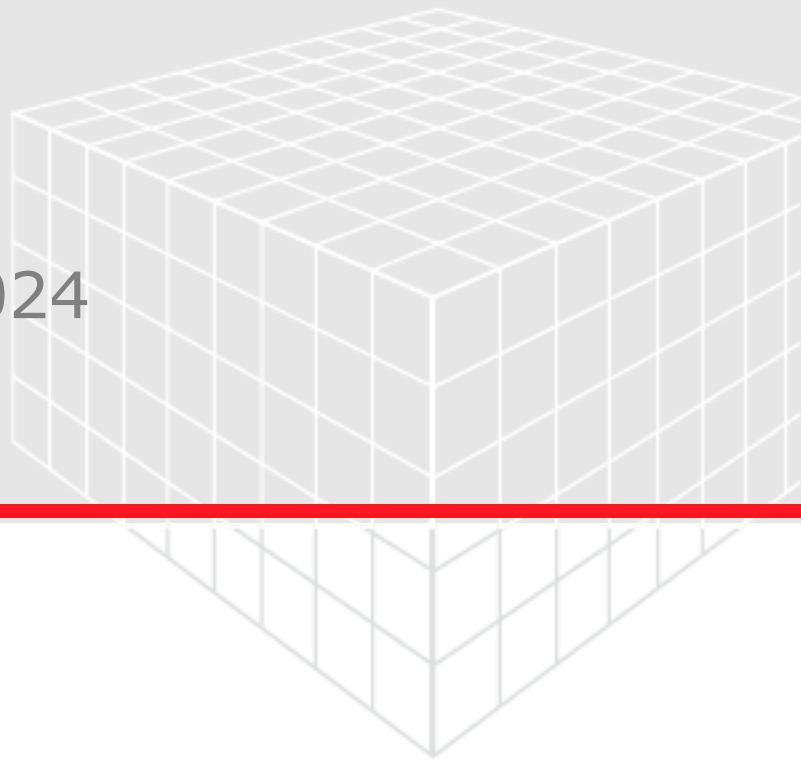


# SATUDICT

User Guide

GeoDict release 2024

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# ASSESSING SATURATION-DEPENDENT MATERIAL PROPERTIES IN POROUS MEDIA 1

## PORE MORPHOLOGY METHODS 3

QUASI-STATIC PORE MORPHOLOGY METHOD 4

DYNAMIC PORE-MORPHOLOGY METHOD WITH MONOTONIC CAPILLARY PRESSURE 5

DYNAMIC PORE-MORPHOLOGY METHOD WITH NON-MONOTONIC CAPILLARY PRESSURE 6

## MODEL FITS 7

THOMEER MODEL 7

LET MODEL 7

THIN FILM MODEL 8

## SATUDICT COMPUTATIONS 9

### SATUDICT SECTION 11

CAPILLARY PRESSURE CURVE 12

RELATIVE PERMEABILITY 35

RELATIVE GAS DIFFUSIVITY 50

RELATIVE THERMAL CONDUCTIVITY 56

RESISTIVITY INDEX 63

TWO-PHASE FLOW GEOAPPS 69

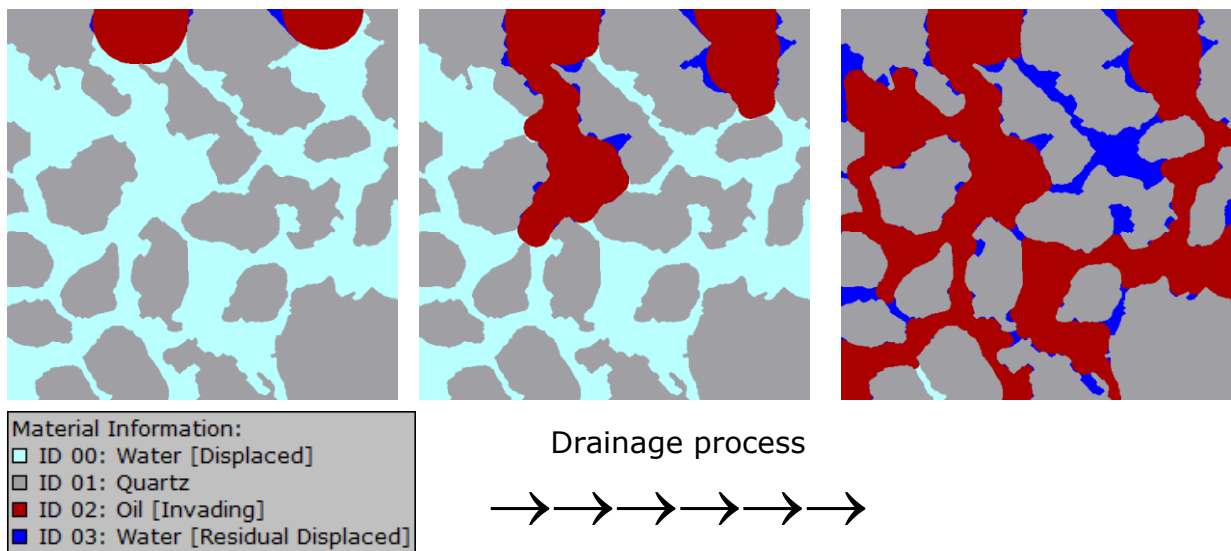
## REFERENCES 72

# ASSESSING SATURATION-DEPENDENT MATERIAL PROPERTIES IN POROUS MEDIA

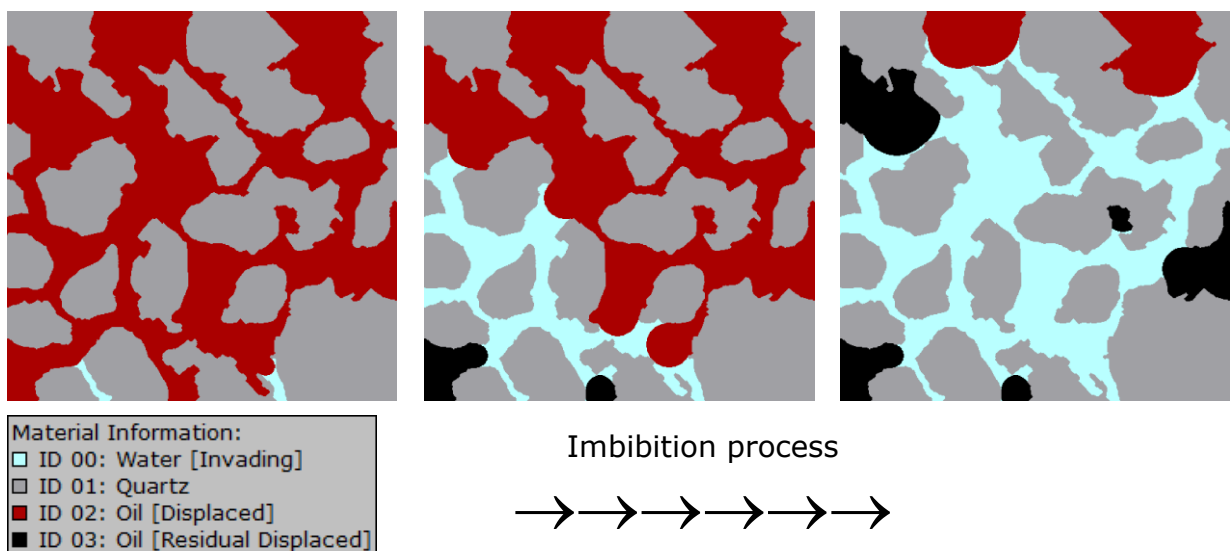
**SatuDict** is the **GeoDict** module for the computation of saturation-dependent material parameters in porous media. In many applications, the porous media is partly saturated, so that part of the pore space is filled with water and part with air, gas, or oil. Oil-water, water-air, or other two-phase 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 fluid.

For example, in a gas-diffusion layer (GDL) with hydrophobic fibers water is the non-wetting phase while air is the wetting phase. In contrast are digital rocks where water is the wetting phase and oil is the non-wetting phase.

**SatuDict** can calculate the phase distribution for the two types of phase displacement, namely Drainage and Imbibition. Below, they are shown with a digital rock.



Drainage displacement occurs when a non-wetting infiltrating fluid enters the porous media and displaces a wetting fluid that has saturated the media.



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.

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 the **Pore Morphology** method to determine the distribution of the two phases inside the porous media.

The **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,

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

where  $\sigma$  is the surface tension,  $\alpha$  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. The contact angle  $\alpha$  can be different at each solid phase inside the porous medium [2] and, thus, variable wettability can be incorporated.

Two versions of the pore morphology method are available in GeoDict: The **Quasi-Static Pore Morphology Method** and the **Dynamic Pore Morphology Method**.

In the **Quasi-Static Pore Morphology Method**, the capillary pressure is increased (or decreased) strictly monotonically. This 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, thin wetting layers can also be considered for imbibition processes by means of 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.

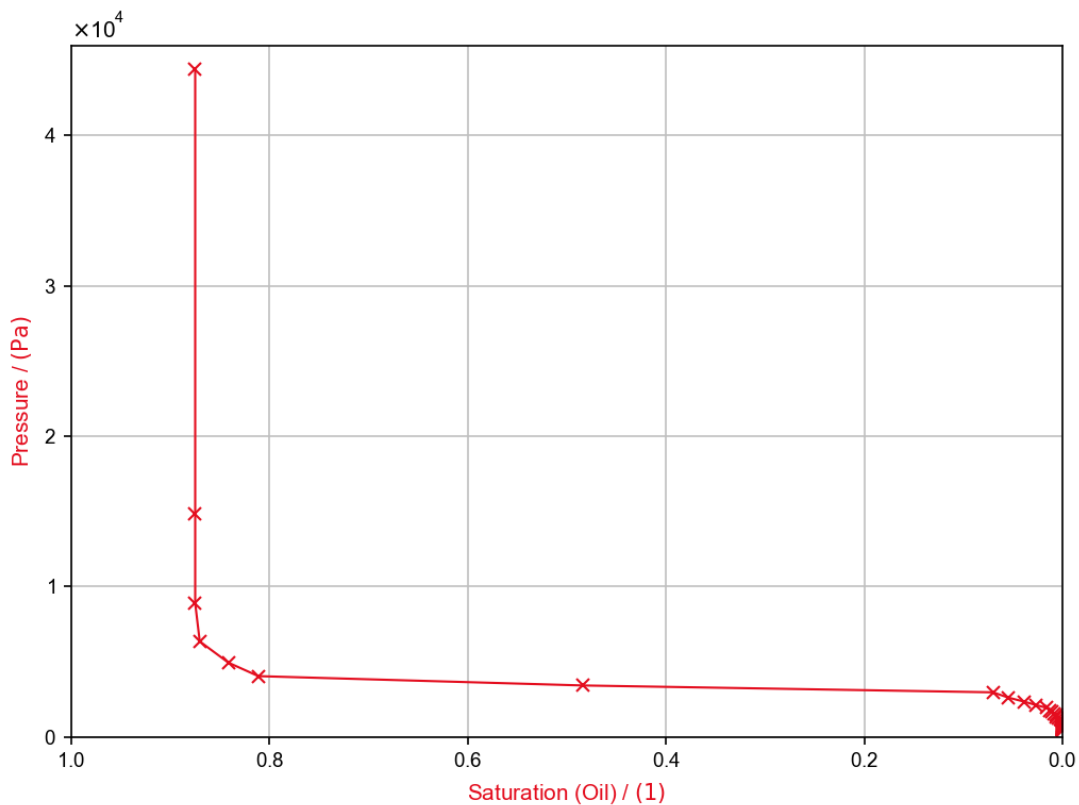
In the following, an example of the resulting capillary pressure curve of a drainage simulation with all three methods is shown below.

## QUASI-STATIC PORE MORPHOLOGY METHOD

With this method, the capillary pressure for a drainage simulation is strictly 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 strictly monotonically decreasing. At each simulation step, the capillary pressure is decreased by a fixed value. This leads to the effect, that small pores beyond big pore bodies are filled at once when the capillary pressure is small enough.

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

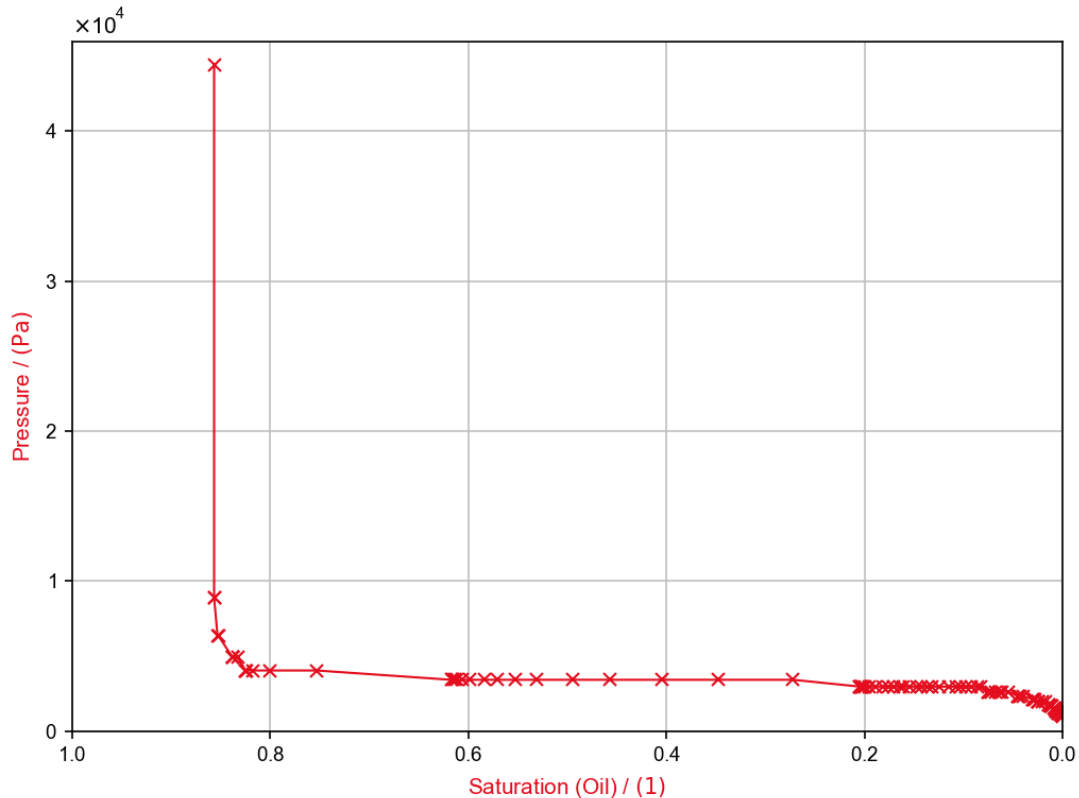


This method is useful for the prediction at which capillary pressure the breakthrough occurs and provides detailed information about fluid distributions for high and low saturated structures. If the detailed fluid distribution at a broad range of saturations is of interest, this method should not be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

## DYNAMIC PORE-MORPHOLOGY METHOD WITH MONOTONIC CAPILLARY PRESSURE

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

For imbibition simulations, the capillary pressure is monotonically decreasing.



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

This method predicts a more accurate fluid movement compared to the quasi-static pore morphology method. It should be used if a detailed fluid distribution at a broad range of saturations is of interest.

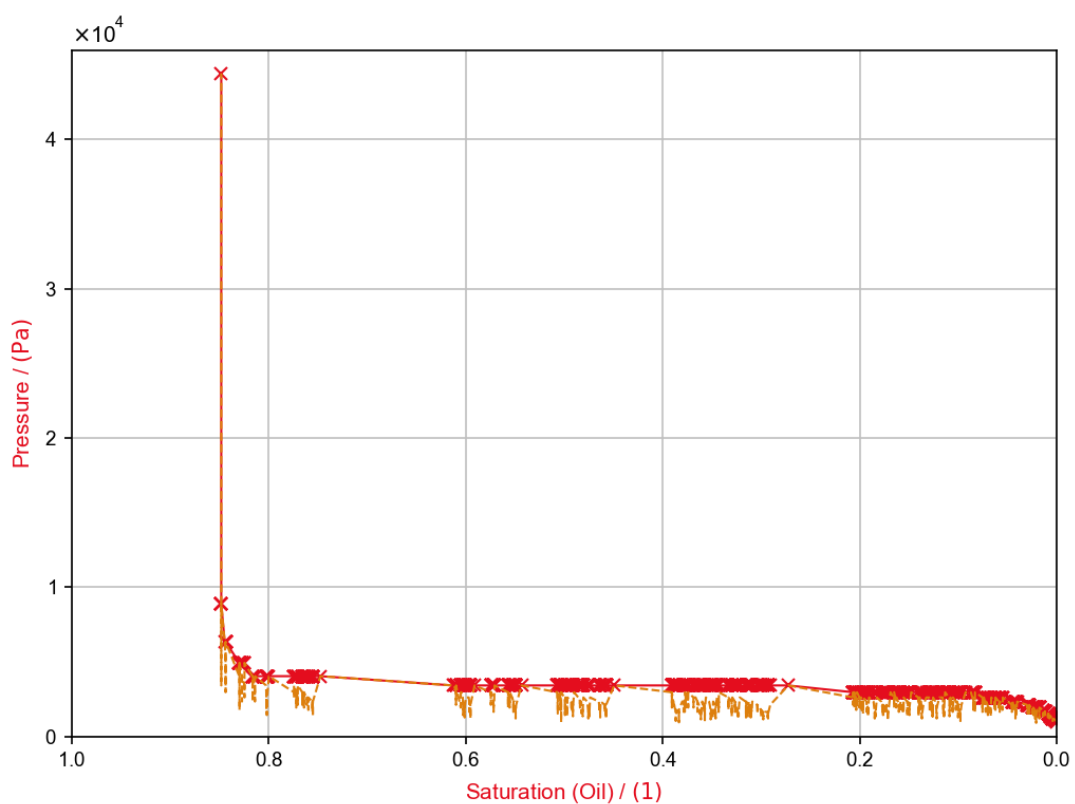
However, certain physical phenomena, e.g., formation of water droplets above a fiber structure with large pore space at the top, cannot be modelled with this method. This requires that the capillary pressure can have a non-monotonic behavior.

### DYNAMIC PORE-MORPHOLOGY METHOD WITH NON-MONOTONIC CAPILLARY PRESSURE

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

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

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



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

## MODEL FITS

### THOMEER MODEL

Since GeoDict 2023, for drainage simulations without residual of the displaced fluid, a **Thomeer Model** [5] can be fitted to the capillary pressure curve.

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

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

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

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

This feature requires a special license. Please contact our support at [support@math2market.de](mailto:support@math2market.de) for more information.

### LET MODEL

For Relative Permeability computations an **LET Model** [20] can be used to approximate relative permeability curves.

The LET-type approximation is described by 3 parameters L, E, T. The correlation for water relative permeability with water injection is thus:

$$K_{rw} = \frac{K_{rwr} S_{wn}^{L_w}}{S_{wn}^{L_w} + E_w (1 - S_{wn})^{T_w}} \quad (3)$$

and

$$K_{row} = \frac{K_{rot} (1 - S_{wn})^{L_o}}{(1 - S_{wn})^{L_o} + E_o S_{wn}^{T_o}} \quad (4)$$

For the oil relative permeability, where:

$$S_{wn} = \frac{S_w - S_{wir}}{S_{wor} - S_{wir}} \quad (5)$$

is the normalized water saturation value  $S_w$ . Only  $S_{wir}$  (irreducible water saturation),  $S_{orw}$  (irreducible oil saturation),  $K_{rot}$  (maximal oil permeability), and  $K_{rwr}$  (maximal water permeability) have direct physical meaning.

The parameters L, E and T are empirical. The parameter L describes the lower part of the curve. The parameter T describes the upper part (or the top part) of the curve in a similar way that the L-parameter describes the lower part of the curve. The parameter E describes the position of the slope (or the elevation) of the curve.

### THIN FILM MODEL

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

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

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

$$K_{ws} = \frac{t \cdot 0.5}{h} K_w + \frac{h - t \cdot 0.5}{h} K_s, \quad K_{wo} = \frac{t \cdot 0.5}{h} K_w + \frac{h - t \cdot 0.5}{h} K_o \quad (6)$$

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

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## SATUDICT COMPUTATIONS

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

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

Regarding the permeability, the values computed with **SatuDict** 2024 and displayed in the GDR result file include the relative permeability and the saturation-dependent permeability (shown as Effective Permeability under the Results-Report tab). See the GDR result file in detail below on page [46](#).

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

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

$$\frac{K_s}{K_1} \in [0,1] \quad (7)$$

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 Flow permeability section of the [FlowDict](#) handbook of the User Guide. 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.

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

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

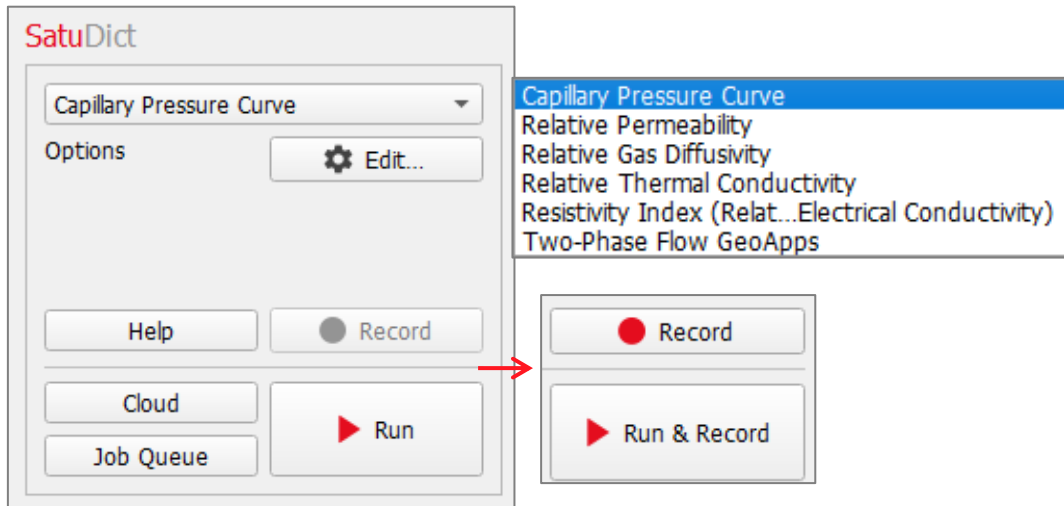
- **Determine saturation-dependent (relative) thermal conductivity, and resistivity index.** **SatuDict** calculates the saturation-dependent thermal conductivity and the resistivity index as in **ConductoDict** (see [\[4\]](#) and the [ConductoDict](#) handbook of the User Guide). The thermal conductivity 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.

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

**SATUDICT SECTION**

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



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

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

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

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



### CAPILLARY PRESSURE CURVE

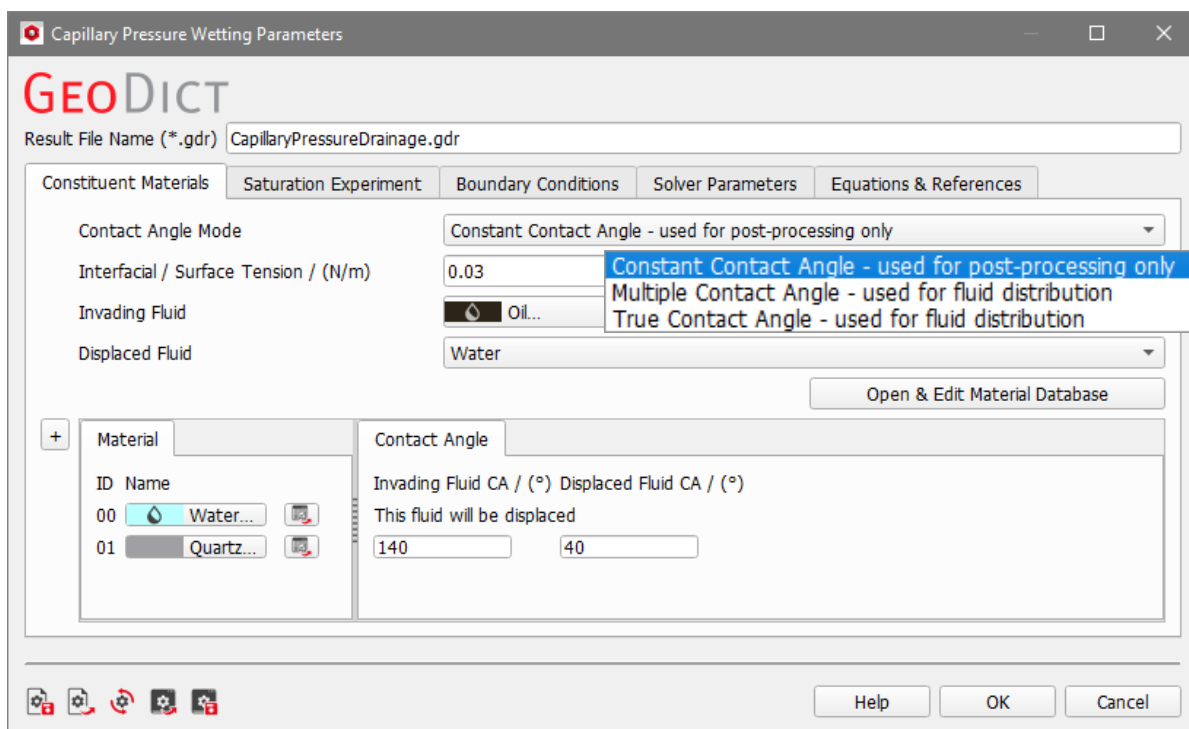
When selecting **Capillary Pressure Curve** from the pull-down menu, the **Wetting Parameters** needed for running this process can be entered (or modified) through the **Edit...** button.

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

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

### CONSTITUENT MATERIALS

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



### CONTACT ANGLE MODE

The **Contact Angle Mode** can be selected as:

- 1. Constant Contact Angle.** In this default setting, for the Pore Morphology method, a single (constant) contact angle is assumed between all solid materials and the invading fluid, and another constant contact angle between all solid materials and the displaced fluid. The given contact angle is considered for the computation of the capillary pressure in the post processing, but a contact angle of  $0^\circ$  is used for the distribution of the fluids!
- 2. Multiple Contact Angle.** For a more general Pore Morphology method, different (multiple) contact angles are specified for every solid material with the invading

fluid and the displaced fluid. The contact angles of every material can be entered under the **Contact Angle** tab on the right-hand side below. The different contact angles are considered for the computation of the capillary pressure and for the distribution of the fluids. Surfaces of solid materials are assumed to be planar for this approach.

3. **True Contact Angle.** In the same way as for **Multiple Contact Angle**, contact angles for every solid material with the invading and the displaced fluid can be defined. To inscribe fluids with a more accurate contact angle, the curvature of the surface of solid materials is considered. For contact angles near 90°, the artefacts occurring for the Multiple Contact Angle method are avoided.

### INTERFACIAL / SURFACE TENSION

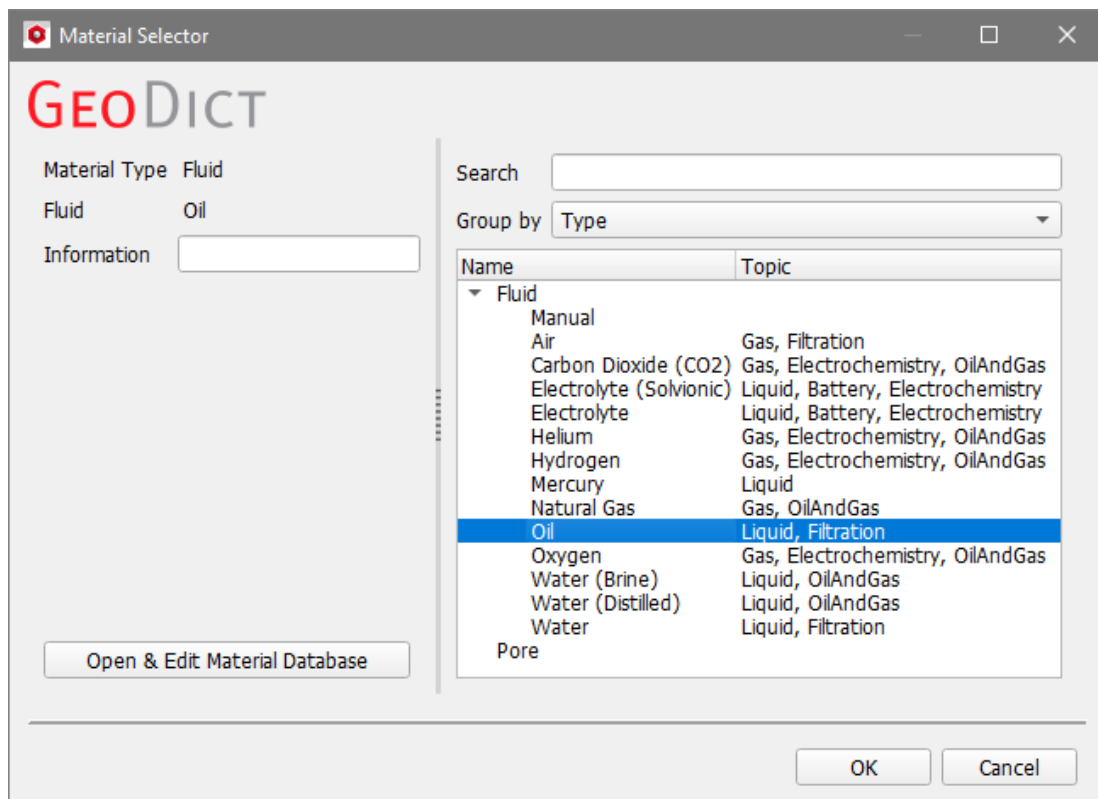
Enter the **Interfacial / Surface Tension** between the invading and displaced fluid or use the default value corresponding to the surface tension between water and air.

