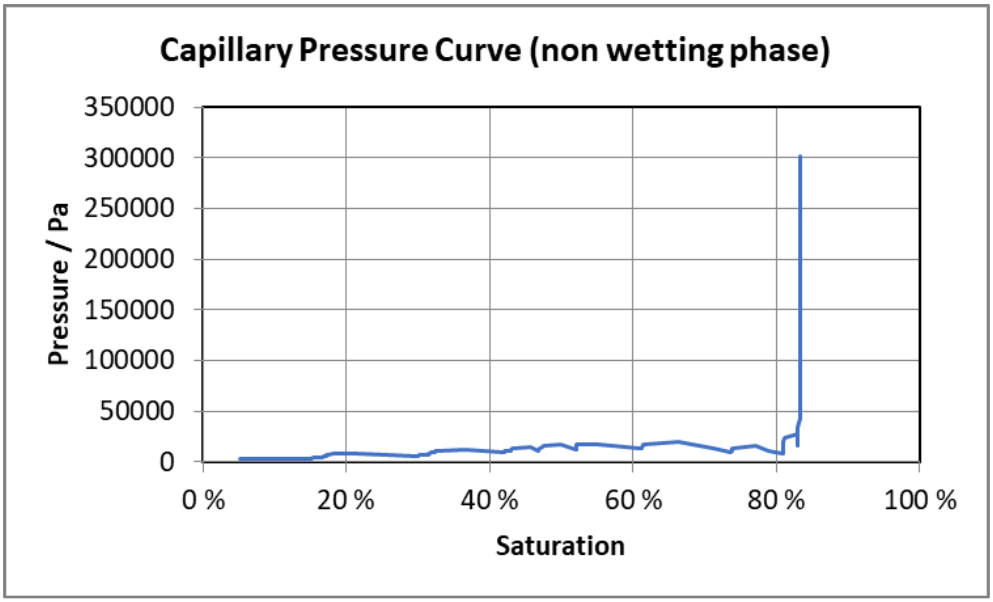
The data are automatically organized as needed to chart the results. The data included under the **Results- Report** subtab in the Result Viewer can be found by scrolling down in the Microsoft Excel® spreadsheet.

Click the **M2M** tab in the menu bar, and then, click **Create GeoDict Charts**.



In the dialog box, select e.g. **Capillary Pressure Curve (non-wetting phase)** from the list and **Active Worksheet** as the origin of the data and click **Create Chart**.

The **Capillary Pressure Curve (non-wetting phase)** data is plotted in a line chart on top of the spreadsheet. This chart corresponds to the plot shown when selecting the Results - Plots subtab of the **CapillaryPressureDrainageII.gdr** file. See page 23.



Charts for the **Capillary Pressure Curve (wetting phase)**, the **Saturation (non-wetting phase)**, or the **Saturation (wetting phase)** are also possible.

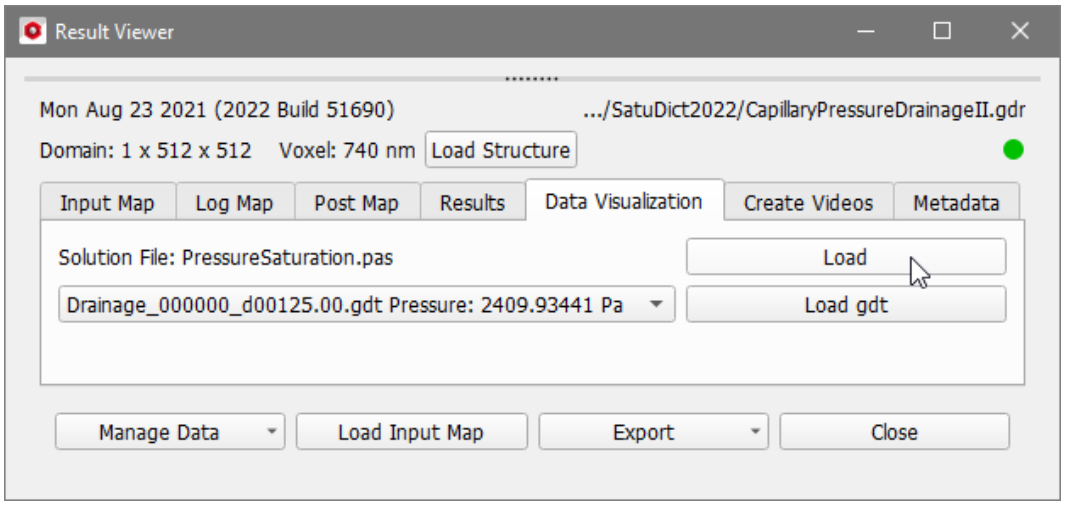
DATA VISUALIZATION

A wide array of visualization options is possible in GeoDict, from which the user can select those that fit for the computations of a particular module.

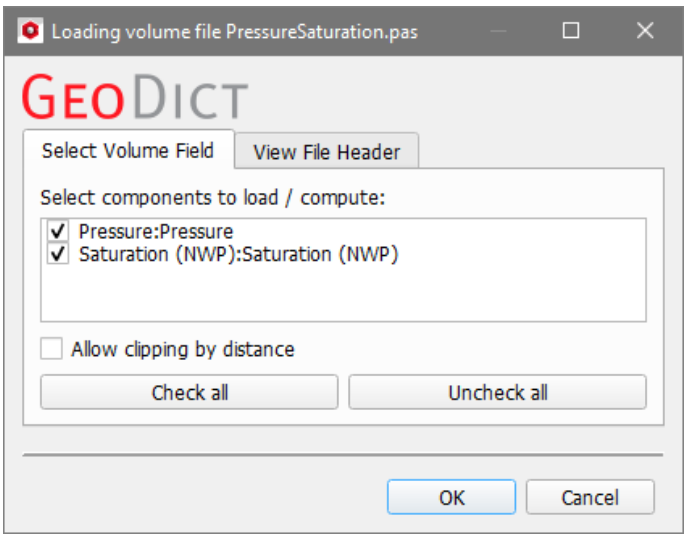
For SatuDict, it makes sense to observe the progress of the drainage (or imbibition) process and the step-by-step images of these processes.

VISUALIZATION OF THE DRAINAGE PROCESS

Under the **Data Visualization** tab, click **Load** to access the pressure and saturation field data saved in the PressureSaturation.pas file. Then, choose the components whose results can be visualized: Pressure and Saturation (NWP).



The values of pressure and saturation of the NWP in the drainage solution file (.pas) are loaded.

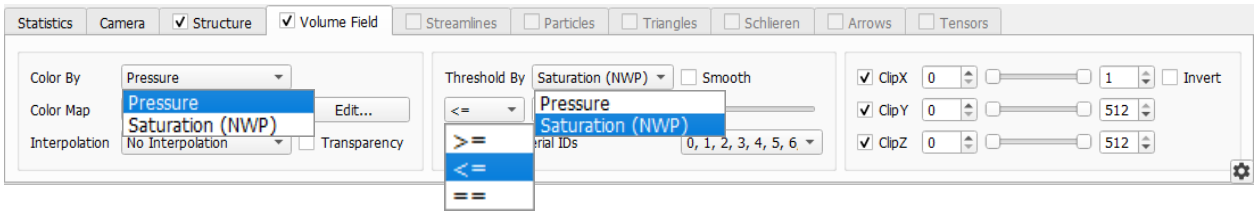


The initial display, in 2D view or 3D rendering, is done using visualization defaults that the user can modify to visualize the imbibition and drainage results obtained with SatuDict. These parameters can be found under the **Volume Field** tab in the **Visualization panel**, above the Visualization 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 (Pressure, Saturation (NWP)) through the **Color By** pull-down menu.

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



With these settings, the visualization is twofold because, for a given NWP 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 drainage process is observed when moving the threshold slider from left to right or entering decreasing values from 0 to 1 in the clip box. This parallels the decreasing saturation of WP (from 100% to 0%) in the porous structure.

  The **beginning** of the drainage process is observed with the slider all the way to the left (Saturation NWP: 0, i.e. 0%, Saturation WP: 1, i.e. 100%). At this point, the pressure is low, and the NWP has not begun displacing the WP.

  By moving the slider to the right or by entering increasing values in the threshold slider box, the drainage process is visualized forward, with the NWP displacing the WP and invading the structure.

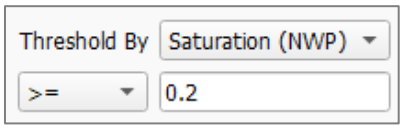
  The drainage process is at the **end** when the clip slider is finally all the way to the right, i.e. the WP has been displaced and the NWP occupies the structure.

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

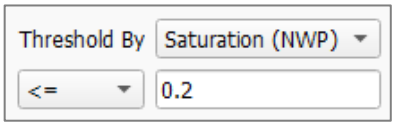
- **Clip Mode**: makes the dual visualization of pressure values and distribution of phases possible because it links them based on the capillary pressure saturation curve (see page 23).

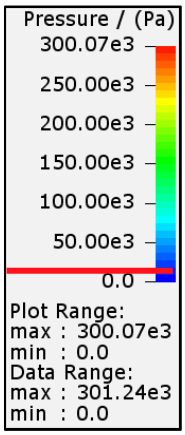
  - By selecting >=, color is shown in the pore space where NWP invades the structure only for a saturation higher than the Saturation (NWP) set in the threshold slider. This shows the locations where the WP is still in the structure at this saturation or below.
  - By selecting <=, color is shown in the pore space where the NWP is already present for a saturation below the value for Saturation (NWP) set in the threshold slider. This shows the locations where the NWP has already invaded the structure and replaced the WP.

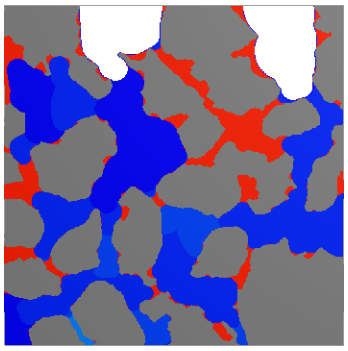
The following are two examples of the effect of setting the **Threshold** slider/box and **Clip Mode** during the visualization of the results in the PressureSaturation.pas file.

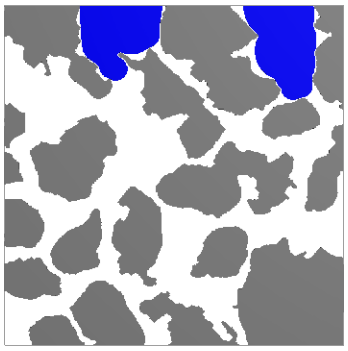


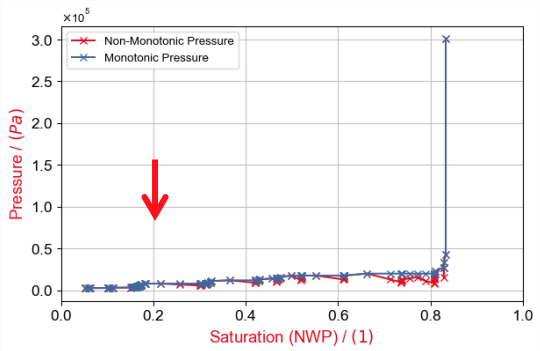
20% NWP

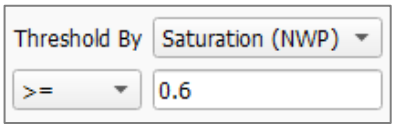




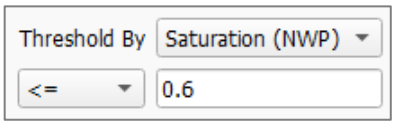


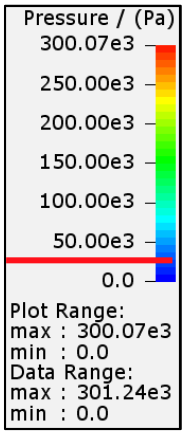


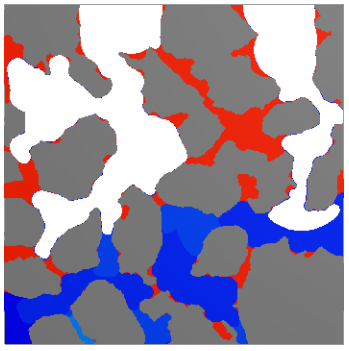


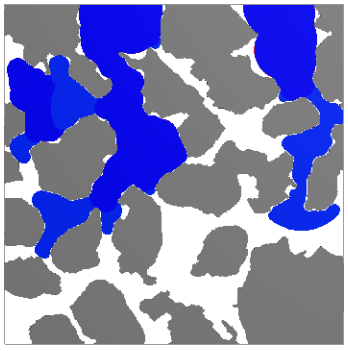


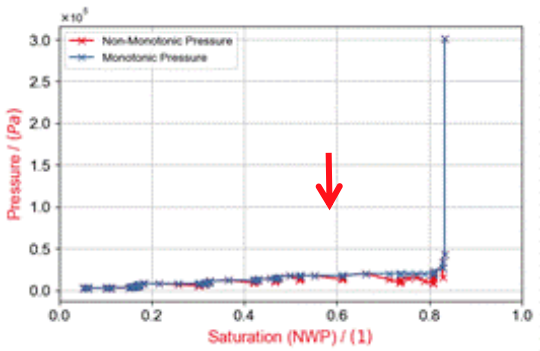
60% NWP











In contrast to the visualization of the drainage process, the imbibition process is visualized backwards after running an imbibition experiment with SatuDict and obtaining a result file. By moving the **Threshold slider** to the left or entering decreasing values in the **Threshold box**, the NWP is being displaced from the structure by the WP.

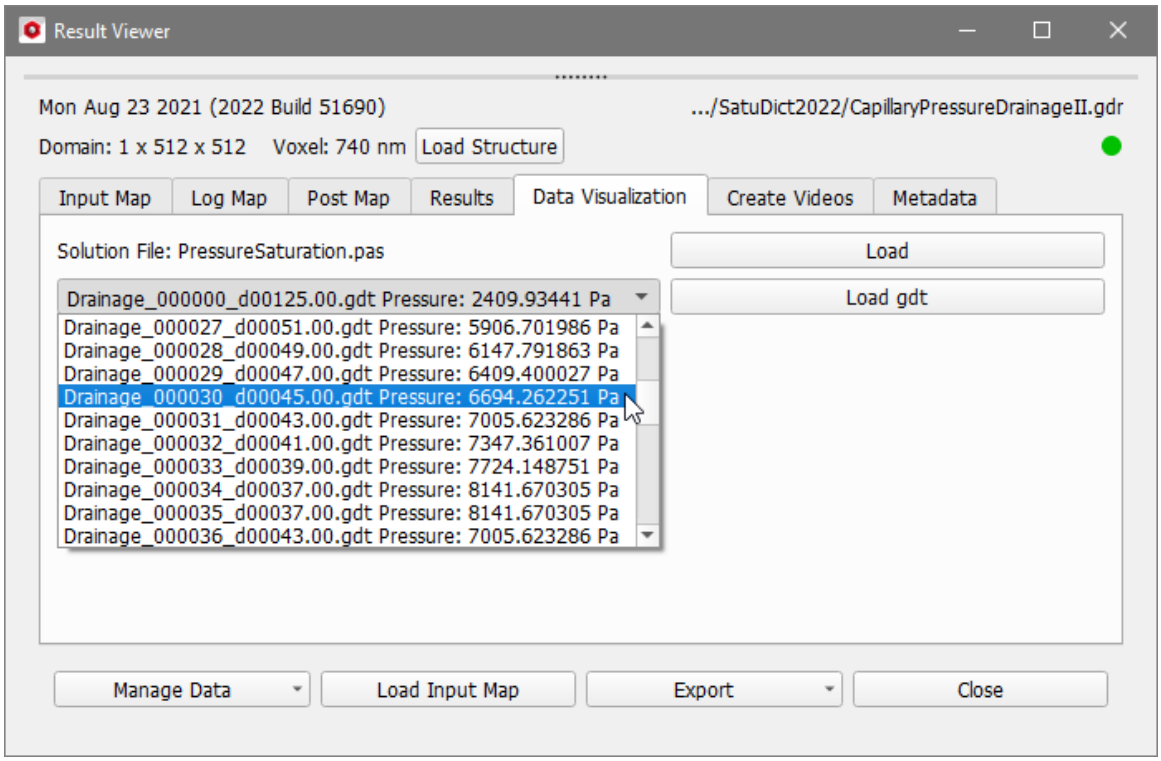
VISUALIZATION OF FREEZE-FRAME SHOTS OF DISPLACEMENT

Finally, use the CapillaryPressureDrainageII.gdr to visualize step-by-step the displacement of NWP by WP in the porous structure during drainage from GDT files saved during the capillary pressure curve calculation.

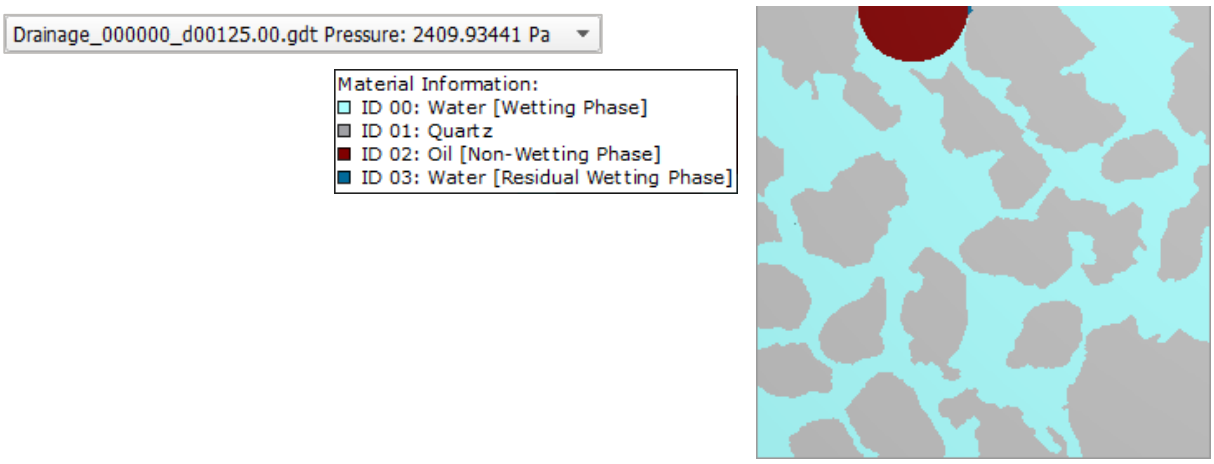
To analyze these images, make sure that the visualization of the Structure is switched on (**View** → **Structure**, in the menu bar).

Select one of the GDT files that are saved for every simulation step. The file names correspond to the inscribed pore diameter and capillary pressures. For example, the file **Drainage_000030_d00045.00.gdt** is the image of the structure at the step corresponding to a pore diameter of 45 voxels (and a capillary pressure of 6694 Pa).

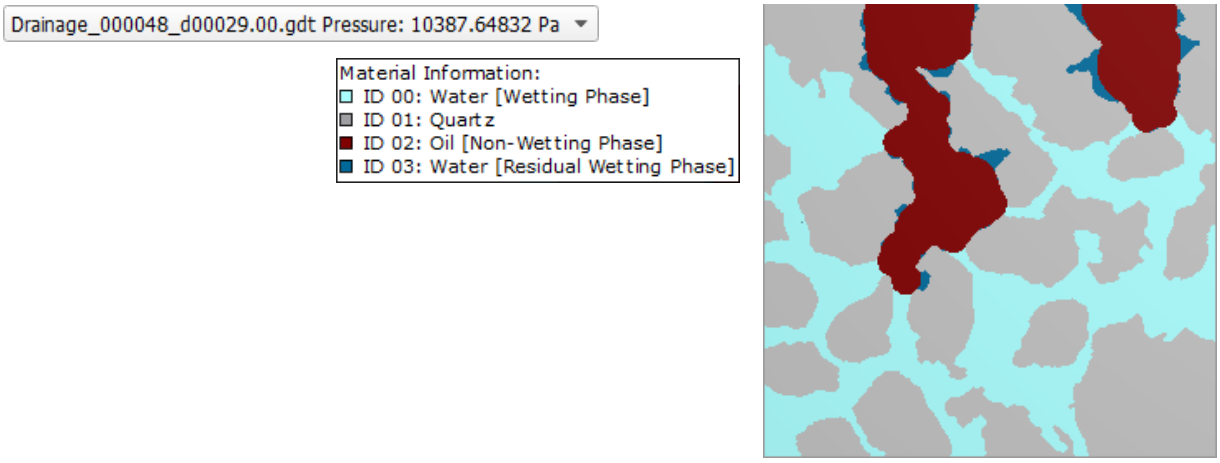
Click **Load gdt** to open the desired file from the **CapillaryPressureDrainageII** folder, inside the project folder. The image from that step is displayed.



The GDT file for largest pore size (here: Drainage_000000_d00125.00.gdt, Pressure: 2410 Pa) corresponds to the beginning of the drainage process. The structure appears (almost fully) saturated by WP.



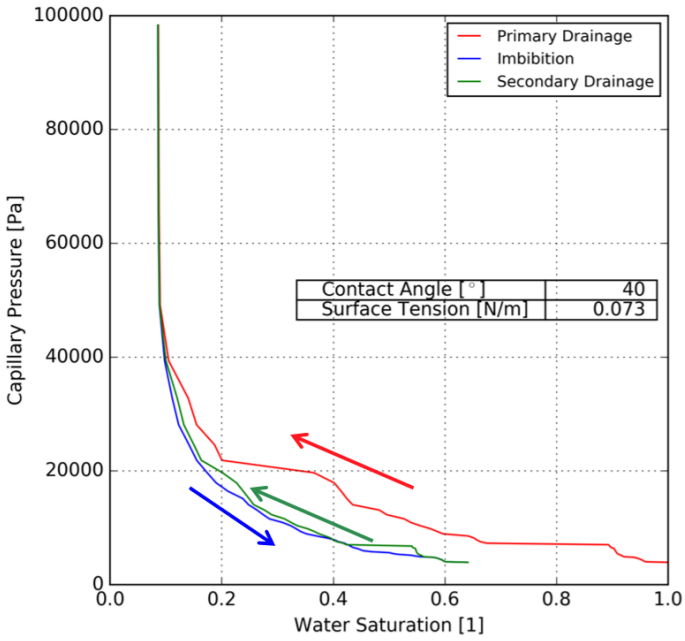
The GDT file for a smaller pore size (here: Drainage_000048_d00029.00.gdt, Pressure: 10388) corresponds to an intermediate part of the drainage process. The structure appears partly saturated by the NWP and the residual WP is visible.



