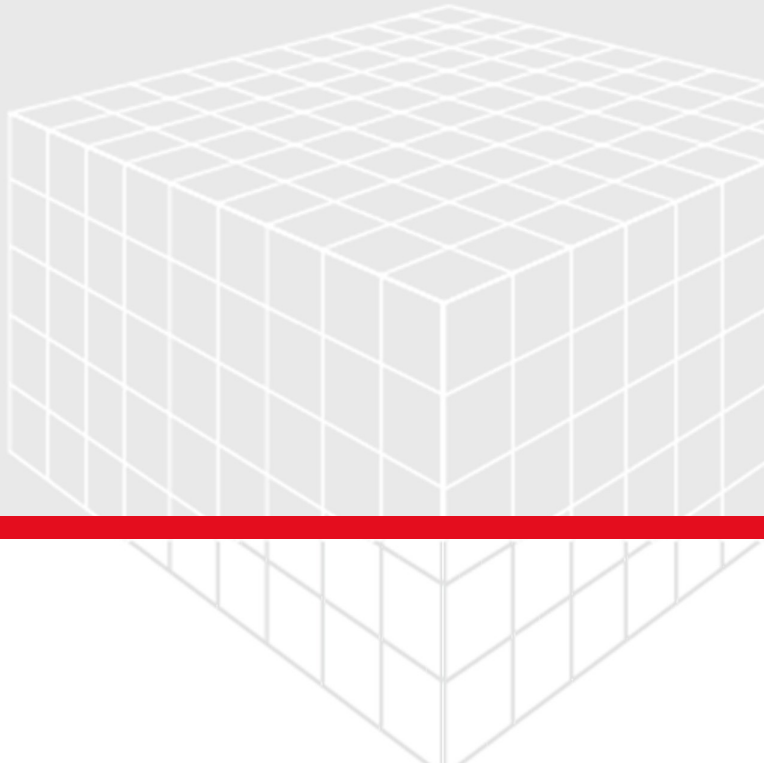
SatuDict

User Guide



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GeoDict

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SatuDict

1 SatuDict

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 rock samples where water is the wetting phase and oil is the non-wetting phase.

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).

This 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 simulation.

New in GeoDict 2026

- It is now possible to simulate Dynamic Contact Angles 9, i.e., advancing and receding contact angles, in the SatuDict Capillary Pressure command. Two models are implemented - one for liquid/gas and one for liquid/liquid systems. These models take the capillary number as input which is evaluated for each simulation step. Therefore, the density, viscosity, surface tension, and flow-rate is now taken into account for distribution of the fluids into the pore space.

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Join the conversation

Visit the Community on GeoDict Forum to be inspired and get answers to top questions.
Find illustrative application examples on the website.
Our tutorials and seminar videos give you a first hands-on experience. They are collected in the Learning Center.
Send your Support Request to our technical Support.

1.1 Theoretical Background

Governing equations and explanations

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  Read more about the Pore Morphology Method used in SatuDict.
- Dynamic Contact Angles 9
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  Find here the equations of different fit models, e.g., fits to the capillary pressure curve.

1.1.1 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** (Hilpert and Miller 185) 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 where fluids do not mix.

For such systems, the pore space accessible to the non-wetting phase is given by the Young-Laplace equation,

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

Young-Laplace equation

where σ is the surface tension, α the contact angle, p_c is the capillary pressure and r defines the minimum radius of accessible pores. Thus, the problem is reduced to a purely geometrical problem. The contact angle α can be different at each solid phase inside the porous medium (Schulz et. al. (2008) 186) 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.

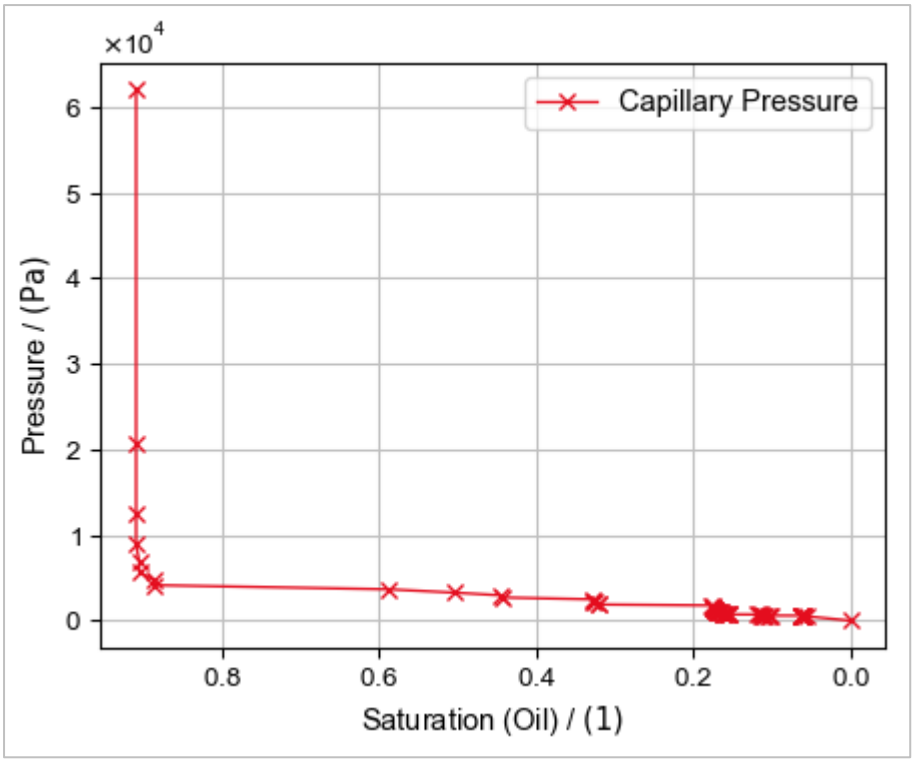
In the following, an example of the resulting capillary pressure curve of a drainage simulation with all three methods is shown below.

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 six saturation points are computed between a saturation of 20% and 80%.