### INVADING FLUID AND DISPLACED FLUID

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

Invading Fluid

Displaced Fluid

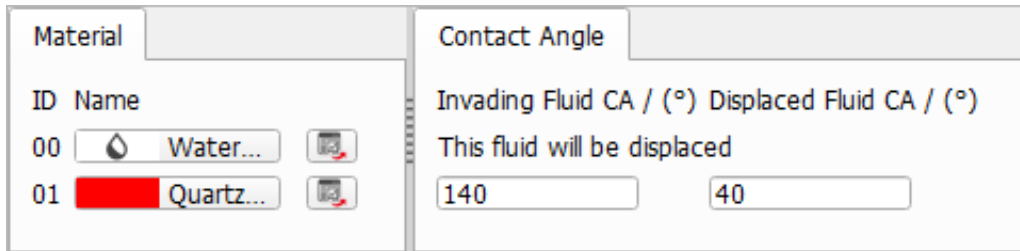


The **Displaced Fluid** must already be present in the model of the structure currently in memory. Choose the displaced fluid from the pull-down menu.

**MATERIAL AND CONTACT ANGLE**

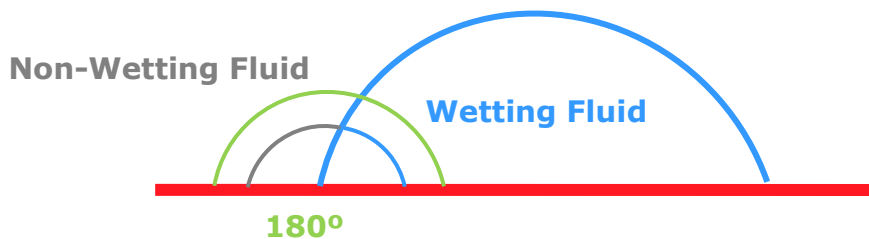
The **Contact Angle** can be entered for all solid materials (after choosing Constant Contact Angle as Contact Angle Mode) or for each solid material separately (after choosing Multiple Contact Angle or True Contact Angle as Contact Angle Mode).

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

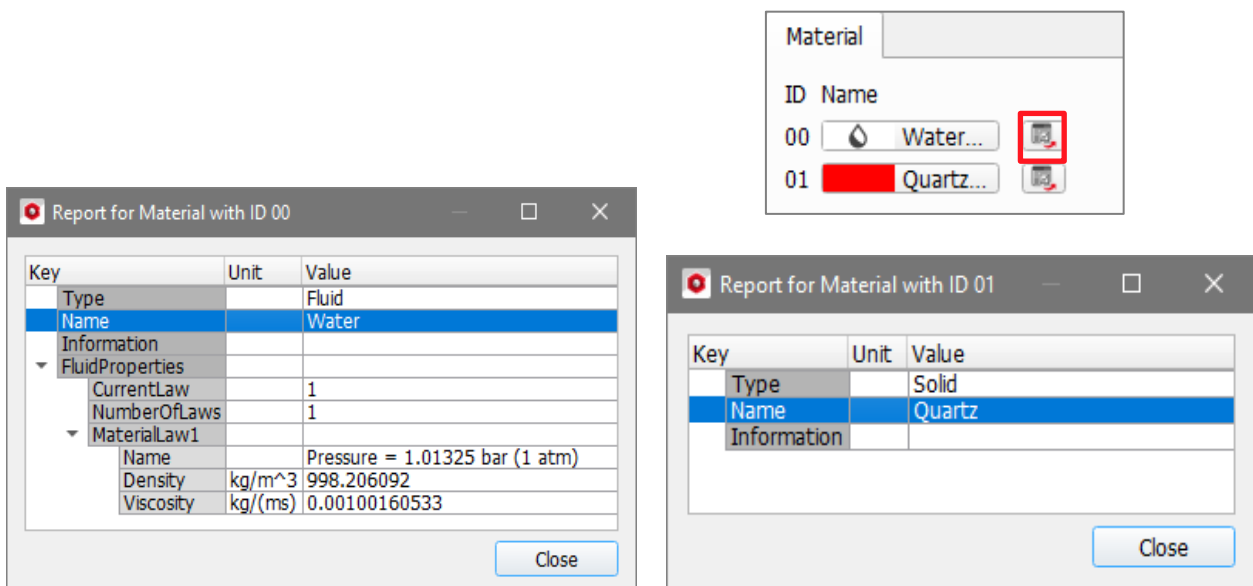


The **Invading Fluid CA** (Contact Angle) and the **Displaced Fluid CA** values add up to 180° and they are adjusted automatically when changing one of the two values. For a given solid material phase, the fluid with a contact angle smaller than 90° is **wetting** and the other fluid (with contact angle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

It is possible to enter contact angles smaller or greater than 90°. For contact angles close to 90° we strongly recommend using the True Contact Angle method. A contact angle equal to 90° is possible but challenging for the Pore Morphology method. For these cases, capillary forces may not be dominant anymore which is a basic assumption of the method.

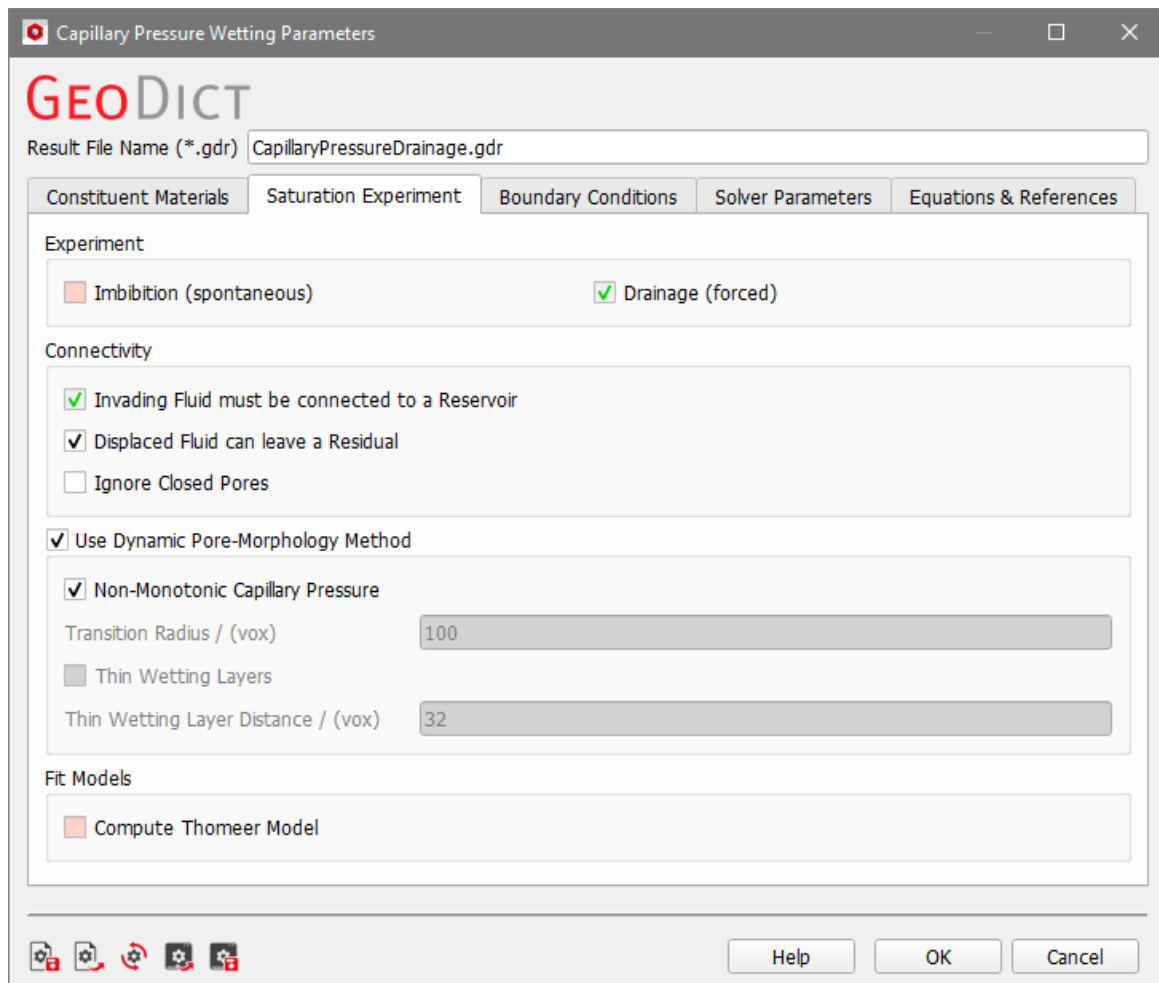


Click the Material Report button to see the relevant parameters for the materials.



## SATURATION EXPERIMENT

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



### EXPERIMENT

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

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

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

### CONNECTIVITY

The pore size and the pore connectivity to the Invading Fluid reservoir or Displaced Fluid reservoir determine the final distribution of the phases.

Check **Invading Fluid must be connected to a Reservoir** to connect the invading fluid continuously to a phase reservoir at a given spatial location outside of the domain (defined in the **Boundary Conditions** tab, see page [17](#)). If this is unchecked, it

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

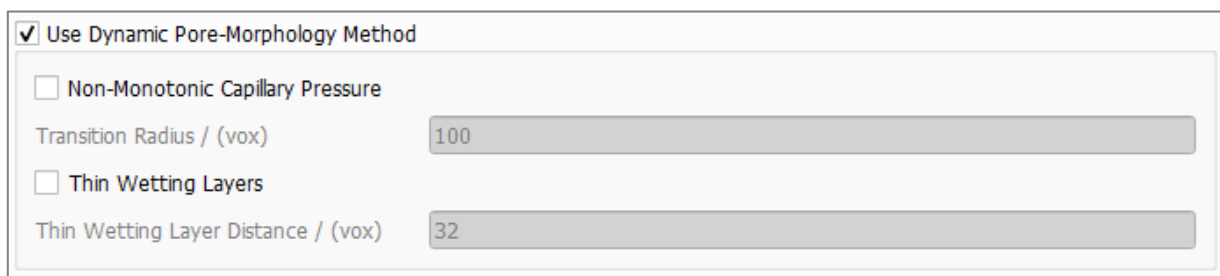
Check **Displaced Fluid can leave a Residual** if the displaced fluid is allowed to leave a residual in pores that are separated from the displaced fluid reservoir, e.g., by the invading fluid. In this case, the displaced fluid needs to be connected to a reservoir, also defined in the **Boundary Conditions** tab, see page [17](#). The residual of the displaced fluid is assigned a new material ID. In general, it is recommended to enable this option. Disable this option for mercury intrusion capillary pressure experiments where mercury invades the pore space and displaces vacuum.

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

### DYNAMIC PORE-MORPHOLOGY METHOD

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Check **Use Dynamic Pore-Morphology Method** to use this method for dynamic simulation of the drainage and imbibition processes (see also page [5ff.](#)).



Use Dynamic Pore-Morphology Method

Non-Monotonic Capillary Pressure

Transition Radius / (vox)

Thin Wetting Layers

Thin Wetting Layer Distance / (vox)

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

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

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

### FIT MODELS

---

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

This option computes the Thomeer Model based on the computed capillary pressure curves, see page 7.

Fit Models

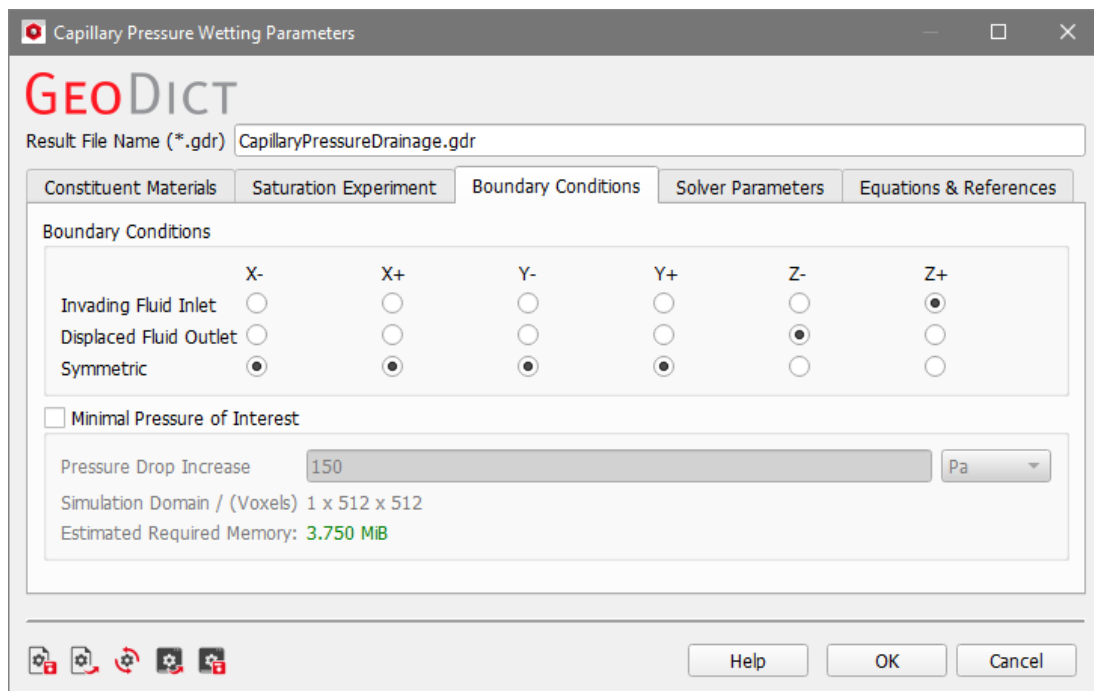
Compute Thomeer Model

## BOUNDARY CONDITIONS

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

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

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



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

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

Minimal Pressure of Interest

Pressure Drop Increase: 300 Pa

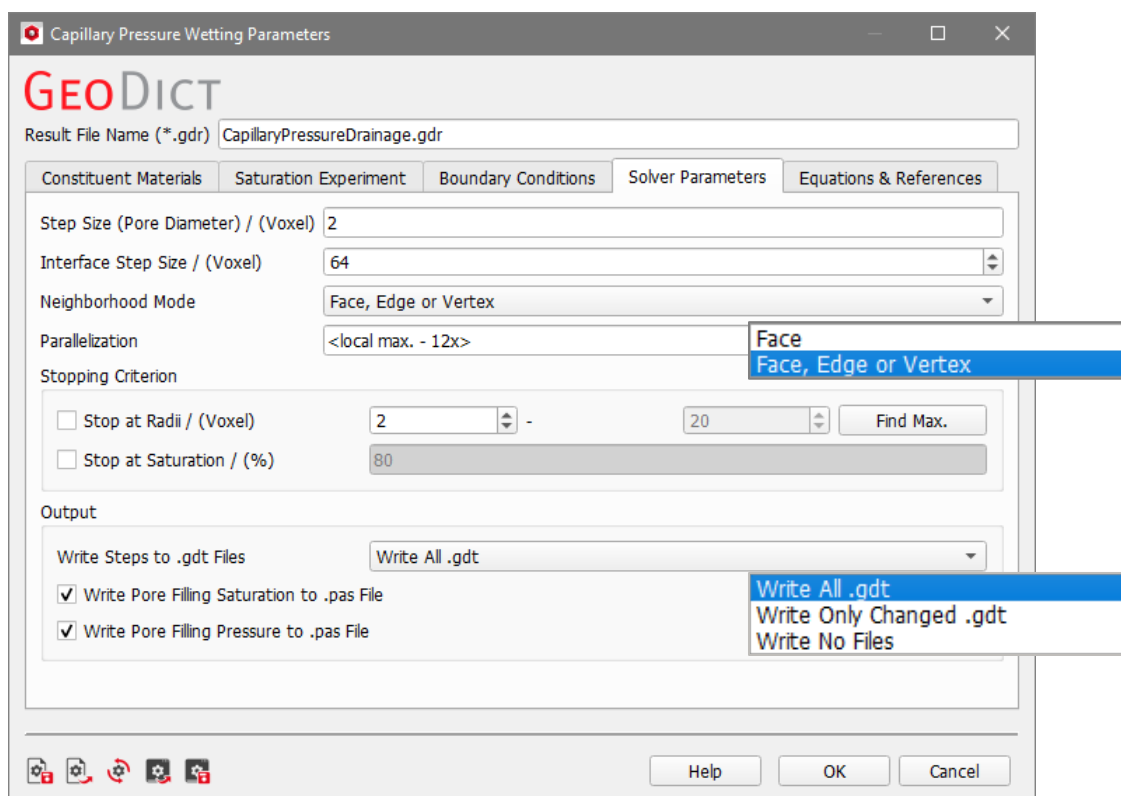
Simulation Domain / (Voxels) 1 x 512 x 1014

Estimated Required Memory: 7.427 MiB

### SOLVER PARAMETERS

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

#### STEP SIZE (PORE DIAMETER)



The pore diameter, together with the connectivity rule based on the Neighborhood Mode and the defined contact angles, determine the distribution of the invading fluid and displaced fluid phases.

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

#### INTERFACE STEP SIZE

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

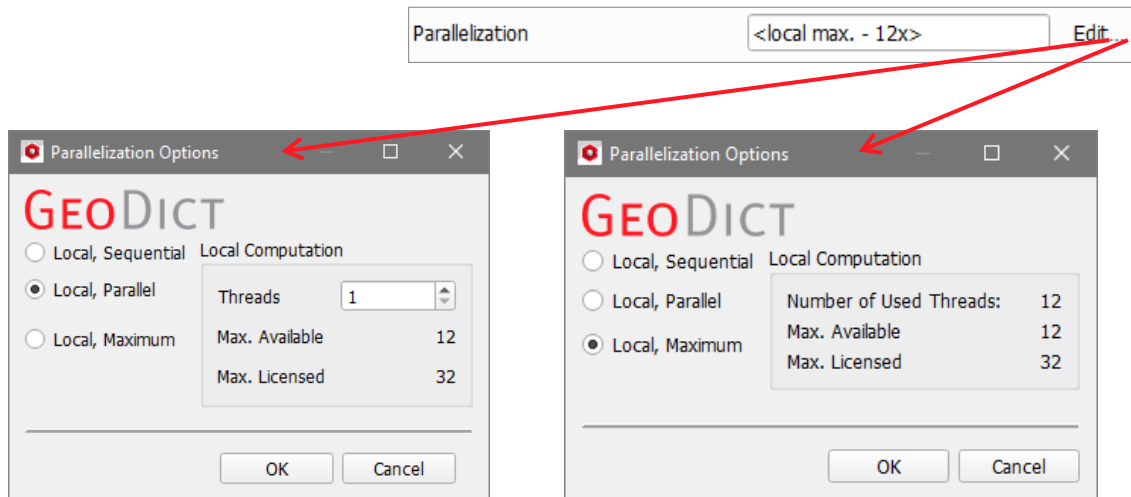
#### NEIGHBORHOOD MODE

The **Neighborhood Mode** determines how the voxels of the material occupying the pore space in the porous media are perceived as belonging to a connected group. Checking **Face** is more restrictive than choosing **Face, Edge, or Vertex**. See more

details on the neighborhood mode in the [MatDict](#) handbook of the User Guide (Connected Components) and the [ProcessGeo](#) handbook of the User Guide (Cleanse command).

## PARALLELIZATION

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



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

When **Local, Parallel** is selected, the number of **Threads** to be used for the calculation can be entered. Then the maximum number of available processors and the maximum number of licensed parallel processes is shown in the dialog.

**Local, Maximum** sets the number of used processes to the maximum possible number, restricted by the hardware and number of licensed processes.

## STOPPING CRITERION

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

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

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

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

## OUTPUT

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

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

Depending on inlet and step size, different steps might lead to the same .gdt file. With **Write Only Changed .gdt** selected, only .gdt files that differ from previous ones are written to the hard drive. The result is a reduction in hard disk space consumption and a slight reduction in battery life.

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

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

## EQUATIONS & REFERENCES

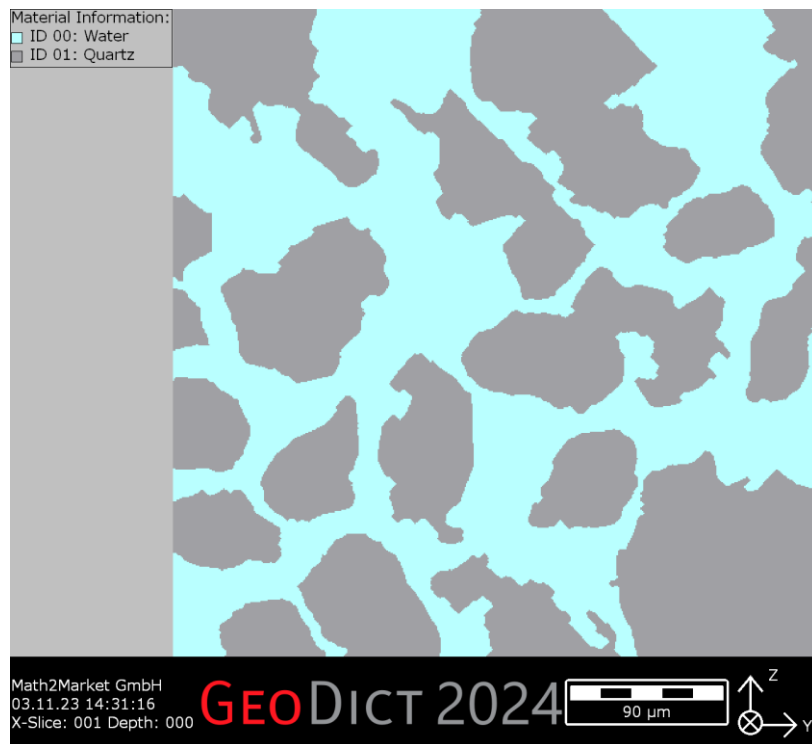
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The **Equations & References** tab provides information about the methods used during this command. The references can also be found at the end of this handbook, in the [References](#) section.

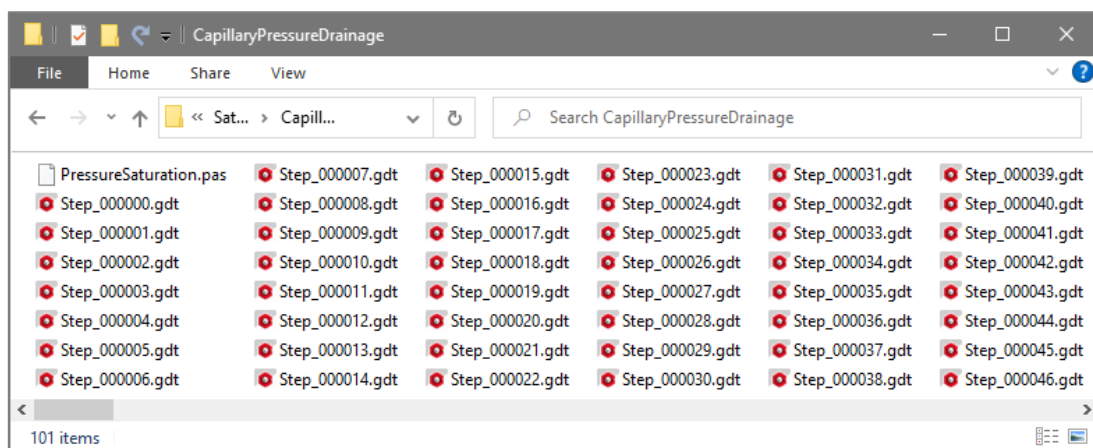
## CAPILLARY PRESSURE CURVE RESULT FILE

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

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

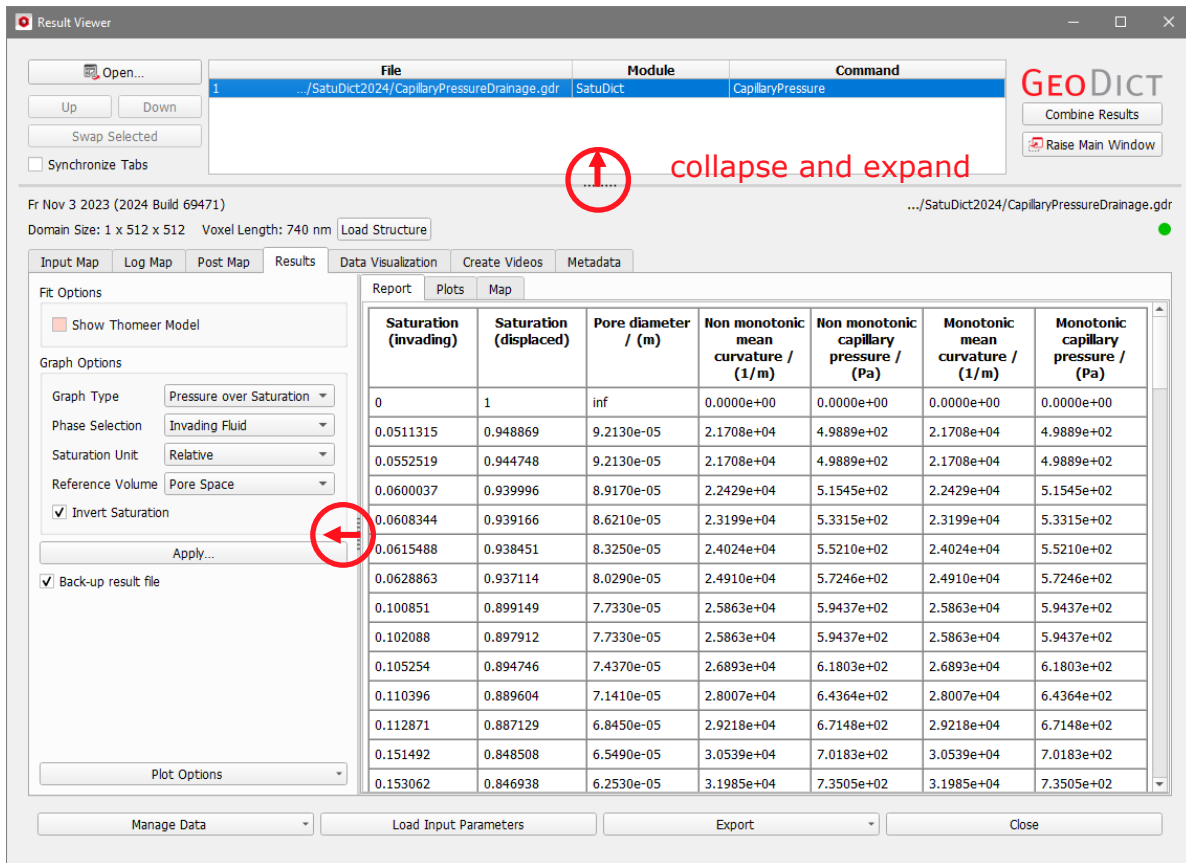


The GDT files corresponding to the computational steps (Step\_000000.gdt, etc.) are stored in the automatically created result folder with the name of the result file name in the project folder.



This is only done if **Write All .gdt** or **Write Only Changed .gdt** was selected in the Solver Parameters tab, see page 19). This folder also contains the **PressureSaturation.pas** file and the Structure.gdt file, with the original structure, before the drainage simulation is started.

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



The results are organized in the tabs **Input Map**, **Log Map**, **Post Map**, **Results**, **Data Visualization**, **Create Videos** and **Metadata**. The computational results can be accessed through the Results tab, additional files to visualize the results can be loaded through the Data Visualization tab and videos of the results can be generated through the Create Videos tab. All these mentioned tabs are explained in the following.

## RESULTS

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

### Report

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

For a typical capillary pressure result file, the table shows the **Saturation** of the invading fluid, the saturation of the displaced fluid, the **Mean curvature** and the calculated corresponding **Capillary pressure** for every step (pore size). The mean curvature approximates the fluid-fluid interface curvature.

If the Dynamic Pore-Morphology Method with the option Non-Monotonic Capillary Pressure was used for the computation, mean curvature and capillary pressure values are shown for both the monotonic and non-monotonic capillary pressure curve.

For computations with the Contact Angle Method **Constant Contact Angle** also the **Pore diameter** is shown in the table. This is the diameter of the pores filled in this saturation step.