Capillary Pressure with Hysteresis Effect

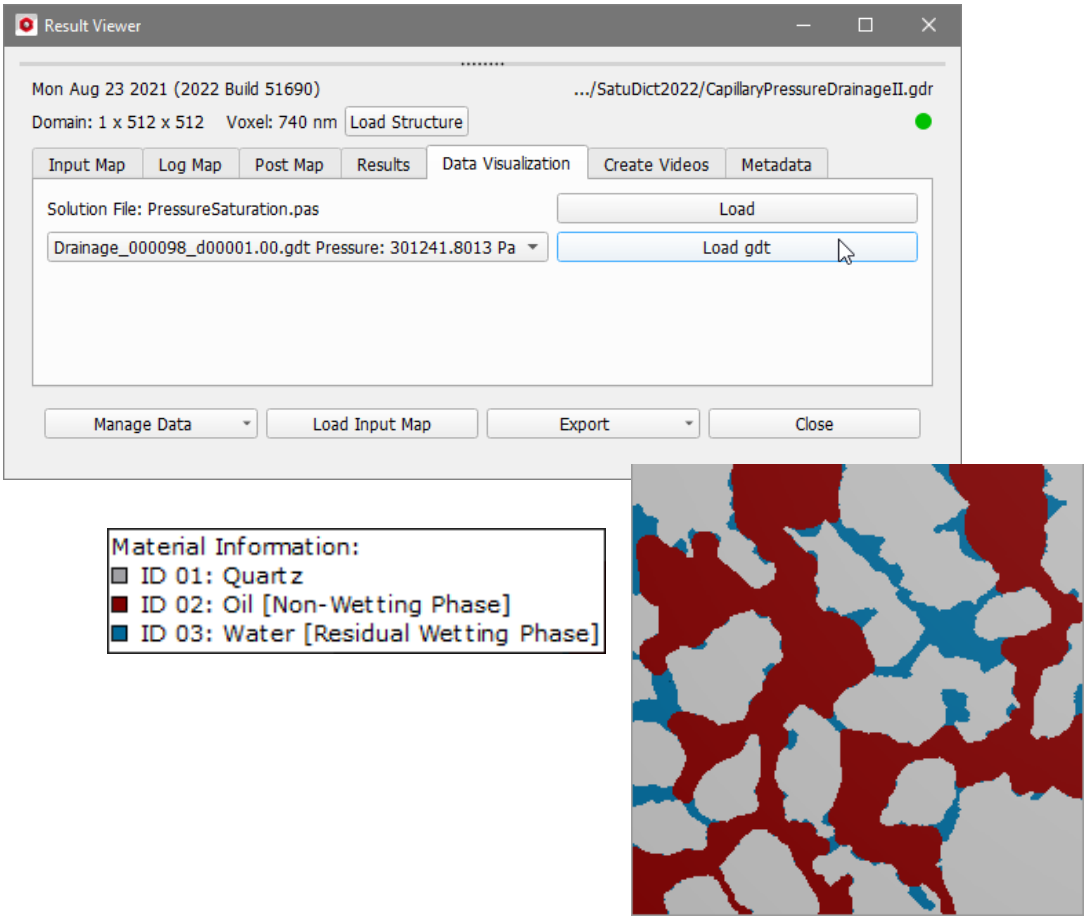
A generalization of the pore morphology method, available since GeoDict 2020, allows considering structures in which the invading fluid is already present in the structure. This allows the simulation of primary and secondary drainage experiments, as well as primary and secondary imbibition experiments.

The image on the right shows a typical graph for primary drainage, imbibition, and secondary drainage.



After the primary drainage simulation shown in pages 18ff. 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 is loaded (Drainage_00098_d00001.00.gdt with 301242 Pa).

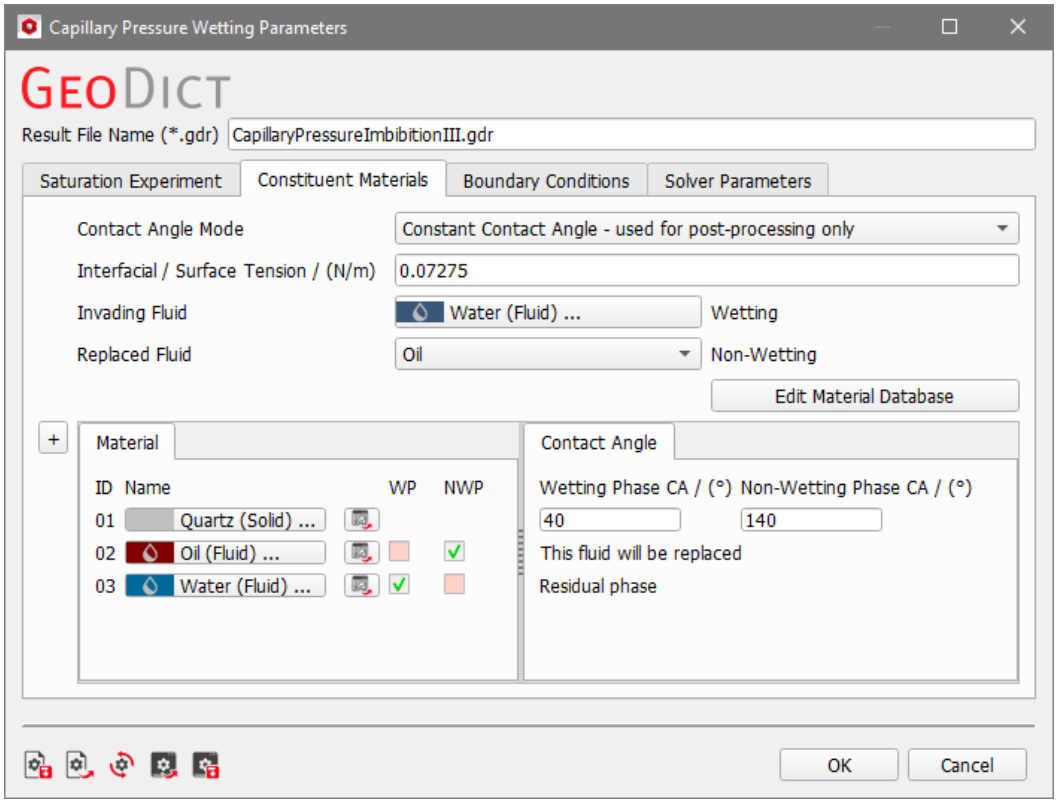


Then, return to the main GeoDict GUI and click the **Solver Options' Edit...** button in the **SatuDict** section to select the wetting parameters for the capillary pressure curve simulation.

Change the name for the result file from **CapillaryPressureDrainageII.gdr** to **CapillaryPressureImbibitionIII.gdr**.

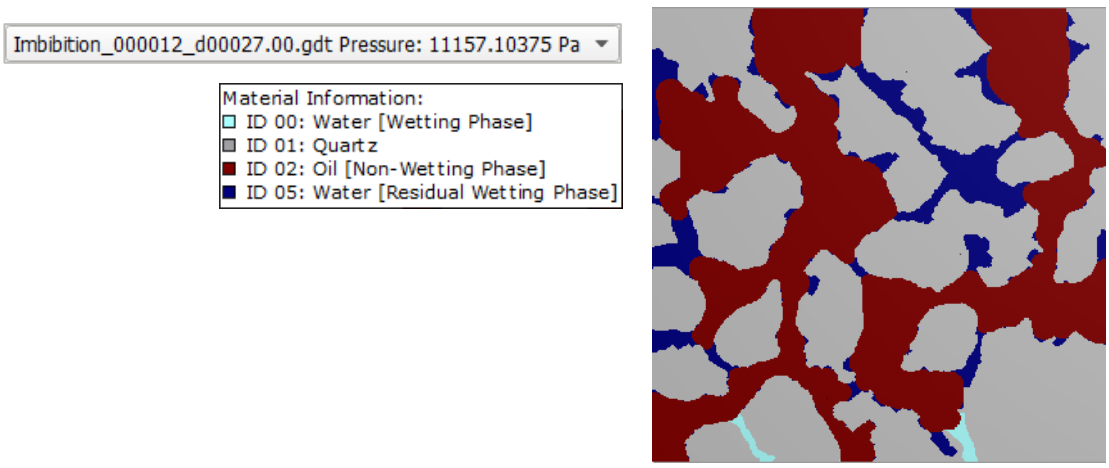
Under the Saturation Experiment tab, set the Experiment to **Imbibition** and check **Invading Fluid must be connected to a reservoir** as well as **Replaced fluid can leave a residual**.

In the Constituent Materials tab, select the **Invading Fluid** to be Water (Water is labelled as Wetting Phase). Automatically, the **Replaced Fluid** is set to be Oil. 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 31ff. 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 (dark blue Residual Wetting Phase) from the earlier drainage simulation.



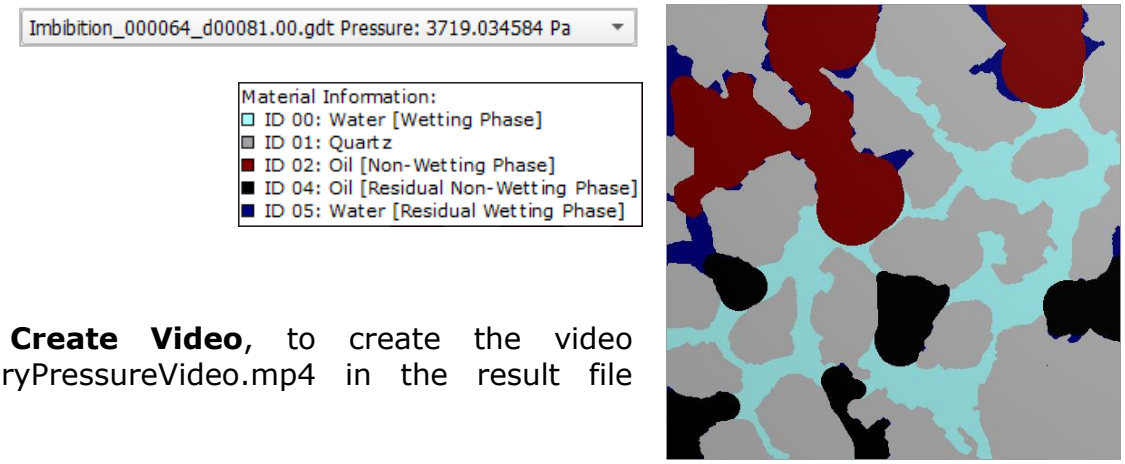
CREATE VIDEOS

On 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:

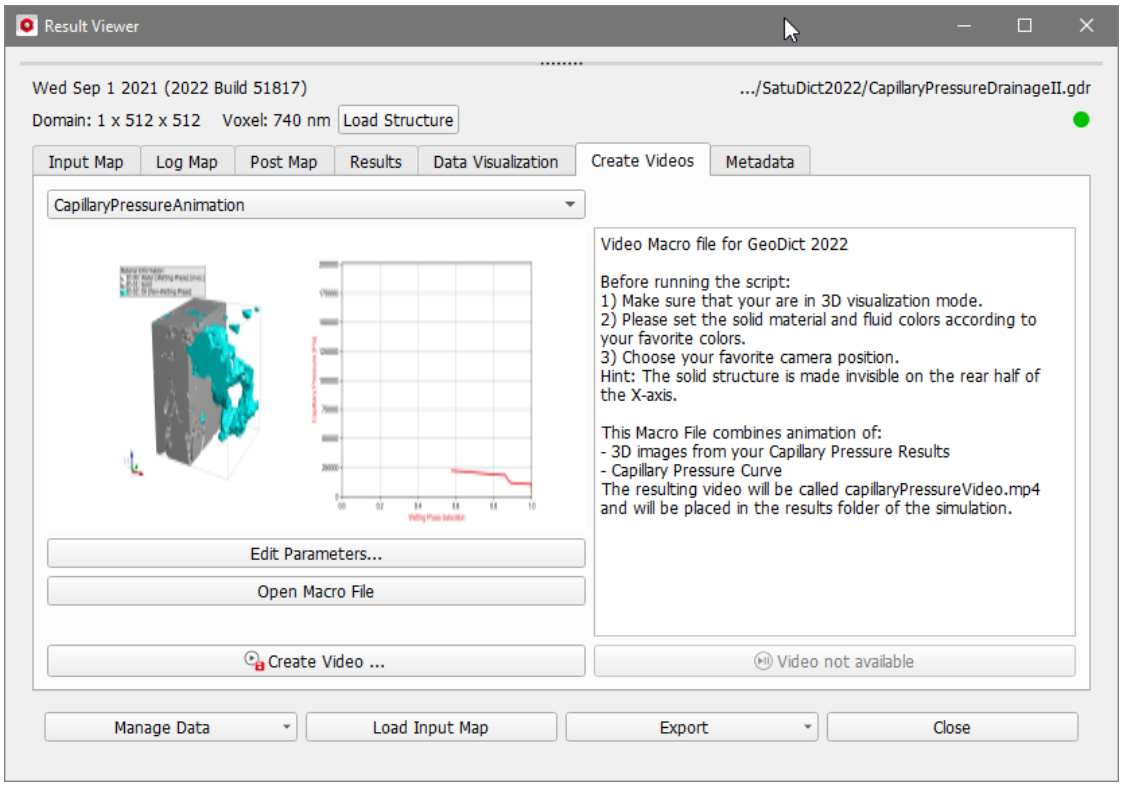
1. Make sure that you are in 3D mode
2. Set the colors of solid and fluid materials to your preferred ones
3. Choose your favorite camera position

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

Select **Open Macro File** to open a text editor with the python file used for the video creation.



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

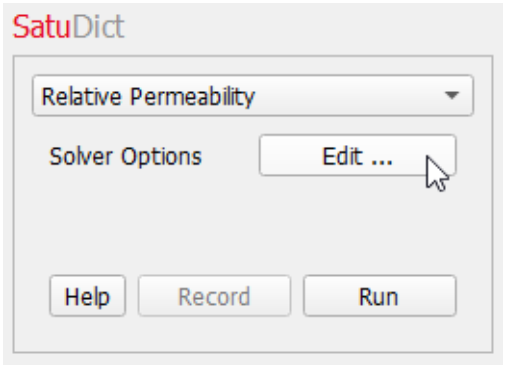


The video shows the capillary pressure curve on the right, and the changing distribution of wetting and non-wetting phase during the saturation simulation on the left. For a better visualization, only part of the structure is shown.

If the video was created successfully, the grayed-out **Video not available** button, is enabled and changes to a **Play Video** button.

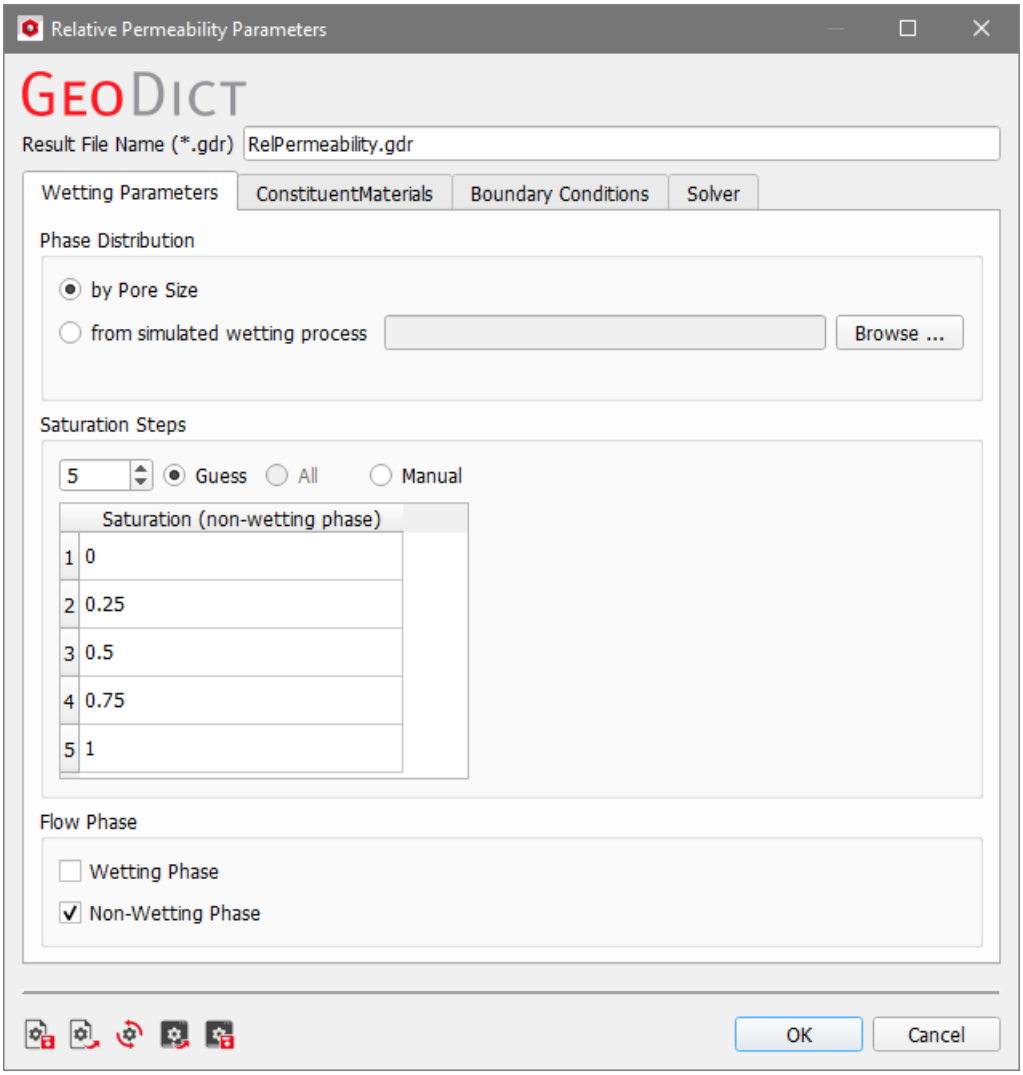
Relative Permeability

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.

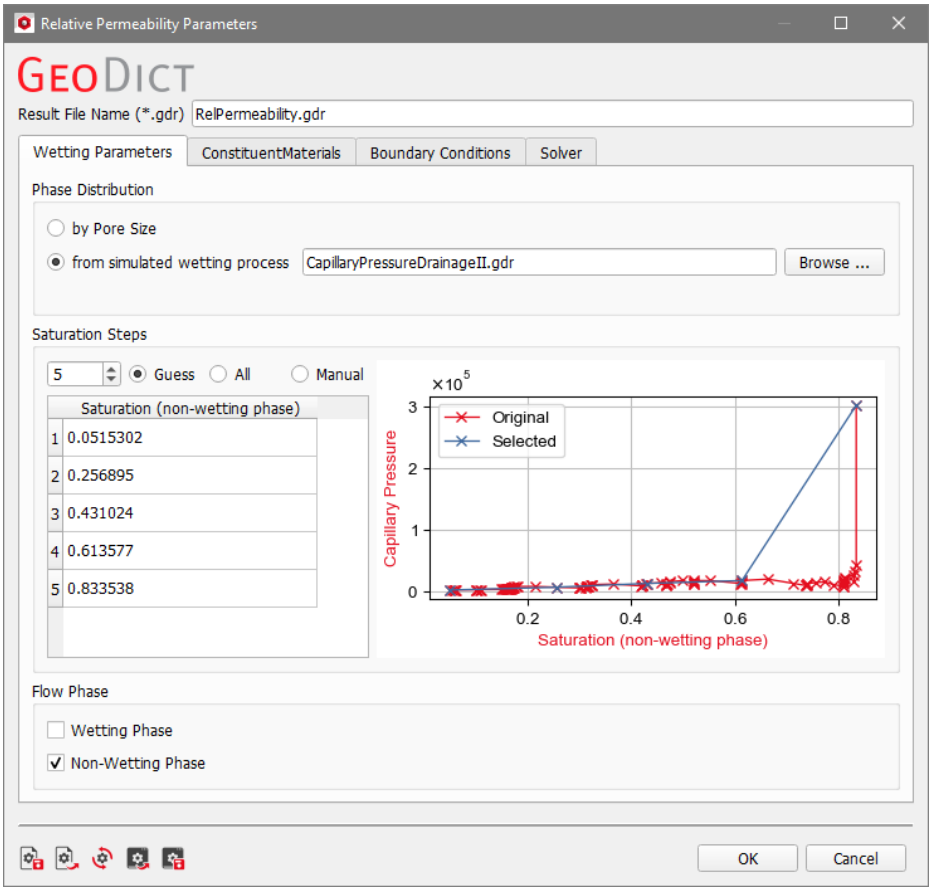


Wetting Parameters

Phase Distribution

The calculation of phase distribution can be based on the pore size alone (**by Pore Size**), corresponding to the Saturation Experiment **Imbibition** with **Invading Fluid must be connected to a Reservoir** unchecked, as applied in the Capillary Pressure Curve calculation (page 10).

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

There are three different modes to select the saturations:

- **Guess**:
  - If the **Phase Distribution** is set to **by Pore Size**, the saturation steps are chosen uniformly based on the number of saturations specified in the box.
  - 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.

- **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.