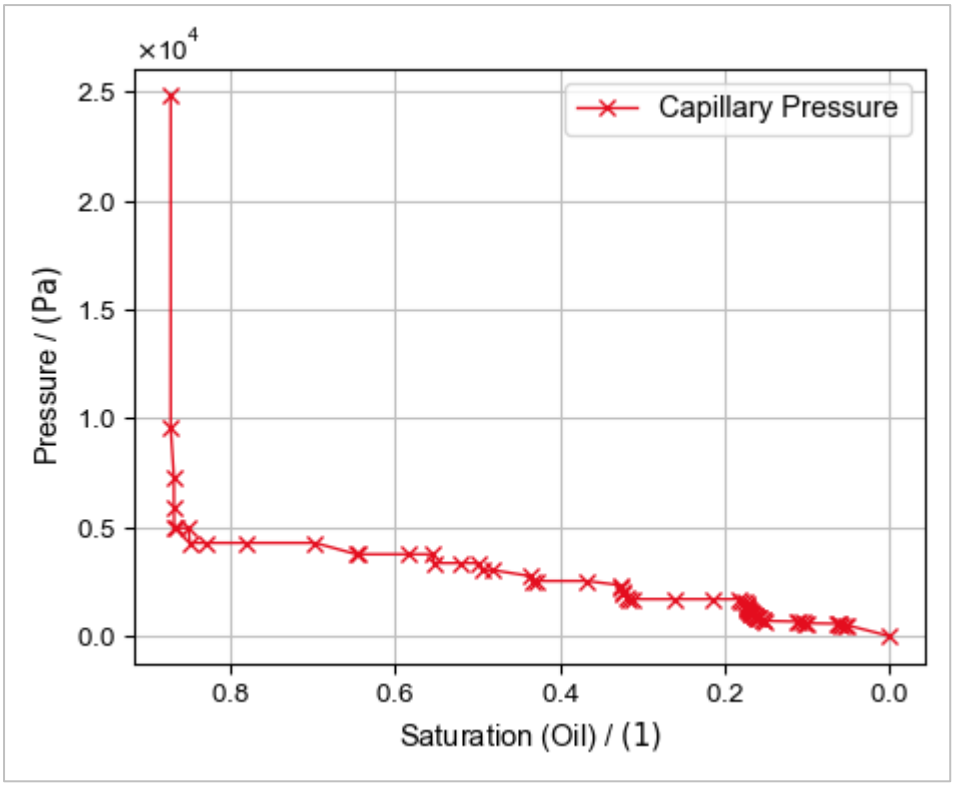


This method is useful for the prediction at which capillary pressure the breakthrough occurs and provides detailed information about fluid distributions for high and low saturated structures. If the detailed fluid distribution at a broad range of saturations is of interest, this method should not be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

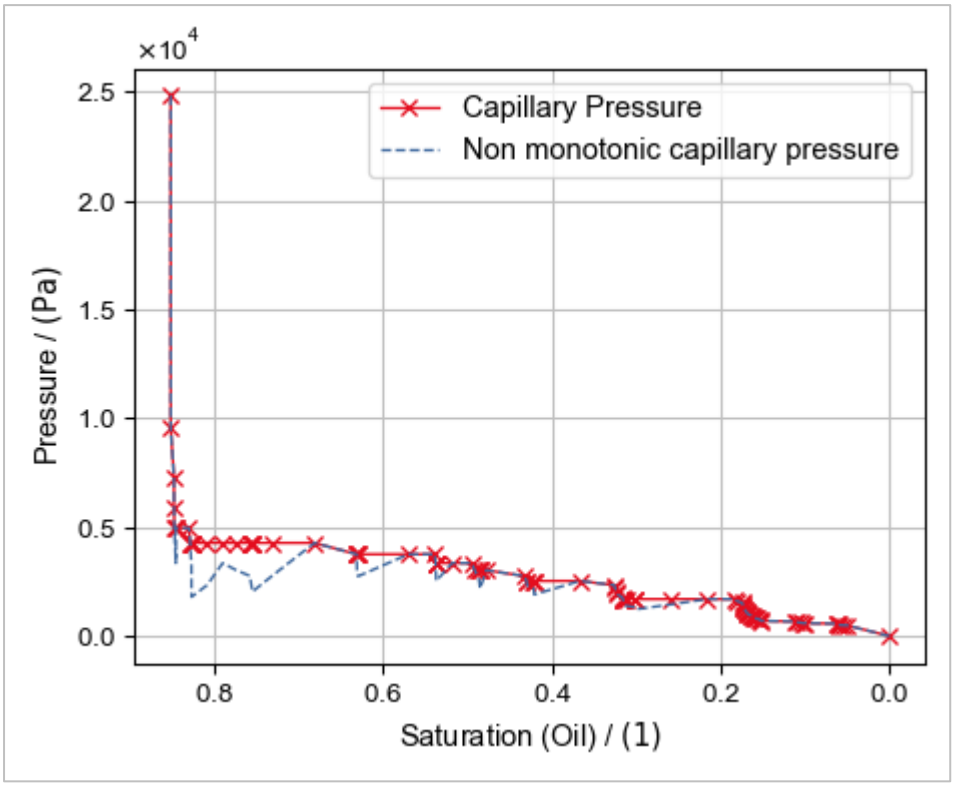
However, certain physical phenomena, e.g., formation of water droplets above a fiber structure with large pore space at the top, cannot be modelled with this method. This requires that the capillary pressure can have a non-monotonic behavior.

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.

1.1.2 Dynamic Contact Angles

If you compare a static two-phase system with a moving two-phase system, you will observe that the interface, defined by the contact line, between the fluids is deformed in the moving system. A simple example would be a water drop running down a wall. The strength of this deformation scales with the Capillary Number

$$Ca = \frac{\eta V}{\gamma}$$

(2) Capillary Number

where η is the viscosity, V is the contact line speed, and γ is the surface tension. It is the ratio of viscous forces to surface tension forces. For capillary numbers near 0 flow through porous media is dominated by capillary forces, while for higher values the viscous forces dominate.

SatuDict with static contact angles assumes that the capillary number is almost zero, which means that the velocity of the contact line is assumed to be almost zero, too (as the viscosity is always positive). Thus, stationary distributions of two fluids are considered.

When checking **Use Dynamic Contact Angles** for the Dynamic Pore Morphology Method[24] in the Capillary Pressure command, non-zero capillary numbers are allowed.

Know how! The option to use dynamic contact angles is new in GeoDict 2026!

This means the velocity of the contact line is not zero anymore which leads to an **advancing contact angle** (maximum angle when the contact line moves forward) and a **receding contact angle** (minimum angle when it retreats). Both differ from the **static contact angle** because viscous stresses bend the interface as it slides over the solid while the surface tension tries to maintain the equilibrium shape. Thus, we now have **dynamic contact angles** which depend on the velocity of the contact line and thus on the capillary number.

If you want to use the dynamic contact angles, you need to enter additional input in the options dialog compared to the static contact angles.

To define the velocity of the contact line you have to give the flow rate on a flow area in the Saturation Experiment[23] tab. Additionaly, you need to predefine the viscosity of the fluids in the Constituent Materials[18] tab. SatuDict always takes the viscosity of the denser fluid, e.g., for both Air-Water and Oil-Water systems, the viscosity of Water is taken.