Saturation (invading)	Saturation (displaced)	Pore diameter / (m)	Non monotonic mean curvature / (1/m)	Non monotonic capillary pressure / (Pa)	Monotonic mean curvature / (1/m)	Monotonic capillary pressure / (Pa)
0	1	inf	0.0000e+00	0.0000e+00	0.0000e+00	0.0000e+00
0.0511315	0.948869	9.2130e-05	2.1708e+04	4.9889e+02	2.1708e+04	4.9889e+02
0.0552519	0.944748	9.2130e-05	2.1708e+04	4.9889e+02	2.1708e+04	4.9889e+02
0.0600037	0.939996	8.9170e-05	2.2429e+04	5.1545e+02	2.2429e+04	5.1545e+02
0.0608344	0.939166	8.6210e-05	2.3199e+04	5.3315e+02	2.3199e+04	5.3315e+02
0.0615488	0.938451	8.3250e-05	2.4024e+04	5.5210e+02	2.4024e+04	5.5210e+02
0.0628863	0.937114	8.0290e-05	2.4910e+04	5.7246e+02	2.4910e+04	5.7246e+02
0.100851	0.899149	7.7330e-05	2.5863e+04	5.9437e+02	2.5863e+04	5.9437e+02
0.102088	0.897912	7.7330e-05	2.5863e+04	5.9437e+02	2.5863e+04	5.9437e+02
0.105254	0.894746	7.4370e-05	2.6893e+04	6.1803e+02	2.6893e+04	6.1803e+02
0.110396	0.889604	7.1410e-05	2.8007e+04	6.4364e+02	2.8007e+04	6.4364e+02
0.112871	0.887129	6.8450e-05	2.9218e+04	6.7148e+02	2.9218e+04	6.7148e+02
0.151492	0.848508	6.5490e-05	3.0539e+04	7.0183e+02	3.0539e+04	7.0183e+02
0.153062	0.846938	6.2530e-05	3.1985e+04	7.3505e+02	3.1985e+04	7.3505e+02
0.154499	0.845501	5.9570e-05	3.3574e+04	7.7157e+02	3.3574e+04	7.7157e+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,  $(\text{Pore Diameter})/(\text{Structure Diameter})$  should always be smaller than  $2 \cdot \cos(\theta)/(1 - \cos(\theta))$ , where  $\theta$  is the wetting phase contact angle.  
 For the current geometry, this requirement is not met and the solution may contain numerical artifacts!  
 Recommendation: Use smaller contact angles or use the true contact angle method so resolve that issue.

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

Two main components of the multiple contact angle method are a dilation and an erosion process. At high contact angles, the dilation radius can become much larger than the erosion radius. For solid objects in the structure with diameters much smaller than the maximum pore diameter, this can lead to artifacts in the fluid distribution

## Assessing saturation-dependent material properties

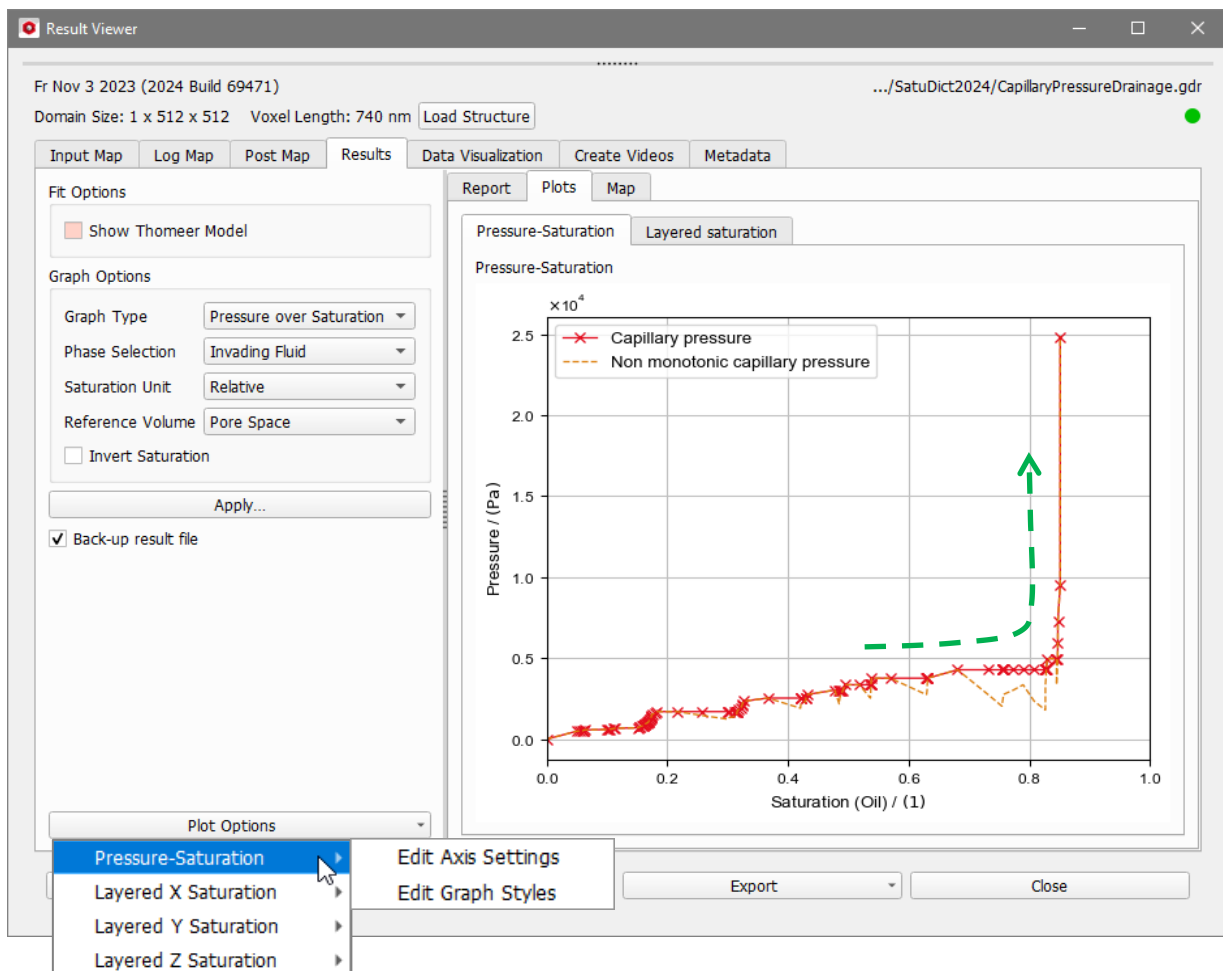
such as higher than desired contact angles, larger saturation steps and fewer saturation steps.

This happens if the ratio between pore diameter and diameter is larger than  $2 * \frac{\cos(\theta)}{1 - \cos(\theta)}$ .  
With the **True Contact Angle** method, this problem can be avoided.

### Plots

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

At the left side of the Result Viewer, the user can modify the way the graph is displayed by selecting **Graph Type** (Pressure over Saturation or Saturation over Pressure), **Phase Selection** (Invading Fluid or Displaced Fluid), **Saturation Unit** (Relative or Absolute) and Reference Volume (Pore Space, Pore Space (Thomeer), or Total Sample Volume). The option Pore Space (Thomeer) is only available after a Drainage simulation without residual of the displaced fluid was performed.



If a Thomeer Model is fitted, see page [7](#), this model can be shown by checking **Show Thomeer Model** under **Fit Options**.

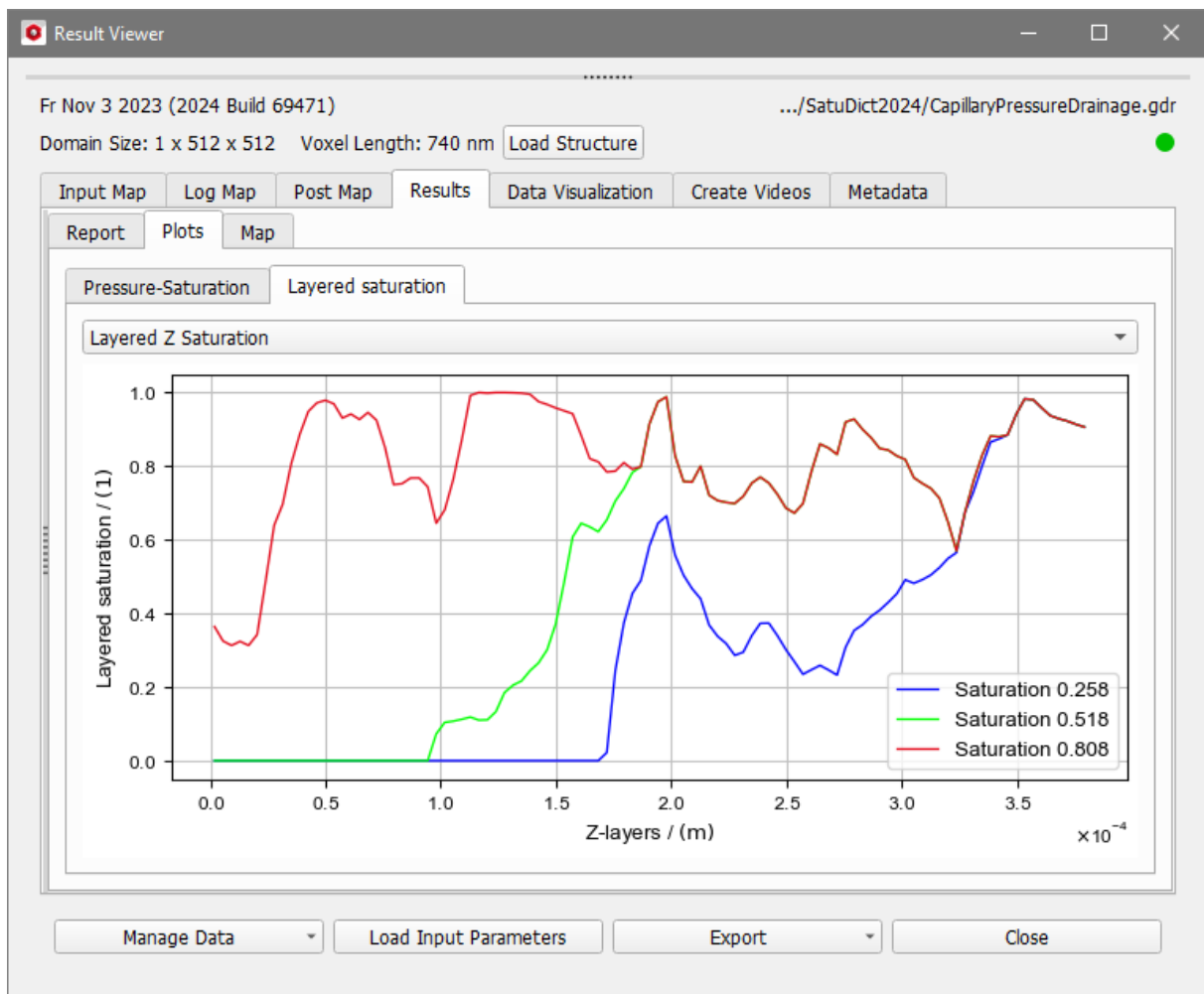
Check **Invert Saturation** to show the values of the saturation in decreasing instead of increasing order.

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

options **Edit Axis Settings** and **Edit Graph Styles** can also be accessed by choosing **Plot Options** → **Pressure-Saturation** at the bottom of the left panel.

In the example, at the beginning of the drainage process, the porous structure does not contain the invading fluid Oil. It is saturated (100%) with Water. As the pressure increases, the Oil starts invading the structure and forces the Water out of it. Thus, the saturation of the Oil is increasing. By the end of the drainage process, where the pressure is at its highest level, the structure is 83% saturated with Oil and 17% saturated with Water (Residual). The non-monotonic increase of the pressure value for the simulation with the Dynamic Pore-Morphology Method is visible, especially for saturation values between 70% and 80%.

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



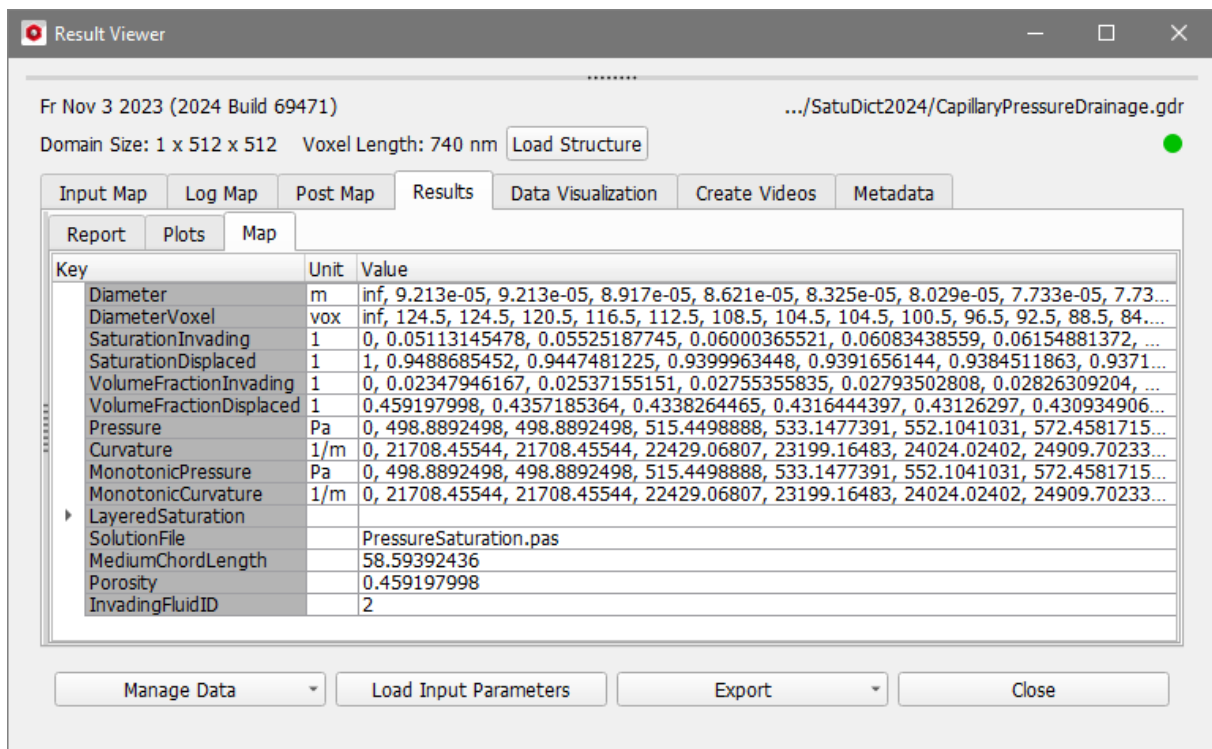
From the drop-down menu choose the direction to observe. For each layer, the occupied space of the invading fluid relative to the pore volume of this layer is plotted. This can be done for several steps of the calculation, which corresponds to different saturations of the whole structure. By right-clicking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

## Map

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

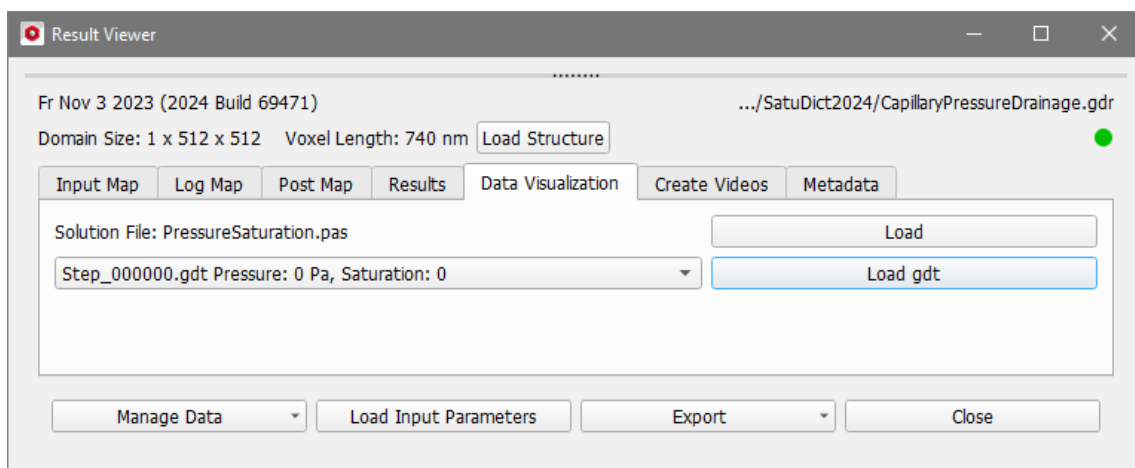
## Assessing saturation-dependent material properties

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



## DATA VISUALIZATION

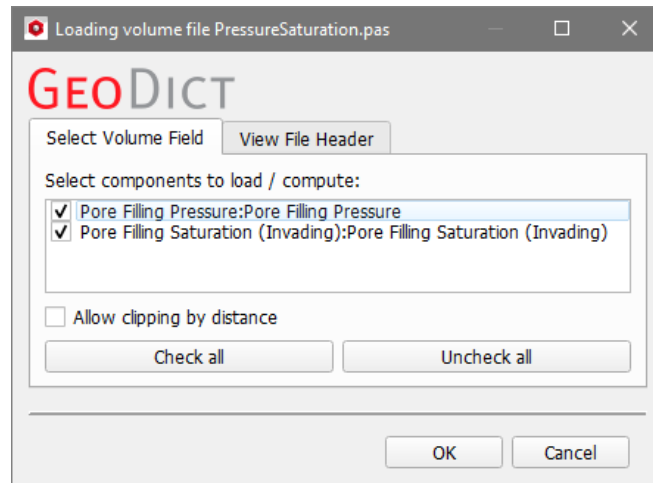
In the **Data Visualization** tab, the \*.pas file and the step-by-step images of the computed process can be loaded.



## Visualization of Pressure and Saturation

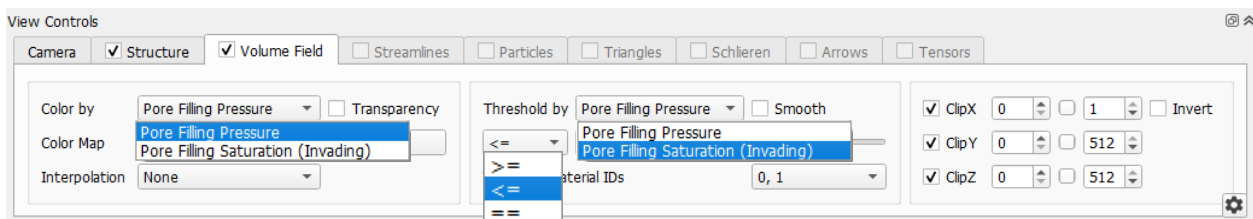
Under the **Data Visualization** tab, click **Load** to access the pressure and saturation field data saved in the **PressureSaturation.pas** file.

Depending on the choice made in the Solver Parameters tab under the output options (see page 19) the **Pore Filling Pressure** and the **Pore Filling Saturation (Invading)** can be selected for the visualization. Click **OK** to load the selected fields.



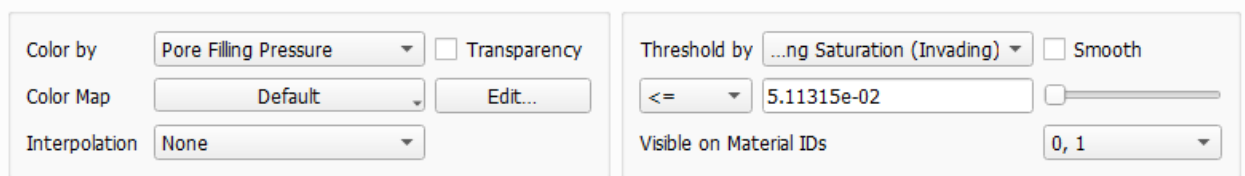
The initial visualization, in 2D view or 3D rendering, is done using default settings that the user can modify to visualize the imbibition and drainage results obtained with **SatuDict**.

These parameters can be found under the **Volume Field** tab in the **Visualization Panel**, above the Visualization Area. For more information on a particular visualization setting, see the [Visualization](#) handbook of the User Guide.



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

For the 3D rendering, we now present a clever way to visualize the data in the pressure and saturation solution file. Select Pore Filling Pressure from the **Color by** and Pore Filling Saturation (Invading) from the **Threshold by** pull down menus.



With these settings, the voxels are displayed in the color corresponding to the pressure at which this voxel was filled. The volume field legend shows which color represents which pressure value. The pressure values are shown dependent on the saturation level of the invading fluid, because Threshold by Pore Filling Saturation is chosen. The Threshold slider combined with the Clip mode determines in which voxels the pressure is displayed:

■ **Threshold Slider / Box**

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

The **beginning** of the process is observed with the slider all the way to the left. By moving it to the right or by entering increasing values in the threshold slider

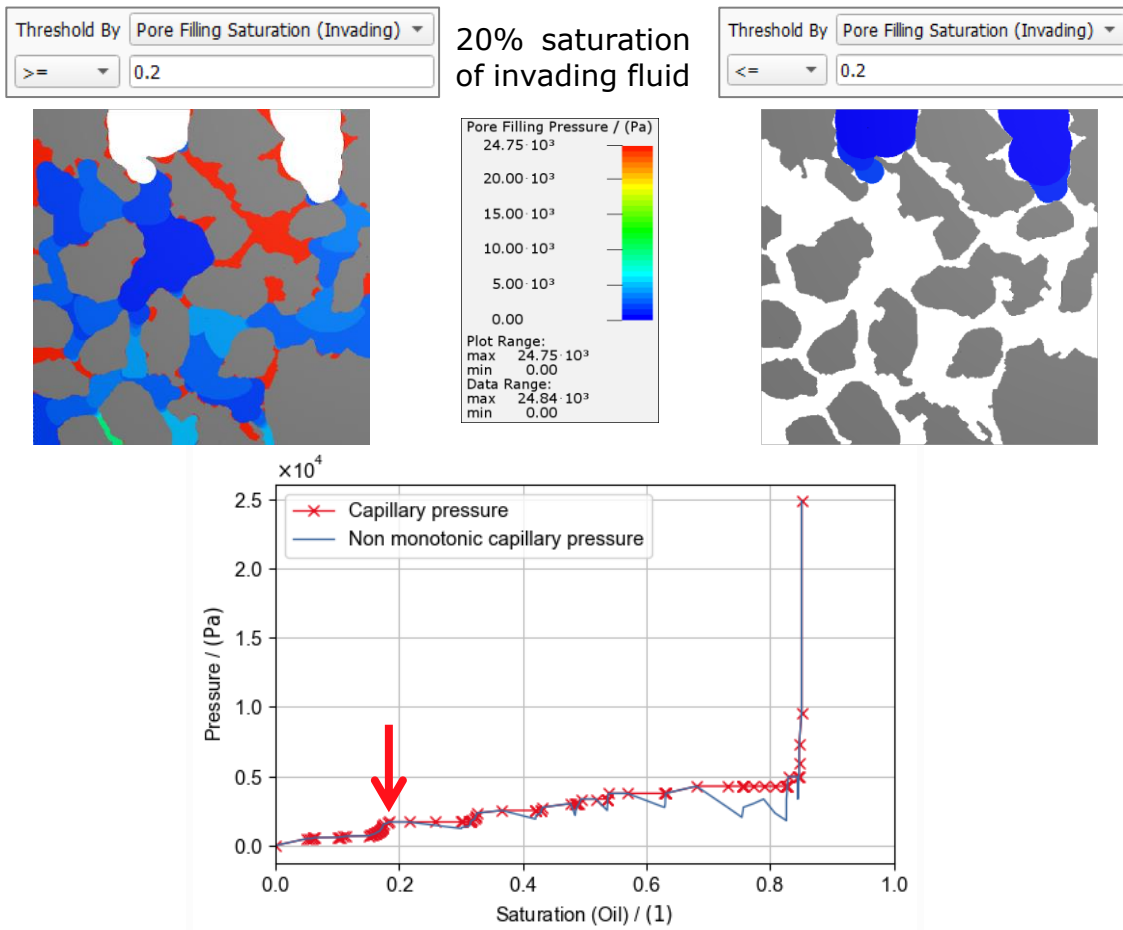
box, the intrusion process is visualized forward and at the **end** the clip slider is all the way to the right.

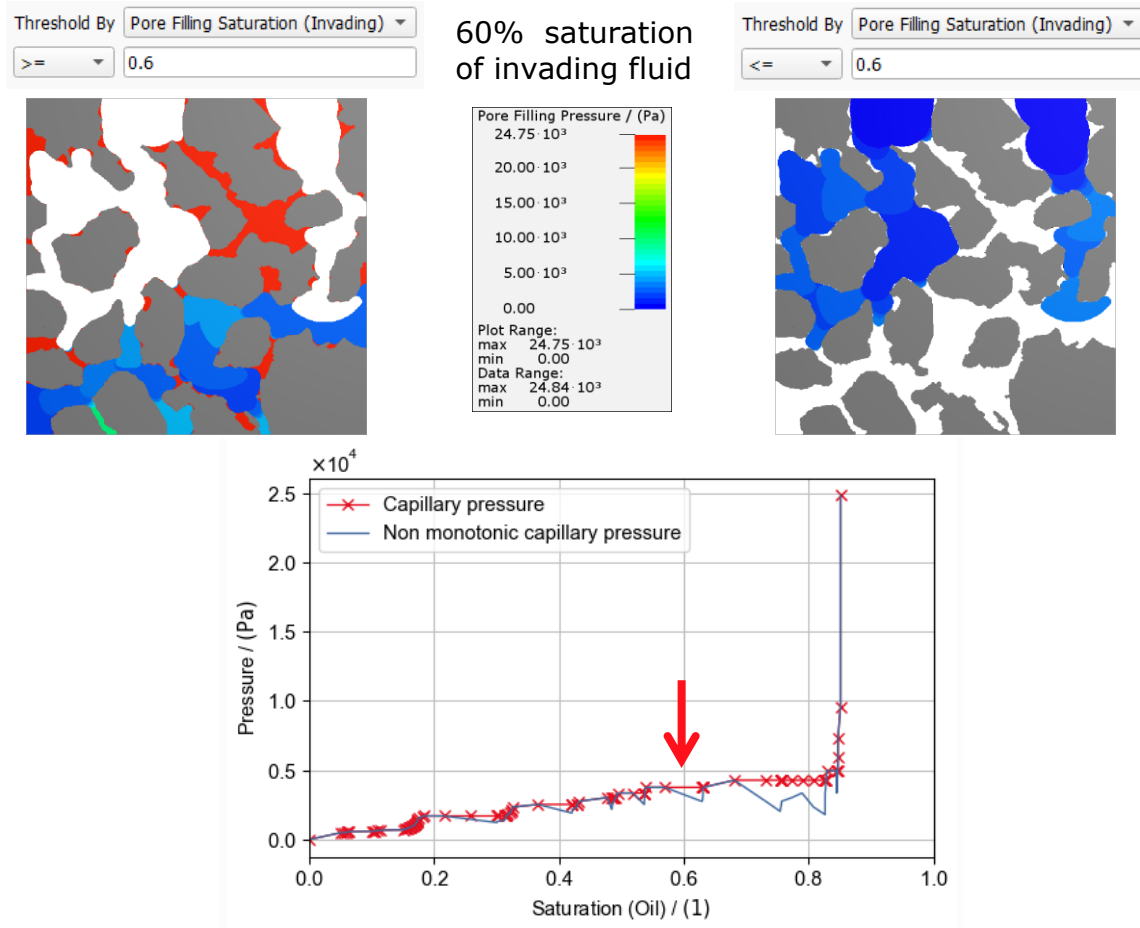
Observe, that in the example shown here, the solution was computed till a saturation of 83%.

- **Clip Mode:** makes the dual visualization of pressure values and distribution of phases possible because it links them based on the capillary pressure saturation curve (see page 24).
  - By selecting  $\geq$ , color is shown in the pore space where the invading fluid occupies the structure only at a higher saturation than the Pore Filling Saturation (Invading) set in the threshold slider. This shows the locations where the displaced fluid is still in the structure at this saturation or below.
  - By selecting  $\leq$ , color is shown in the pore space where the invading fluid is already present for a saturation below the value for Pore Filling Saturation (Invading) set in the threshold slider. This shows the locations where the invading fluid has already entered the structure and replaced the displaced fluid.

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

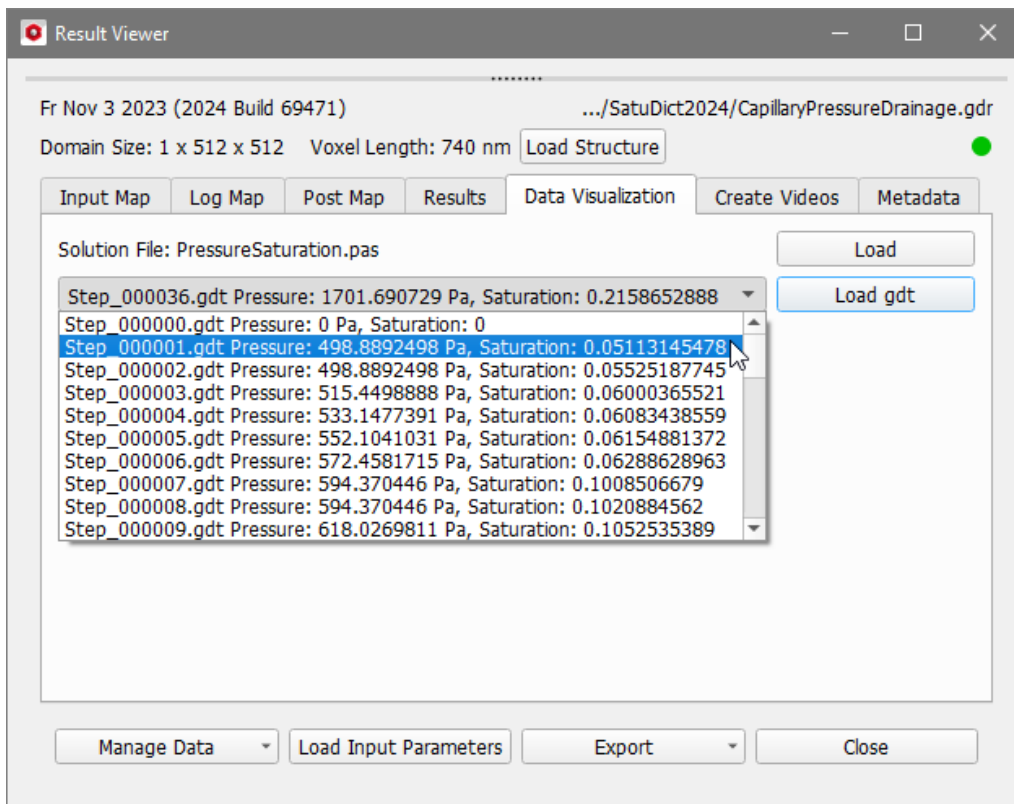
The following are two examples of the effect of setting the **Threshold** slider/box and **Clip Mode**.