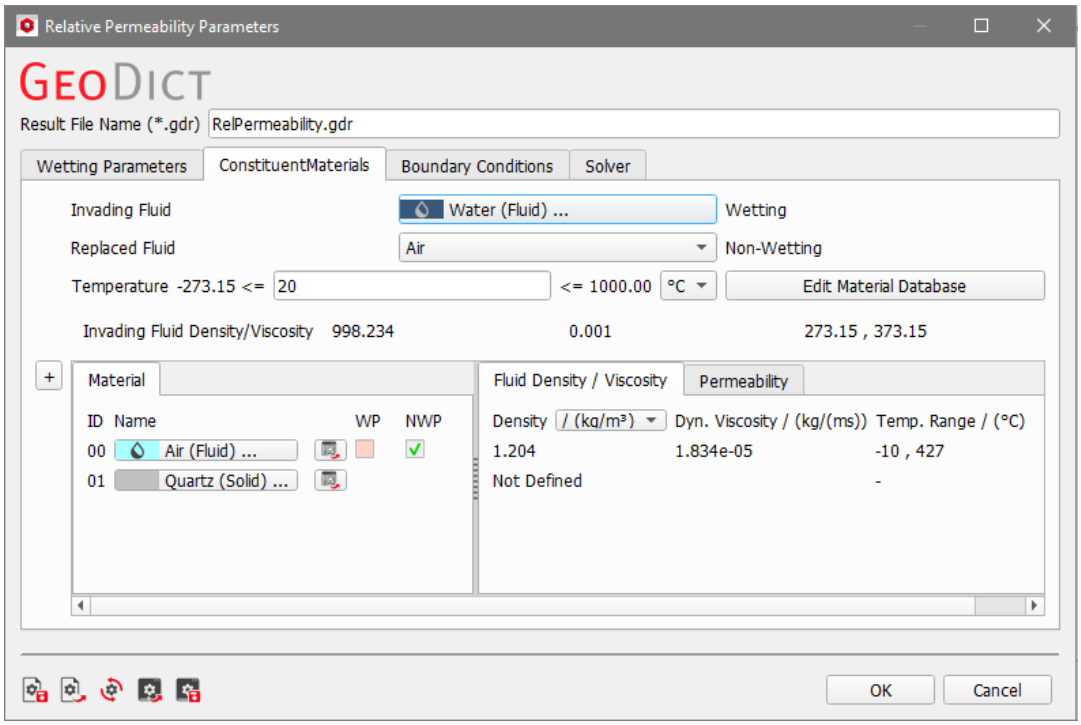
Flow Phase

In the **Flow Phase** panel, choose the phase (Wetting Phase and/or Non-Wetting 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 15) 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

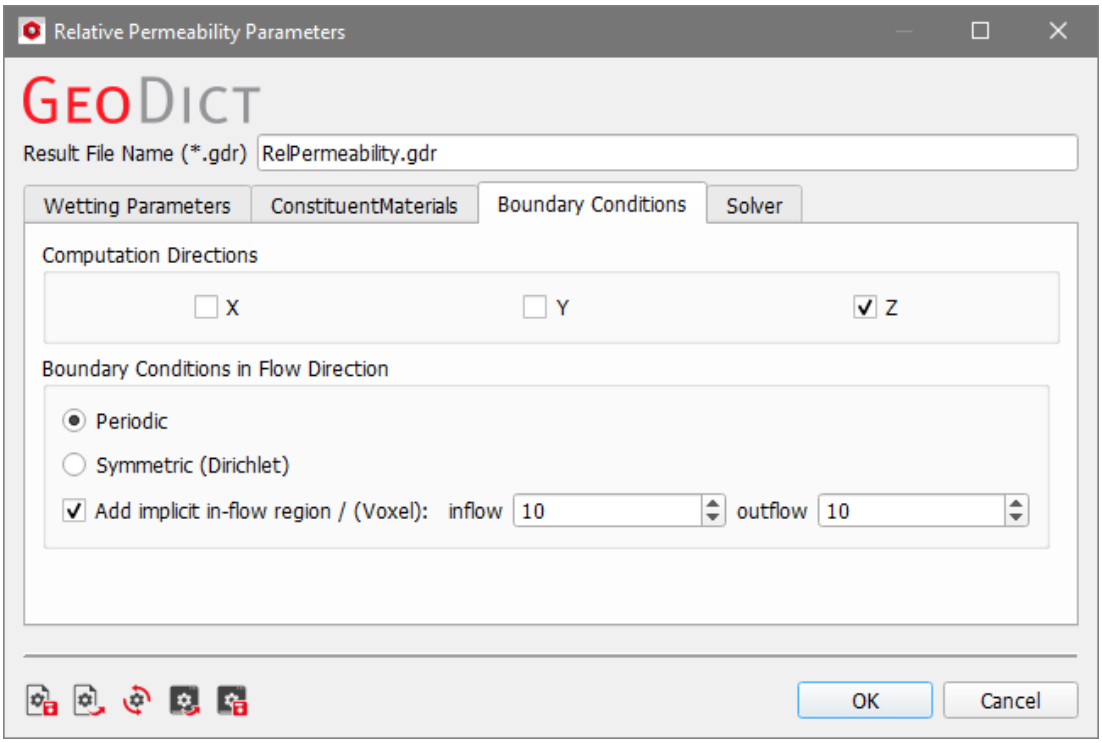
Computation Directions

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 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.



Solver

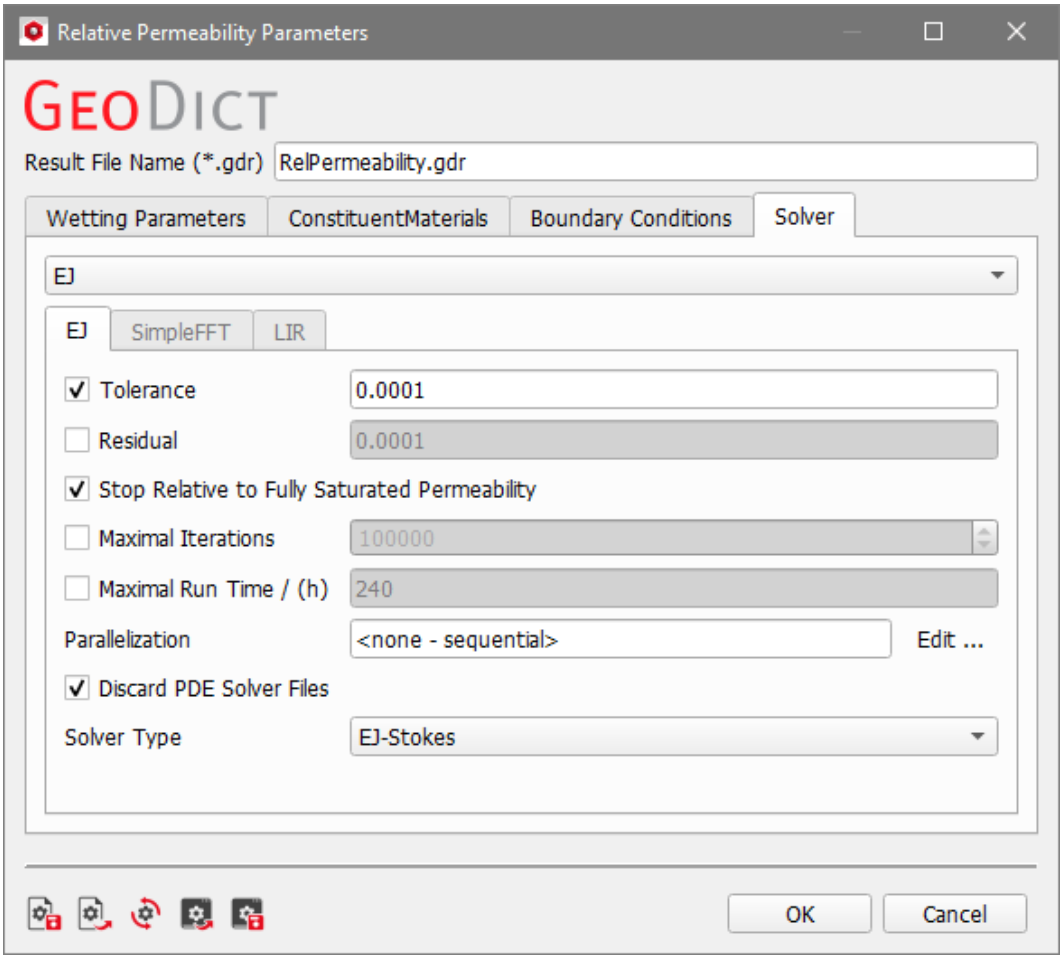
Internally SatuDict solves several equations for values of permeability at each voxel by using an iterative solver. The basic idea of an iterative method is to:

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 additional **Error Bound** stopping criterion is available for **LIR** and **SimpleFFT** only.

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**.

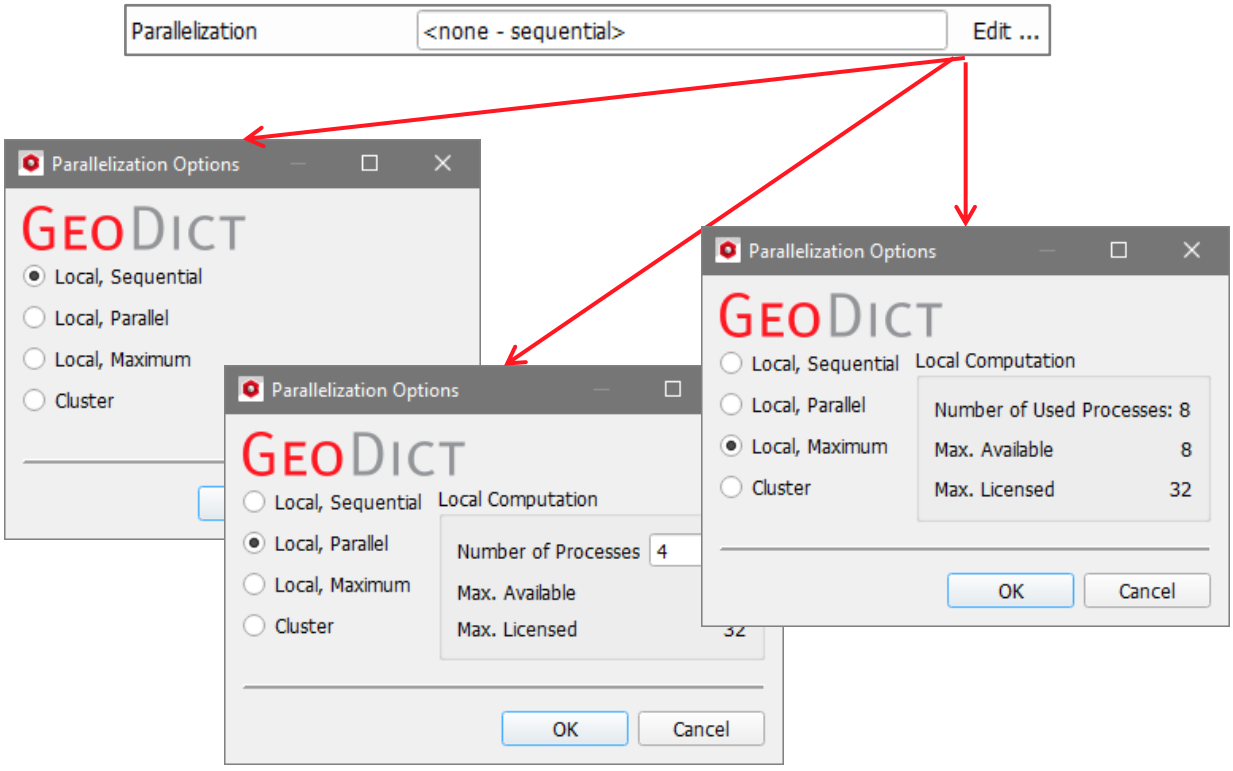
The option to **Stop Relative to Fully Saturated Permeability** alters the chosen stopping criterion such that for low saturated states the solver stops relative to the result of the computation where the structure was fully saturated. The fully saturated structure has the highest permeability and decreases 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. And **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.

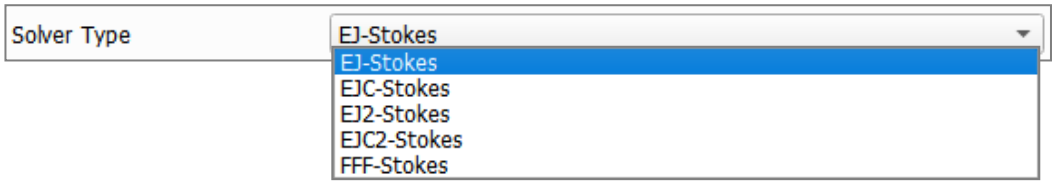
Discard PDE Solver Files

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**.

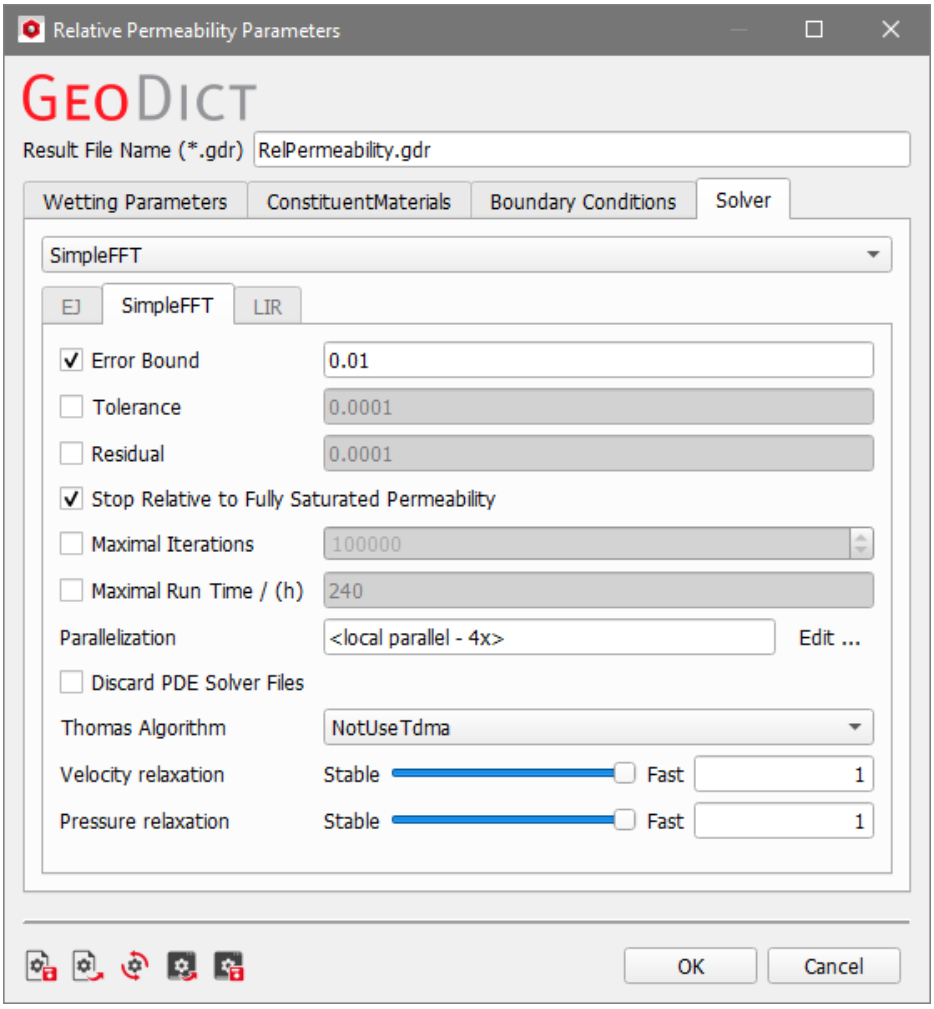


The implementations describe how the no-slip boundary conditions are discretized, i.e., at which discrete point the tangential velocity reaches zero.

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 40ff 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

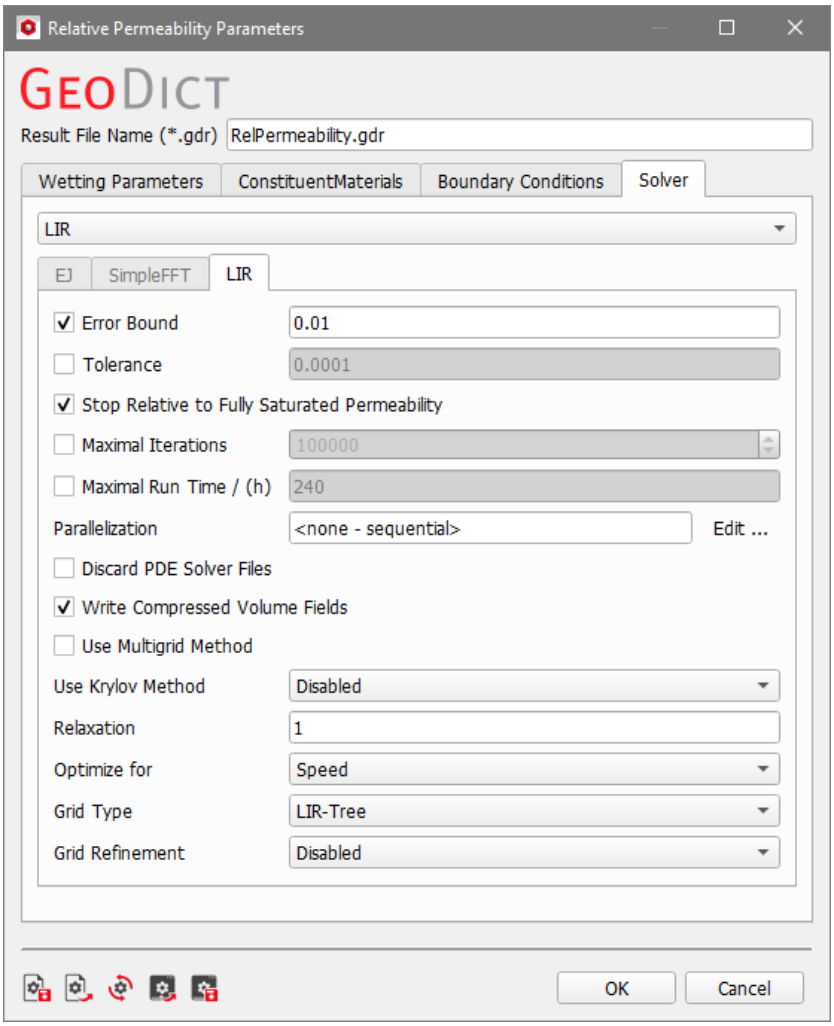
For **Thomas Algorithm**, **Automatic**, **NotUseTdma** or **UseTdma** can be selected. The tridiagonal matrix algorithm (Tdma) can help to improve the convergence for structures with high porosity and therefore speedup the computation with SimpleFFT. With **UseTdma** / **NotUseTdma** it can be switched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

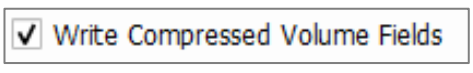
LIR

The explanations given in pages 40ff. 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 2022 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

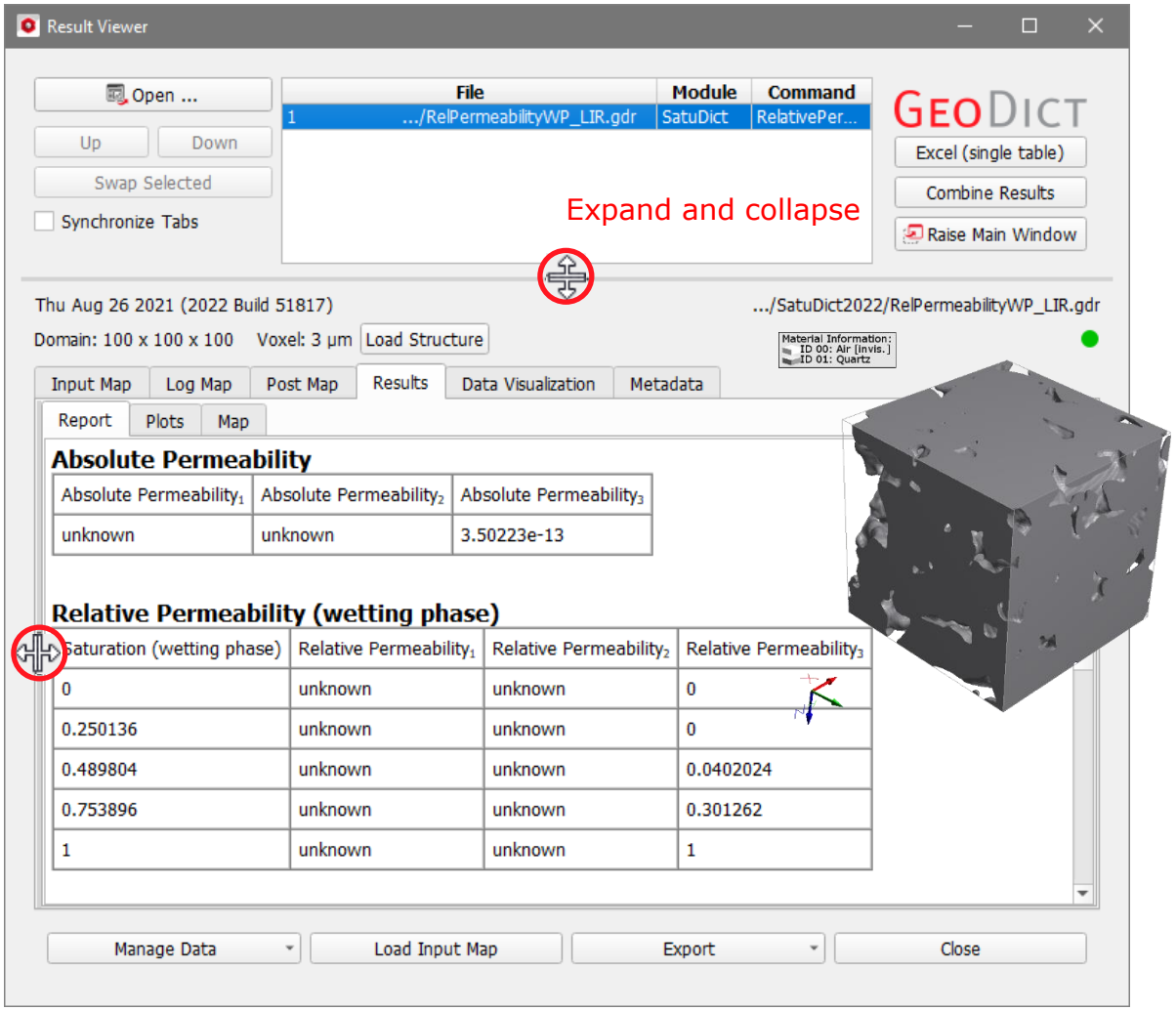
The **Optimize for**, **Grid Type**, and **Grid Refinement** parameters are special options for the LIR solver. The defaults are already optimal for most applications.