To determine the phase distributions SatuDict computes the resulting dynamic contact angle. As shown by R.L. Hoffmann (1974)[185] by plotting measured dynamic contact angles, the dynamic contact angle θ_d can be written as a function of the capillary number Ca and a shift factor related to the static contact angle θ_s.

$$\theta_d = F(Ca + G(\theta_s)) \tag{3}$$

The fact that for $Ca = 0$ the static and dynamic contact angles have to be the same, yields that $G = F^{-1}$ has to be the inverse function of F. The function F is called the Hoffmann function and the dynamic contact angle θ_d can now be written as

$$\theta_d = F\left(Ca + F^{-1}(\theta_s)\right) \tag{4}$$

(4) Hoffmann model

with F^{-1} being the inverse function of F.

Important! Hoffmann's correlation matches well at low to moderate capillary numbers (e.g., $Ca < \sim 0.01$) but can deviate at higher velocities (e.g., due to inertial effects) which was found in experimental studies.

There are two methods implemented to determine the dynamic contact angle based on the above described input parameters. They are developed by Kistler (1993)[185] and Cox (1986)[185] and depend on the aggregate state of the two incorporated fluids.

Kistler (gas-liquid systems)

Kistler has found an expression for the Hoffmann function F by fitting the original graph in Hoffmann's paper:

$$F(x) = \arccos\left\{1 - 2\tanh\left[5.16\left(\frac{x}{1 + 1.31\,x^{0.99}}\right)^{0.706}\right]\right\} \quad (5)$$

Kistler model

This model is only valid for liquid-gas interfaces.

Cox (liquid-liquid systems)

Cox uses different formulas describing the dynamics at the contact line and, with some assumptions such as very small capillary number, derives another formula. We use the formula simplified by Chan (2020)[185], which gives an expression for the inverse of the Hoffmann function:

$$F^{-1}(\theta) = \int_0^{\theta} -\frac{\sin^2\phi}{3\,G(\phi, M)}\,d\phi \quad (6)$$

Cox model

The function G depends on the viscosity ratio M

$$M = \frac{\eta_{\text{displaced}}}{\eta_{\text{invading}}} \quad (7)$$

Viscosity ratio

of invading and displaced fluid and is defined as

$$G(\theta, M) = -\frac{2\sin^3\theta}{3}\,\frac{M^2F_1(\theta) + 2MF_3(\theta) + F_1(\pi - \theta)}{MF_1(\theta)F_2(\pi - \theta) + F_1(\pi - \theta)F_2(\theta)} \quad (8)$$

with the additional functions

$$F_1(\theta) = \theta^2 - \sin^2\theta \quad (9)$$

$$F_2(\theta) = \theta - \sin\theta\cos\theta \quad (10)$$

and

$$F_3(\theta) = \theta(\pi - \theta) + \sin^2\theta \quad (11)$$

Moreover, the Hoffmann model is slightly modified:

$$\theta_d = F\left(Ca \cdot \ln\left(\frac{R}{\lambda}\right) + F^{-1}(\theta_s)\right) \quad (12)$$

where R is the outer macroscopic scale (e.g., radius related to the interface curvature) and λ is the inner microscopic scale (e.g., slip length of the more viscous fluid).

This model is only valid for liquid-liquid systems.

1.1.3 Model Fits

Thomeer Model

The **Thomeer Model** (Thomeer (1960)[186]) is designed for Mercury Intrusion Capillary Pressure[49] (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:

$$S_{NWP} = S_d \cdot \exp\left(-\frac{G}{\log\left(\frac{P_c}{P_d}\right)}\right) \quad (13)$$ Thomeer Model

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

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

LET Model

For Relative Permeability computations an **LET Model** (Lomeland and Ebeltoft[185]) can be used to approximate relative permeability curves.

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

$$K_{rw} = \frac{K_{rwr}(S_{wn})^{L_w}}{(S_{wn})^{L_w} + E_w(1 - S_{wn})^{T_w}} \quad (14)$$

and

$$K_{row} = \frac{K_{rot}(1 - S_{wn})^{L_o}}{(1 - S_{wn})^{L_o} + E_o(S_{wn})^{T_o}} \quad (15)$$

for the oil relative permeability, where:

$$S_{wn} = \frac{S_w - S_{wir}}{S_{wor} - S_{wir}} \quad (16)$$

Normalization of water saturation

is the normalized water saturation value S_w. Only S_{wir} (irreducible water saturation), S_{wor} (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.

Corey Model

The Corey correlations of the relative permeability for oil and water are

$$K_{row}(S_w) = K_{rot}(1 - S_{wn})^{N_o} \quad (17)$$

and

$$K_{rw}(S_w) = K_{rwr}(S_{wn})^{N_w} \quad (18)$$

The empirical parameters N_o and N_w are called **Corey exponent**.

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:

$$K_{ws} = \frac{t \cdot 0.5}{h} K_w + \frac{h - t \cdot 0.5}{h} K_s$$

(19) New conductivity at solid boundary

$$K_{wo} = \frac{t \cdot 0.5}{h} K_w + \frac{h - t \cdot 0.5}{h} K_o$$

(20) New conductivity invading fluid

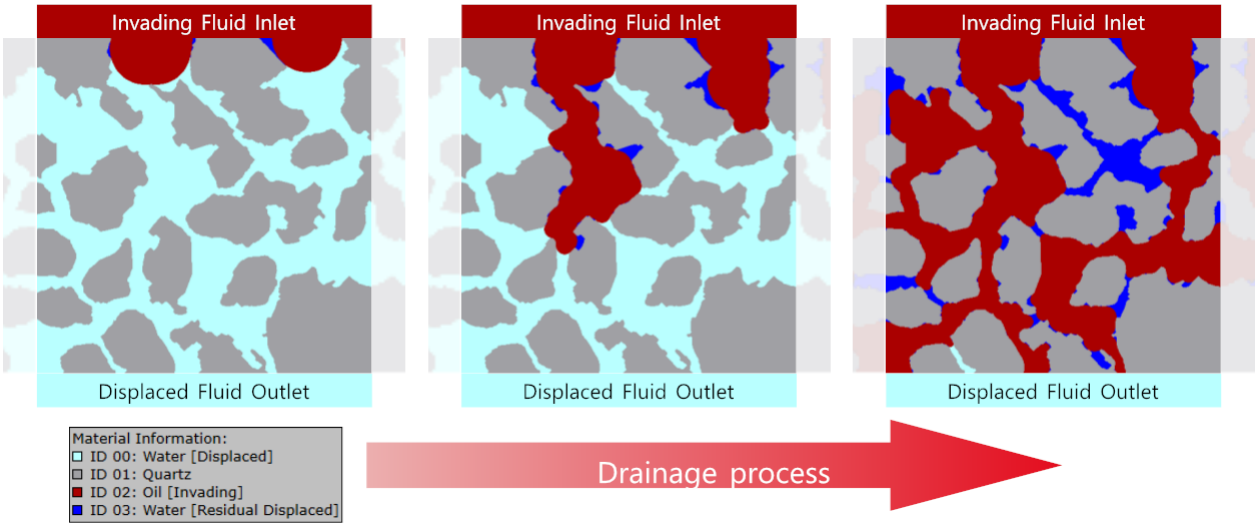
where K_w is the conductivity of the displaced fluid (e.g., 5 S/m), K_s is the conductivity of the solid, K_o is the conductivity of the invading fluid (e.g., 0 S/m), h is the voxel length and t is the thickness of the thin film (e.g., 5 nm).