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

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



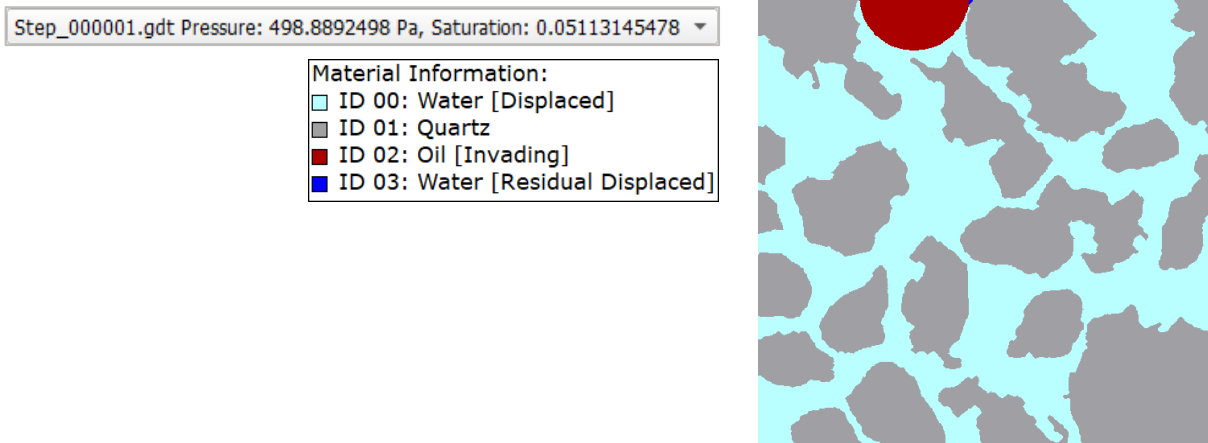
## Assessing saturation-dependent material properties

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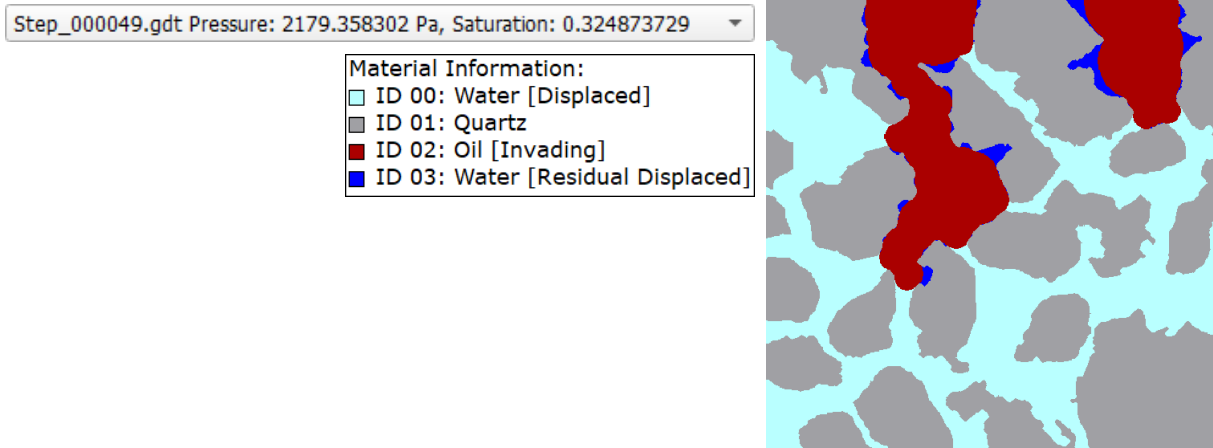
Select one of the GDT files, where the file names correspond to the simulation step in which the GDT file was saved. Also, the pressure and saturation of the invading fluid in this step are shown, which is the same as in the corresponding row of the table in the Results-Report tab.

Click **Load gdt** to open the desired file which is displayed in the visualization area.

The GDT file Step\_000001.gdt (Pressure: 499 Pa, Saturation: 0.0511) corresponds to the beginning of the intrusion process. The structure appears (almost fully) saturated by the displaced fluid.



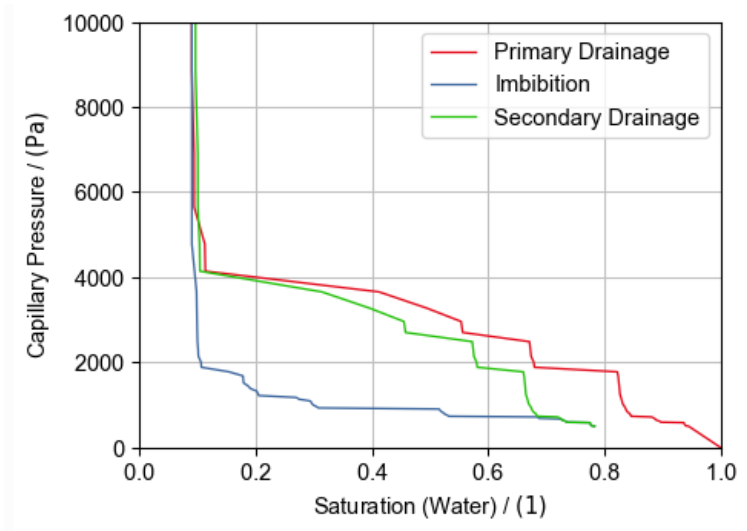
The GDT file Step\_000049.gdt (Pressure: 2179 Pa, Saturation: 0.325) corresponds to an intermediate part of the intrusion process. The structure appears partly saturated by the invading fluid and the displaced fluid.



Capillary Pressure with Hysteresis Effect

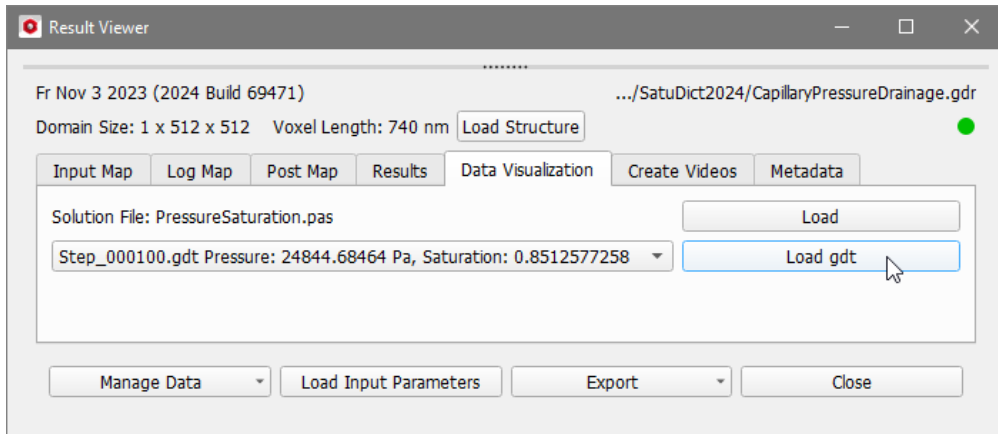
A generalization of the pore morphology method allows considering structures in which the invading fluid is already present in the structure. This makes the simulation of primary and secondary drainage experiments possible, as well as primary and secondary imbibition experiments.

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

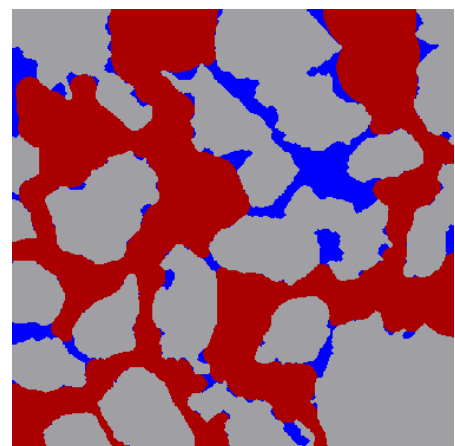


After the primary drainage simulation shown in pages 21ff. with the result file obtained, perform a follow-up imbibition simulation.

First, the final state of the previous drainage simulation (Step\_000100.gdt with 24845 Pa) is loaded as starting state for the imbibition simulation.



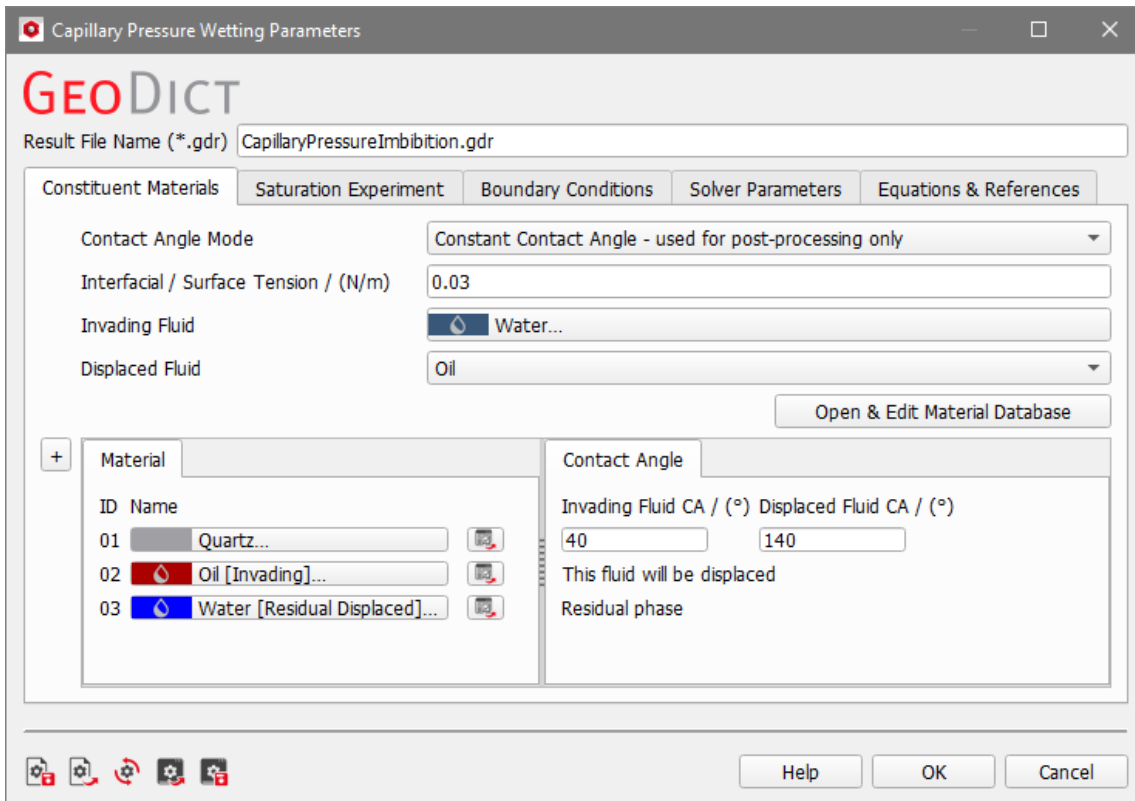
**Material Information:**  
 ■ ID 01: Quartz  
 ■ ID 02: Oil [Invading]  
 ■ ID 03: Water [Residual Displaced]



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

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

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



Under the **Saturation Experiment** tab, the Experiment has automatically changed to **Imbibition**. Check that **Invading Fluid must be connected to a Reservoir** as well as **Displaced Fluid can leave a Residual** are selected. In this example we uncheck the Dynamic Pore Morphology Method.

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

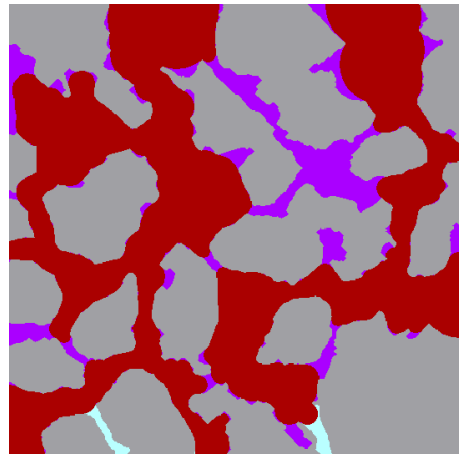
Confirm the settings with **OK** and click **Run** in the **SatuDict** section to start the simulation.

The Result Viewer of the result file opens at the end of the computations. Load the GDT files as explained in pages [30ff.](#) to visualize the imbibition process.

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

Step\_000012.gdt Pressure: 2484.468464 Pa, Saturation: 0.158445205

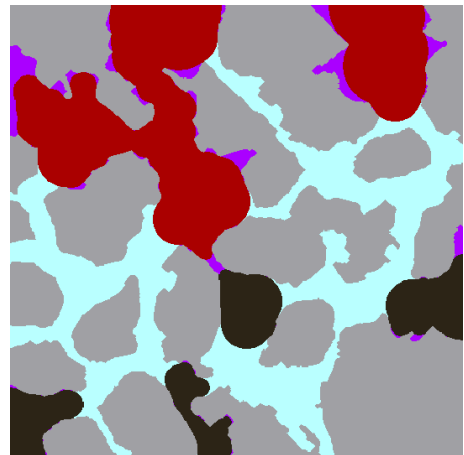
- Material Information:
- ID 00: Water [Invading]
  - ID 01: Quartz
  - ID 02: Oil [Displaced]
  - ID 05: Water [Residual Invading]



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

Step\_000029.gdt Pressure: 1052.740875 Pa, Saturation: 0.4595185087

- Material Information:
- ID 00: Water [Invading]
  - ID 01: Quartz
  - ID 02: Oil [Displaced]
  - ID 04: Oil [Residual Displaced]
  - ID 05: Water [Residual Invading]



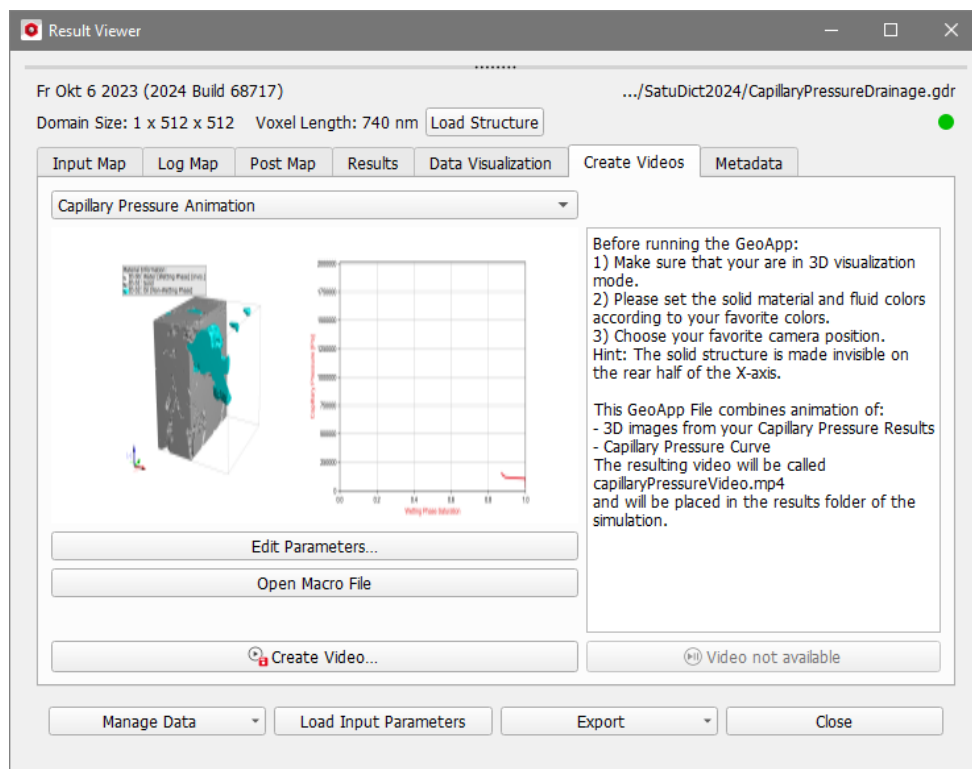
### CREATE VIDEOS

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

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

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

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



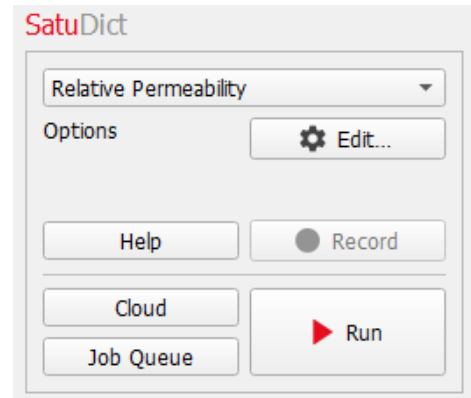
The video shows the capillary pressure curve on the right, and the changing distribution of invading and displaced fluid during the saturation simulation on the left. For a better visualization, only part of the structure is shown.

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

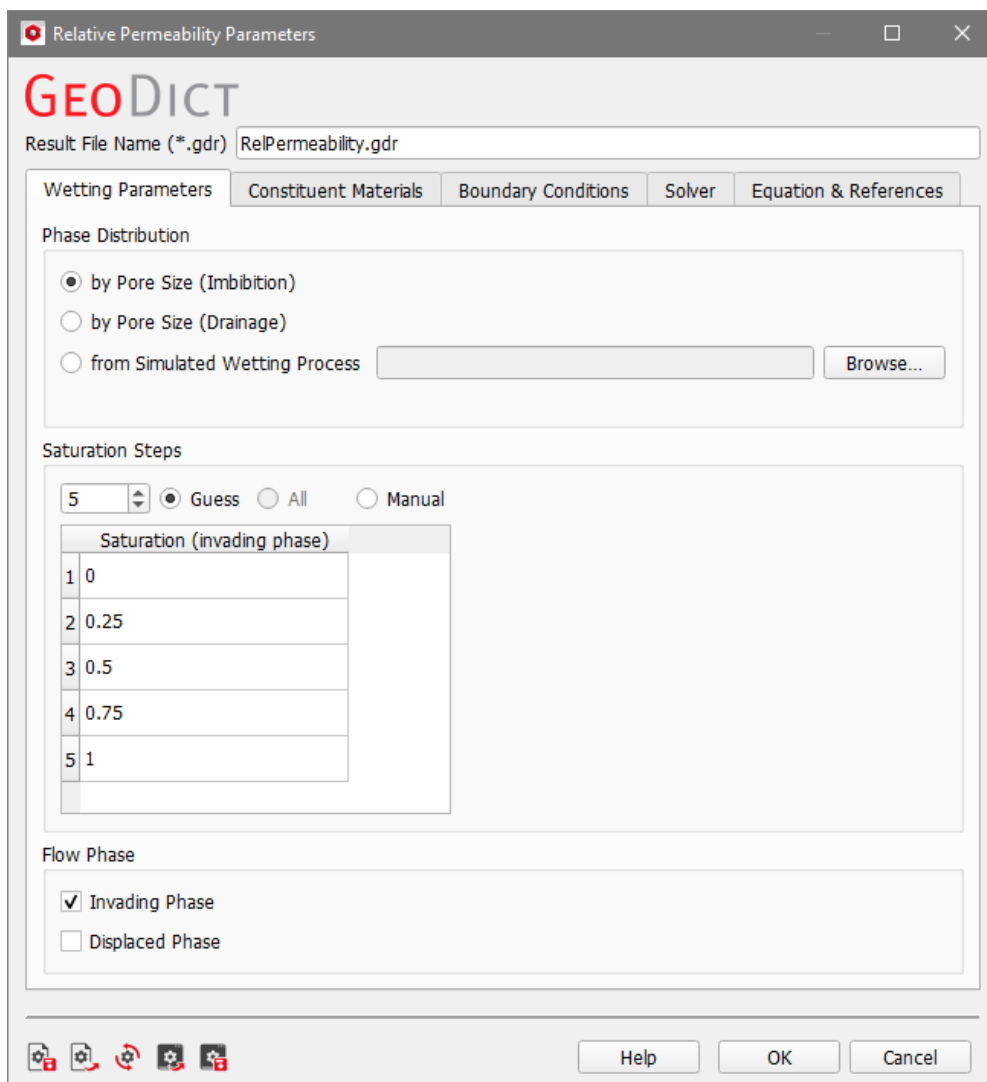
## RELATIVE PERMEABILITY

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

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



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

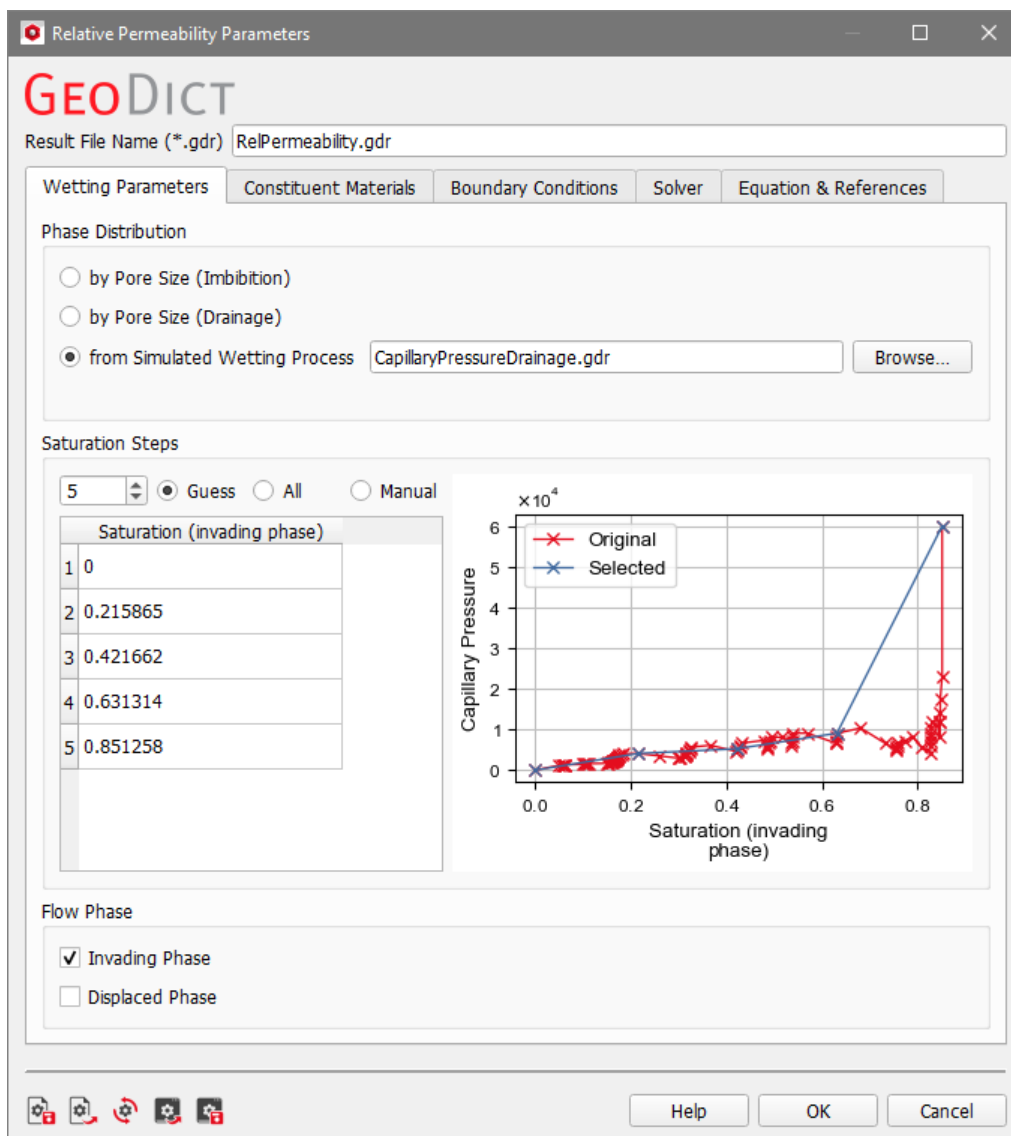


## WETTING PARAMETERS

### PHASE DISTRIBUTION

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

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



### SATURATION STEPS

The permeability is calculated at different saturation steps of the invading fluid. In the **Saturation (invading phase)** table the chosen steps are shown or can be edited. There are three different modes to select the saturations:

- **Guess:** The number of guessed saturation points is specified in the box to the left.
  - If the **Phase Distribution** is set to **by Pore Size**, the saturation steps are chosen uniformly between 0 and 1.
  - If the **Phase Distribution** is set to **from Simulated Wetting Process**, the saturation steps are chosen from the provided GDR file. An internal selection process tries to find representative saturation steps based on the saturation and capillary pressure. A plot shows the original saturation points and the selected saturation points. With a right-click the plot can be modified with the usual options from the result viewer (see also the [Result Viewer](#) handbook of the User Guide). This way the user can control if the guessed saturation points are indeed representative.
- **All** is only available when the **Phase Distribution** is set to **from Simulated Wetting Process**. Then all saturation steps provided in the GDR file are used.
- **Manual:** In manual mode, the table can be modified at will, and the desired saturation steps can be entered.

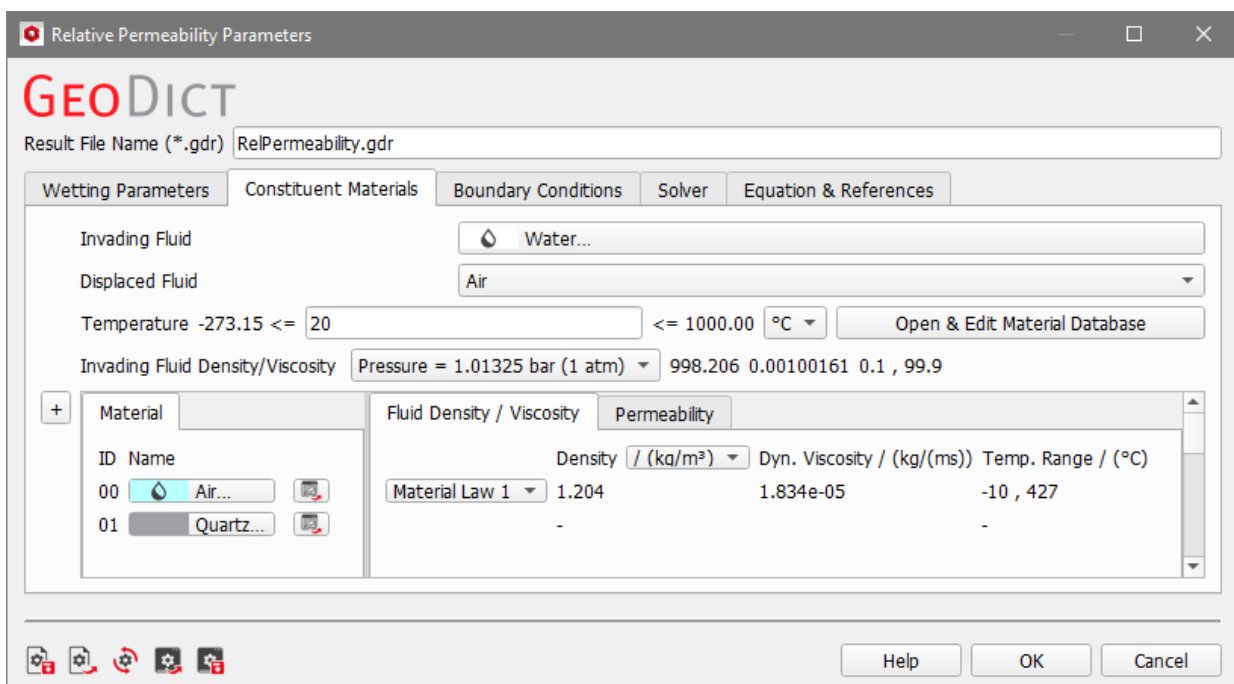
## FLOW PHASE

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

## CONSTITUENT MATERIALS

Under the **Constituent Materials** tab, the **Invading Fluid** and **Displaced Fluid** can be entered. The tab is similar to the one for capillary pressure (see page [12](#)) but some properties cannot be entered (e.g. surface tension and contact angle).

If the phase distribution under the Wetting Parameters tab is chosen **by Pore Size**, the displaced 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.