A detailed explanation of these parameters can be found in the section **Solver Options** of the FlowDict 2022 handbook.

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 Wetting 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, RelPermeabilityWP_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 18ff.).

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 WP 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 Wetting Phase as the flow phase under the Wetting Parameters tab, it is the permeability depending on the saturation of the flowing WP that is shown in the tables.

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

Report | Plots | Map

Absolute Permeability

Absolute Permeability$_1$	Absolute Permeability$_2$	Absolute Permeability$_3$
unknown	unknown	3.50223e-13

Relative permeability (0 to 1)

Relative Permeability (wetting phase)

Saturation (wetting phase)	Relative Permeability$_1$	Relative Permeability$_2$	Relative Permeability$_3$
0	unknown	unknown	0
0.250136	unknown	unknown	0
0.489804	unknown	unknown	0.0402024
0.753896	unknown	unknown	0.301262
1	unknown	unknown	1

Effective permeability / m^2

Effective Permeability (wetting phase)

Saturation (wetting phase)	**K_{11}**	K_{12}	K_{13}	K_{21}	**K_{22}**	K_{23}	K_{31}	K_{32}	**K_{33}**
0	unknown	unknown	0	unknown	unknown	0	unknown	unknown	0
0.250136	unknown	unknown	0	unknown	unknown	0	unknown	unknown	0
0.489804	unknown	unknown	5.00469e-16	unknown	unknown	-2.38875e-16	unknown	unknown	1.40798e-14
0.753896	unknown	unknown	-1.0128e-14	unknown	unknown	-4.01648e-15	unknown	unknown	1.05509e-13
1	unknown	unknown	3.44493e-14	unknown	unknown	-1.05432e-14	unknown	unknown	3.50223e-13

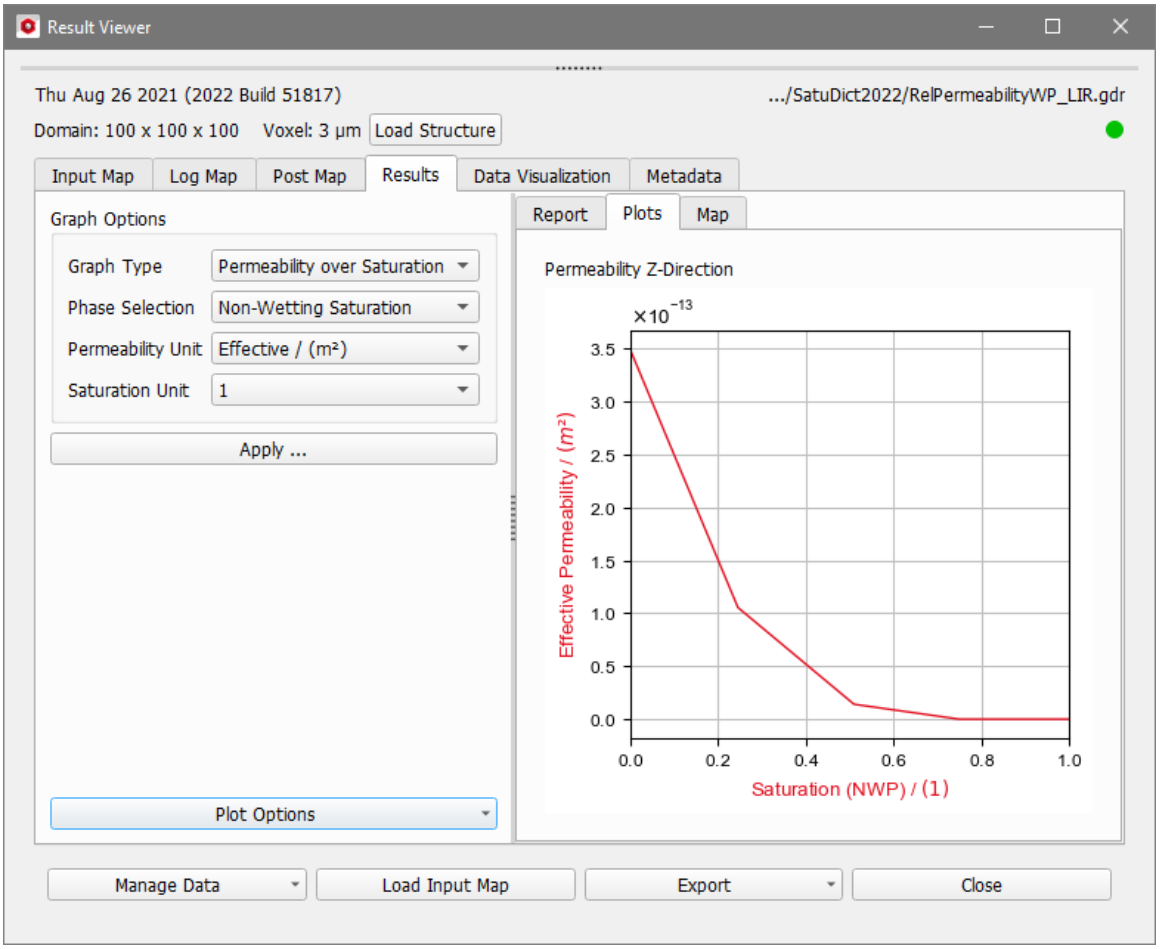
Remark: Permeability values are given in m²

Plots

In the **Results - Plots** subtab, the values of the **Relative Permeability** or **Effective Permeability** table are shown in a graph.

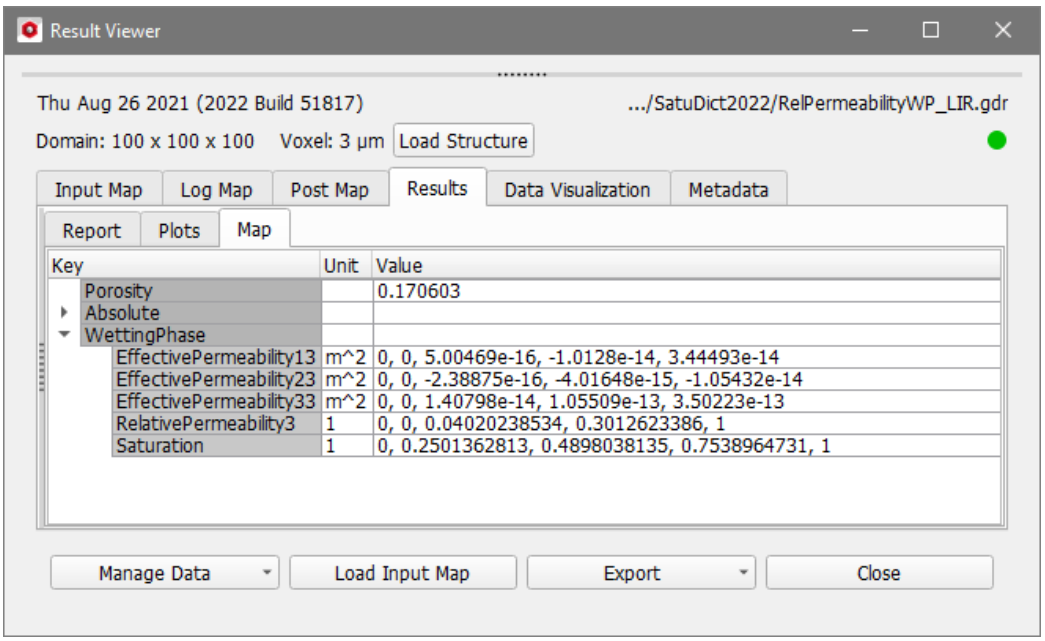
On the left side, the user can modify the way the graph is displayed by selecting the **Graph Type** (Permeability over Saturation, Saturation over Permeability), the **Phase Selection** (Non-Wetting Saturation, Wetting Saturation), the Permeability

Unit (**Effective** permeability in m^2, **Relative** permeability between 0 and 1), and the **Saturation Unit** (1, %, mL). Click **Apply** to change the graph shown according to the options selected. Choose **Plot Options**, to change axis and graph settings.



Map

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

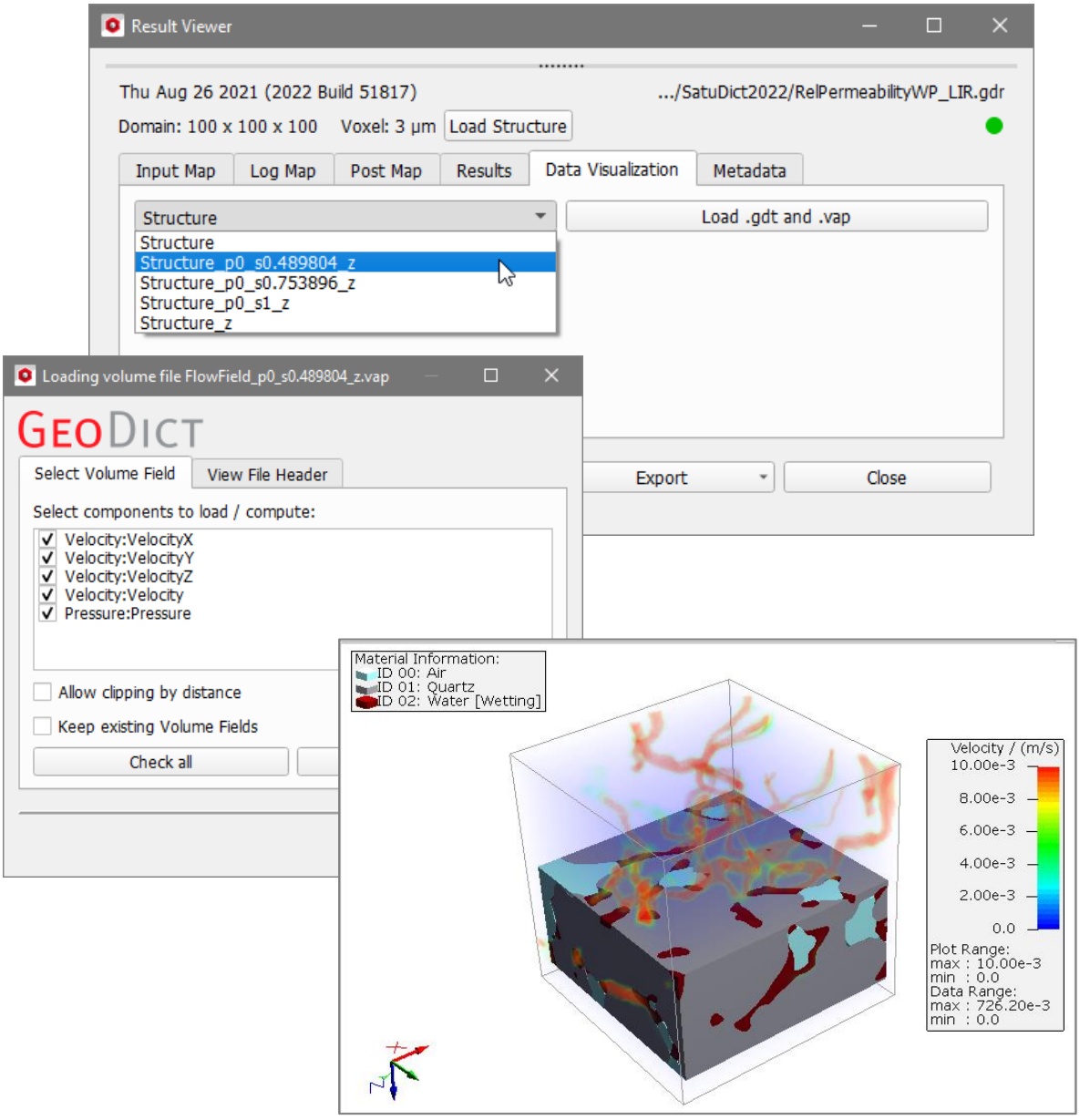


Data Visualization

Under the **Data Visualization** tab, the .gdt and .vap files, corresponding to the saturation levels computed, can be opened, as explained above in pages 31ff. Here shown is the GDT file for a 49% WP saturation level.

The solid phase (Quartz) is shown together with the Non-Wetting phase (Air) and the Wetting phase (Water). The upper part of the image shows the velocity field of the WP (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.

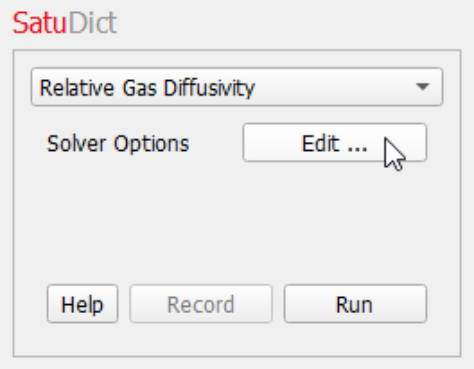


Export of Results

The result file **RelPermeabilityWP_LIR.gdr** can be loaded into a Microsoft Excel™ spreadsheet with GeoDexcel in the same way as explained above (pages 26f.) for the analysis of the capillary pressure curve.

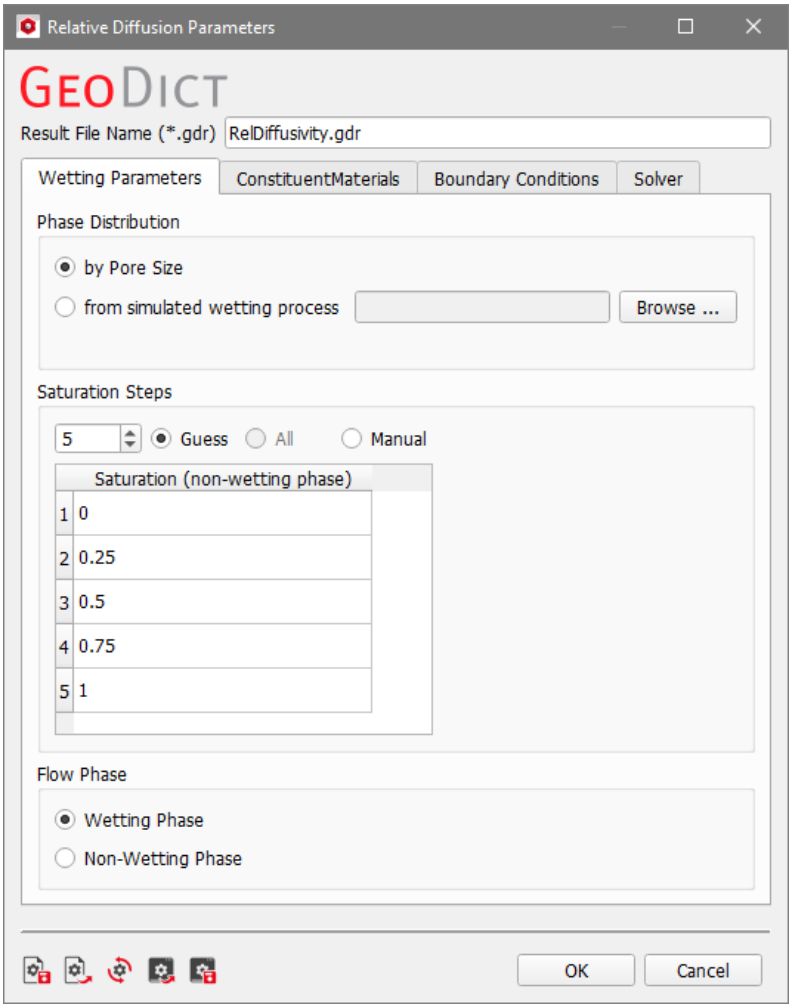
Relative Gas Diffusivity

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.



Wetting Parameters

The wetting parameters for the calculation of the Relative Diffusivity are the same as seen above (pages 37f.) 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

The **Constituent Materials** tab for the calculation of the Relative Diffusivity are analogous to those seen above (page 38) for the Relative Permeability.

Boundary Conditions

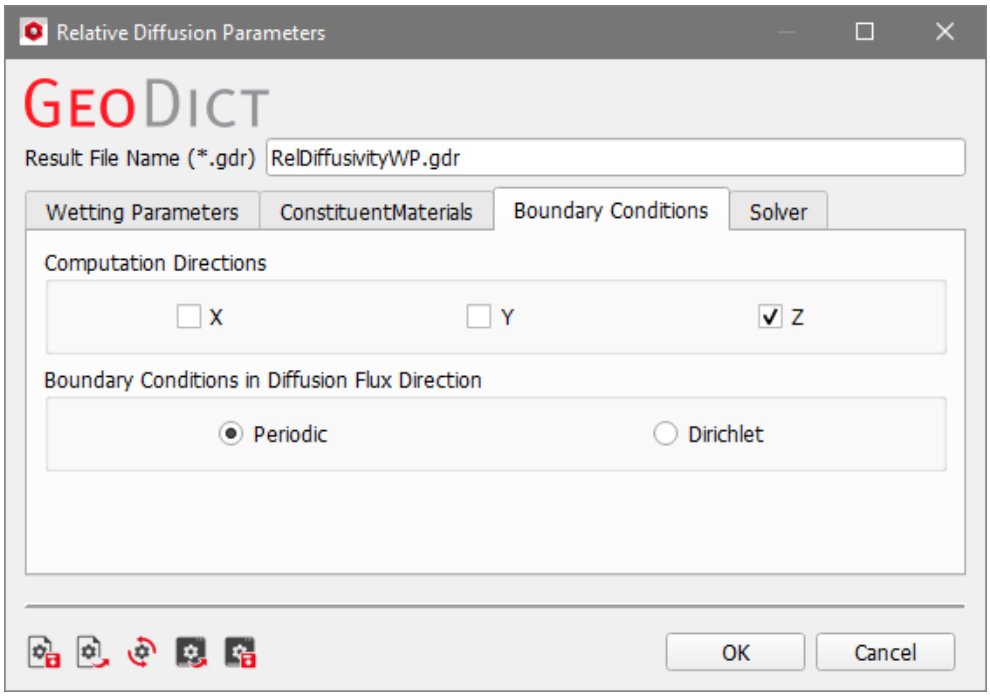
For the **Computation Directions**, choose the direction of the calculated flow. To obtain the whole diffusivity matrix in the result file, it is necessary to choose all three directions.

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).

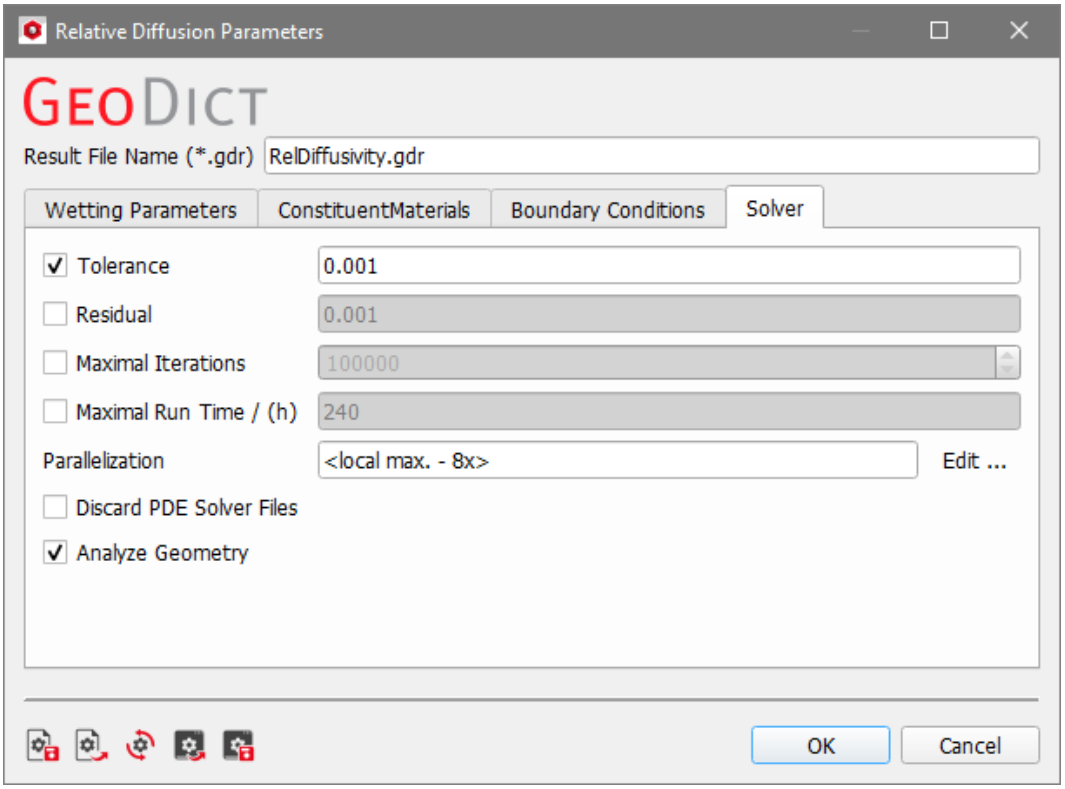
If **Dirichlet** is checked, a constant concentration is ensured along both border planes in the diffusion direction. The use of Dirichlet boundary conditions approximately doubles the computational costs.

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

The parameters for the calculation of the relative gas diffusivity under the **Solver** tab are the same as for the **EJ** solver for the computations of the Relative Permeability (see pages 40ff.). The options **Stop Relative to Fully Saturated Permeability** and **Solver Type** are not available for the diffusivity computations.



Checking **Analyze Geometry** enables the geometrical analysis of the structure model if the user deems it necessary.

When checked, the analysis is carried out before the solver computations to determine the existence of a through path, and to fill up unconnected empty spaces.