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

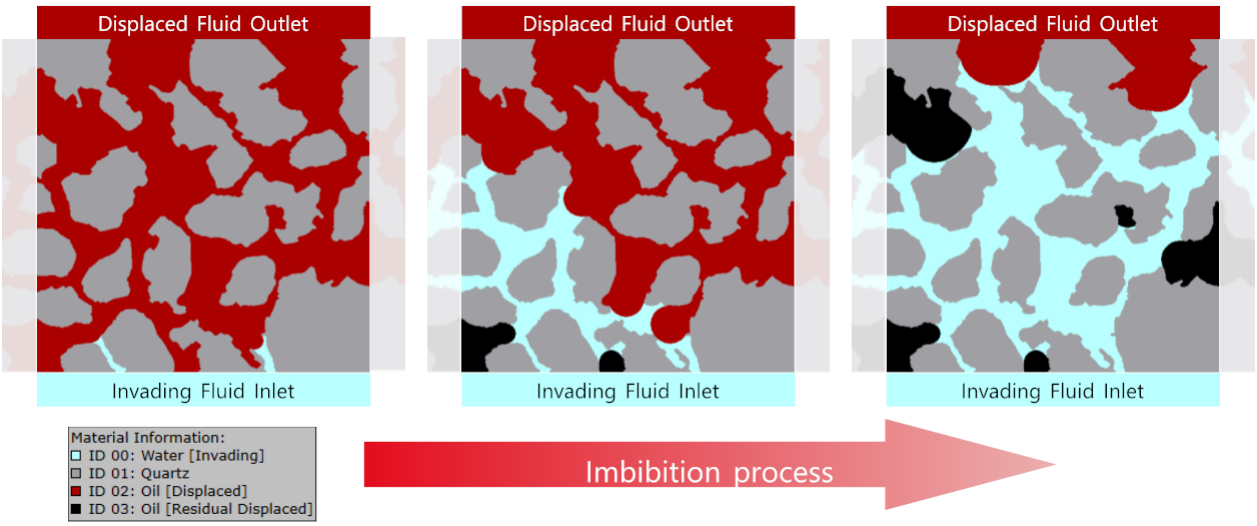
1.2 Capillary Pressure Curve

Determine the **Capillary Pressure Curve** using a pore morphology method [5] 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.

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, where the Oil reservoir is at the top and the Water reservoir is at the bottom. The left and right sides of the structure have symmetric boundary conditions.



Drainage displacement occurs when a **non-wetting** infiltrating fluid (here Oil) enters the porous media and displaces a **wetting** fluid (here Water) 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, displaces it (here, Water displaces Oil).

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 or, after Imbibition, a residue of the non-wetting phase can remain trapped in the porous media as **Residual Displaced**. The **Residual** is the part of the displaced fluid that is not connected to the displaced fluid outlet anymore during the simulated process.

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.

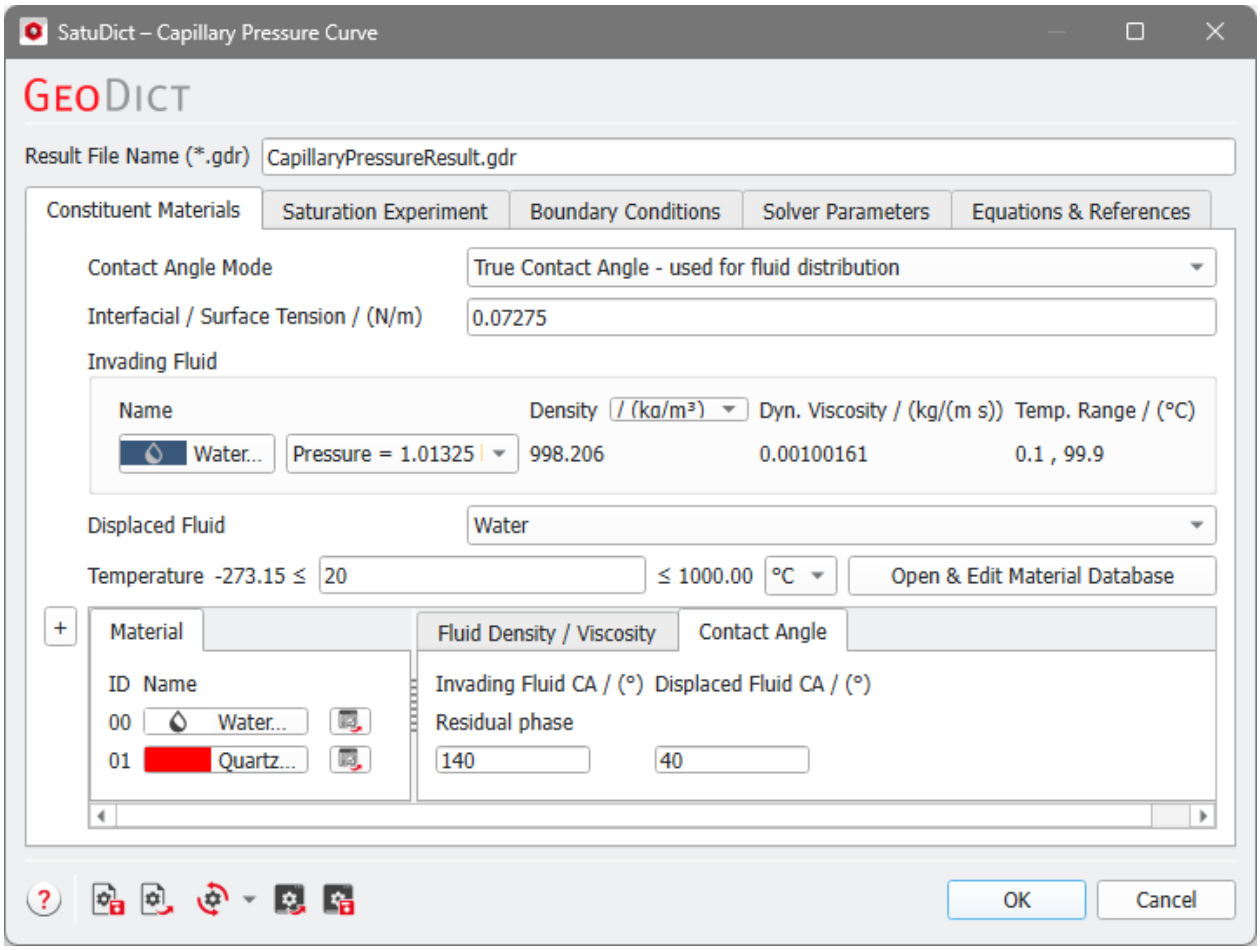
The Capillary Pressure Curve command

- Options 16
  Set the parameters for the calculation.
- Results 31
  View the computed results.
- Capillary Pressure with Hysteresis Effect 44
  We explain how you can manually set up a Hysteresis where Drainage and Imbibition simulations are performed alternately.