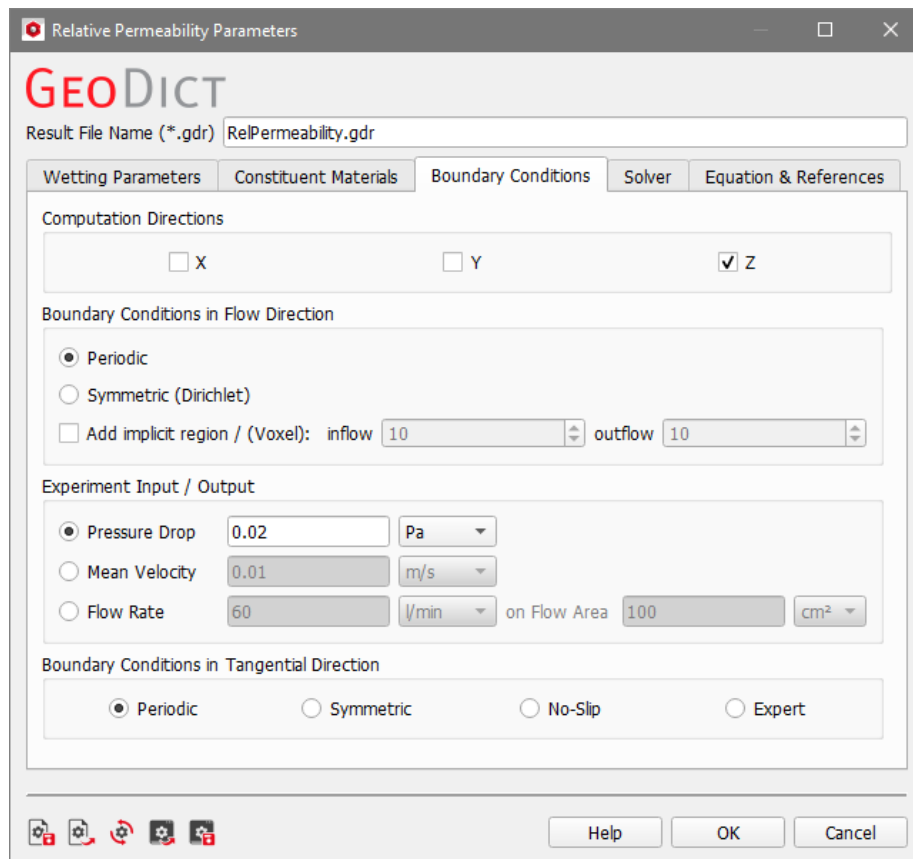


## Assessing saturation-dependent material properties

Set the temperature applied for the calculation in the selected units below. Click **Open & Edit Material Database** to edit the materials properties in the material database if needed.

The next line with **Invading Fluid Density/Viscosity** and the table below shows the same information, once for the invading fluid and below for the materials present in the structure. The values shown for the selected material law are Density, Dynamic Viscosity and the lower and upper bound of the Temperature Range in which the values are defined. For solid and porous materials in the structure their Permeability is defined in the respective tab.

## 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 (Dirichlet)**. Periodic boundary conditions are recommended for periodically generated structure models and for non-periodic structures with high porosity.

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

## EXPERIMENT INPUT / OUTPUT

In fluid dynamics, three experiments are typical:

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

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

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

## BOUNDARY CONDITIONS IN TANGENTIAL DIRECTION

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

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

Boundary Conditions in Tangential Direction

The screenshot shows a dialog box titled "Boundary Conditions in Tangential Direction". At the top, there are four radio buttons: "Periodic", "Symmetric", "No-Slip", and "Expert". The "Expert" radio button is selected. Below this, there is a section labeled "Expert Settings" which contains a grid of dropdown menus. The grid has three columns and two rows. The first column has a "Y" label and a dropdown menu set to "Periodic". The second column has an "X" label and a dropdown menu set to "Periodic". The third column has an "X" label and a dropdown menu set to "Periodic". The second row has a "Z" label and a dropdown menu set to "Periodic" in the first column, a "Z" label and a dropdown menu set to "Periodic" in the second column, and a "Y" label and a dropdown menu set to "Symmetric" in the third column.

## 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

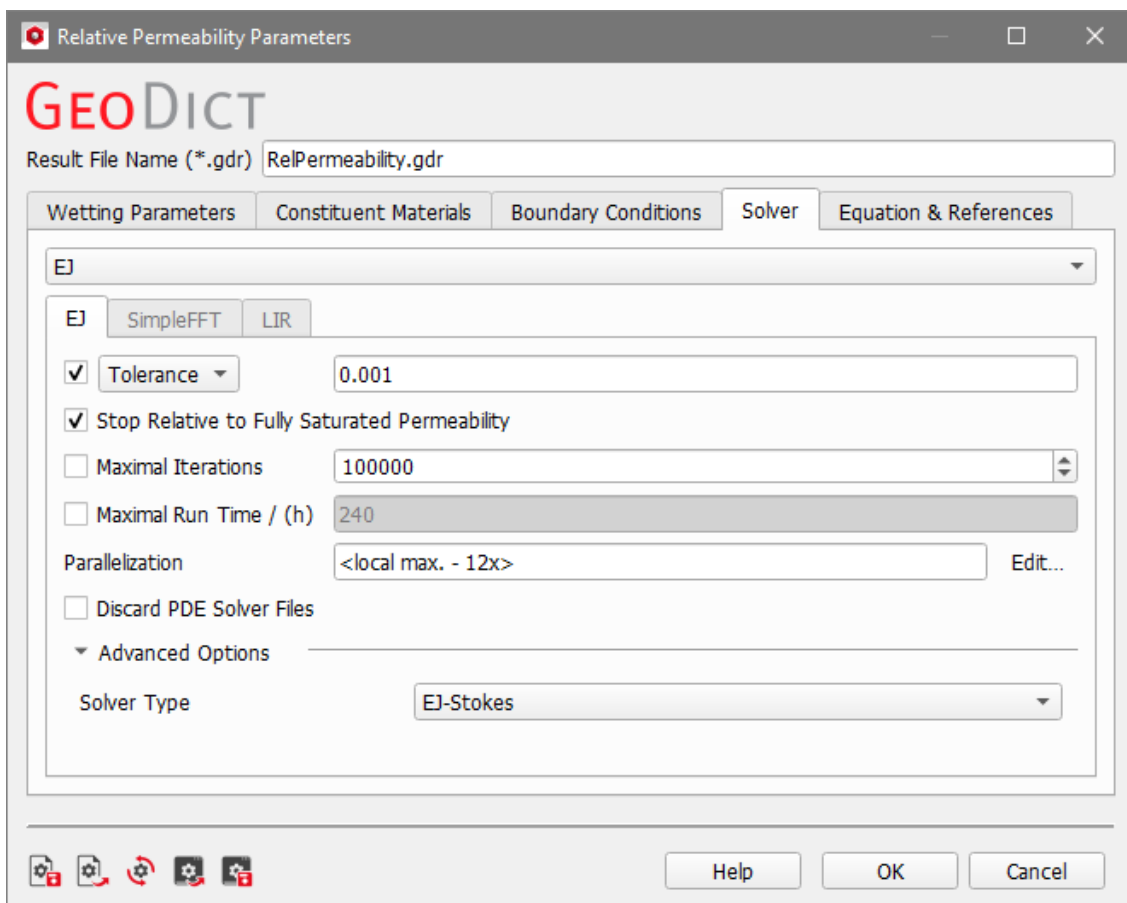
The EJ solver is assigned to compute the flow fields and relative permeability after selecting **EJ** from the pull-down menu.

### Stopping Criteria

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

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

In the pull-down menu switch from tolerance to **Residual** as stopping criterion. Then, 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**.



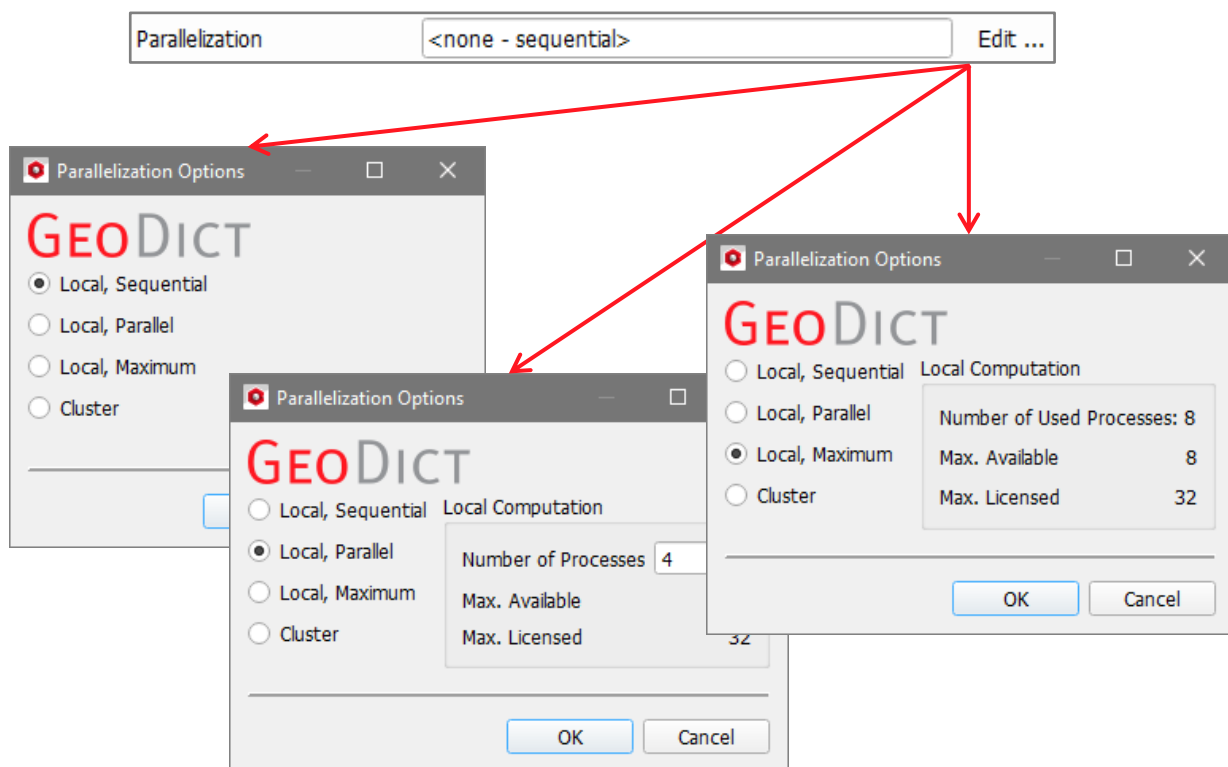
The option to **Stop Relative to Fully Saturated Permeability** alters the chosen stopping criterion such that for low saturated states the solver stops relative to the result of the computation where the structure was fully saturated. The fully saturated structure has the highest permeability and decreases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

Additionally, 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). The solver run will stop when one of the chosen stopping criteria is reached. However, when the solver stops because the **Maximal Iterations** value or the **Maximal Run Time** 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 opens when clicking the **Edit...** button, to choose between **Local, Sequential**, **Local, Parallel** or **Local, Maximum**. When **Local, Parallel** is chosen, the number of **Processes** to run can be entered. **Local, Maximum** sets the number of used processes to the maximum possible number, restricted by the hardware and number of licensed processes.

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



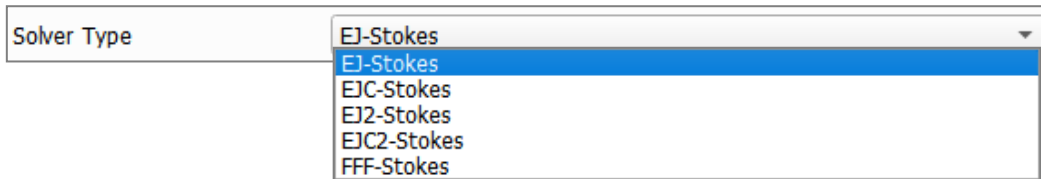
### Discard PDE Solver Files

The result file (\*.gdr) of the permeability computations is 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, volume files, etc.).

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.

### Advanced Options

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.

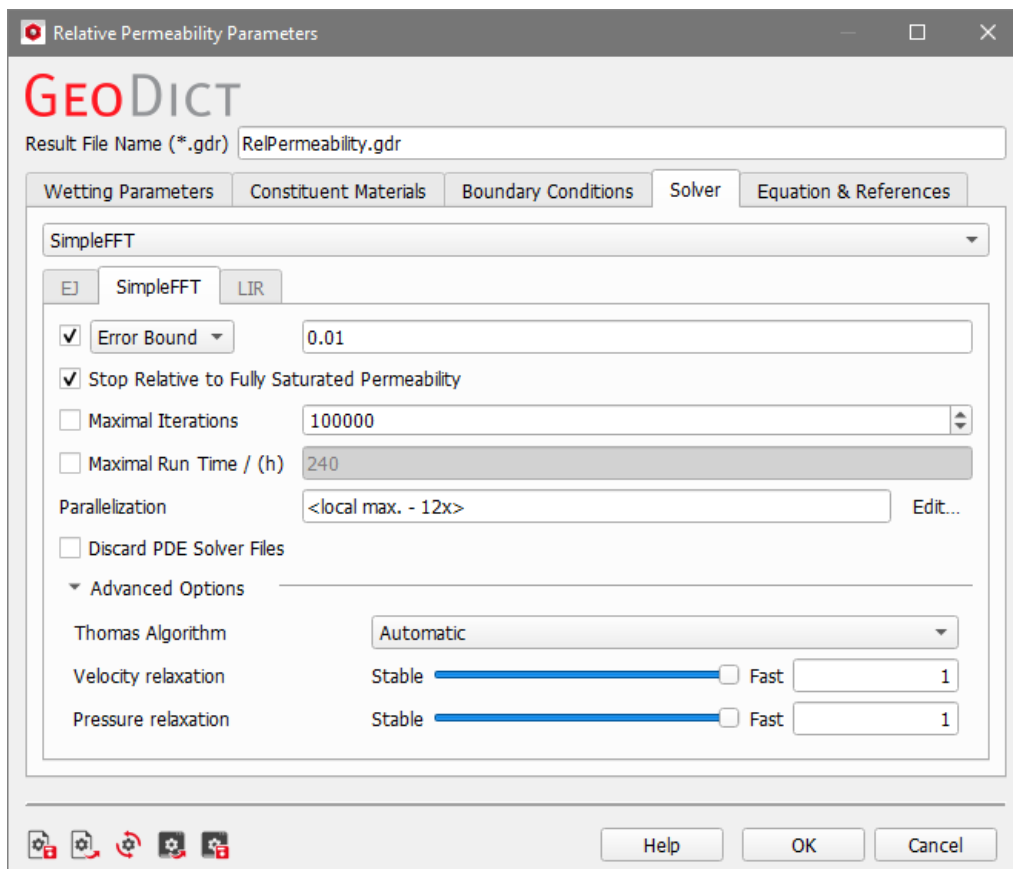
**EJ2-Stokes** sets the tangential velocity to zero at the center of the voxel surfaces and uses a 2nd order approximation of the velocity field.

**EJC2-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.

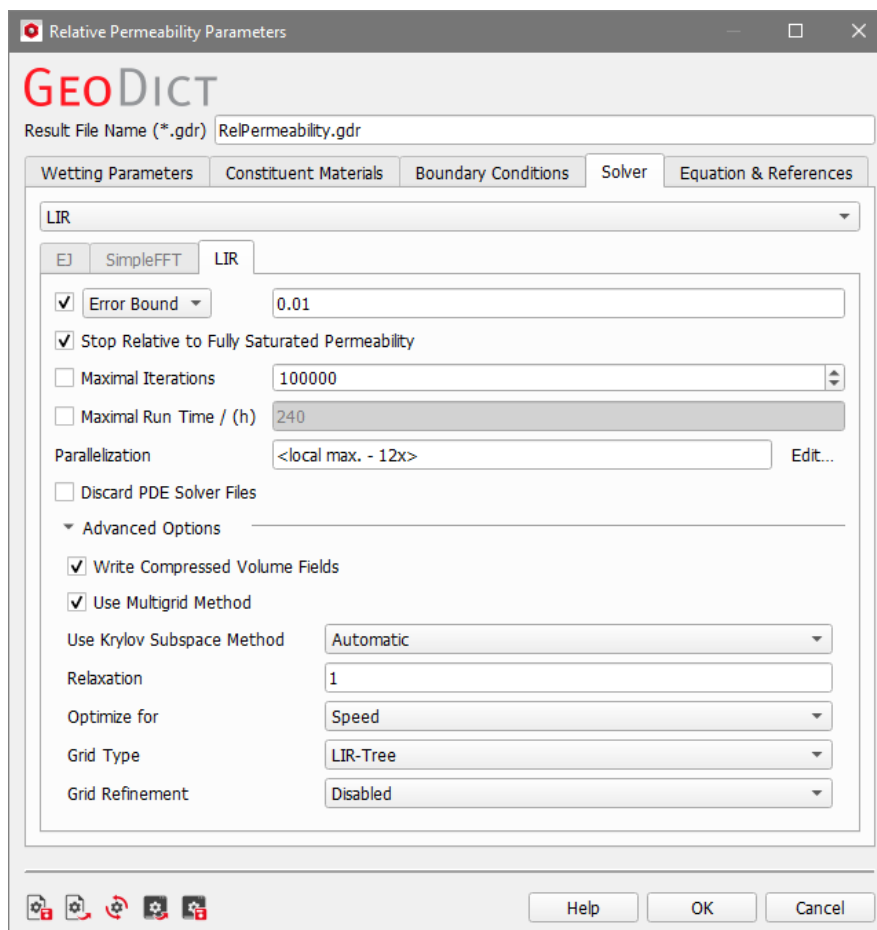
With the pull-down menu choose the stopping criterion between **Error Bound, Tolerance** and **Residual**. The recommended (and default) stopping criterion is **Error Bound** for the SimpleFFT and the LIR solver. The **Error Bound** stopping criterion uses the result of previous iterations and predicts the final solution. The solver stops if the relative difference with respect to the prediction is smaller than the specified error bound.

### Advanced Options

The tridiagonal matrix algorithm (Tdma), also known as the **Thomas Algorithm**, can help to improve the convergence for structures with high porosity and therefore speed up the computation with SimpleFFT. Here, **Automatic, NotUseTdma** or **UseTdma** can be selected. With **UseTdma / NotUseTdma** it can be switched on or off. Choosing **Automatic** makes the selection based on the porosity of the structure and on the partial differential equation for the flow solver. For Stokes equation, which is always solved in the **Relative Permeability** computations in **SatuDict**, Tdma is always switched off for **Automatic** selected.

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

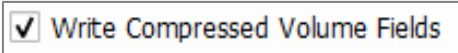


The explanations given in pages 40ff. for the EJ solver and the SimpleFFT solver, regarding **Stopping Criterion**, **Stop Relative to Fully Saturated Permeability**, **Parallelization** (except that running the LIR solver on a cluster is not possible), and **Discard PDE Solver Files** apply also here for the LIR solver. As stopping criterion **Error Bound** or **Tolerance** can be selected from the pull-down menu.

### Advanced Options

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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 can save 80-90% of the hard disk space. 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.

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

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

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 **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.

The **Optimize for**, **Grid Type**, and **Grid Refinement** parameters are special options for the LIR solver. The defaults are already optimal for most applications. A detailed explanation of these parameters can be found in the section **Solver Options** of the [FlowDict](#) handbook of the User Guide.

## EQUATIONS & REFERENCES

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

- Momentum conservation,
- Mass conservation,
- No-slip boundary condition.

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

## RELATIVE PERMEABILITY RESULT FILE

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

The screenshot shows the GeoDict Result Viewer window. At the top, there is a file list with columns for File, Module, and Command. Below this, there are navigation buttons (Open..., Up, Down, Swap Selected) and a checkbox for Synchronize Tabs. The main area displays the results for the file RelPermeability\_Inv\_LIR.gdr. The results are organized into three sections:

**Absolute Permeability**

Absolute Permeability <sub>1</sub>	Absolute Permeability <sub>2</sub>	Absolute Permeability <sub>3</sub>
unknown	unknown	3.50223e-13

**Relative Permeability (Invading fluid)**

Saturation (Invading fluid)	Relative Permeability <sub>1</sub>	Relative Permeability <sub>2</sub>	Relative Permeability <sub>3</sub>
0	unknown	unknown	0
0.250136	unknown	unknown	0
0.489804	unknown	unknown	0.0402024
0.753896	unknown	unknown	0.301242
1	unknown	unknown	1

**Effective Permeability (Invading fluid)**

Saturation (Invading fluid)	K <sub>11</sub>	K <sub>12</sub>	K <sub>13</sub>	K <sub>21</sub>	K <sub>22</sub>	K <sub>23</sub>	K <sub>31</sub>	K <sub>32</sub>	K <sub>33</sub>
0	unknown	unknown	0	unknown	unknown	0	unknown	unknown	unknown

At the bottom right, there is a 3D visualization of a porous material structure. A tooltip for the material information is visible, showing ID 00: Air [invis.] and ID 01: Quartz.

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

In this handbook of the User Guide we explain how to access the results in the **Results** and **Data Visualization** tabs. The other tabs are explained in the [Result Viewer](#) handbook of the User Guide.

RESULTS

Report

Under the **Results-Report** subtab, the **Relative Permeability** (dimensionless relative permeability) and **Effective Permeability** (saturation-dependent permeability) tables are shown for the chosen invading fluid saturation rates (here, 0.25, 0.50, 0.75) and the start and end saturations (0.0 and 1.0) in the chosen computation directions (here, K13, K23, K33 for the computation in Z-direction). The chosen saturation rates are approximated as best as possible (here, 0.25, 0.49, 0.75). Additionally, the **Absolute Permeability** of the structure is shown at the top. This value is the same as the effective permeability for the fully saturated structure.

Having selected the Invading Fluid as the flow phase under the Wetting Parameters tab, the saturation-dependent permeability of the invading fluid is shown in the tables.

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

**Absolute Permeability**

Absolute Permeability <sub>1</sub>	Absolute Permeability <sub>2</sub>	Absolute Permeability <sub>3</sub>
unknown	unknown	3.50223e-13

**Relative Permeability (Invading fluid)**

Saturation (Invading fluid)	Relative Permeability <sub>1</sub>	Relative Permeability <sub>2</sub>	Relative Permeability <sub>3</sub>
0	unknown	unknown	0
0.250136	unknown	unknown	0
0.489804	unknown	unknown	0.0402024
0.753896	unknown	unknown	0.301242
1	unknown	unknown	1

**Effective Permeability (Invading fluid)**

Saturation (Invading fluid)	K <sub>11</sub>	K <sub>12</sub>	K <sub>13</sub>	K <sub>21</sub>	K <sub>22</sub>	K <sub>23</sub>	K <sub>31</sub>	K <sub>32</sub>	K <sub>33</sub>
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	5.00657e-16	unknown	unknown	-2.38831e-16	unknown	unknown	1.40798e-14
0.753896	unknown	unknown	-1.0129e-14	unknown	unknown	-4.01622e-15	unknown	unknown	1.05502e-13
1	unknown	unknown	3.44493e-14	unknown	unknown	-1.05432e-14	unknown	unknown	3.50223e-13

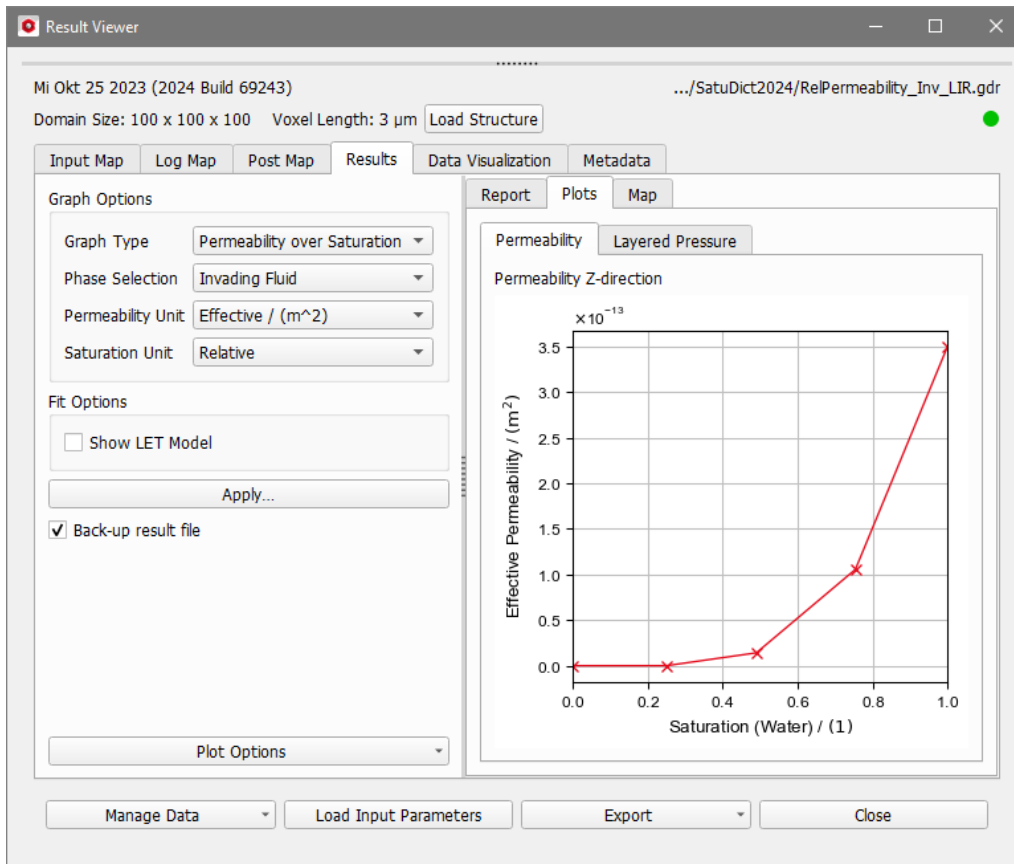
Remark: Permeability values are given in m<sup>2</sup>

Plots

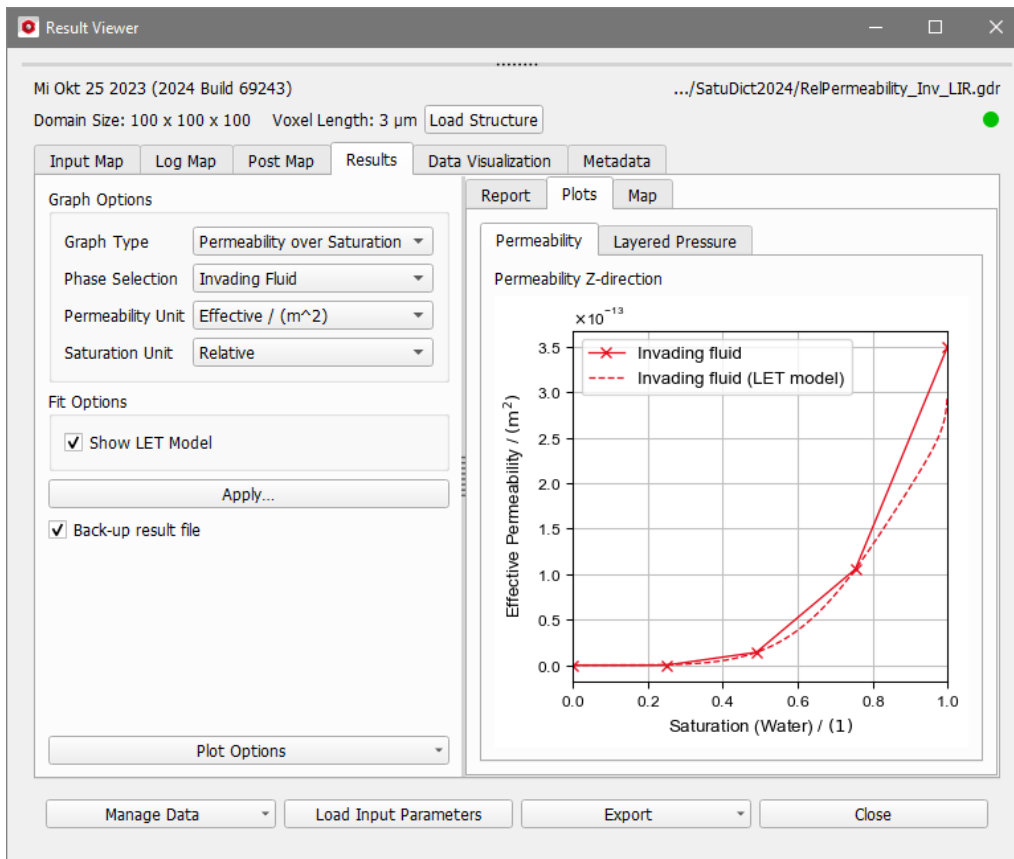
In the **Results - Plots** subtab, the values of the **Relative Permeability** or **Effective Permeability** table are shown in a graph. Also, the **Layered Pressure** in the computed directions is given.

On the left side in the expandible **Graph Options**, the user can modify the way the permeability graph is displayed by selecting the **Graph Type** (Permeability over Saturation or Saturation over Permeability), the **Phase Selection** (Invading Fluid or Displaced fluid), the **Permeability Unit** (Effective permeability in m<sup>2</sup>, Relative

permeability between 0 and 1), and the **Saturation Unit** (Relative or Absolute). Click **Apply** to change the graph shown according to the options selected. Choose **Plot Options**, to change axis and graph settings.