Relative Gas Diffusivity result file

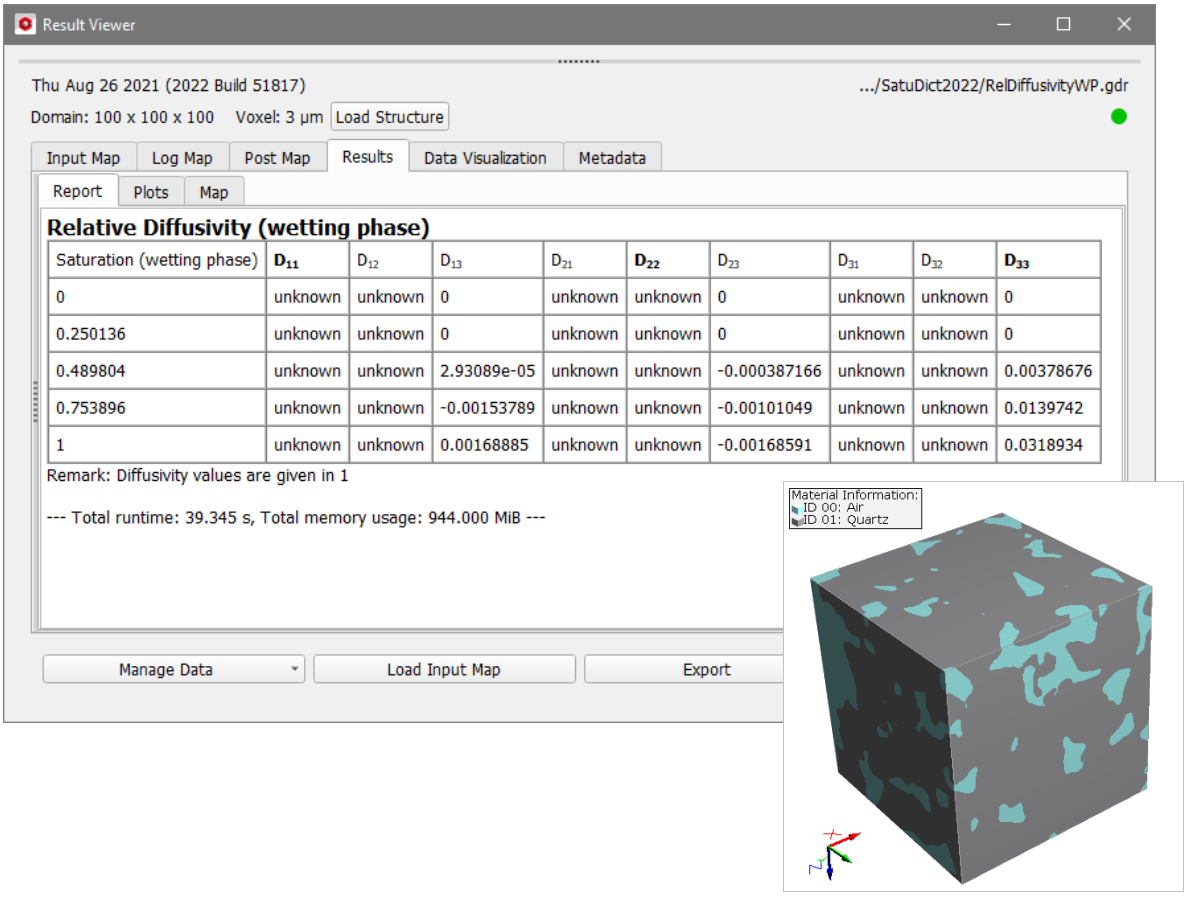
Here, the results of the computation of the relative diffusivity of a partially saturated porous media with 17% porosity (83% SVF) are explained.

The Wetting Phase 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, RelDiffusivityWP.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 18ff.).

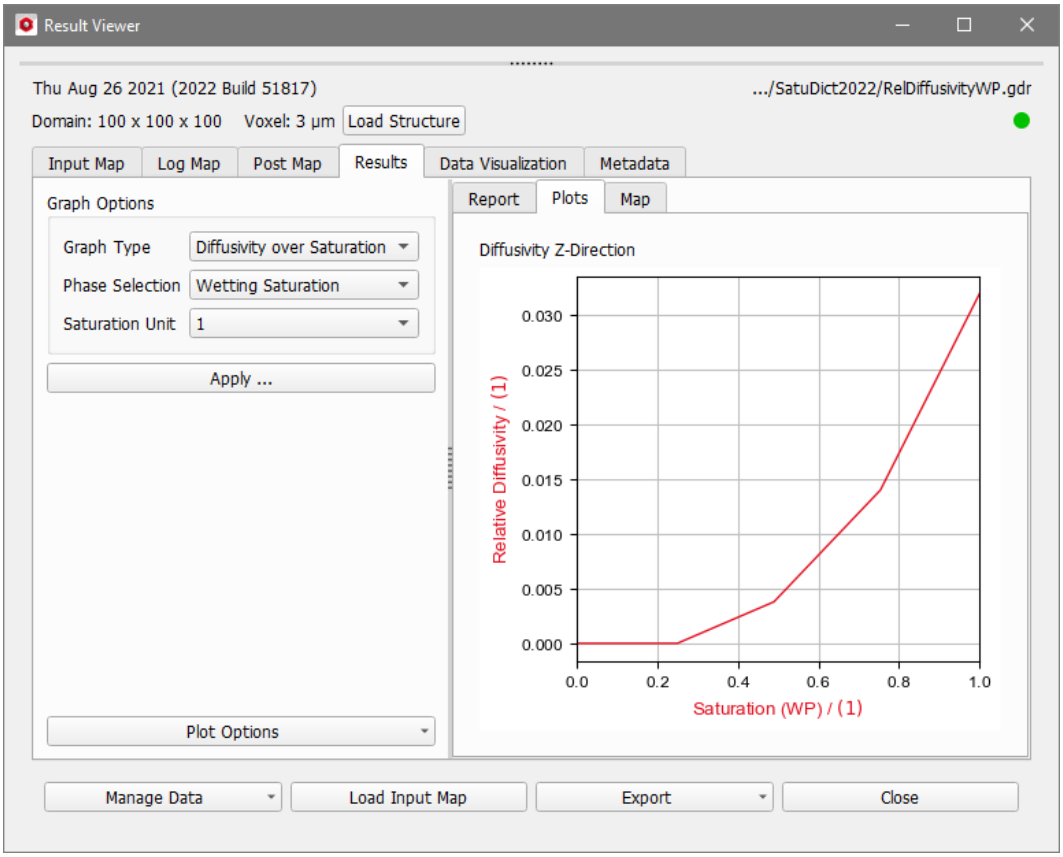
Under the **Results-Report** subtab, the **Relative Diffusivity** table (saturation-dependent diffusivity) is shown for the chosen saturation rates (0.00, 0.25, 0.49, 0.75, 1.00) in the chosen directions (here, D13, D23, D33 for the diffusion in z - direction). The chosen saturation rates are approximated as good as possible. The Wetting Phase was selected as the flow phase in the Wetting Parameters dialog box. Thus, it is the diffusivity depending on the saturation of the WP that is shown in the **Relative Diffusivity** table.



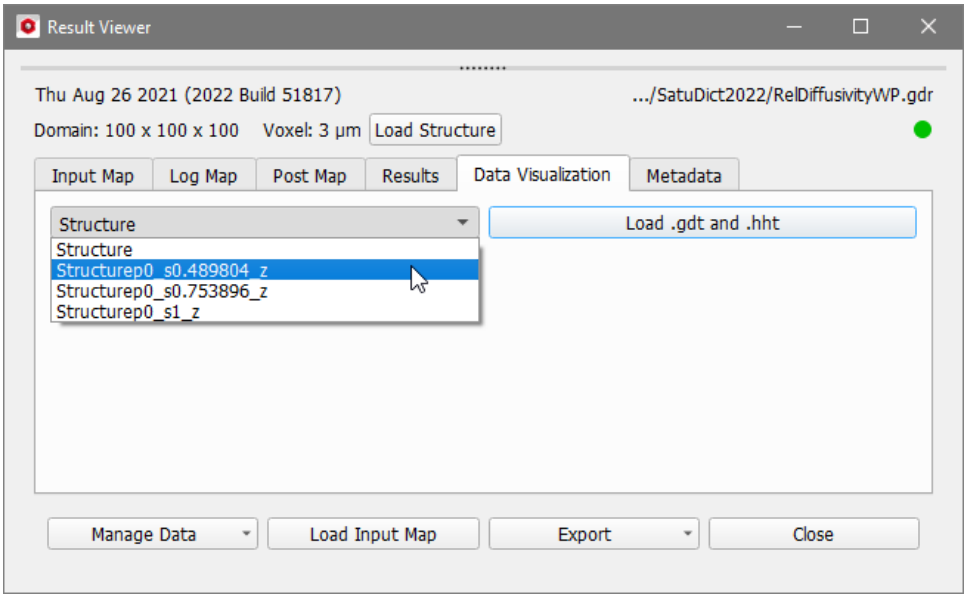
Observe how, similar to what occurred with the relative permeability, the diffusivity is zero at 0% and 25% saturation of the WP, indicating that before the structure is 49% saturated with the WP, no through path of the WP is available.

In the **Results-Plots** subtab, the values in the **Relative Diffusivity** table of the **Report** tab are shown in a graph.

On the left panel, the user can modify the way the graph is displayed by selecting **Graph Type** (Diffusivity over Saturation, or Saturation over Diffusivity), **Phase Selection** (Non-Wetting Saturation, Wetting Saturation), and **Saturation Unit** (1, %, mL).

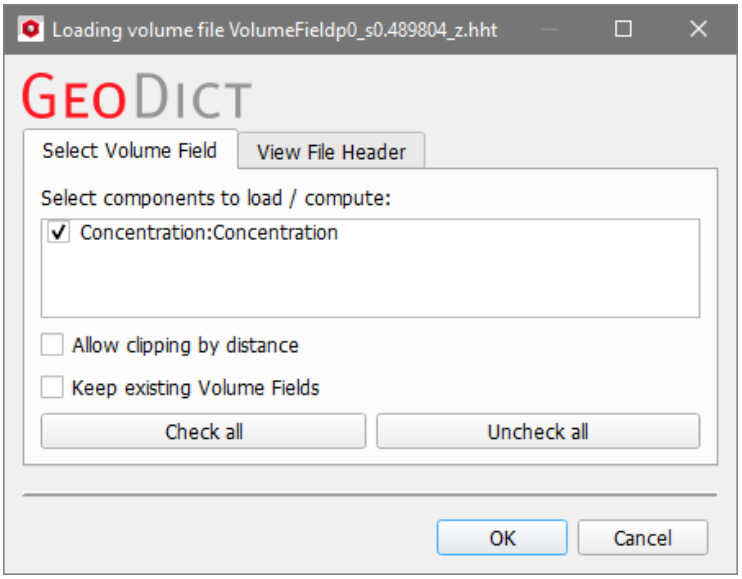


The **RelDiffusivityWP.gdr** result file that opens at the end of the computation is saved in the project folder, together with the **RelDiffusivityWP** result folder. The result folder contains various files for the saturation levels entered in the wetting parameters dialog box.



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

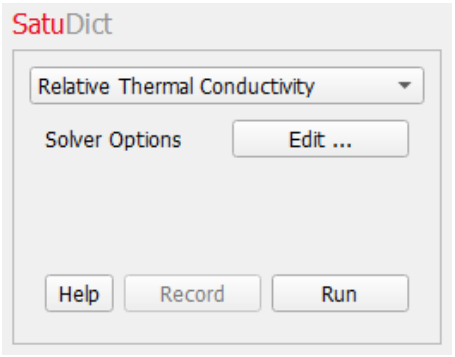
Click **Load .gdt and .hht** to load the structure for a certain saturation of the WP and the corresponding concentration field in the same way as explained in pages 31ff. for the relative permeability results.



The result file **RelDiffusivityWP.gdr** can be loaded into a Microsoft Excel™ spreadsheet with GeoDexcel in the same way as explained above (pages 26f.) for the analysis of the capillary pressure curve.

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.

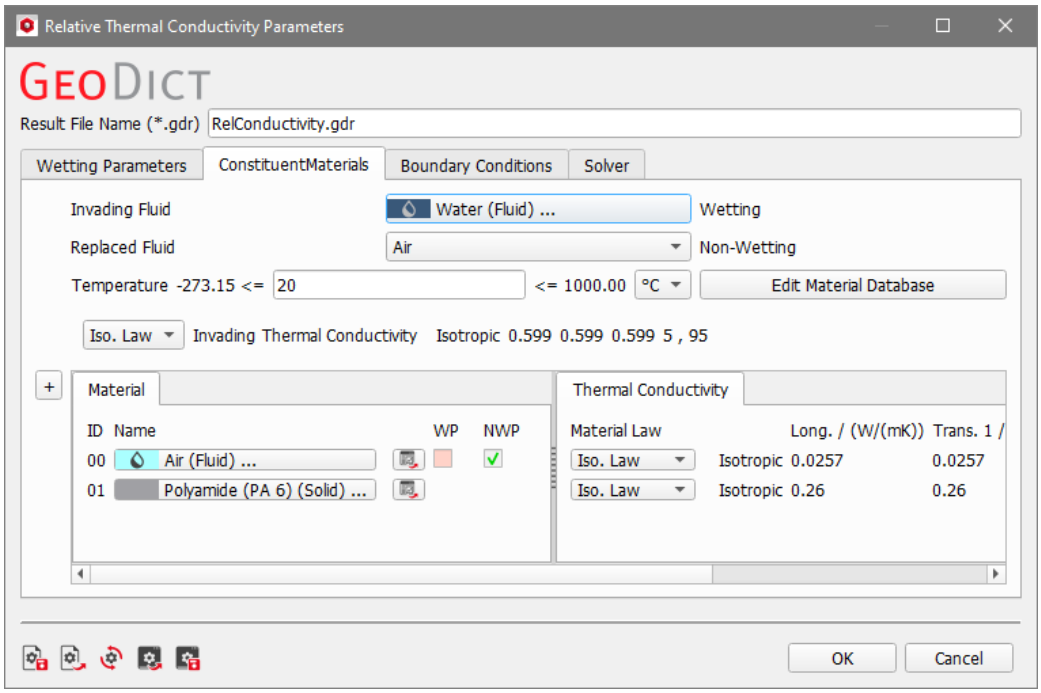
Clicking the **Wetting Parameters**, **Constituent Materials**, **Boundary Conditions**, and **Solver** tabs, the parameters necessary to run the Relative Thermal Conductivity calculations can be entered.

Wetting Parameters

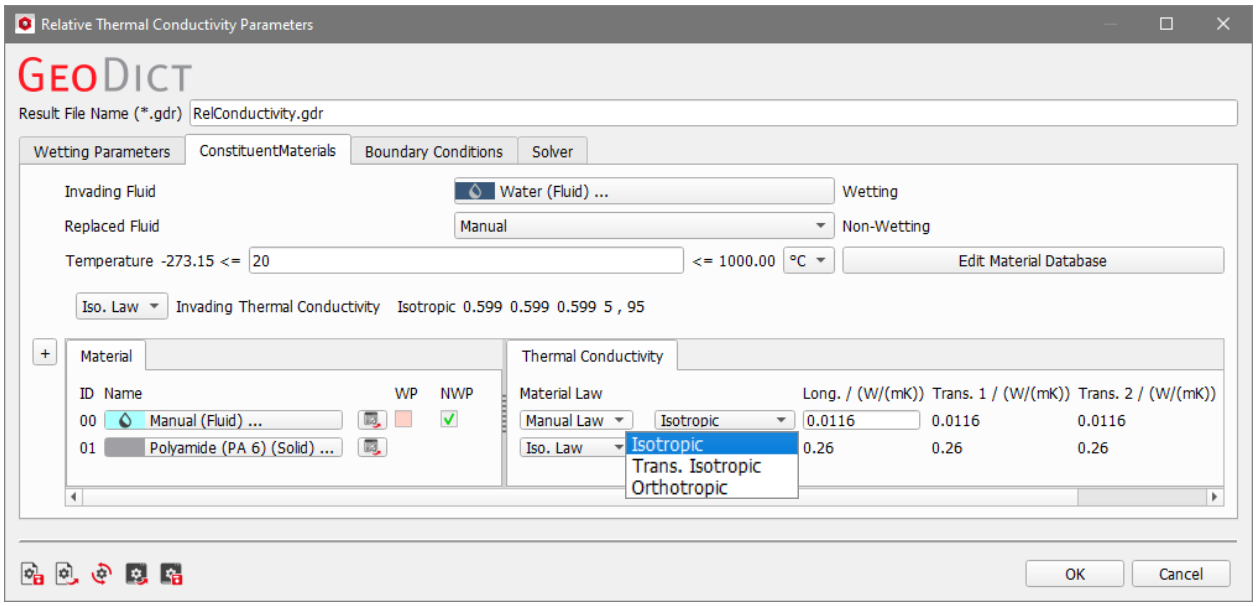
The wetting parameters for the calculation of the Relative Thermal Conductivity are the same as seen above (pages 37f.) for the Relative Permeability. No Flow Phase needs to be selected for thermal conductivity computations.

Constituent Materials

Under the **Constituent Materials** tab, the Wetting Phase fluid (in the Pore space), all constituent materials of the structure, and the Non-Wetting Phase fluid can be selected and their thermal conductivity (W/(m K)) can be defined. 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. The properties of the invading fluid appear above the thermal conductivity tab. The replaced fluid must be present in the current structure.



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

The parameters for the calculation of the Relative Thermal Conductivity under the **Solver** tab are the same as for the **EJ** solver for the Relative Permeability (see pages 40ff.). The options **Stop Relative to Fully Saturated Permeability** and **Solver Type** are not available for thermal conductivity computations.

Checking **Analyze Geometry** enables the geometrical analysis of the structure model if the user deems it necessary.

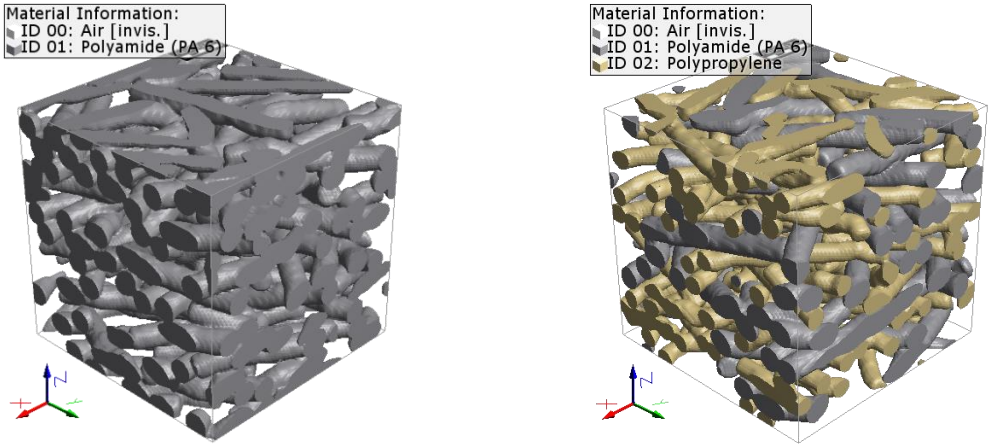
When checked, the analysis is carried out before the solver computations to determine the existence of a through path, and to fill up unconnected empty spaces.

RELATIVE THERMAL CONDUCTIVITY RESULT FILE

Here, the saturation-dependent effective thermal conductivity is computed at various NWP saturation levels (0%, 25%, 50%, 75%, and 100%) for two structures, both with 70% porosity, but different constituent materials. The WP is water, and the NWP is air. The relative thermal conductivity is calculated in z-direction.

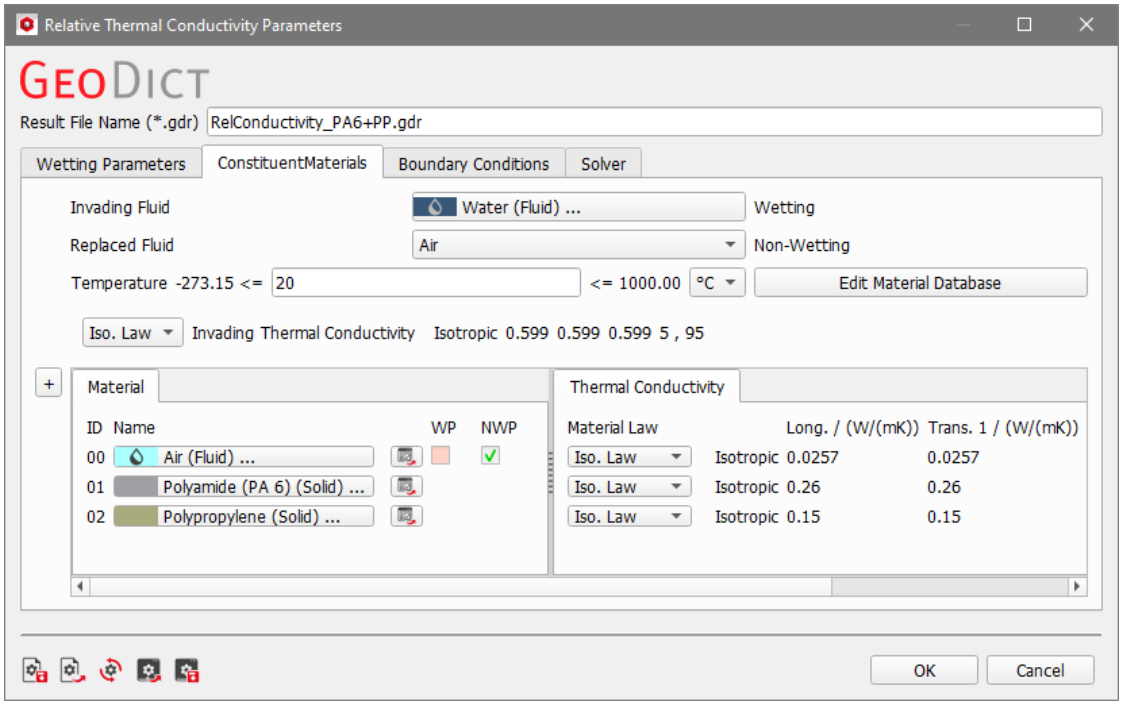
In the **first experiment**, the only fiber material in the structure is 100% polyamide PA6 (Material ID 01, grey).