1.2.1 Options

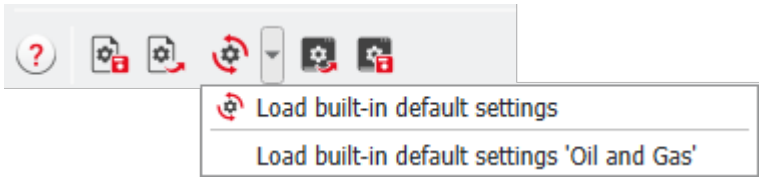
The **Capillary Pressure Curve** dialog opens when clicking the **Edit...** button and includes the **Constituent Materials** tab, the **Saturation Experiment** tab, the **Boundary Conditions** tab, the **Solver Parameters** tab, and the **Equations & References** tab, which cites several references 185.

At the top of the dialog, enter the **Result File Name (*.gdr)**. The result file is saved in the chosen project folder (**File → Choose Project Folder** in the menu bar).



The built-in default icon comes with a selection of different presets. Clicking on the little arrow shows several additional preset options.

The usual built-in default settings will load the settings according to the current GeoDict edition. You can change the current GeoDict edition from the **Settings menu** as described in the Graphical User Interface chapter.



In **SatuDict - Capillary Pressure** find edition-specific presets for the **Standard Edition** and the **Oil and Gas Edition**.

In the Oil and Gas edition, the default **Invading Fluid** is changed from Water to Oil, which means that the surface tension is adjusted accordingly. In the **Solver Parameters** tab, the **Step Size** is reduced from 2 to 1.

Tabs of the Capillary Pressure Curve dialog

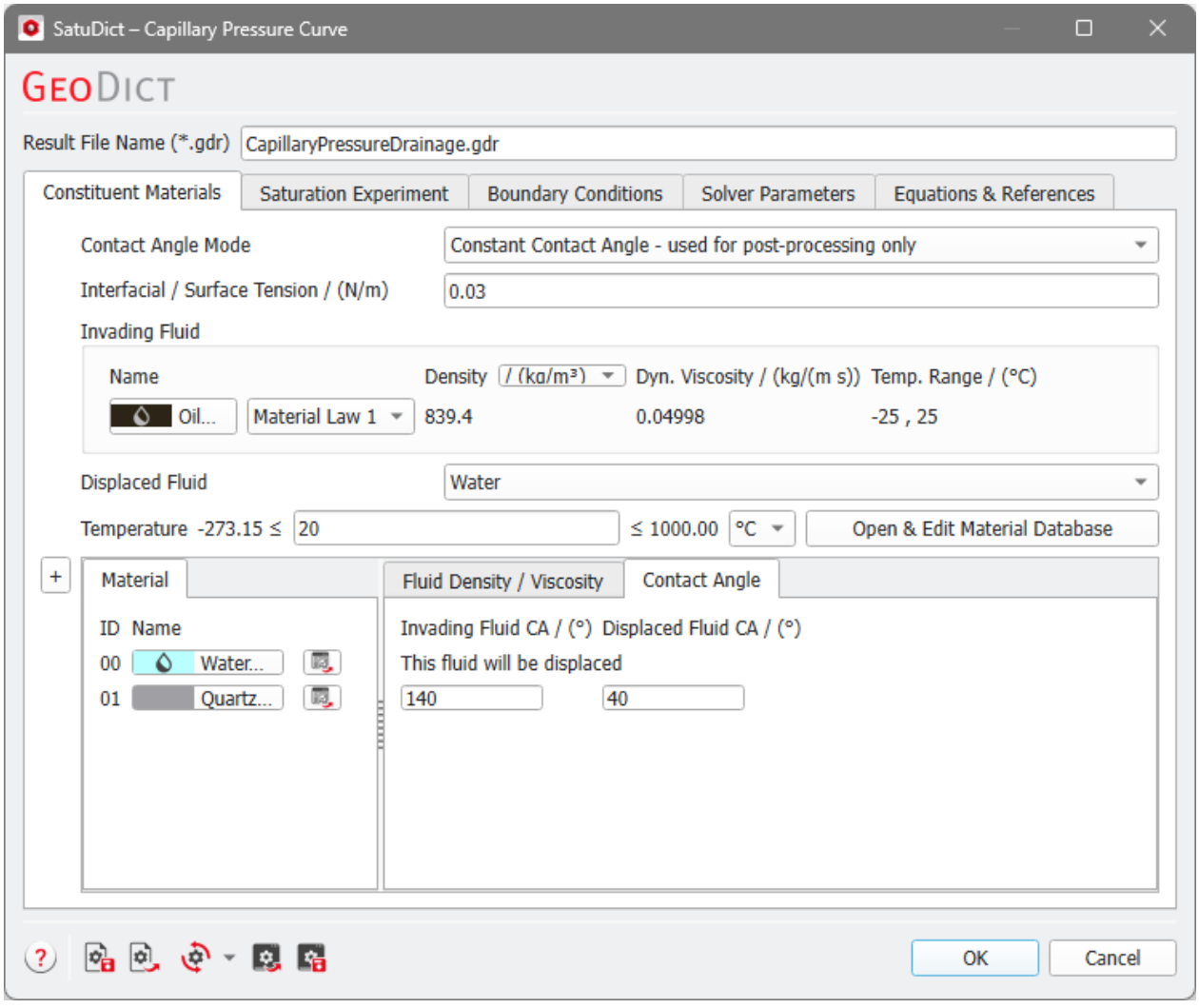
- Constituent Materials 18
  Select the materials in the structure and their properties, including the selection of invading and displaced fluid.

Tabs of the Capillary Pressure Curve dialog

- Saturation Experiment 23
  Choose the settings for the conducted saturation experiment.
- Boundary Conditions 25
  Set the domain boundary conditions.
- Solver Parameters 27
  Define the settings for the solver and the output files.