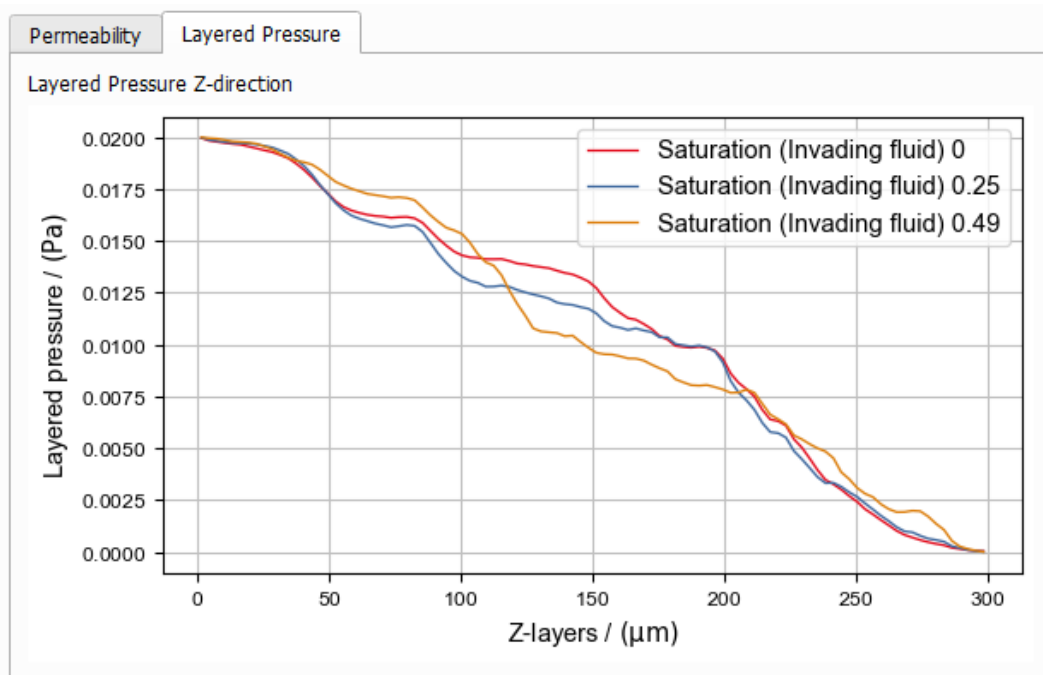


Check **Show LET Model** under Fit Options to additionally show an LET fit in the permeability plot (see also page 7).



## Assessing saturation-dependent material properties

In the **Layered Pressure** tab for each computational direction the pressure in each layer is shown in a graph. The axis settings and graph styles can be changed under **Plot Options**.



Map

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

Result Viewer

Mi Okt 25 2023 (2024 Build 69243) .../SatuDict2024/RelPermeability\_Inv\_LIR.gdr

Domain Size: 100 x 100 x 100 Voxel Length: 3  $\mu\text{m}$

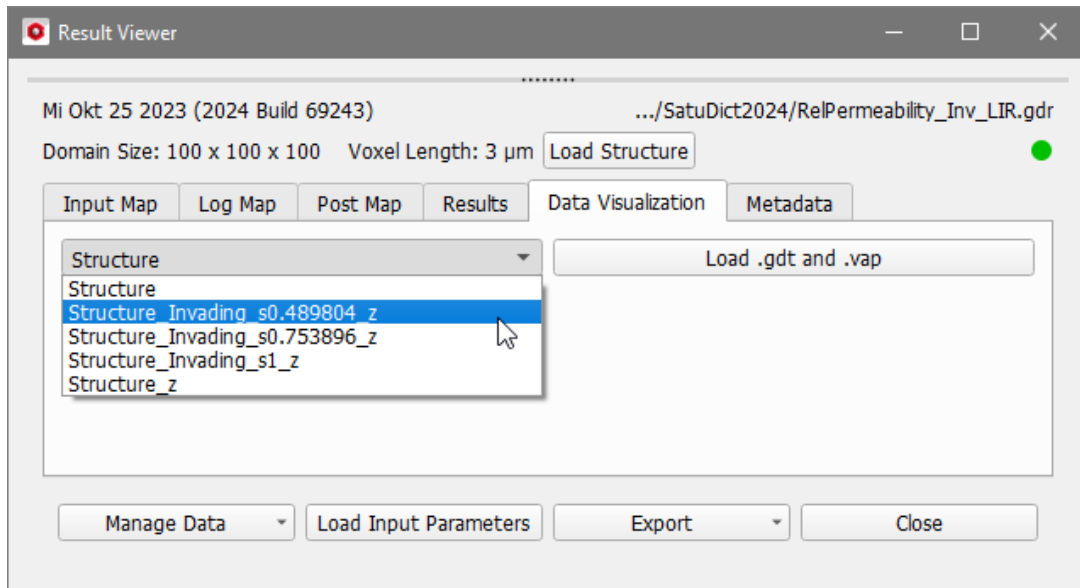
Input Map | Log Map | Post Map | **Results** | Data Visualization | Metadata

Report | Plots | **Map**

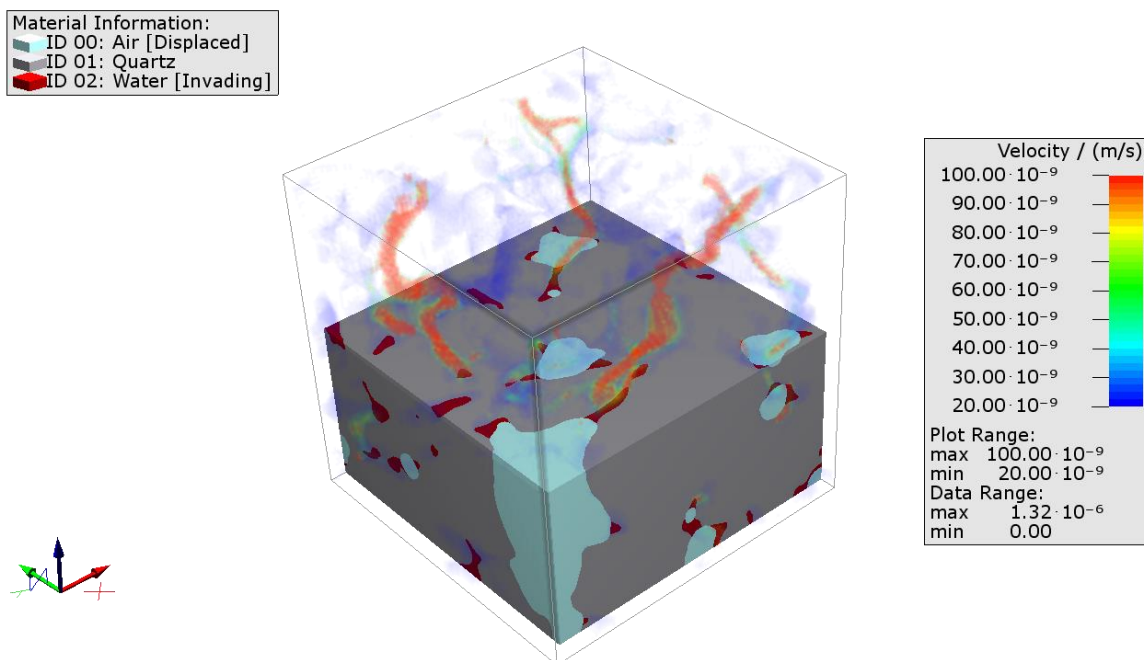
Key	Unit	Value
Porosity		0.170603
Absolute		
AbsolutePermeability3	$\text{m}^2$	3.50223e-13
InvadingFluid		
EffectivePermeability13	$\text{m}^2$	0, 0, 5.00657e-16, -1.0129e-14, 3.44493e-14
EffectivePermeability23	$\text{m}^2$	0, 0, -2.38831e-16, -4.01622e-15, -1.05432e-14
EffectivePermeability33	$\text{m}^2$	0, 0, 1.40798e-14, 1.05502e-13, 3.50223e-13
RelativePermeability3	1	0, 0, 0.04020238534, 0.3012423513, 1
Saturation	1	0, 0.2501362813, 0.4898038135, 0.7538964731, 1
LayeredPressureValues13		0.0199581, 0.0198257, 0.0197707, 0.0197168, 0.0196697, 0...
LayeredPressureSteps3		1.5e-06, 4.5e-06, 7.5e-06, 1.05e-05, 1.35e-05, 1.65e-05, 1.9...
LayeredPressureValues23		0.0199772, 0.0198652, 0.0198139, 0.0197586, 0.0197194, 0...
LayeredPressureValues33		0.0199896, 0.0199467, 0.0199209, 0.0198555, 0.0197875, 0...
LETModelL3		5.077262878
LETModelE3		0.7291030884
LETModelT3		0.197593689

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 26ff.



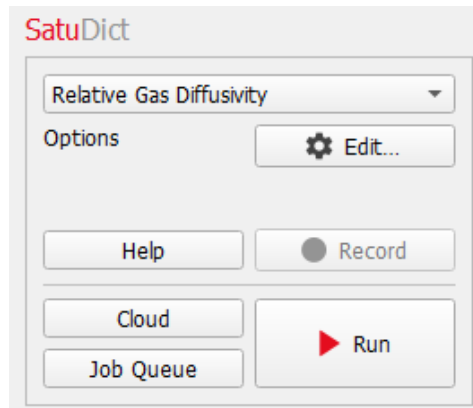
Here shown is the GDT file for a 49% invading fluid saturation level. The solid phase (Quartz) is shown together with the Displaced fluid (Air) and the Invading Fluid (Water). The upper part of the image shows the velocity field of the Water with transparent effect on the clipped structure model.



A detailed explanation of the procedure to obtain this kind of visualization can be found in the [Visualization](#) handbook of the User Guide.

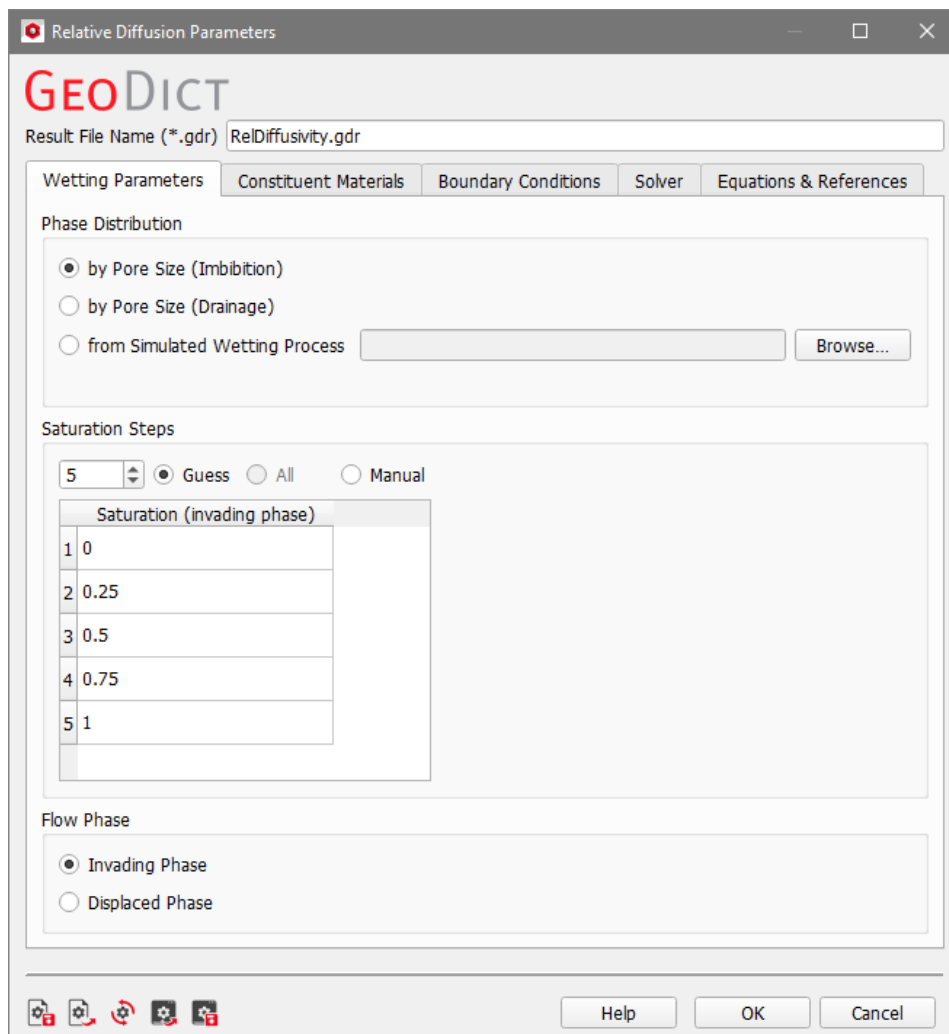
## RELATIVE GAS DIFFUSIVITY

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



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

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



## WETTING PARAMETERS

The wetting parameters for the calculation of the Relative Diffusivity are the same as seen above (pages 36ff.) for the Relative Permeability.

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

## CONSTITUENT MATERIALS

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

## BOUNDARY CONDITIONS

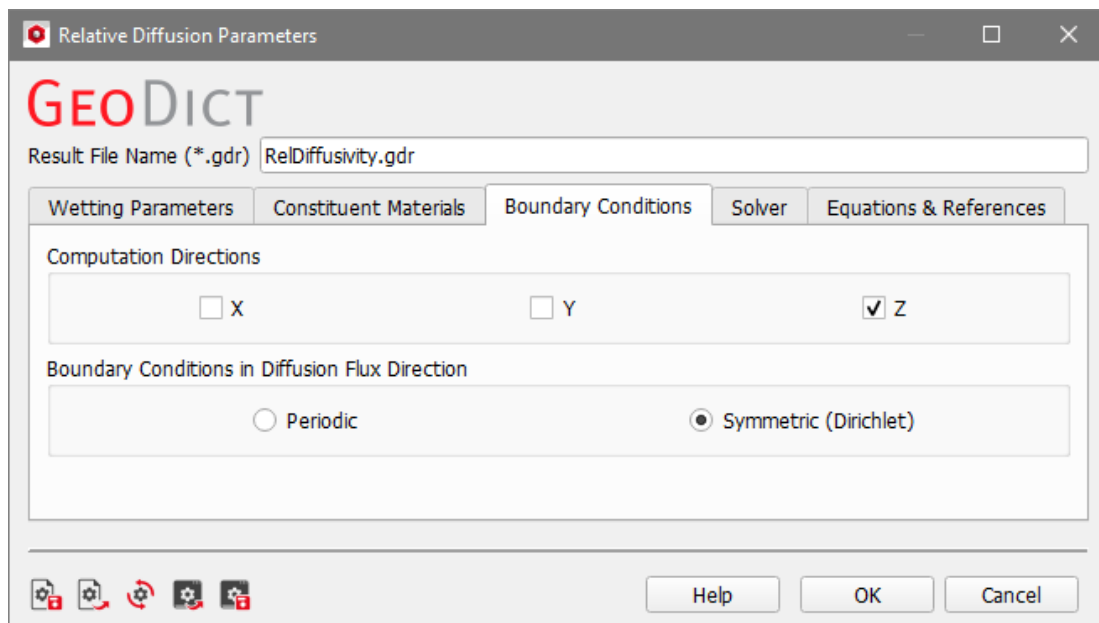
For the **Computation Directions**, choose the direction of the calculated flow. To obtain the whole diffusivity matrix in the result file, it is necessary to choose all three directions.

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

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

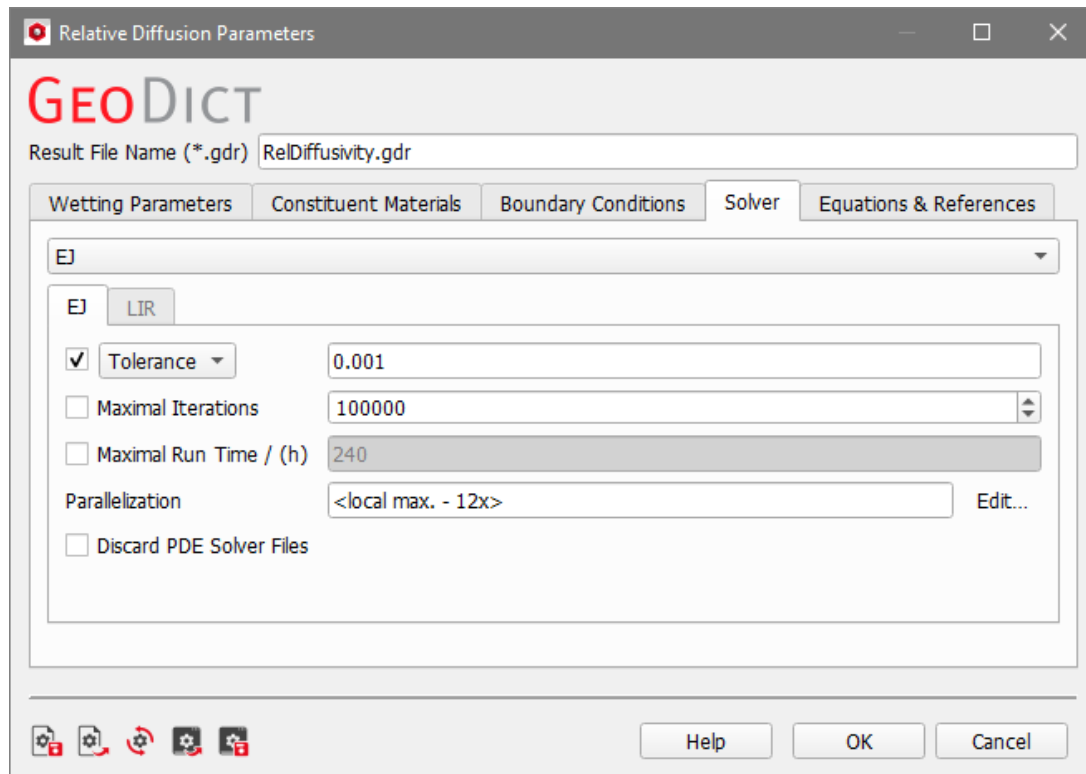
If **Symmetric (Dirichlet)** is selected, a constant concentration is ensured along both border planes in the diffusion direction.

For highly porous structures, the difference between these two settings is not significant and but it gets significant for low porous structures (e.g. digital rocks). In general, we suggest using symmetric boundary conditions.



### SOLVER

For **Relative Gas Diffusivity**, the two flow solvers **EJ** and **LIR** are available and can be chosen from the pull-down menu. The parameters for the **EJ** solver and the **LIR** solver are the same as for the computations of the Relative Permeability (see pages 40ff.). The options **Stop Relative to Fully Saturated Permeability** and **Solver Type** (for EJ) are not available for the diffusivity computations.



### EQUATIONS & REFERENCES

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

- Laplace equation,
- Fick's first law,
- Tortuosity Definition.

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

### RELATIVE GAS DIFFUSIVITY RESULT FILE

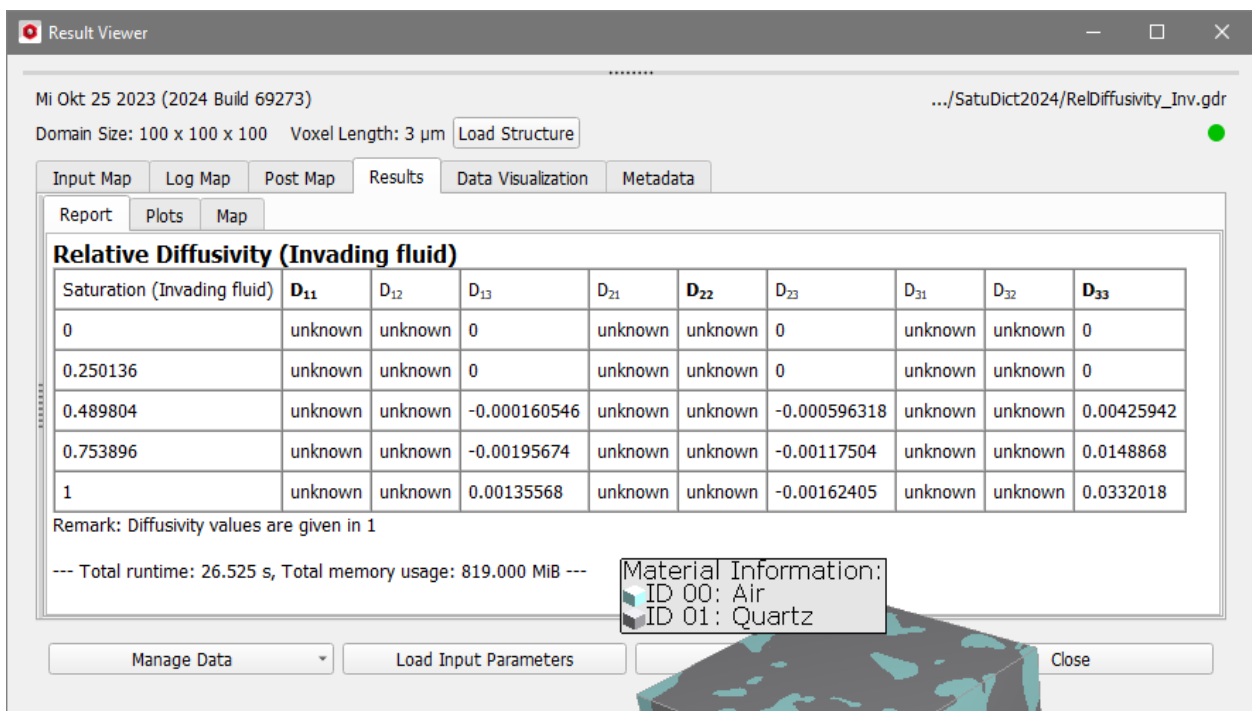
After the solver has finished, the calculation results are immediately displayed in the Result Viewer and saved into a GDR file in the chosen project folder (**File** → **Choose Project Folder...**). The entered **Result File Name** (here, RelDiffusivity\_Inv.gdr) appears at the top.

Here, the results of the computation of the relative diffusivity of a partially saturated porous media with 17% porosity (83% SVF) are explained. This is the same structure that was used for computing the relative permeability.

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

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 21ff.).

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

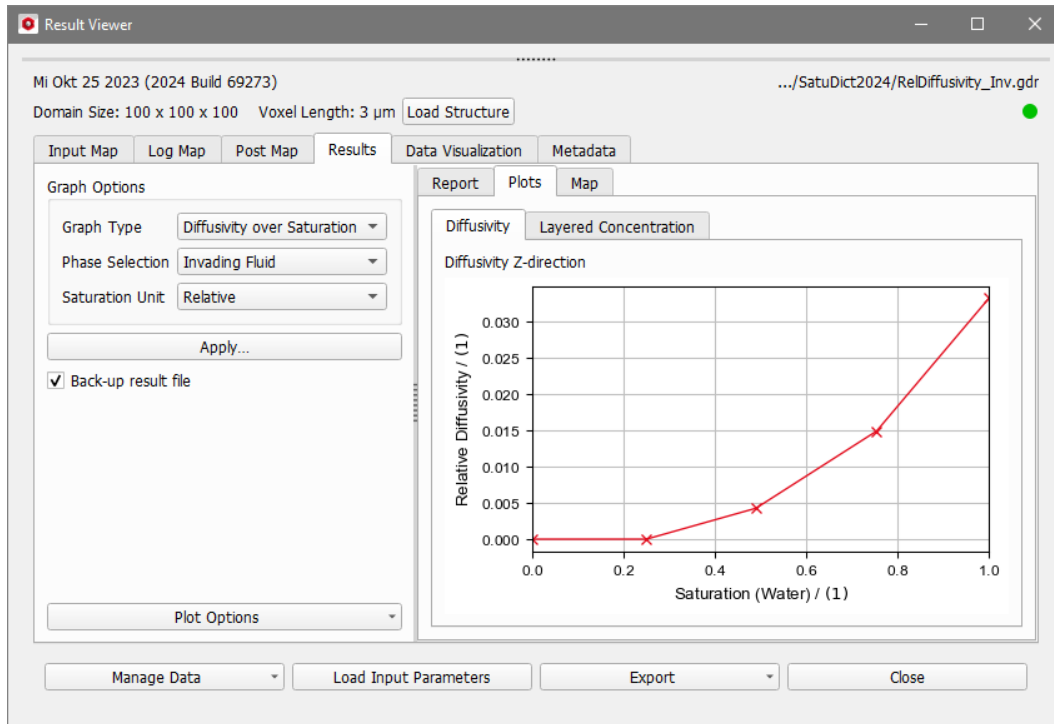


Observe how, similar to what occurred with the relative permeability, the diffusivity is zero at 0% and 25% saturation of the invading fluid. This indicates that before the structure is 49% saturated with water, no through path of this fluid is available.

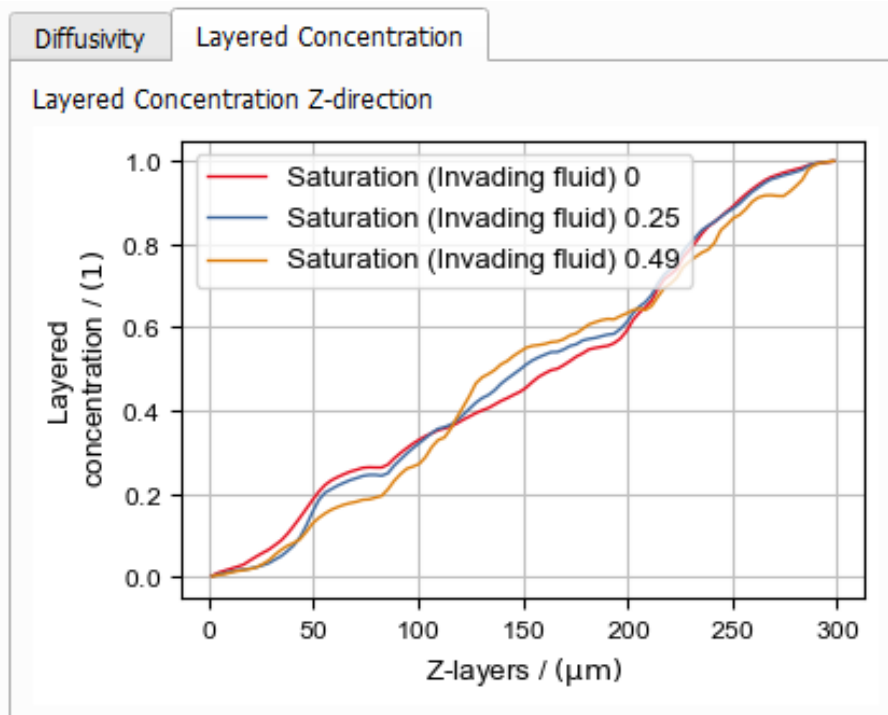
In the **Results-Plots** subtab, the values in the **Relative Diffusivity** table of the **Report** tab are shown in the **Diffusivity** graph. Also, the **Layered Concentration** in the computed directions is given.

## Assessing saturation-dependent material properties

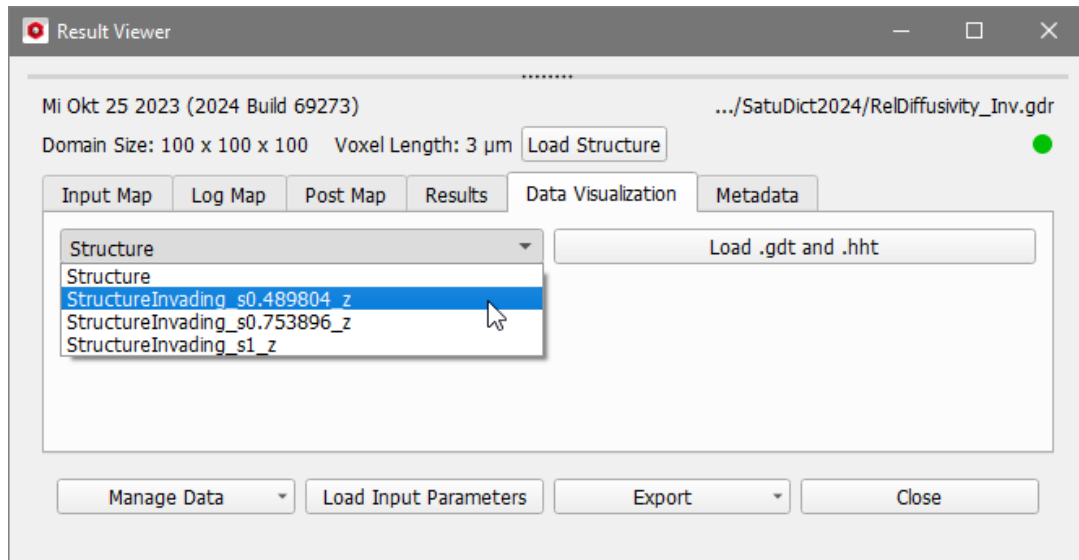
On the left panel in the expandible **Graph Options**, the user can modify the way the graph is displayed by selecting **Graph Type** (Diffusivity over Saturation or Saturation over Diffusivity), **Phase Selection** (Invading Fluid or Displaced Fluid), and **Saturation Unit** (Relative or Absolute).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



For each computational direction the concentration in each layer is shown in a graph in the **Layered Concentration** tab. The settings made under the **Graph Options** do not apply for these plots, but the axis settings and graph styles can be changed under **Plot Options**.