In the **second experiment**, the structure is made of 20% polyamide (Material ID 01, grey) and 80% polypropylene (Material ID 02, brown) fibers

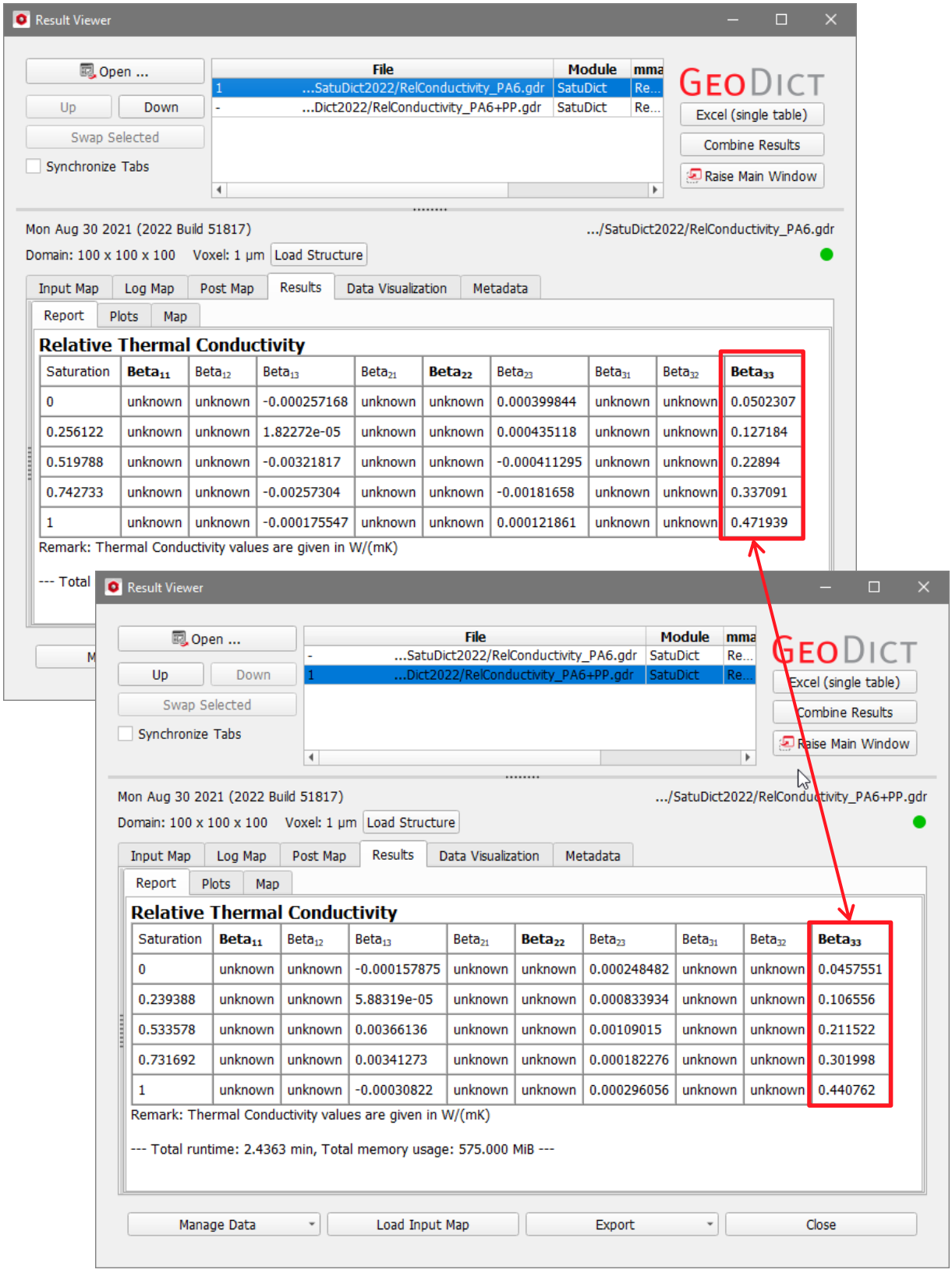


PA6 and PP have different thermal conductivities.

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). The thermal conductivity of the materials included in the database is automatically considered. For other materials, the material database can be edited, or the thermal conductivity can be entered manually.



After the computations for the first experiment and the second experiment are finished, the Result Viewer opens. The result data contained in the result file are 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.

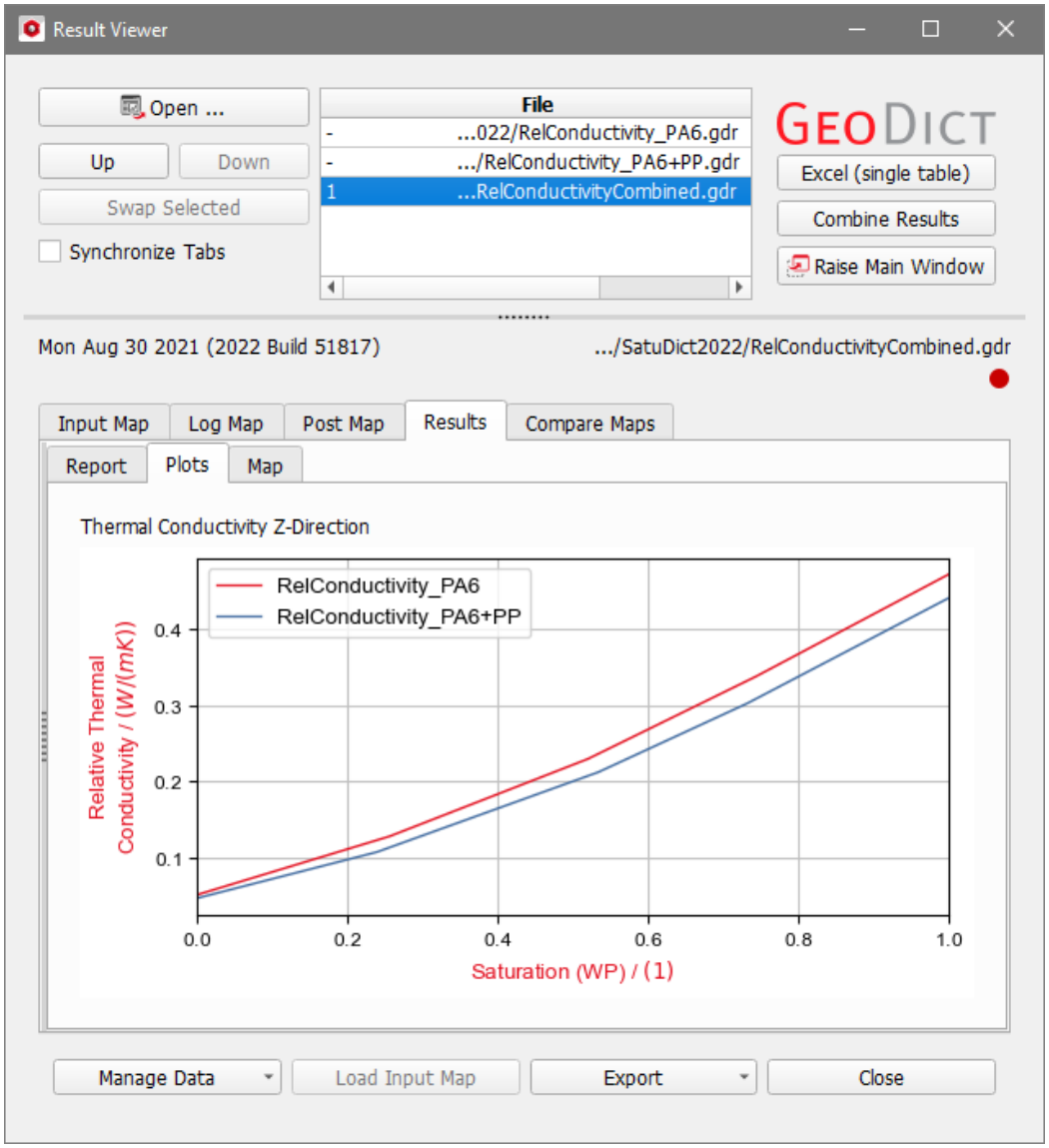
By highlighting the names of both result files and clicking the **Combine Results** button, the results of both files are combined and saved into a GDR file in the chosen project folder. The combining process enables post-processing on the combined results.

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 2022 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 (WP). The relative thermal conductivity of the PA6+PP structure is always lower.

The parameters for the graphs can be modified (see pages 23f.) 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.

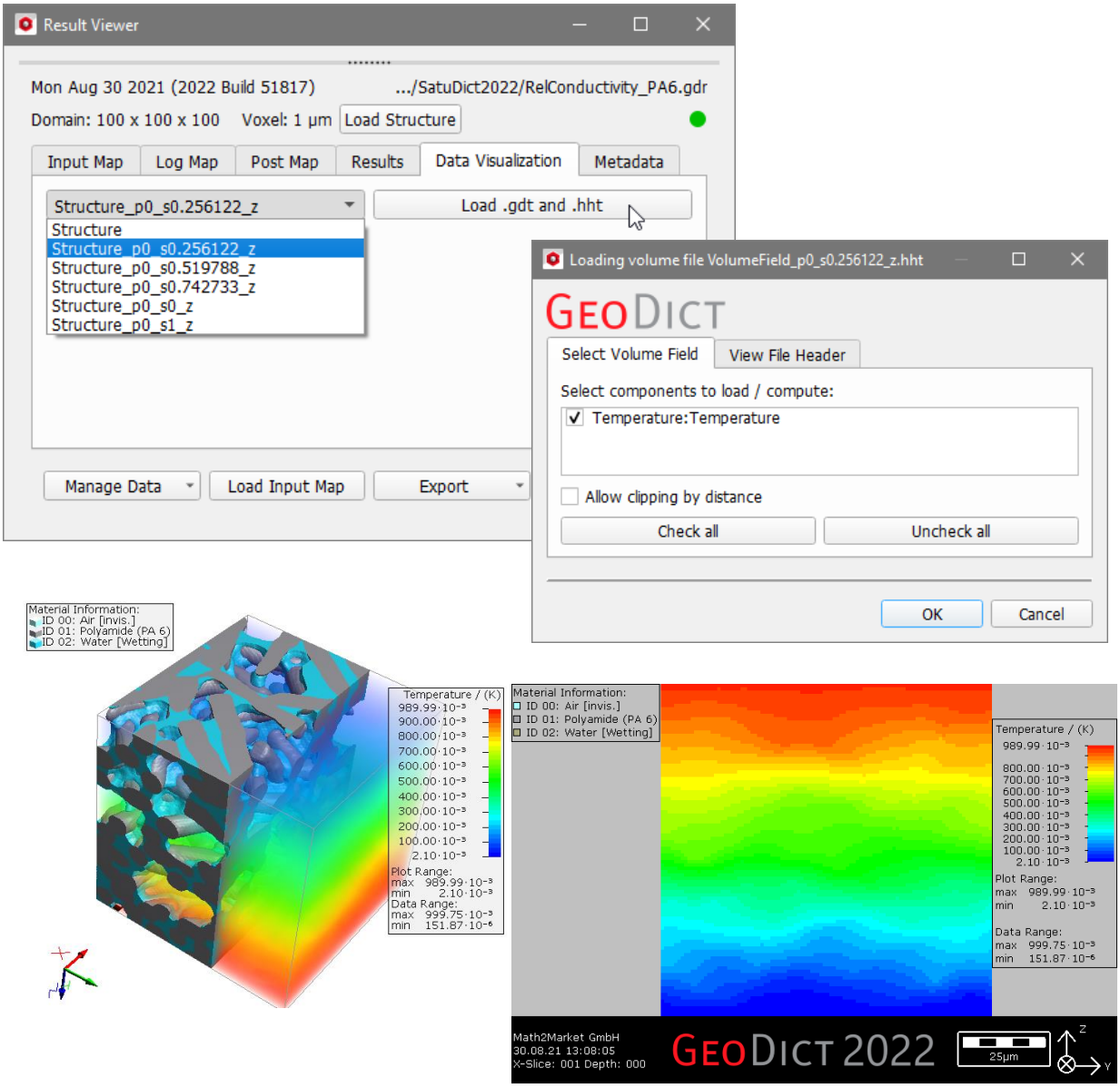


The HHT files (homogenized heat file; containing the temperature distribution) corresponding to the five saturation levels entered under the Wetting Parameters tab (0.00, 0.25, 0.50, 0.75, 1.00) are stored for each computation in the result folder, here **RelConductivity_PA6** and **RelConductivity_PA6+PP,**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

Under the **Data Visualization** tab, click **Load .gdt and .hht**, to access the .hht files and visualize the results.

This is similar to opening GDT files (see pages 31ff.) for the visualization of the phase distribution for results of Capillary Pressure Curve and Relative Permeability directly from the result file (GDR).

For example, open the RelConductivity_PA6_p0_s0.256122_z.hht file that corresponds to a 25% NWP saturation in Z-direction from the experiment with the **100% PA6 structure**.

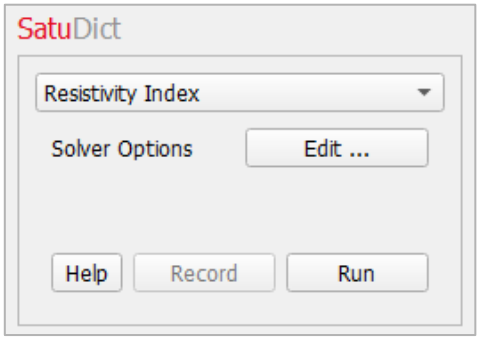


To better observe the results, clip the structure (in 3D Rendering) or switch off the visualization of the structure (in 2D cross-section, **View** → **Structure** in the menu bar), and adjust the Color Map values in the Visualization panel.

Observe how the heat is distributed in the structure.

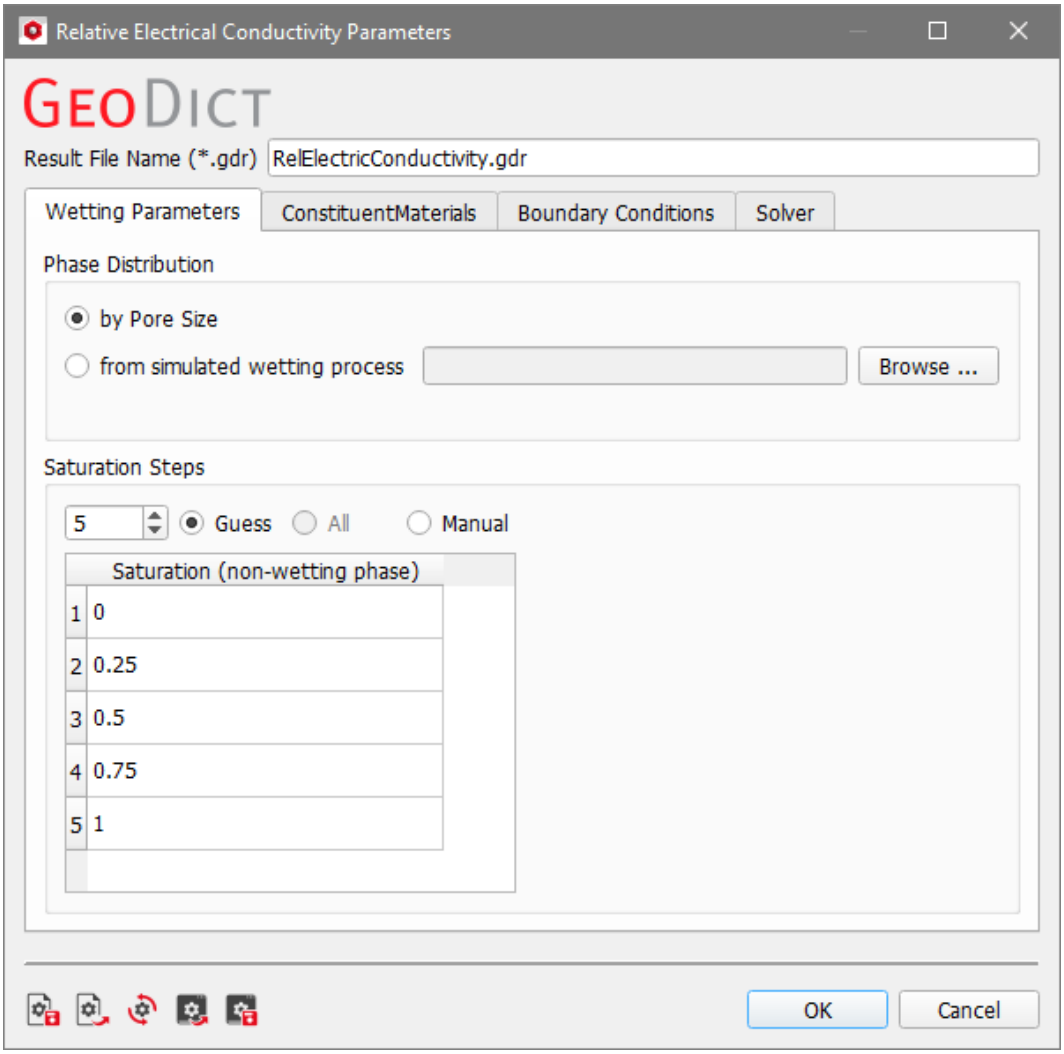
Resistivity Index (relative electrical conductivity)

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, Normalized Electrical Conductivity, and Relative Electrical Conductivity. All parameters are similar to those explained for the Relative Thermal Conductivity computation starting on page 56.



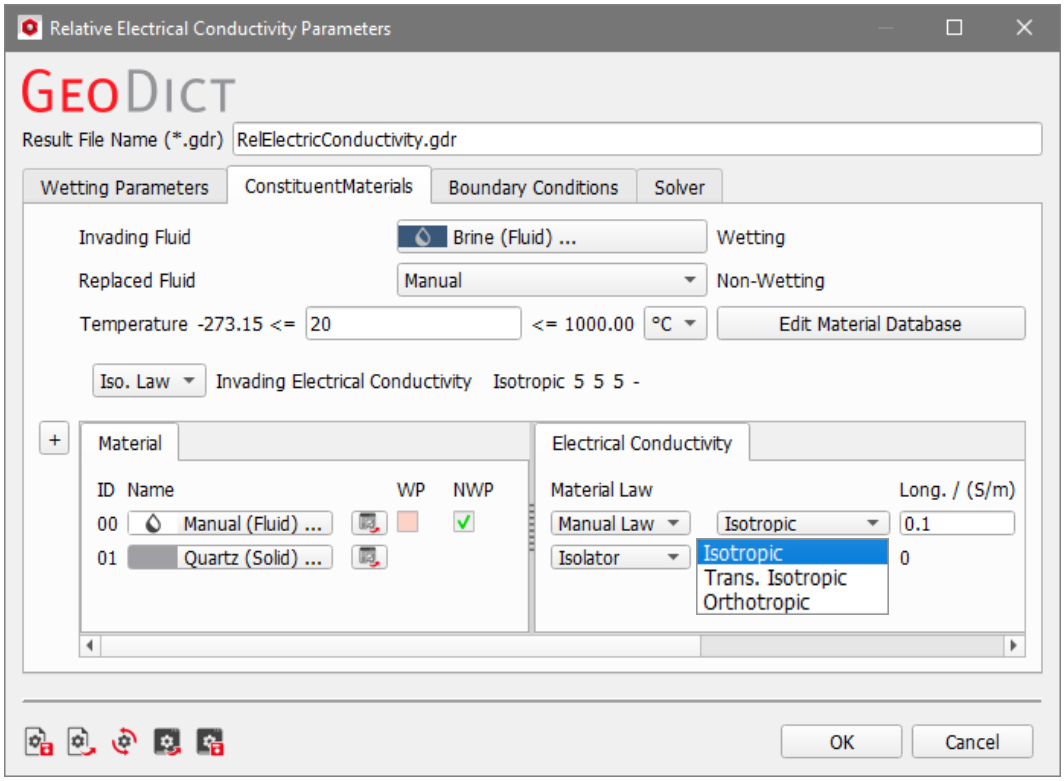
Wetting Parameters

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 56).

Constituent Materials

Under the **Constituent Materials** tab, the Wetting Phase fluid (in the Pore space), all constituent materials of the structure, and the Non-Wetting Phase 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).



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

The parameters for the calculation of the Relative Electrical Conductivity under the **Solver** tab are the same as for the **EJ** solver seen above (pages 40f.) for the Relative Permeability. The options **Stop Relative to Fully Saturated Permeability** and **Solver Type** are not available for electrical conductivity computations.

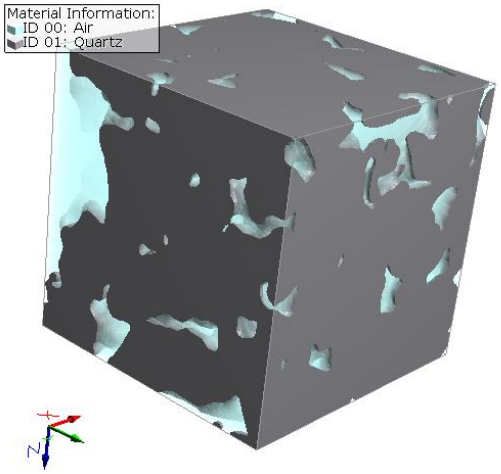
Checking **Analyze Geometry** enables the geometrical analysis of the structure model if the user deems it necessary.

When checked, the analysis is carried out before the solver computations to determine the existence of a through path, and to fill up unconnected empty spaces.