Constituent Materials

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



Contact Angle Mode

Three options for the **Contact Angle Mode** are available:

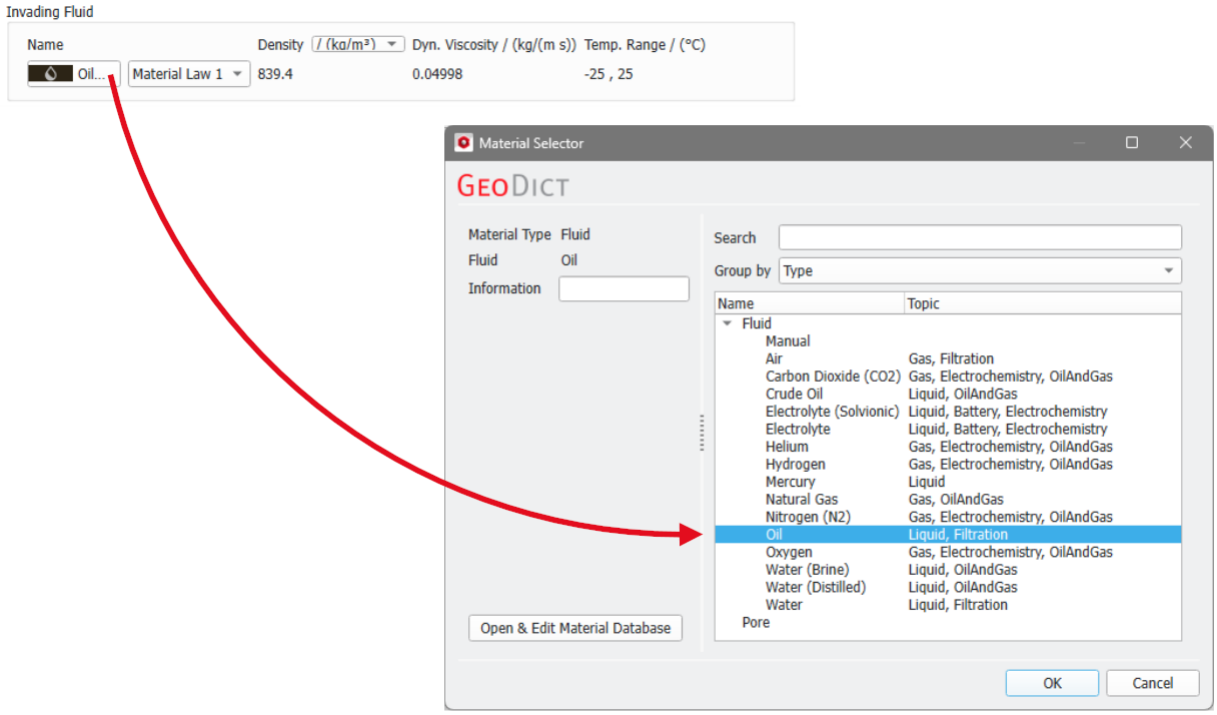
1. **Constant Contact Angle**: For the Pore Morphology method, a single (constant) contact angle is assumed between all solid materials and the invading fluid, and another constant contact angle between all solid materials and the displaced fluid. The given contact angle is considered for the computation of the capillary pressure in the post processing, but a contact angle of 0° 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 this default setting, 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

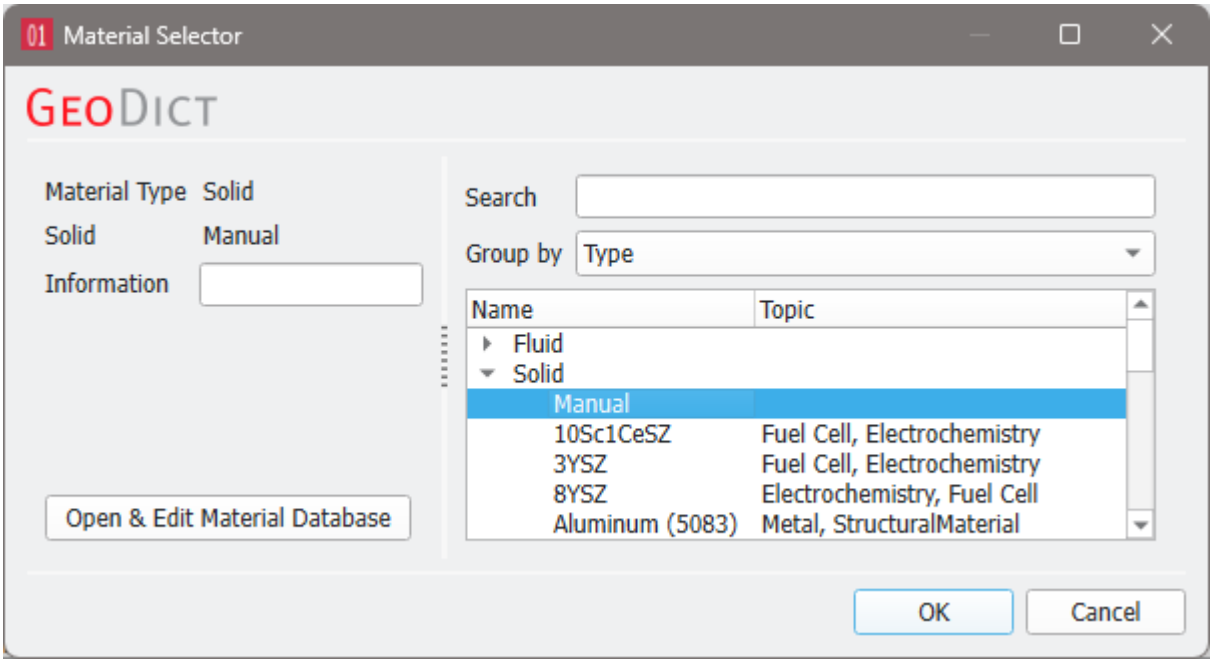
Enter the **Interfacial / Surface Tension** in N/m between the invading and displaced fluid or use the (standard edition) default value of 0.07275 N/m corresponding to the surface tension between water and air at 20°C. For the Oil and Gas edition, the default value of 0.03 N/m corresponds to the surface tension of oil and water at 20°C.

Invading 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.



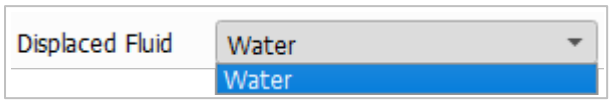
The pull-down menu gives access to selecting the desired material from the GeoDict **Material Database**. When none of the materials available in the database fit the preferred specifications, **Manual** should be chosen. Alternatively, a new material with the desired specifications can be added to the **Material Database** (see the Material Database chapter).