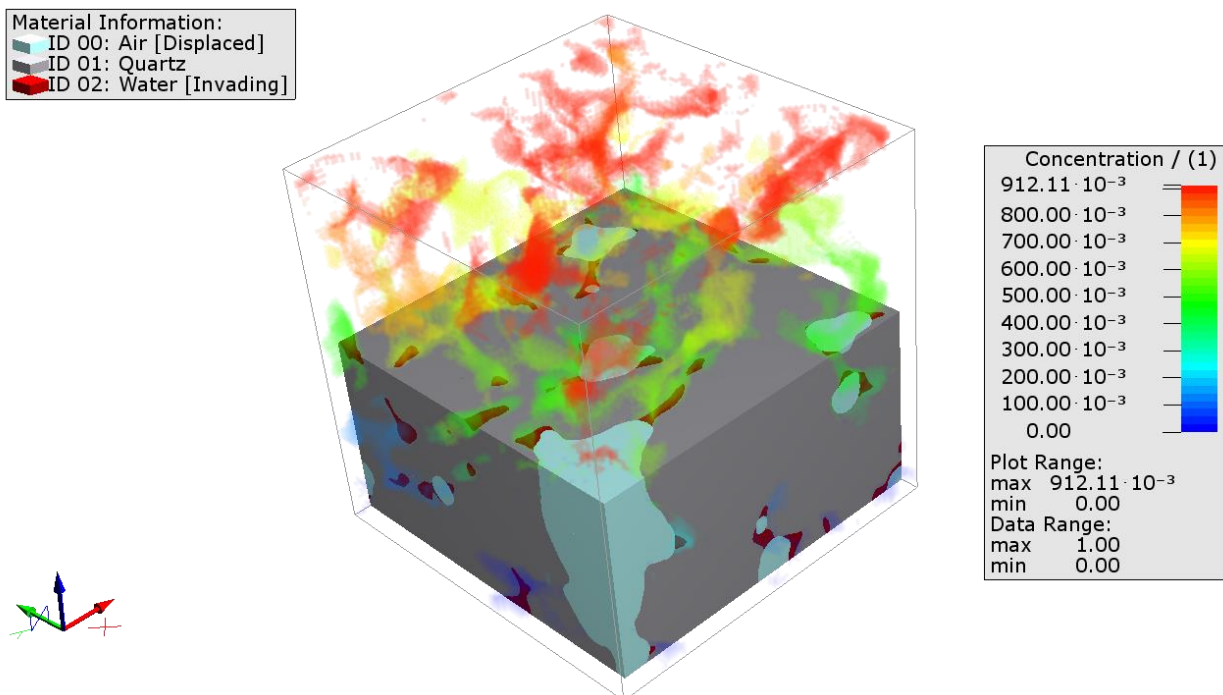


The **RelDiffusivity\_Inv.gdr** result file that opens at the end of the computation is saved in the project folder, together with the **RelDiffusivity\_Inv** result folder. If **Discard PDE Solver Files** was unchecked, the result folder contains various files for the saturation levels entered in the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



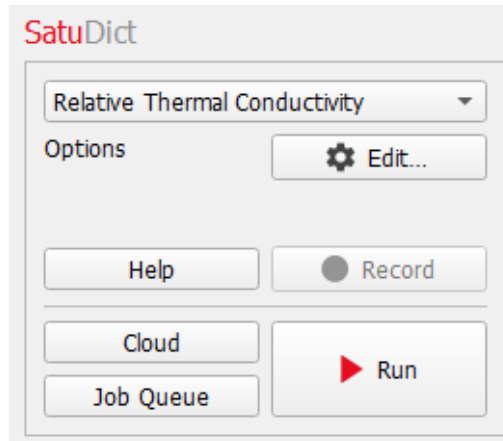
Among these files, the GDT and HHT (homogenized heat file; containing the concentration values) files can be opened in the **Data Visualization** tab.

Click **Load .gdt and .hht** to load the structure for a certain saturation of the invading fluid and the corresponding concentration field in the same way as explained in pages [49ff.](#) for the relative permeability results.

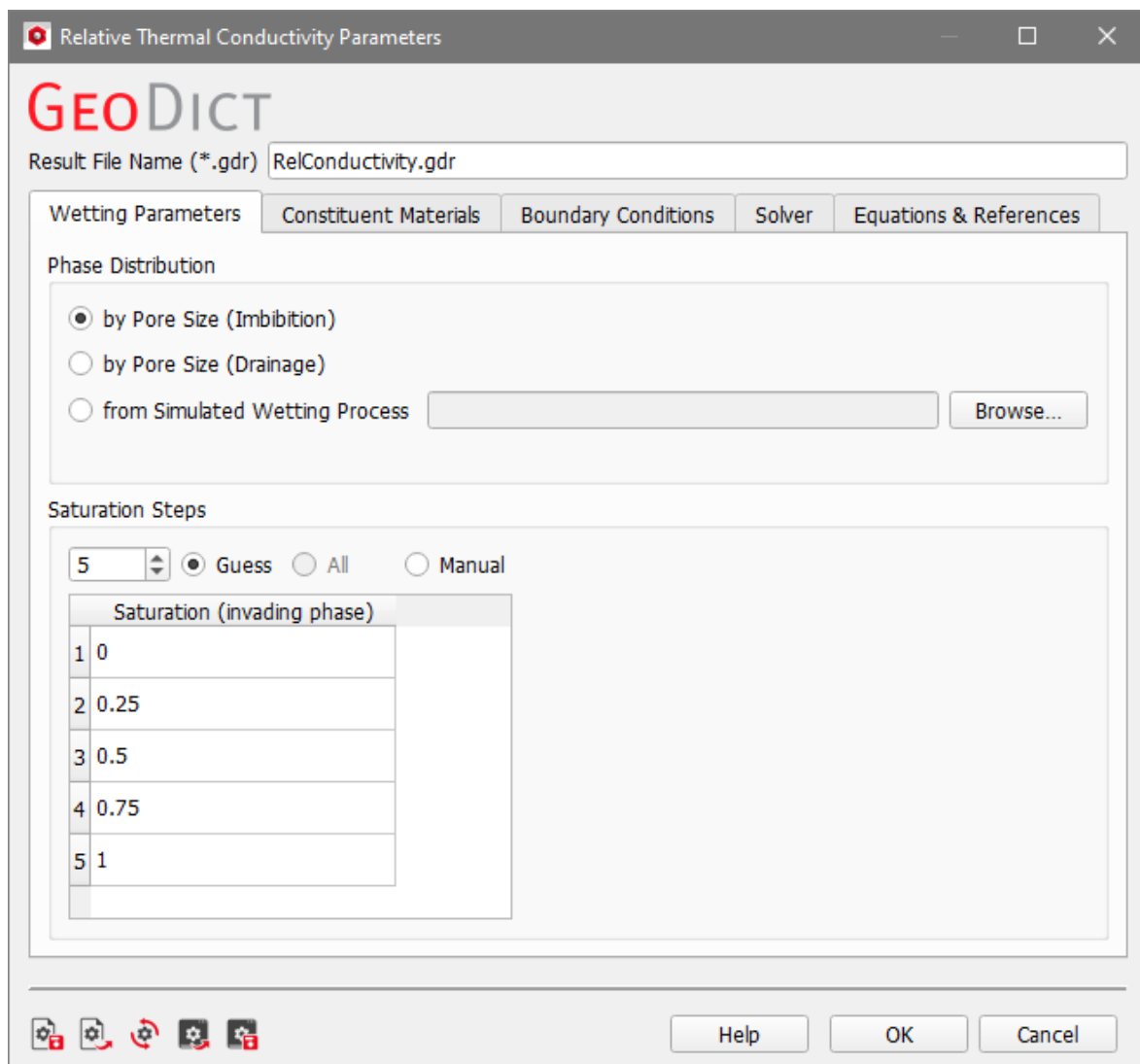


## RELATIVE THERMAL CONDUCTIVITY

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



Keep the default **Result File Name** (RelConductivity.gdr) or rename it according to your current project.



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

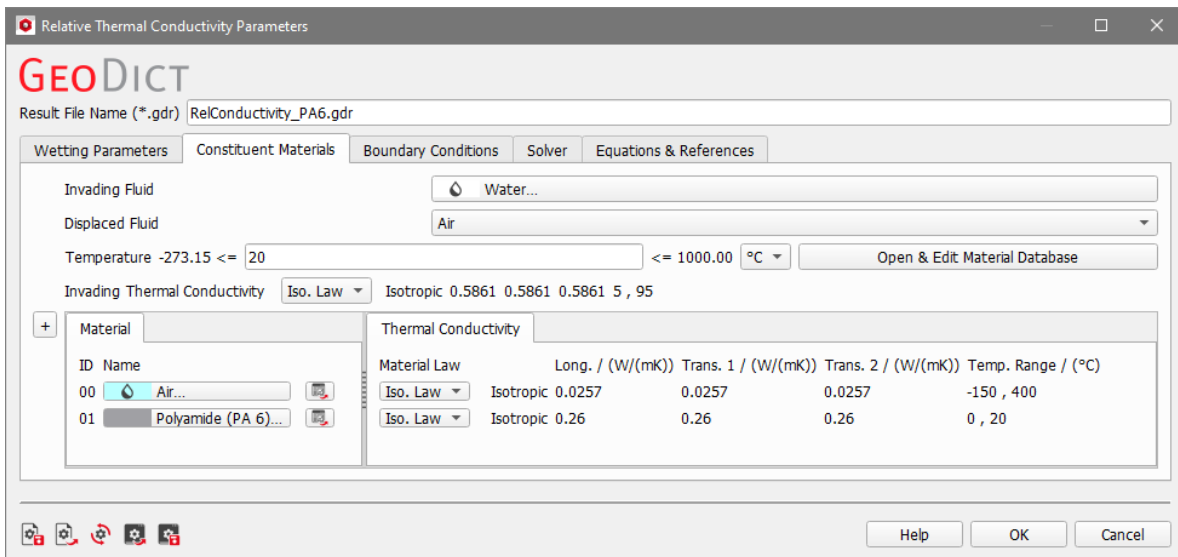
calculations can be entered. The last tab **Equations & References** provides further information about the equations used in this calculation.

## WETTING PARAMETERS

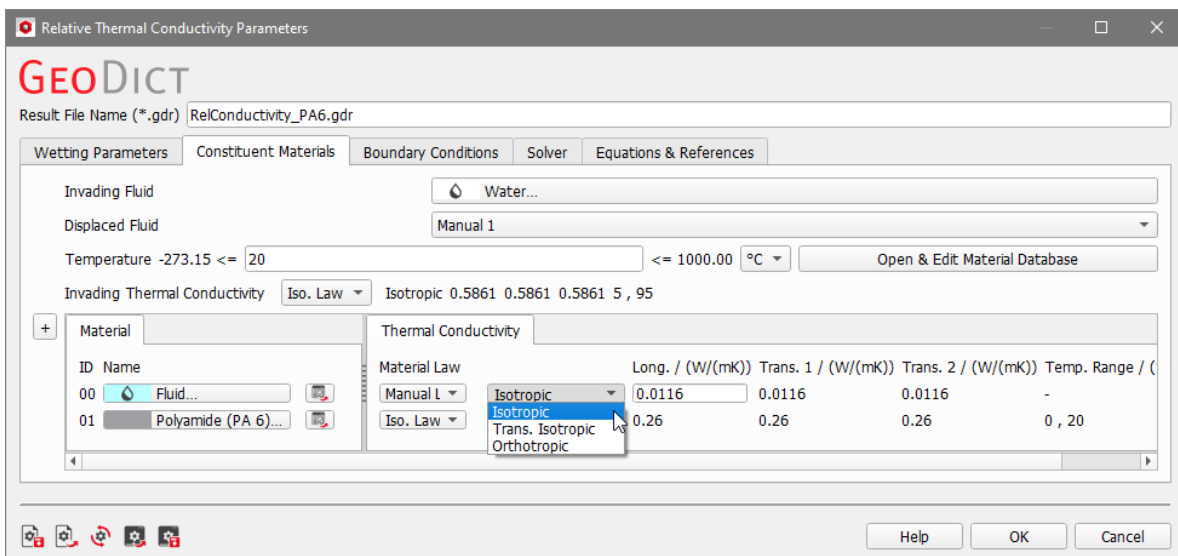
The wetting parameters for the calculation of the Relative Thermal Conductivity are the same as seen above (pages 36ff.) for the Relative Permeability. No Flow Phase needs to be selected for thermal conductivity computations.

## CONSTITUENT MATERIALS

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



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



## Assessing saturation-dependent material properties

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

## BOUNDARY CONDITIONS

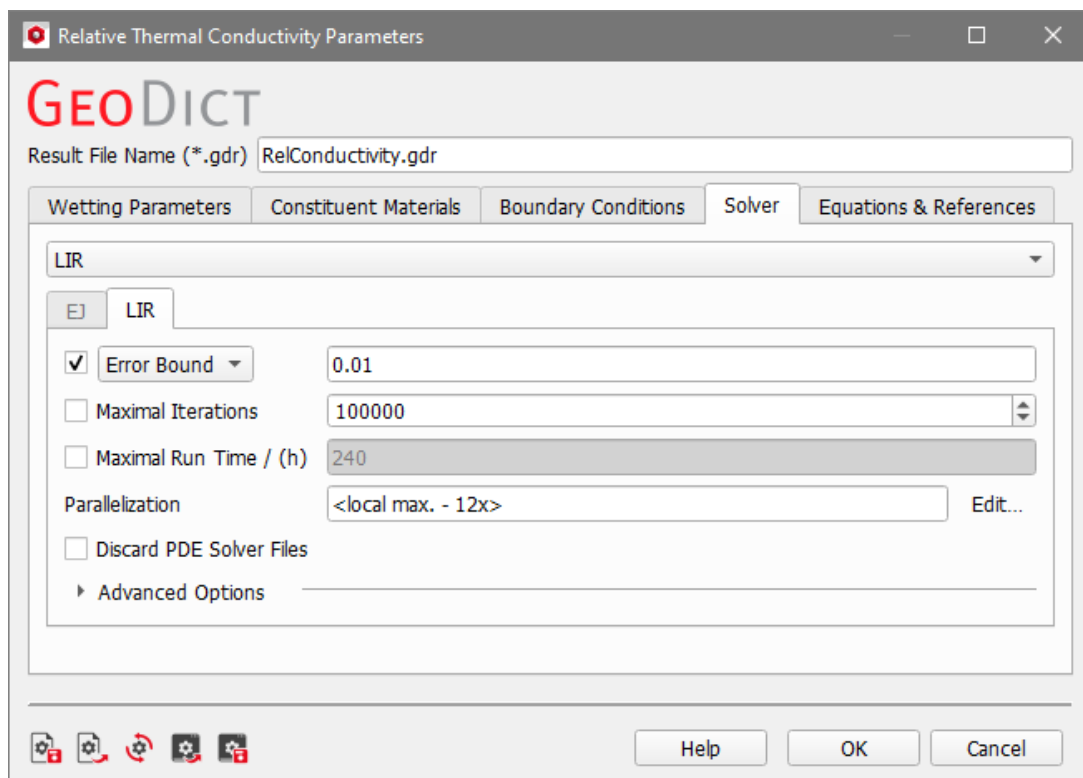
---

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 (page 51) for the Relative Diffusivity.

## SOLVER

---

For **Relative Thermal Conductivity**, the two flow solvers **EJ** and **LIR** are available and can be chosen from the pull-down menu. The parameters for the **EJ** solver and the **LIR** solver are the same as for the computations of the Relative Permeability (see pages 40ff.). The options **Stop Relative to Fully Saturated Permeability** and **Solver Type** (for EJ) are not available for the diffusivity computations.



## EQUATIONS & REFERENCES

---

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

- Poisson equation,
- Fourier's law.

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

## RELATIVE THERMAL CONDUCTIVITY RESULT FILE

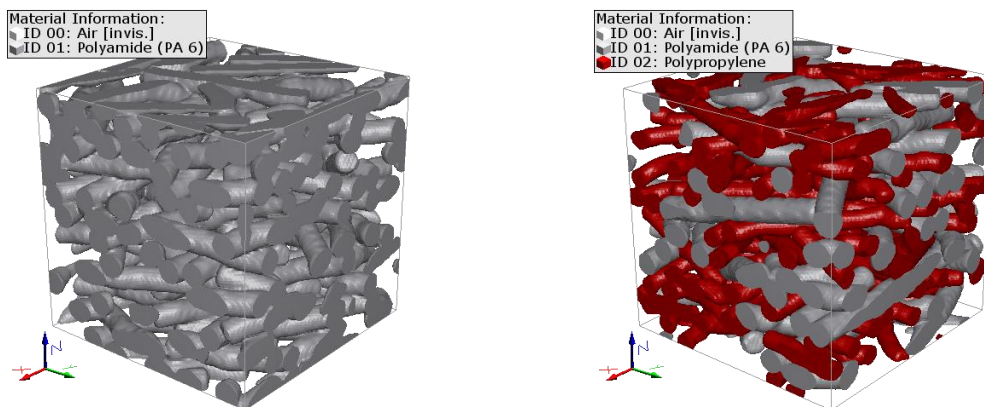
---

The Result File for the Relative Thermal Conductivity is very similar to the Result File of the Relative Gas Diffusivity. The settings described on pages 52ff. apply also here, but with Thermal Conductivity instead of Diffusivity. In the Plots subtab, the **Layered Temperature** is shown.

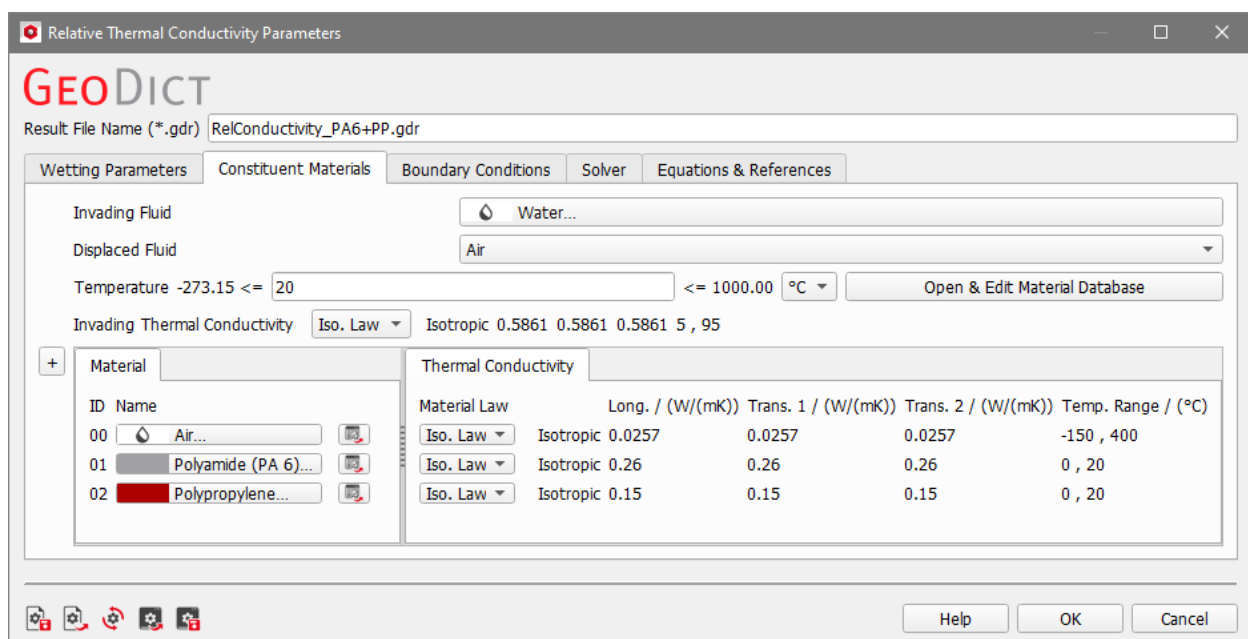
Additionally, we show here how to set-up and compare two result files, where the saturation-dependent relative thermal conductivity is computed at various invading fluid saturation levels (0%, 25%, 50%, 75%, and 100%) for two structures, both with 70% porosity, but different constituent materials. The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

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

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



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



## Assessing saturation-dependent material properties

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

The image shows two screenshots of the GEO DICT Result Viewer interface. The top screenshot shows the first experiment with the file 'RelConductivity\_PA6.gdr' selected. The bottom screenshot shows the second experiment with the file 'RelConductivity\_PA6+PP.gdr' selected. Both screenshots display a table of relative thermal conductivity values for various saturation levels. A red box highlights the  $\beta_{33}$  column in both tables, and a red arrow points from the value in the first table to the value in the second table.

**Relative Thermal Conductivity (Experiment 1)**

Saturation (Invading fluid)	$\beta_{11}$	$\beta_{12}$	$\beta_{13}$	$\beta_{21}$	$\beta_{22}$	$\beta_{23}$	$\beta_{31}$	$\beta_{32}$	$\beta_{33}$
0	unknown	unknown	-0.000257168	unknown	unknown	0.000399844	unknown	unknown	0.0502307
0.256122	unknown	unknown	1.79212e-05	unknown	unknown	0.000421221	unknown	unknown	0.126325
0.519788	unknown	unknown	-0.00315651	unknown	unknown	-0.000406753	unknown	unknown	0.226314
0.742733	unknown	unknown	-0.00252221	unknown	unknown	-0.00178244	unknown	unknown	0.332337
1	unknown	unknown	-0.000164613	unknown	unknown	0.000115047	unknown	unknown	0.464421

Remark: Thermal Conductivity values are given in W/(mK)

**Relative Thermal Conductivity (Experiment 2)**

Saturation (Invading fluid)	$\beta_{11}$	$\beta_{12}$	$\beta_{13}$	$\beta_{21}$	$\beta_{22}$	$\beta_{23}$	$\beta_{31}$	$\beta_{32}$	$\beta_{33}$
0	unknown	unknown	-0.000157875	unknown	unknown	0.000248482	unknown	unknown	0.0457551
0.239388	unknown	unknown	5.90432e-05	unknown	unknown	0.000824768	unknown	unknown	0.105868
0.533578	unknown	unknown	0.00357936	unknown	unknown	0.00107653	unknown	unknown	0.20898
0.731692	unknown	unknown	0.00334945	unknown	unknown	0.000181945	unknown	unknown	0.297647
1	unknown	unknown	-0.000299994	unknown	unknown	0.000281147	unknown	unknown	0.433536

Remark: Thermal Conductivity values are given in W/(mK)

--- Total runtime: 12.097 s, Total memory usage: 1.115 GiB ---

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.

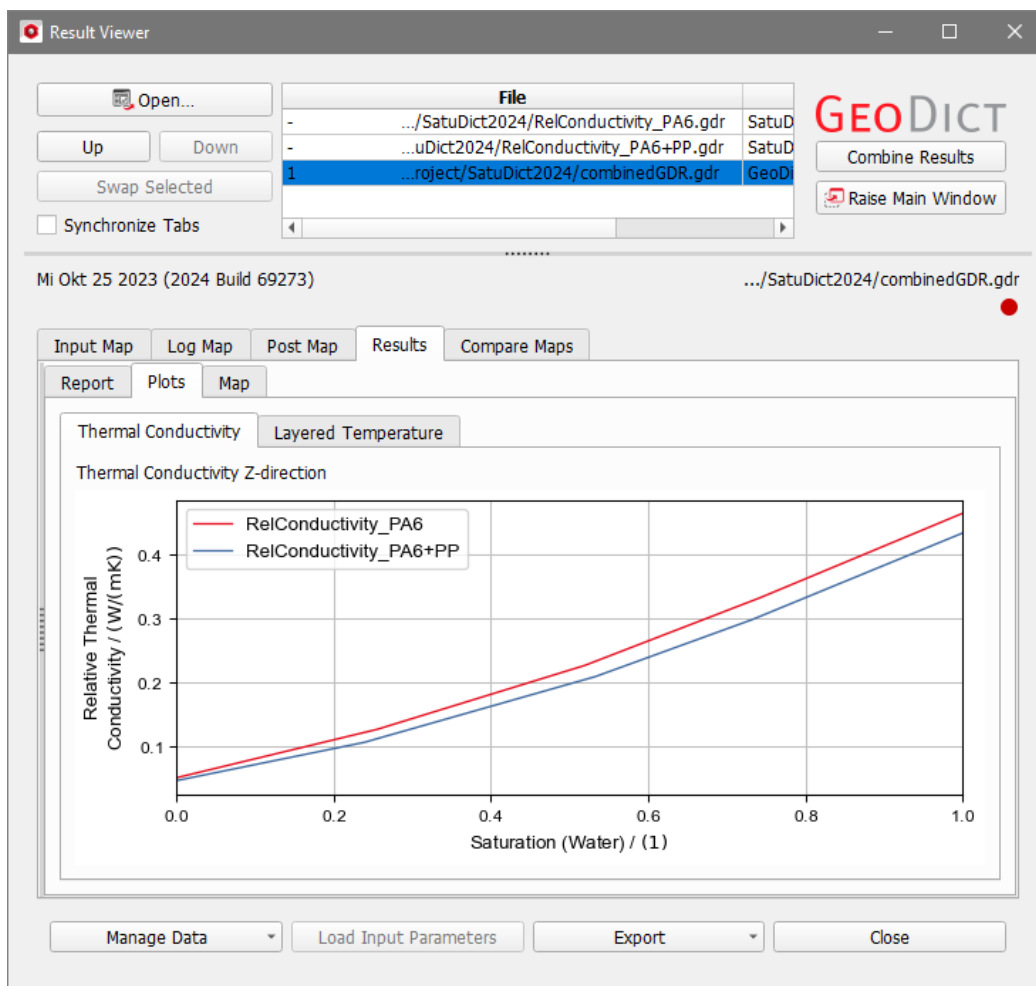
By highlighting the names of both result files and clicking the **Combine Results** button, the results of both files are combined and saved into a GDR file in the chosen project folder. The combining process allows post-processing on the combined results.

The combined result file contains the **Input Map, Log Map, Post Map, Results** and **Compare Maps** tabs. The **Results – Report** subtab, shows the names of the files that were used to create the combined result file (RelConductivity\_PA6.gdr and RelConductivity\_PA6+PP.gdr).

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

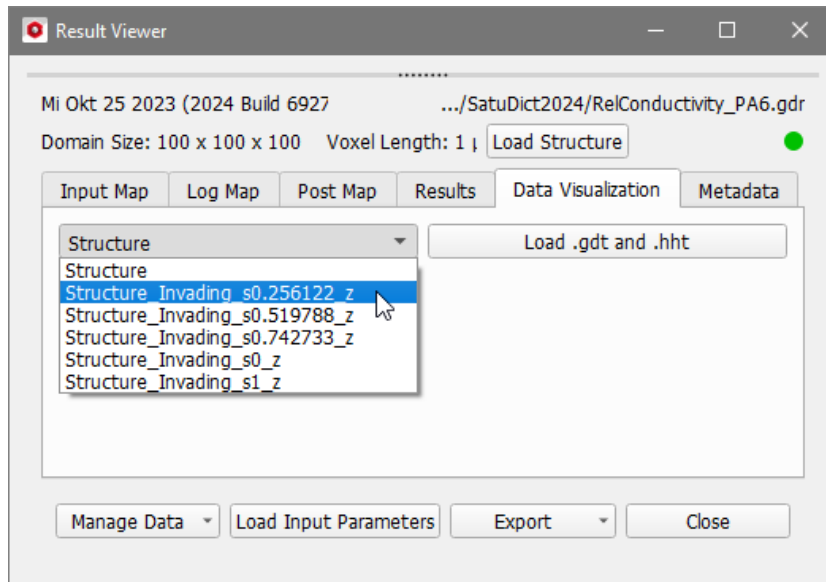
In the combined plot, the **Relative Thermal Conductivity** of the structures (Y-axis) increases with increasing saturation levels of water (Invading Fluid, X-axis). The relative thermal conductivity of the PA6+PP structure is always lower.

The parameters for the graphs can be modified (see pages 24ff.) in the Result Viewer of the original result files before combining them. The modification of the plot settings can be synchronized in both original files.



The HHT files (homogenized heat file; containing the temperature distribution) corresponding to the five saturation levels entered under the Wetting Parameters tab (0.00, 0.25, 0.50, 0.75, 1.00) are stored for each computation in the result folder, here **RelConductivity\_PA6** and **RelConductivity\_PA6+PP**, in the project folder.