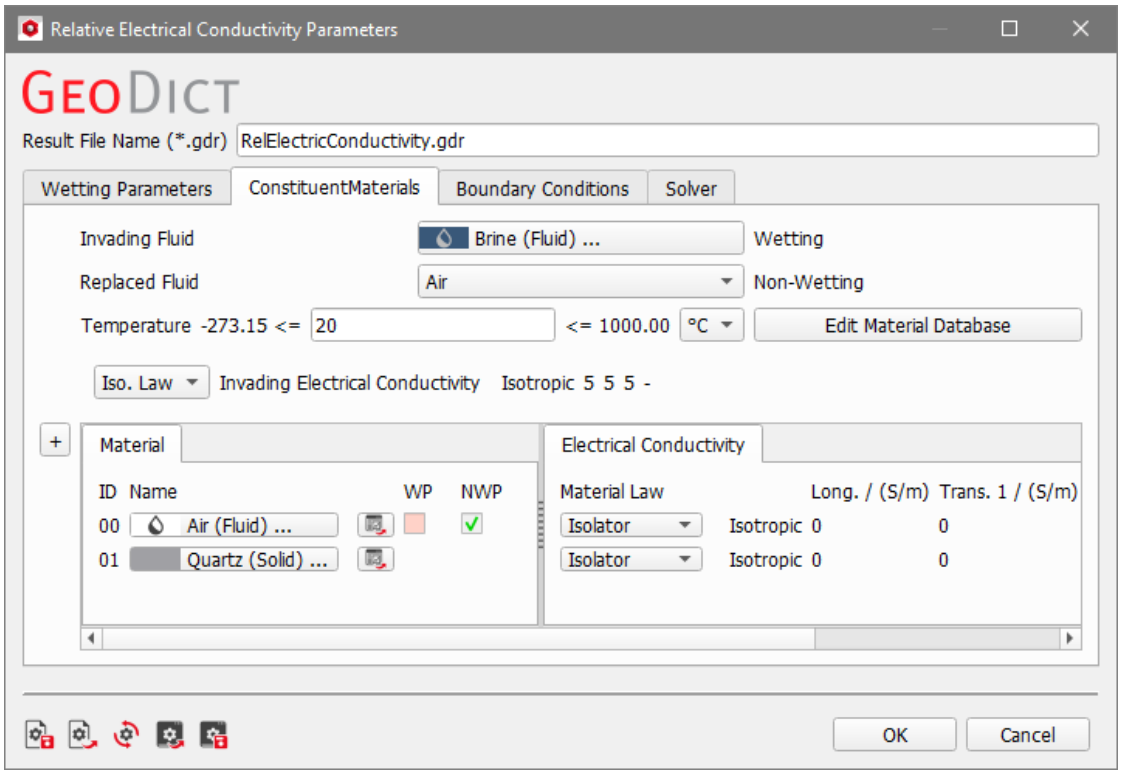
RESISTIVITY INDEX RESULT FILE

Here, the resistivity index is computed at various NWP saturation levels (0%, 25%, 50%, 75% and 100%) for a porous medium with 17% porosity. The invading fluid is brine (5 S/m, WP) and the replaced fluid is air (0 S/m, NWP). 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.

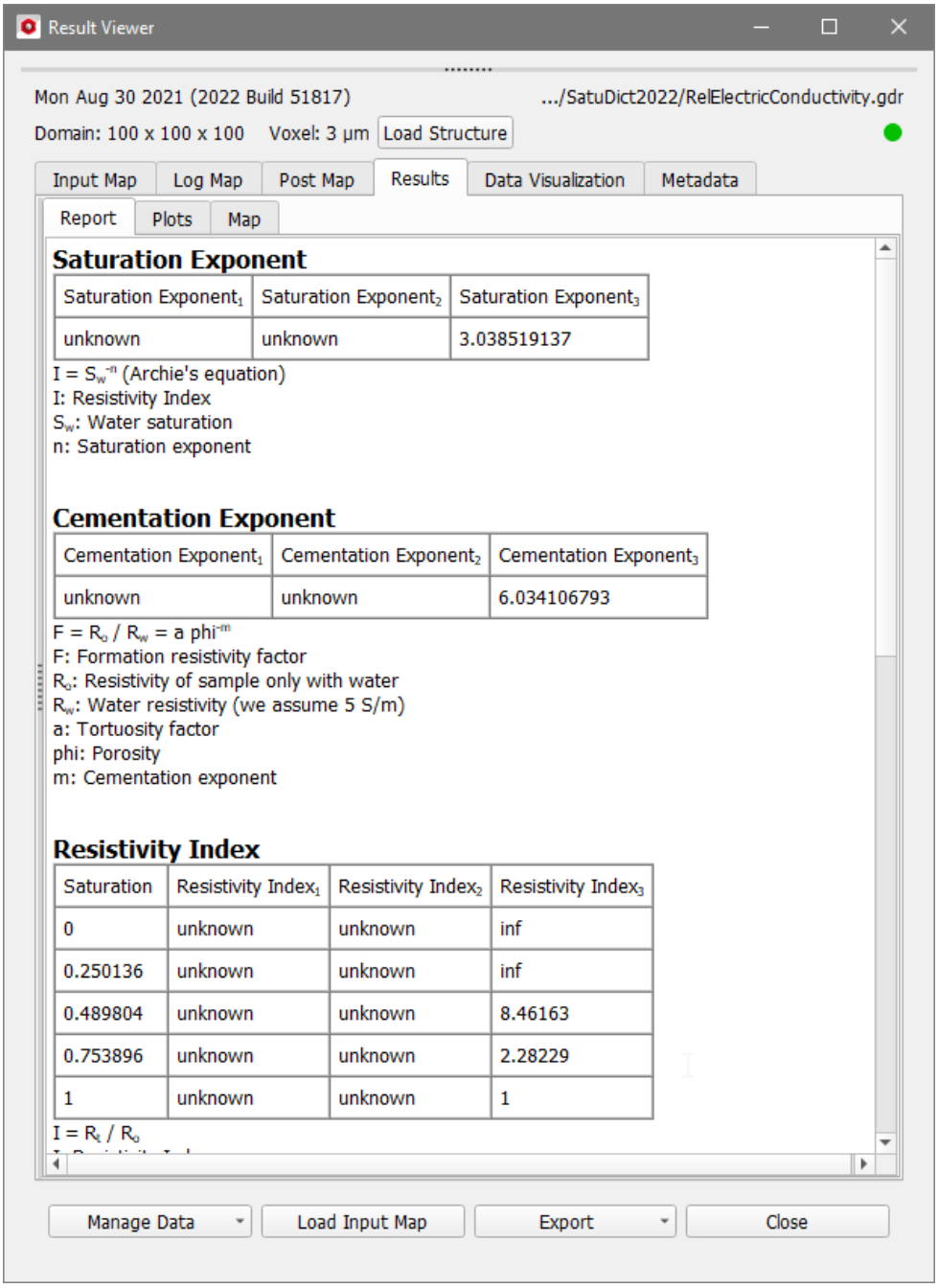


After the computations are finished, the Result Viewer of the result file opens, and the results are saved into a GDR file in the chosen project folder (**File → Choose Project Folder...**). In this example, the **RelElectricConductivity.gdr** result file is saved in the project folder together with 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 18ff.).

Under the **Results - Report** subtab, the tables for **Saturation Exponent**, **Cementation Exponent**, **Resistivity Index**, **Normalized Electrical Conductivity**, 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.

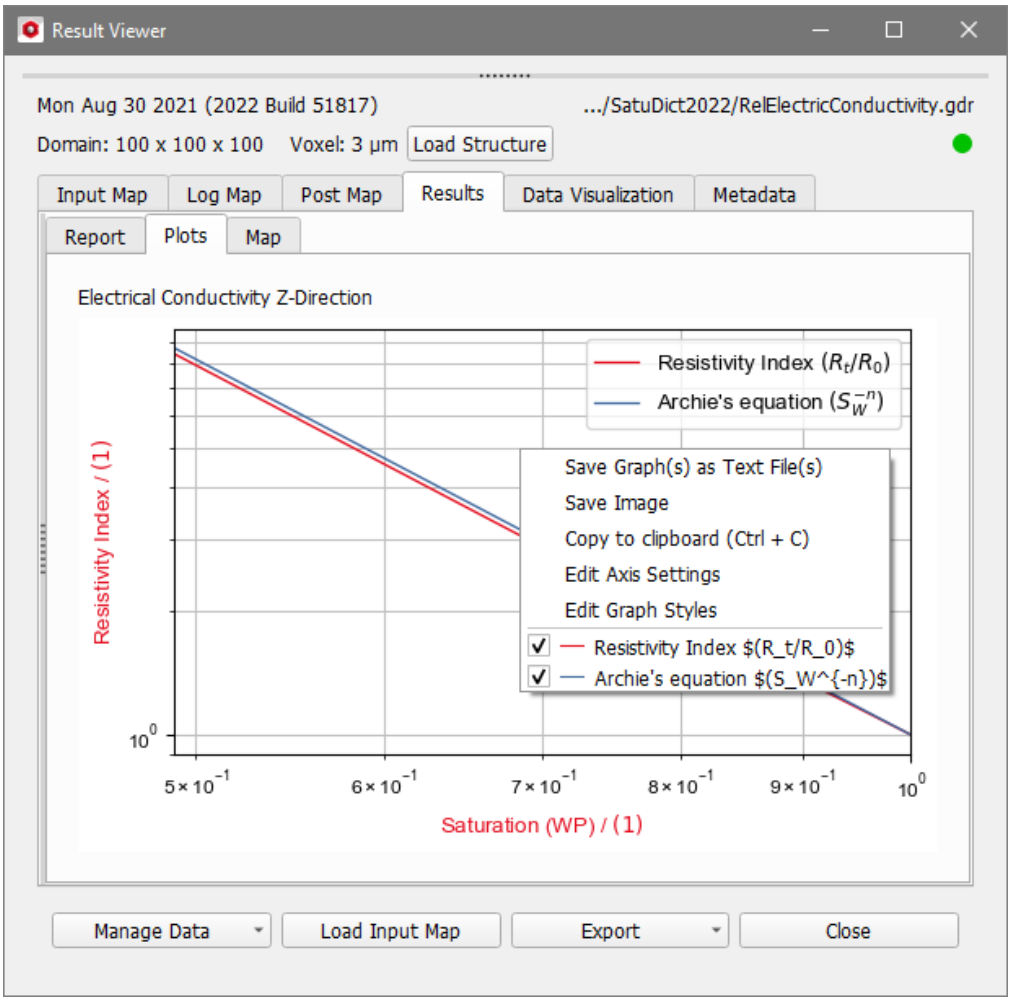
The values of the **Resistivity Index** table are the inverted values of the **Normalized Electrical Conductivity** table.



Under the **Results** - **Plots** subtab, these values are shown in graphs.

The parameters of the graphs can be changed as seen in pages 23f

By right-clicking inside the graph and opening the **Edit Axis Settings** dialog box, the range and scaling of the y-axis can be changed.

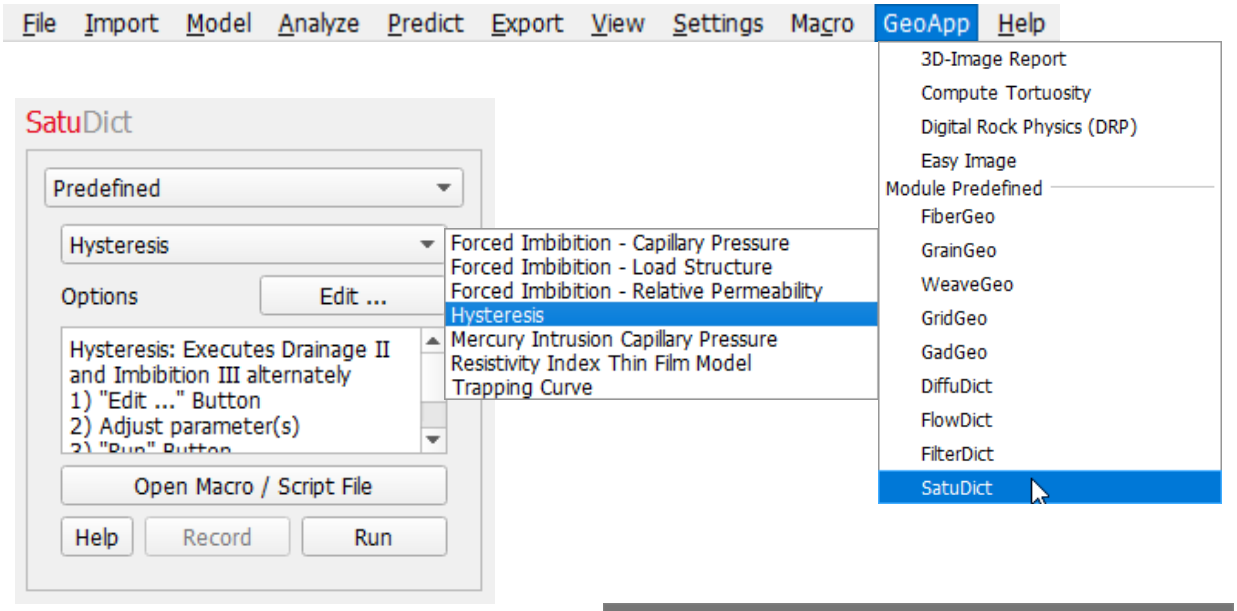


The interpretation of the result tables and the visualization of the corresponding created files are like for the results of the **Relative Thermal Conductivity,** see page 62.

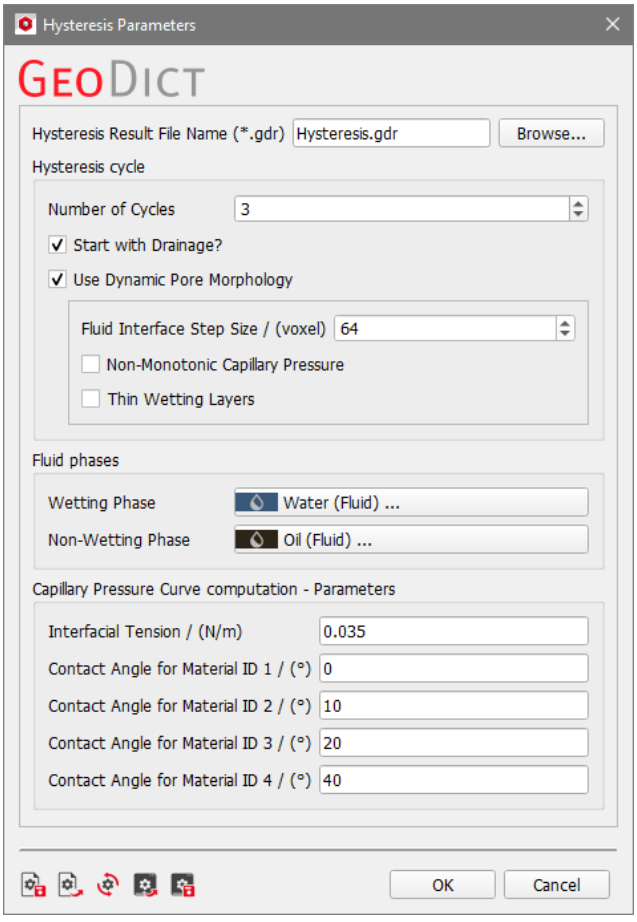
PREDEFINED

When **Predefined** is selected in the **SatuDict** section, predefined computation settings can be chosen from the pull-down menu in the **Predefined** panel: **Hysteresis**, **Mercury Intrusion Capillary Pressure**, **Resistivity Index Thin Film Model**, and **Trapping Curve**.

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



The SatuDict **Predefined** 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.

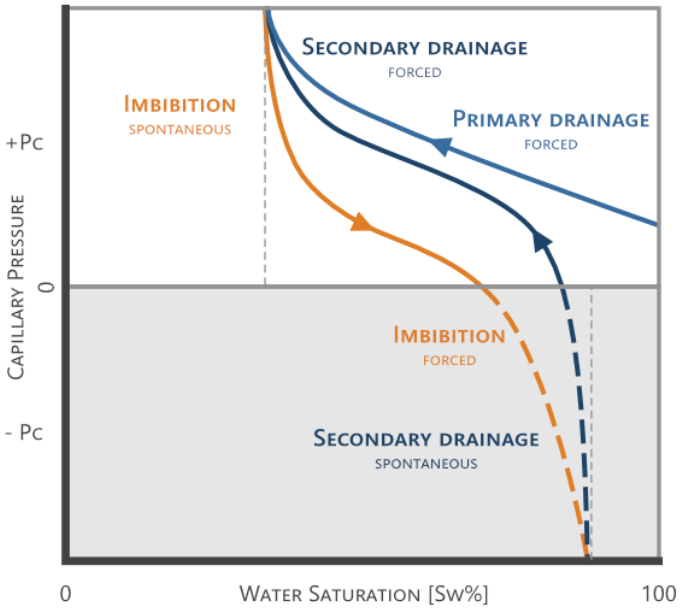
Click **OK** to close the dialog, and then **Run** to execute the computation.

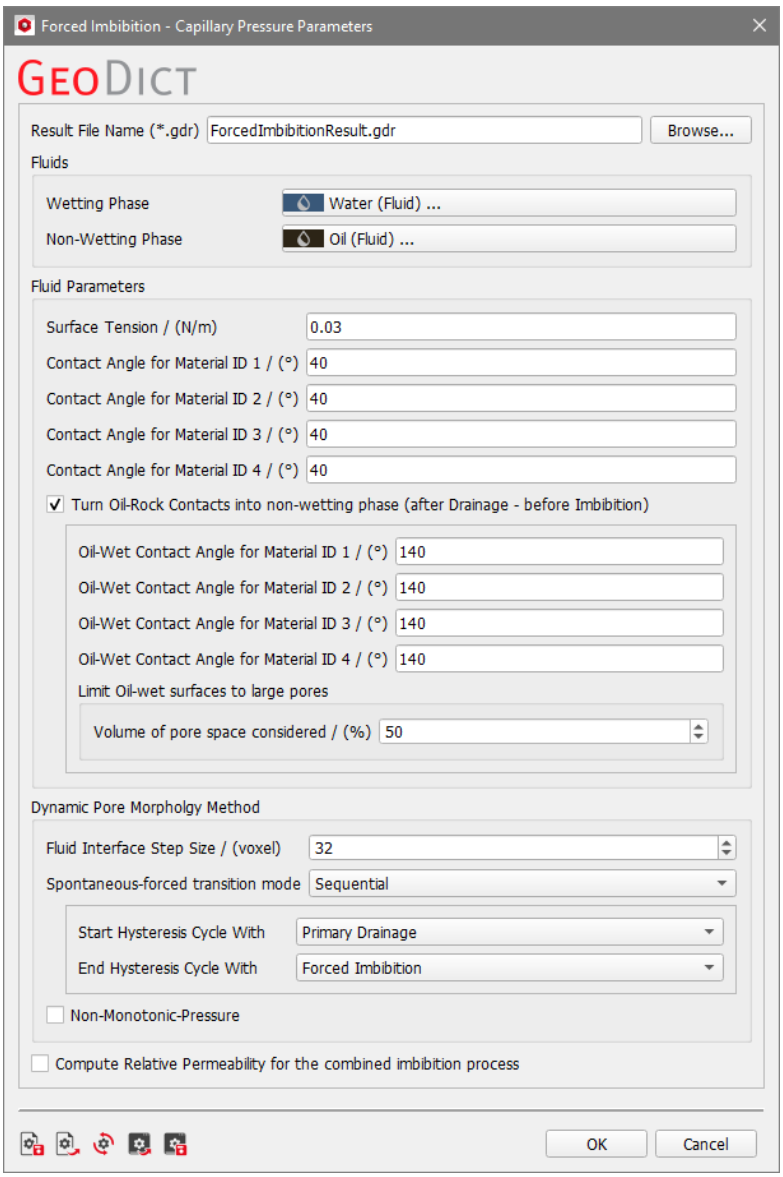
Forced Imbibition – Capillary Pressure

This script allows to simulate the capillary pressure curve in the case of mixed wettability of the considered structure e.g. if the fluid phases are water and oil. Both spontaneous and forced drainage and imbibition can be simulated, as shown in the figure on the right.

GeoDict predicts a capillary pressure hysteresis cycle with

1. Primary drainage simulation
2. Spontaneous and forced imbibiton
3. Spontaneous and forced drainage simulation.





The wetting-phase contact angle for up to four materials at the start of the simulation can be defined. After the drainage simulation, the app will turn some of the water-wet grain surfaces (i.e. where the contact angle is less than 90°) into oil-wet surfaces (i.e. where the contact angle is larger than 90°) where oil is in contact with a grain surface. Like this, water is non-wetting for this part of the structure for the following imbibition simulation. Check **Turn Oil-Rock Contact into non-wetting phase** and define now the contact angles larger than 90° for water.

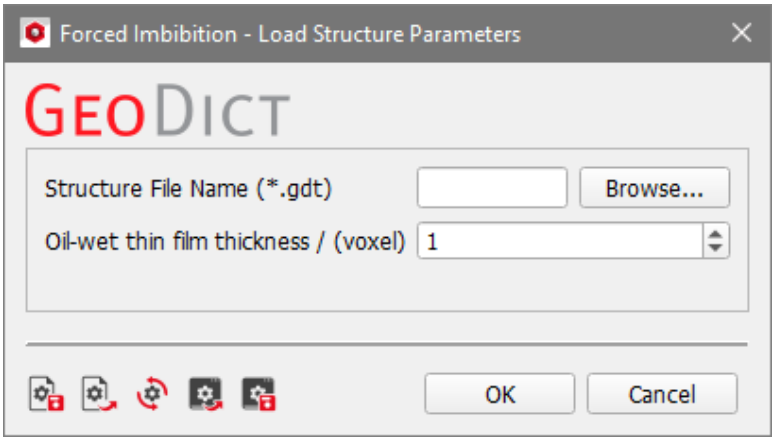
The simulation uses the Dynamic Pore Morphology Method. Start and End Hysteresis Cycle can be defined, and the computation of Non-Monotonic Pressure Curves can be selected. The tooltips in the **Forced Imbibition – Capillary Pressure Parameters** dialog show a more detailed explanation of the parameters selectable.

To compute the relative permeability for the combined imbibition process, check this option at the bottom of the dialog or compute the relative permeability later with the predefined script **Forced Imbibition – Relative Permeability**, see page 72.