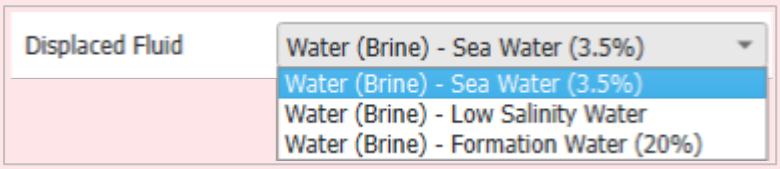
To match realistic material colors for visualization in a certain application, the default material colors can be changed through the **Color & Visibility** tab of the GUI sidebar. For more visualization options, see the Visualization chapter.

Displaced Fluid

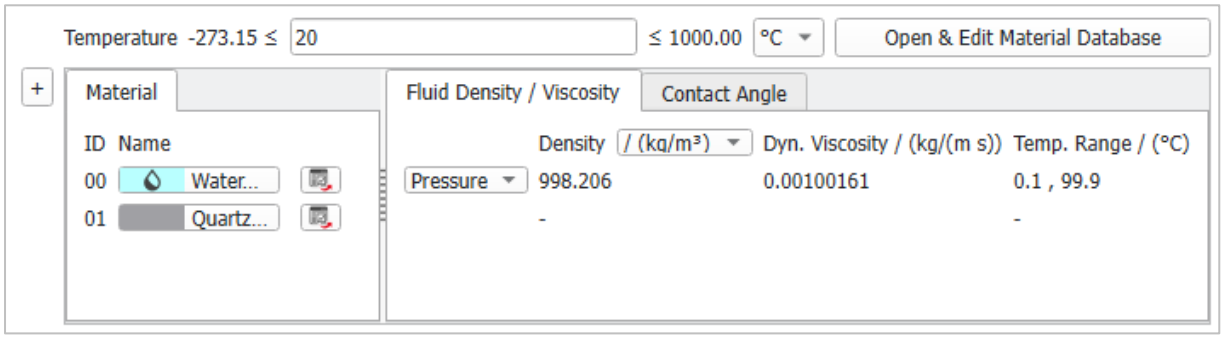
The **Displaced Fluid** must already be present in the model of the structure currently in memory. Choose the displaced fluid from the drop-down menu. To change the fluid to another one, select a different fluid in the Material panel below. The changes apply automatically to the selection in this menu.



Important! For materials with different material laws, the selection of a material law is not updated. In this case, you have to choose the material law manually from the drop-down menu.



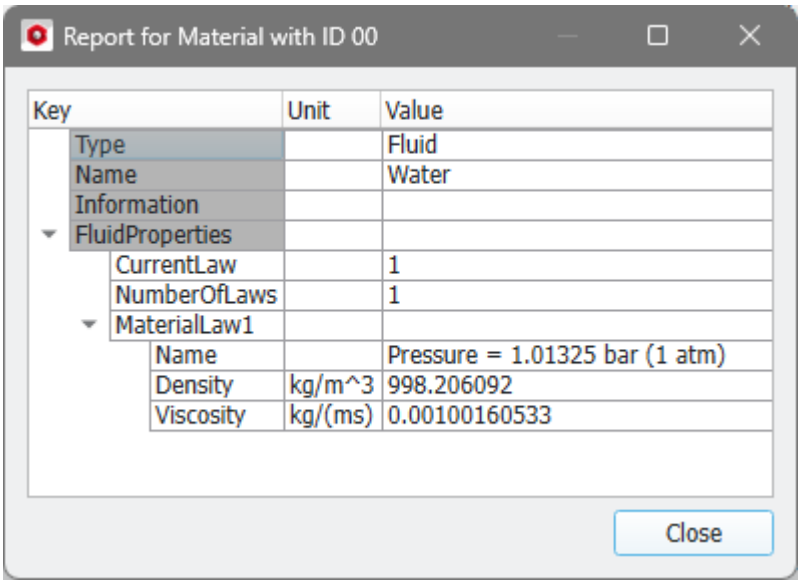
Material, Fluid Density / Viscosity and Contact Angle



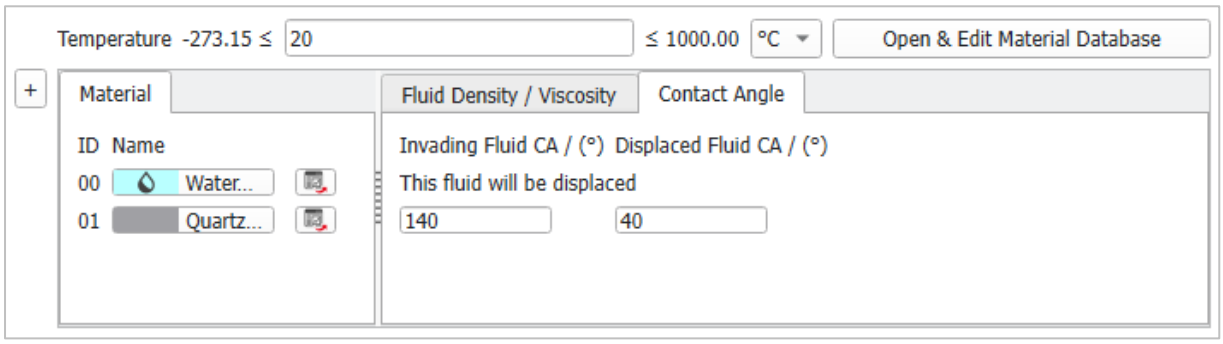
Set the **Temperature** applied for the calculation in the selected units below. Click **Open & Edit Material Database** to edit the material properties in the Material Database if needed.

Underneath, the **Material** panel contains the Material IDs of the constituent materials present in the current structure. By default, Material IDs that are not present in the structure are not displayed under the **Material** tab, but they can be displayed by clicking on the "+" symbol to the left of the **Material** tab. Click on the name of a material to change the material of the corresponding Material ID in the Material Selector as explained above for Invading Fluid.

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



In the **Fluid Density / Viscosity** panel you can see the physical properties density and viscosity of the fluids in the structure. If available, you can select between different material laws. For manual materials, define their properties directly in this panel.