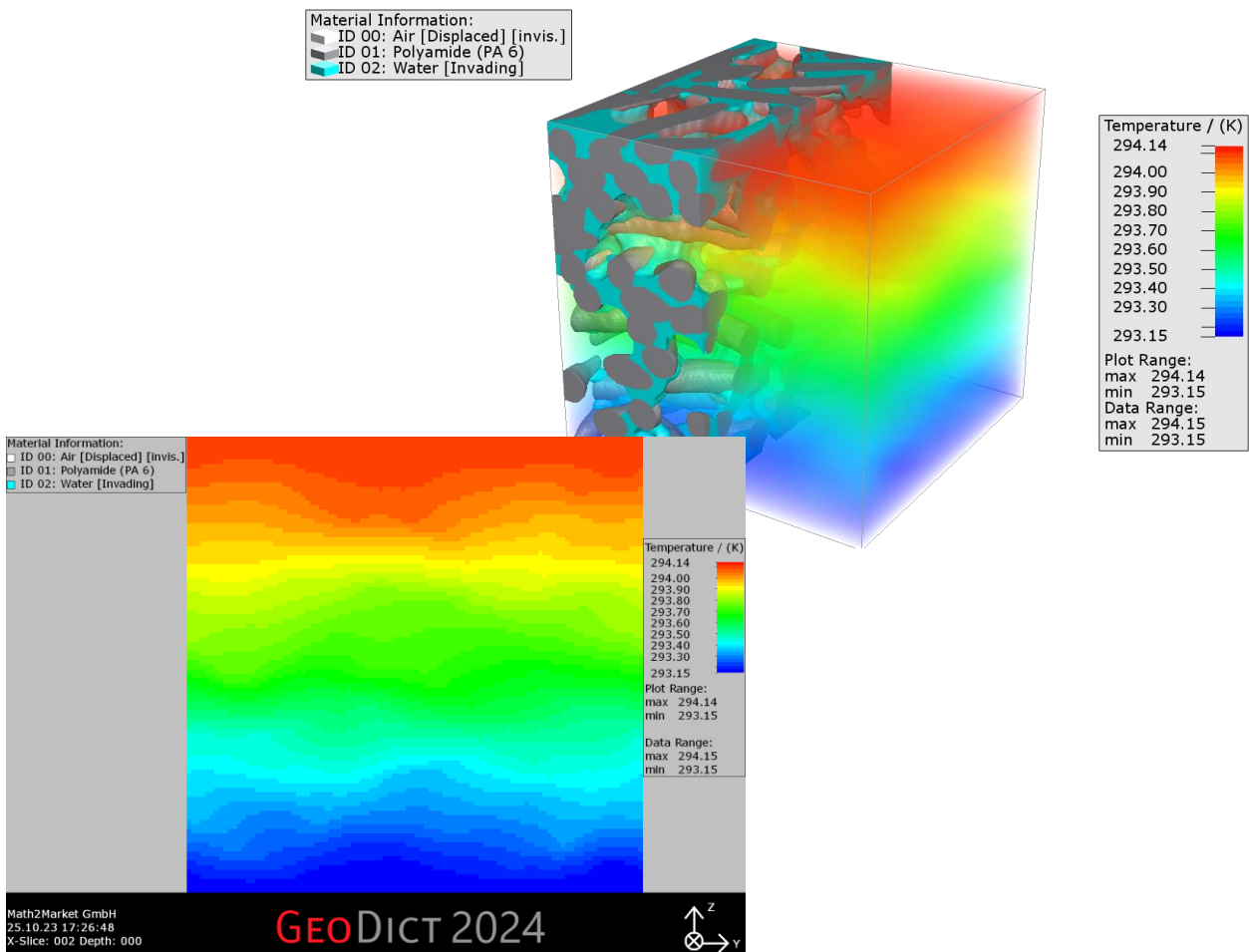
Under the **Data Visualization** tab, click **Load .gdt and .hht**, to access the .hht files and visualize the results. This can only be done for each of the result files individually and not for the combined result file.



This is similar to opening .gdt and .vap files (see pages 49ff.) to visualize the phase distribution for Relative Permeability results directly from the result file (GDR).

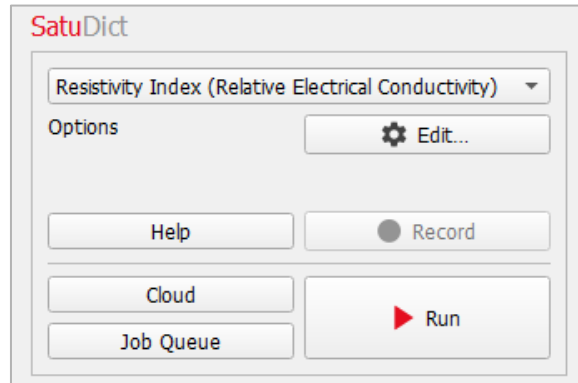
For example, we show the Structure\_p0\_s0.256122\_z files that correspond to a 25% invading fluid saturation in Z-direction from the experiment with the **100% PA6 structure**.

To better observe the results, we clip the structure (in 3D Rendering). An Alternative is to change to the 2D cross-section view (**View** → **Structure** in the menu bar) and to switch off the visualization of the structure. Observe how the heat is distributed in the structure.

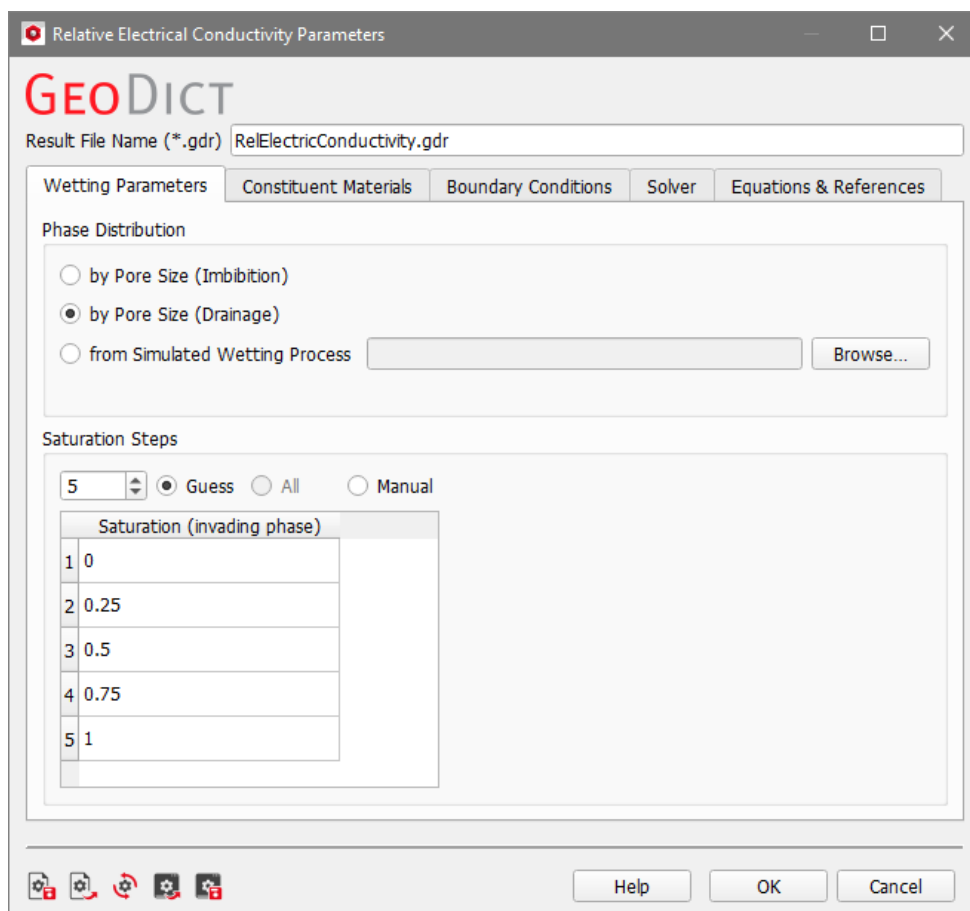


## RESISTIVITY INDEX

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



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



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

## Assessing saturation-dependent material properties

All parameters are similar to those explained for the Relative Thermal Conductivity computation starting on page [57](#).

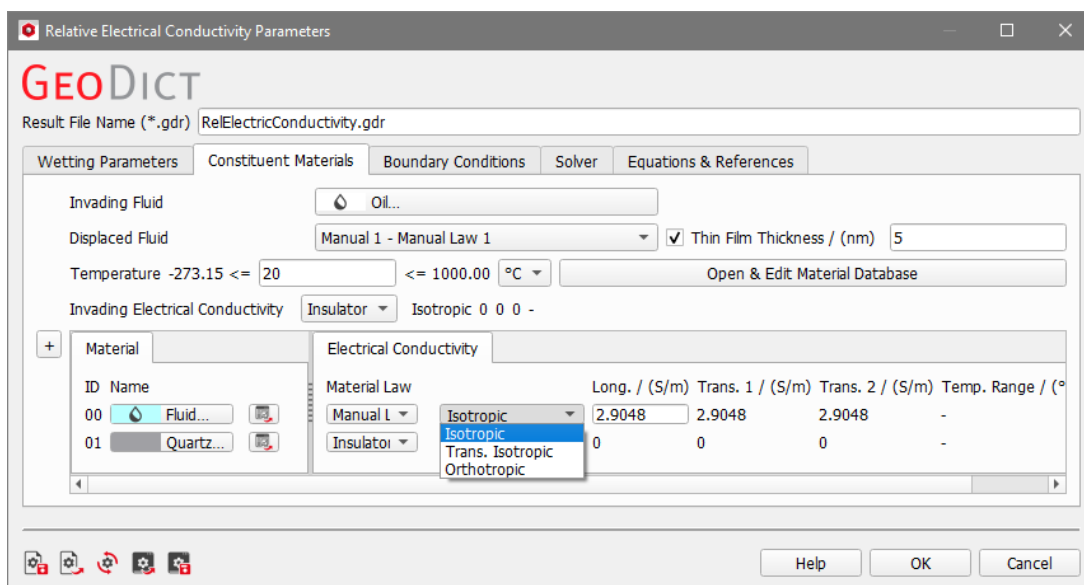
## WETTING PARAMETERS

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

## CONSTITUENT MATERIALS

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

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



Additionally, by checking **Thin Film Thickness**, the thin film model (see page [8](#)) can be used. The thickness of the thin film must be smaller than the current voxel length.

## BOUNDARY CONDITIONS

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

## SOLVER OPTIONS

For **Relative Electrical Conductivity**, the **EJ** and **LIR** flow solvers are available and can be chosen from the pull-down menu. The parameters for the **EJ** solver and the **LIR** solver are the same as for the computations of the Relative Permeability (see pages 40ff.).

The options **Stop Relative to Fully Saturated Permeability** and **Solver Type** (for EJ) are not available.

## EQUATIONS & REFERENCES

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

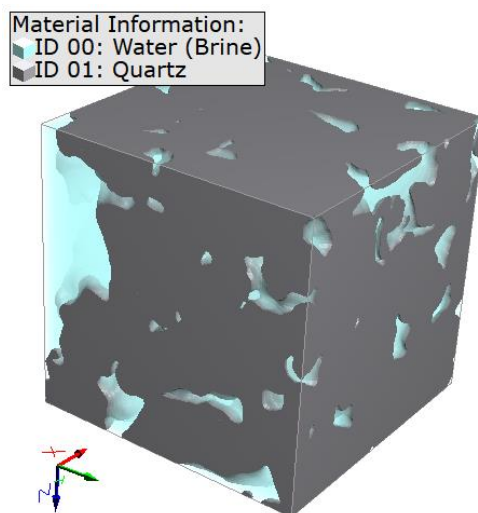
- Poisson equation,
- Ohm's law.

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

## RESISTIVITY INDEX RESULT FILE

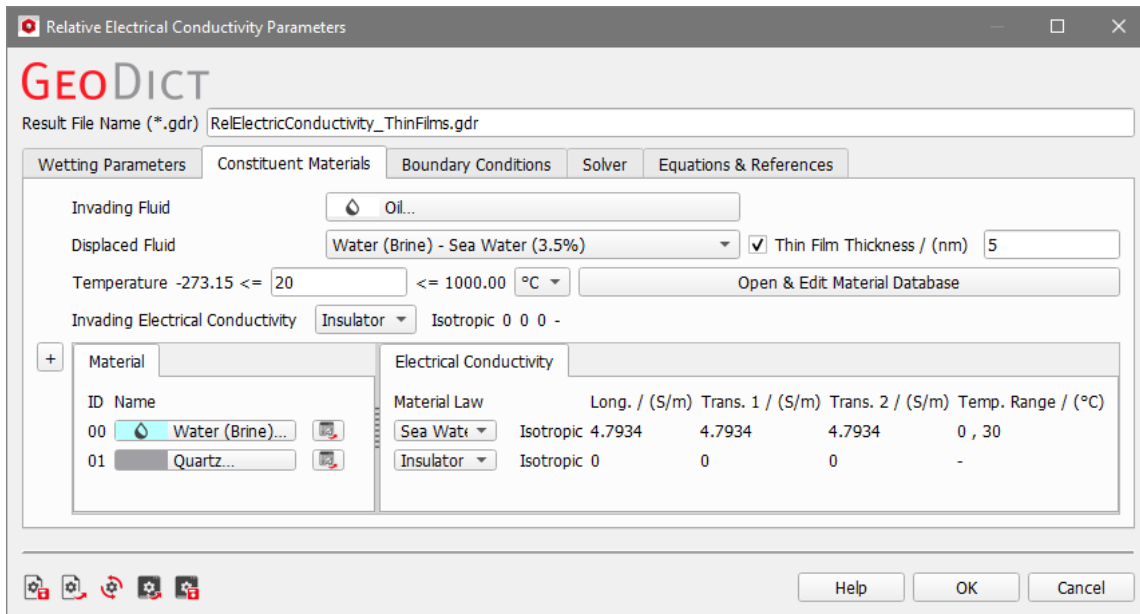
Here, the resistivity index is computed at various invading fluid saturation levels (0%, 25%, 50%, 75% and 100%) for a porous medium with 17% porosity. The invading fluid is Oil (0 S/m) and the displaced fluid is Water (Brine) (5 S/m). The relative electrical conductivity is calculated in Z-direction.

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



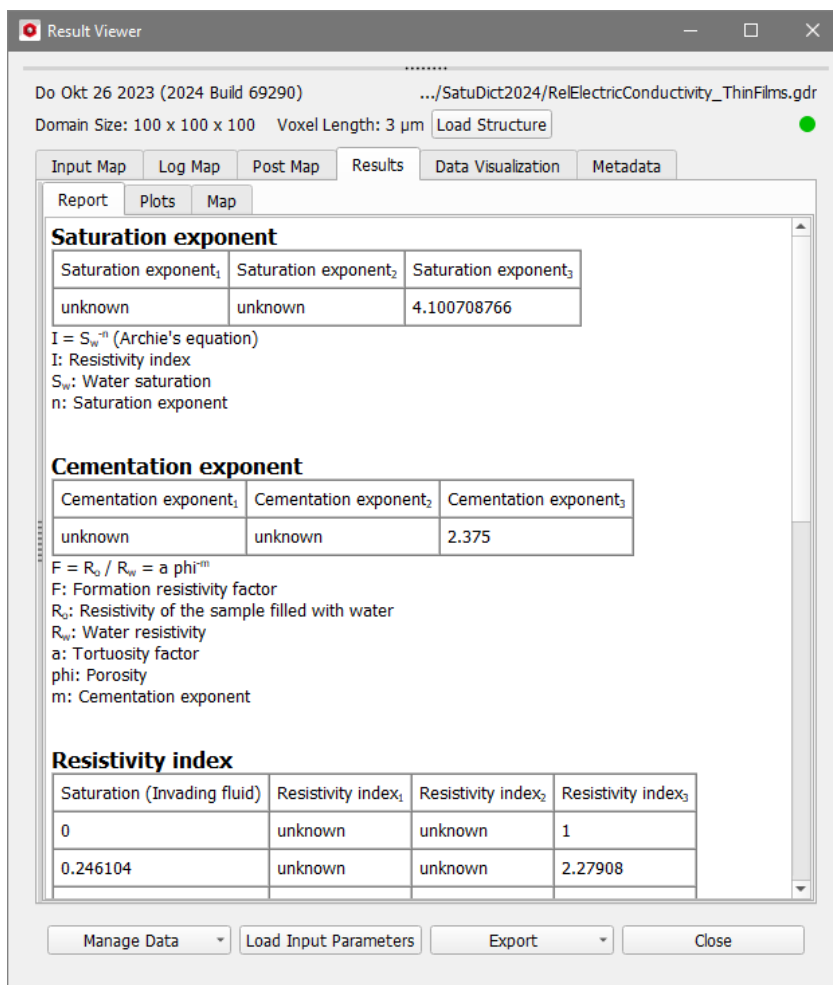
The selected materials and their electrical conductivity are entered under the **Constituent Materials** tab by selecting them from the material database.

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

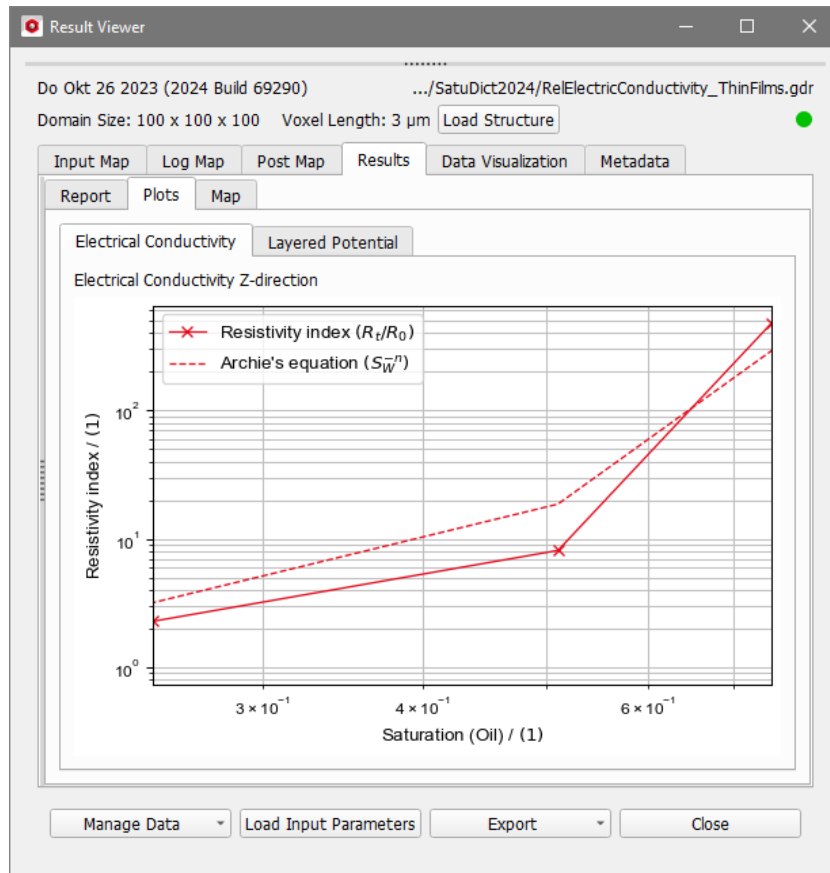


After the computations are finished, the Result Viewer of the result file opens, and the results are saved into a GDR file in the chosen project folder (**File → Choose Project Folder...**). In this example, the **RelElectricConductivity.gdr** result file is saved in the project folder together with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

Under the **Results - Report** subtab, the tables for **Saturation exponent**, **Cementation exponent**, **Resistivity index**, and **Relative Electrical Conductivity** are shown for the chosen saturation rates (0.25, 0.5, 0.75) and the start and end saturations (0 and 1) in the directions for which results were calculated.



Under the **Results - Plots** subtab, these values are shown in graphs and the **Layered Potential** is shown. The parameters of the graphs can be changed as seen in pages [24ff.](#)



## Assessing saturation-dependent material properties

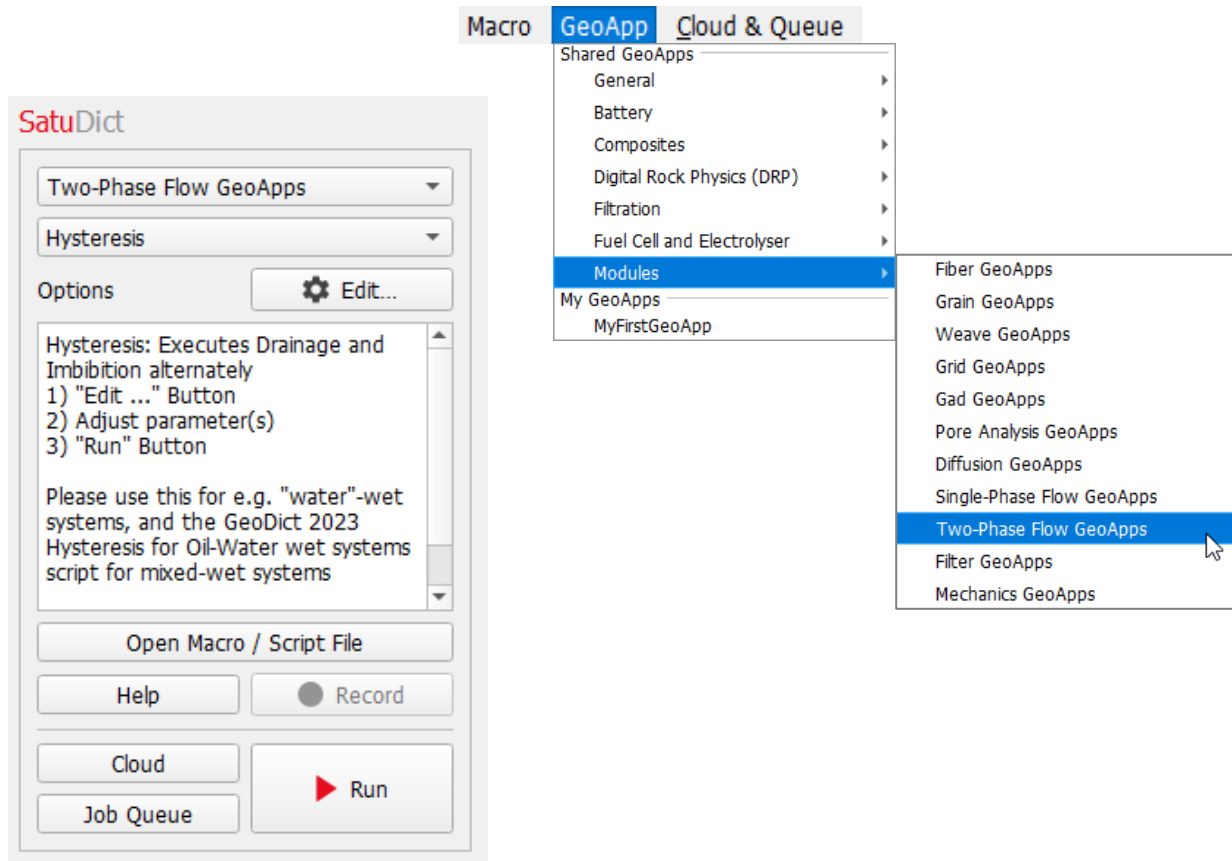
We redo the computations, but without adding thin film voxels and compare the plots of the resistivity index using a combined gdr file. Observe that for the structure without thin film voxels there is no conductivity above an oil saturation of about 50%.



## TWO-PHASE FLOW GEOAPPS

When **Two-Phase Flow GeoApps** is selected in the **SatuDict** section, predefined computation settings can be chosen from the pull-down menu. In **GeoDict 2024** only the **Hysteresis** GeoApp is available.

The **Predefined SatuDict** computations are also accessible directly from the menu bar as one of the **GeoApps**.



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

## ADD PREDEFINED COMPUTATIONS

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



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

### EDIT AND EXECUTE PREDEFINED COMPUTATIONS

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

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

### HYSTERESIS

The **Hysteresis** GeoApp performs a Hysteresis simulation of the **SatuDict** functionalities Drainage and Imbibition (both with invading fluid connected to a reservoir and the displaced fluid can leave a residual) in succession. This GeoApp repetitively runs the Capillary Pressure command in the same way as it was explained on page 31ff. until the chosen **Number of Cycles** is reached. After clicking **Edit...**, enter the **Hysteresis Result File Name**, **Number of Cycles**, **Interfacial Tension**, and **Contact Angle**.

The screenshot shows the 'Hysteresis Parameters' dialog box. It features the 'GEO DICT' logo at the top left. The parameters are organized into several sections:

- Hysteresis Result File Name (\* .gdr):** A text field containing 'Hysteresis.gdr' and a 'Browse...' button.
- Hysteresis cycle:** A section containing:
  - Number of Cycles:** A spin box set to '3'.
  - Start with Drainage?**
  - Use Dynamic Pore Morphology**
- Fluid phases:** A section containing:
  - Wetting Phase:** A dropdown menu showing 'Water (Brine) (Fluid)...'.
  - Non-Wetting Phase:** A dropdown menu showing 'Oil (Fluid)...'.
- Capillary Pressure Curve computation - Parameters:** A section containing:
  - Interfacial Tension / (N/m):** A text field with '0.035'.
  - Contact Angle Mode:** A dropdown menu set to 'True Contact Angle'.
  - Contact Angle for Material ID 1 / (°):** A text field with '30'.
  - Contact Angle for Material ID 2 / (°):** A text field with '40'.
  - Contact Angle for Material ID 3 / (°):** A text field with '50'.
  - Contact Angle for Material ID 4 / (°):** A text field with '60'.
- Boundary conditions:** A section containing:
  - Drainage - invading phase boundary:** A dropdown menu set to 'z-'.
  - Imbibition - invading phase boundary:** A dropdown menu set to 'z+'.
- Parallelization:** A dropdown menu set to 'Maximum'.

At the bottom of the dialog, there are several small icons (a folder, a document, a refresh arrow, a gear, and a lock) and two buttons: 'OK' and 'Cancel'.

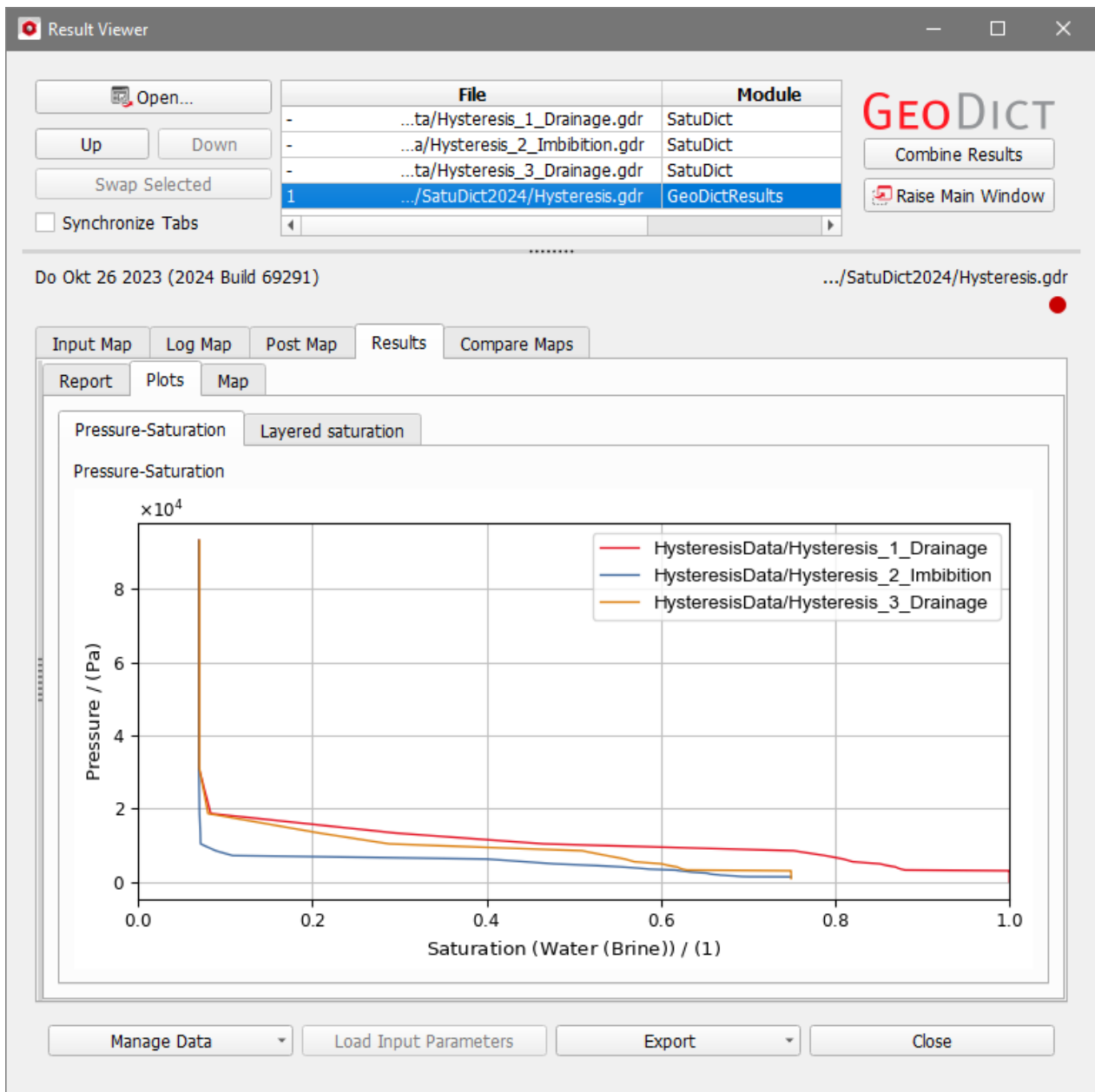
Additionally, the **Wetting Phase** and **Non-Wetting Phase** can be chosen and whether to start with Drainage or with Imbibition.

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

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

Tooltips describe all those options in more detail.

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



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