Forced Imbibition – Load Structure

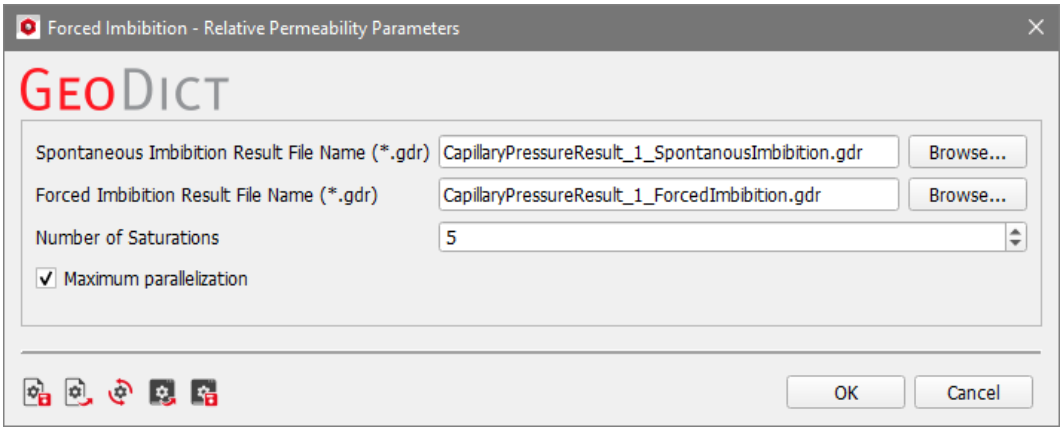
This script adjusts Material IDs and Material Colors to forced imbibition script defaults upon loading geometries (*.gdt).

Like all Forced Imbibition scripts, it is dedicated to oil and water setups!



Forced Imbibition – Relative Permeability

This script performs relative permeability computations for mixed wettability imbibition results obtained via the predefined function **Forced Imbibition – Capillary Pressure**, see page 71.



HYSTERESIS

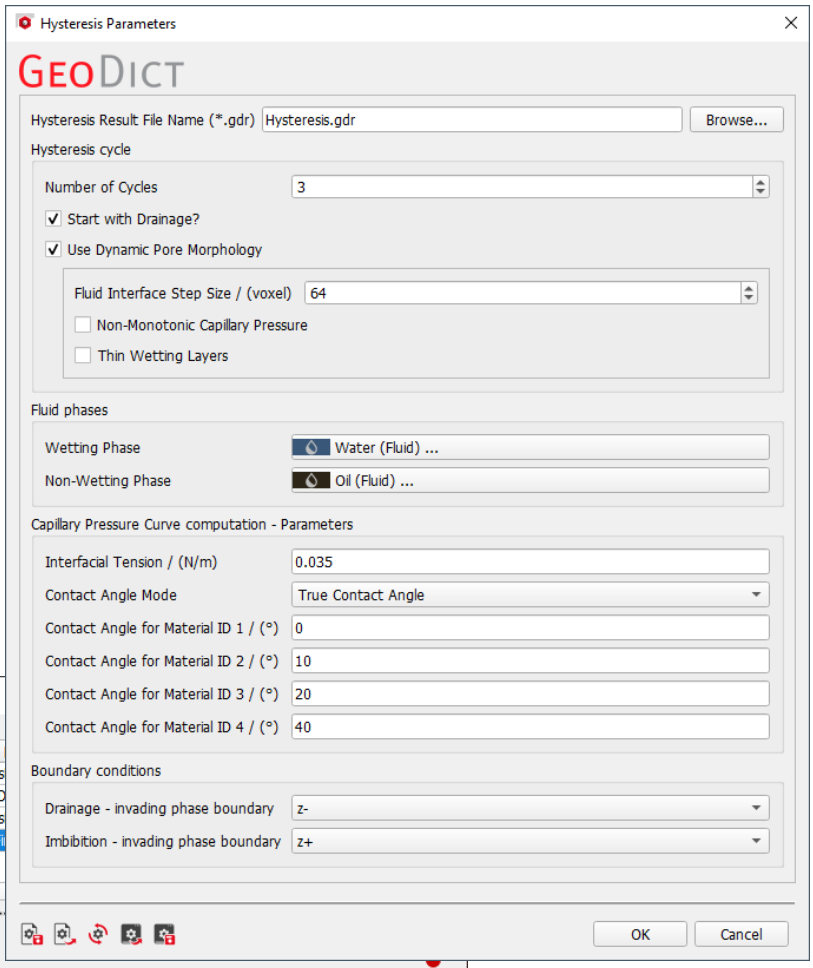
The **Hysteresis** predefined computation performs a Hysteresis simulation of the SatuDict functionalities Drainage and Imbibition (both with invading fluid connected to a reservoir and the replaced fluid can leave a residual) in succession.

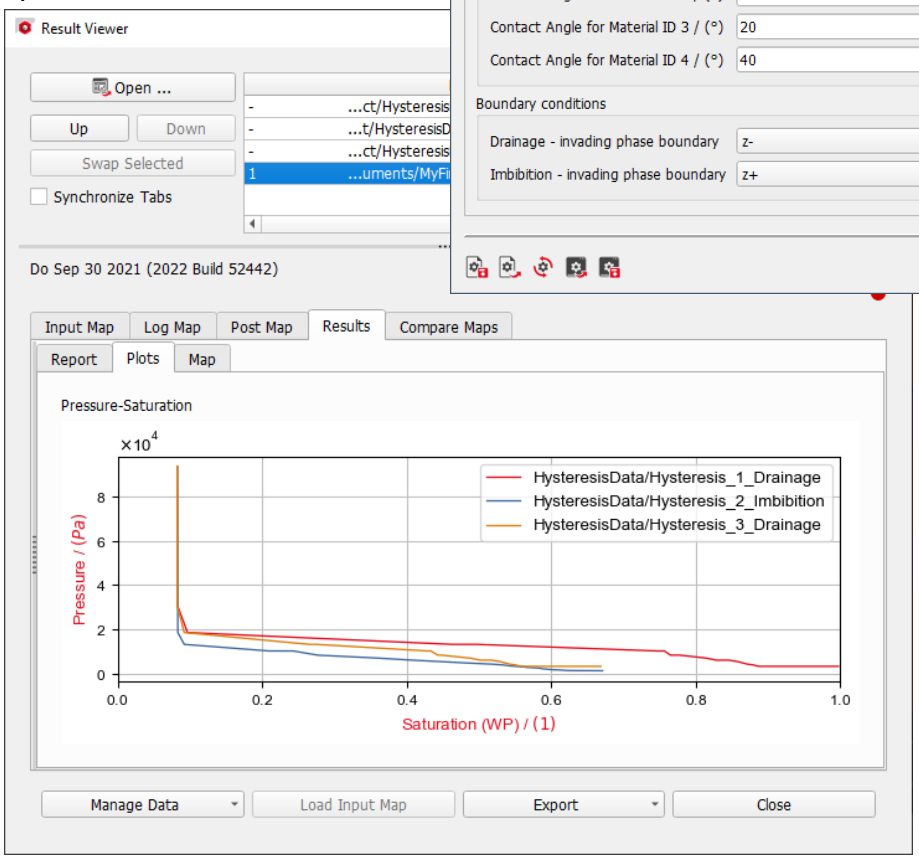
After clicking **Edit...**, enter the **Hysteresis Result File Name**, **Number of Cycles**, **Interfacial Tension**, and **Contact Angle**.

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.

Tooltips describe all those options in more detail.



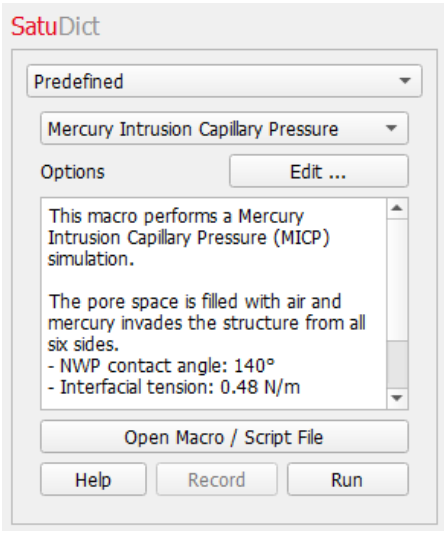


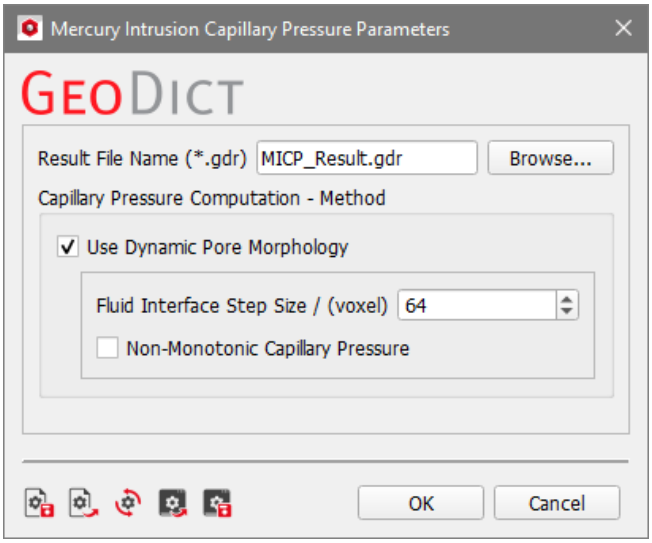
After the **Predefined - Hysteresis** has finished, the Result Viewer opens. The Header section box lists all the Imbibition and Drainage result files of each cycle. The hysteresis result file is an automatically combined result file showing the Pressure-Saturation curves in a single plot.

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 (Drainage I, see page 11), 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.

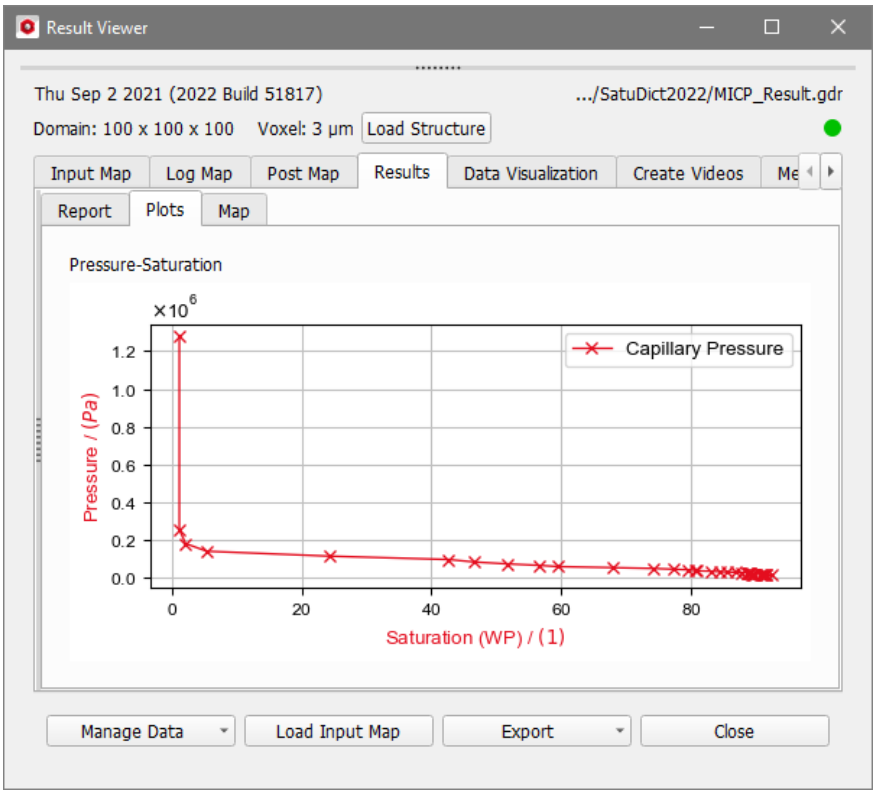
After clicking **Edit...**, the Result File Name can be changed. If **Use Dynamic Pore Morphology** is checked, parameters for this method can be defined.





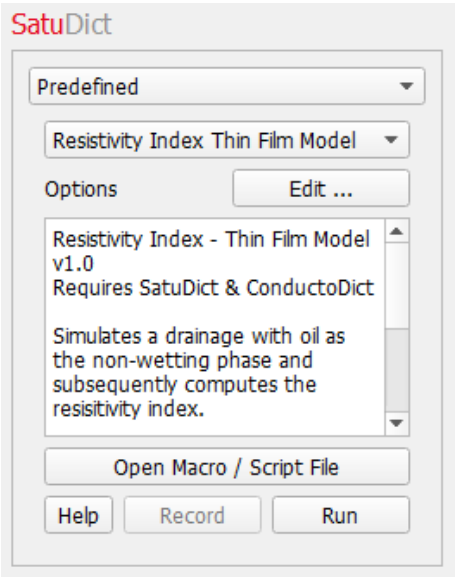
After the predefined simulation is finished, the Result Viewer opens showing the results from SatuDict Drainage simulation as seen on pages 18ff..

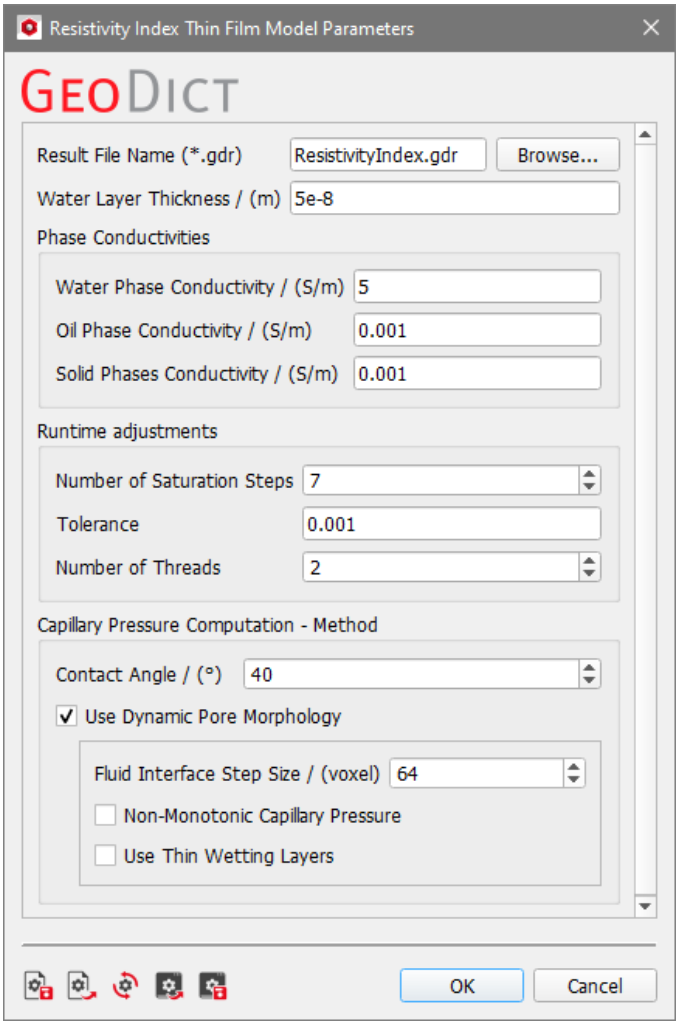
The saturation table and the capillary pressure curve are seen under the **Results – Report** and the **Results – Plots** tabs.



Resistivity Index Thin Film Model

The **Resistivity Index Thin Film Model** predefined computation accounts for thin water films on the mineral phase(s) by computing the effective fluid properties for voxels containing oil and the water film. This model simulates a drainage with oil as the non-wetting phase and subsequently computes the resistivity index.





After clicking **Edit...**, it is possible to modify the **Result File Name**, **Water Layer Thickness**, **Phase Conductivities**, **Number of Saturation Steps**, **Tolerance**, **Number of Threads** and the **Contact Angle**.

If **Use Dynamic Pore Morphology** is selected, parameters for this method can be defined as well.

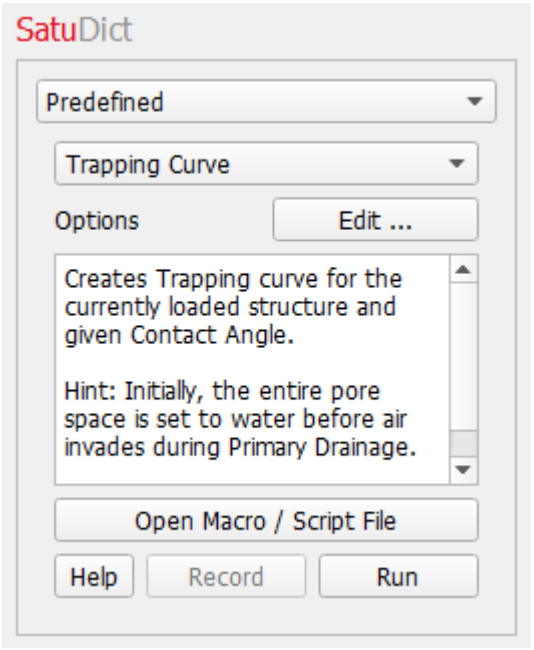
Tooltips describe all those options in more detail.

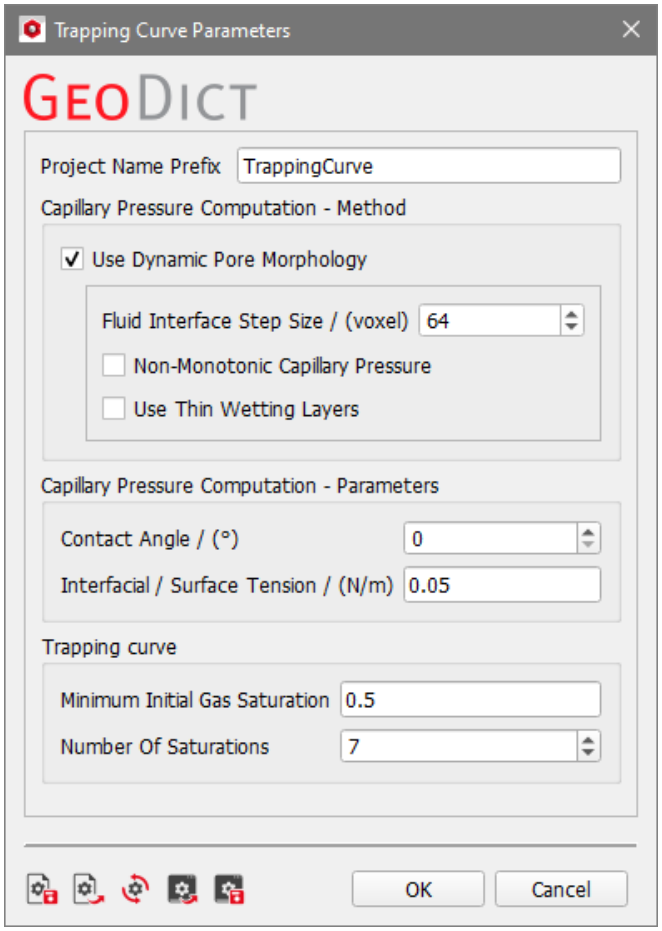
Results for the electrical conductivity computed, are shown in the same way as explained on page 66ff.

TRAPPING CURVE

The **Trapping Curve** predefined computation computes the trapping curve for the currently loaded structure and the given contact angle.

Initially, the entire pore space is set to water before air invades during a primary drainage simulation. For the **Number Of Saturations** defined in the **Trapping Curve Parameters** dialog, imbibition processes are simulated for different gas saturations and the residual gas saturation is computed.

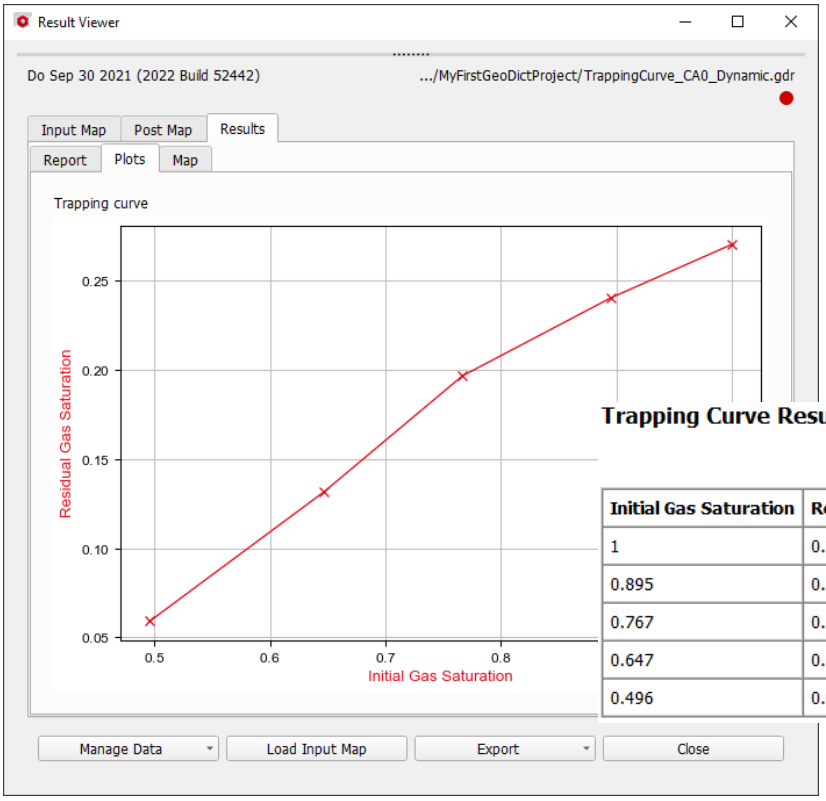




A **Project Name Prefix** for the result files created can be set in the **Trapping Curve Parameters** dialog, as well as the **Contact Angle**, **Interfacial / Surface Tension** and the **Minimum Initial Gas Saturation**.

If **Use Dynamic Pore Morphology** is selected, parameters for this method can be set as well.

In the **Results – Plots** tab of the Result Viewer, the Residual Gas Saturation is plotted over the Initial Gas Saturation. In the **Results - Report** tab, a table with the corresponding values is available.



Trapping Curve Results

Initial Gas Saturation	Residual Gas Saturation
1	0.27
0.895	0.24
0.767	0.197
0.647	0.132
0.496	0.059

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