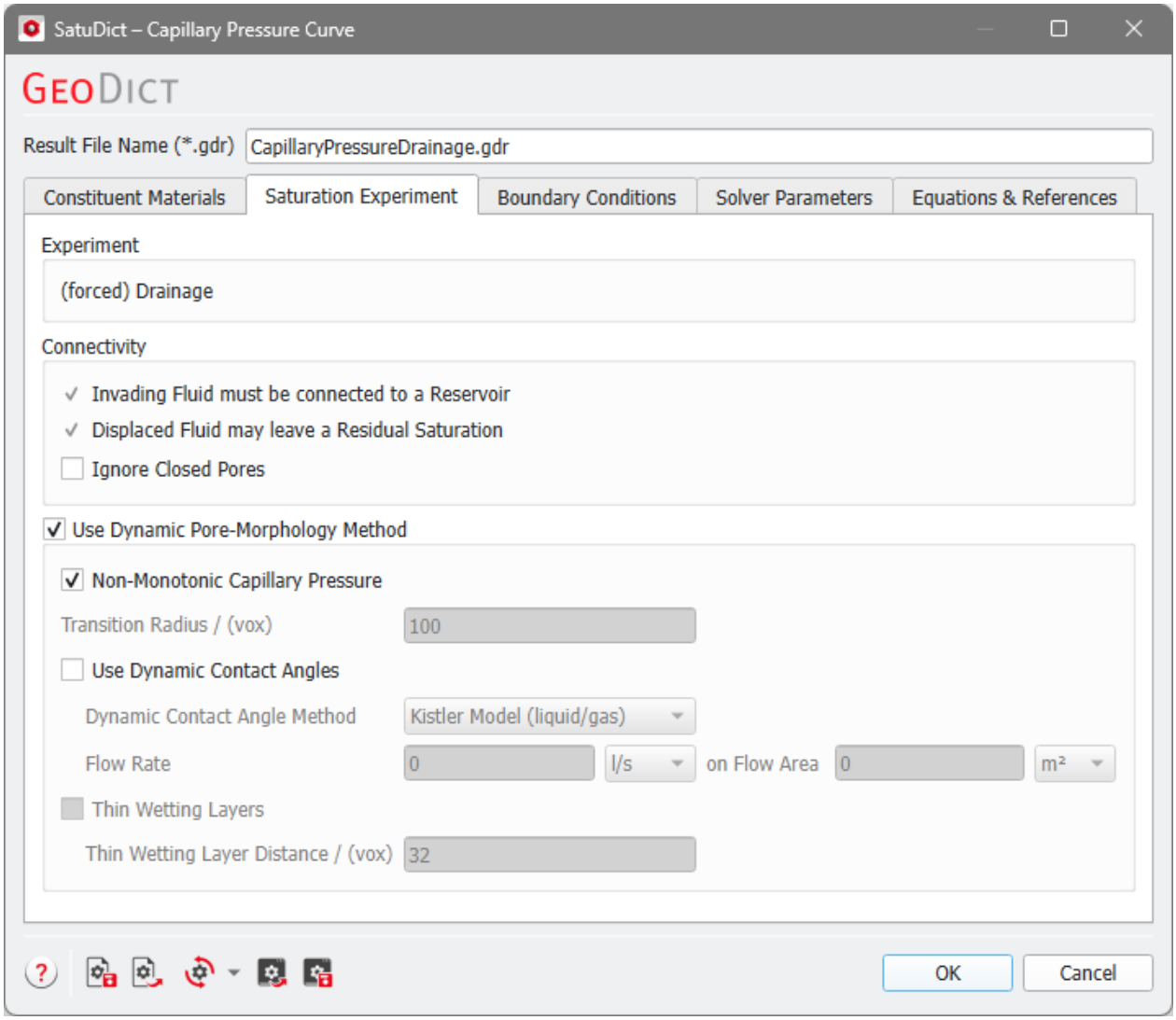
In the **Contact Angle** panel, enter the contact angle for all solid materials (after choosing **Constant Contact Angle** as Contact Angle Mode) or for each solid material separately (after choosing **Multiple Contact Angle** or **True Contact Angle** as Contact Angle Mode). For fluids, it will be displayed if it has a role in the simulation, e.g., in this simulation 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**.

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

Saturation Experiment

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



Experiment

Observe which kind of experiment is performed. This depends on the choice of the contact angles made in the **Constituent Materials** 18 tab.

If all contact angles of the invading fluid are above 90° then a **Drainage** experiment will be performed, where the invading fluid is forced into the structure.

If all contact angles of the invading fluid are below 90° then an **Imbibition** experiment is performed, where the invading fluid enters the structure spontaneously.

In mixed-wet cases, where the contact angles of the invading fluid are above and below 90°, then **spontaneous + forced Imbibition** are computed.

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 enforce that the invading fluid is continuously connected to a phase reservoir at a given spatial location outside of the domain (defined in the **Boundary Conditions** 25 tab). 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.

The option **Displaced Fluid may leave a Residual Saturation** allows 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** 25 tab. The residual of the displaced fluid is assigned a new Material ID. In general, it is recommended to enable this option.

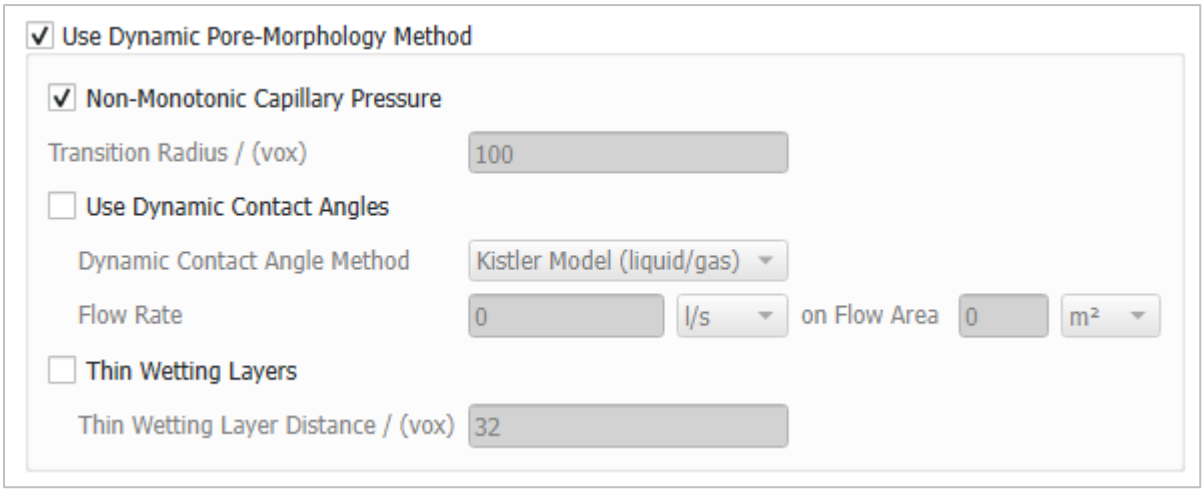
Know how! Disabling this option is done for mercury intrusion capillary pressure experiments where mercury invades the pore space and displaces vacuum. Use the Mercury Porosimetry & Capillary Pressure 49 command for simulating MICP experiments.

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

Check **Use Dynamic Pore-Morphology Method** to use this method for dynamic simulation 5 of the drainage and imbibition processes.

Important! This option is required for mixed-wet cases! If you enter mixed-wet contact angles, the dynamic pore-morphology method is automatically activated.



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.

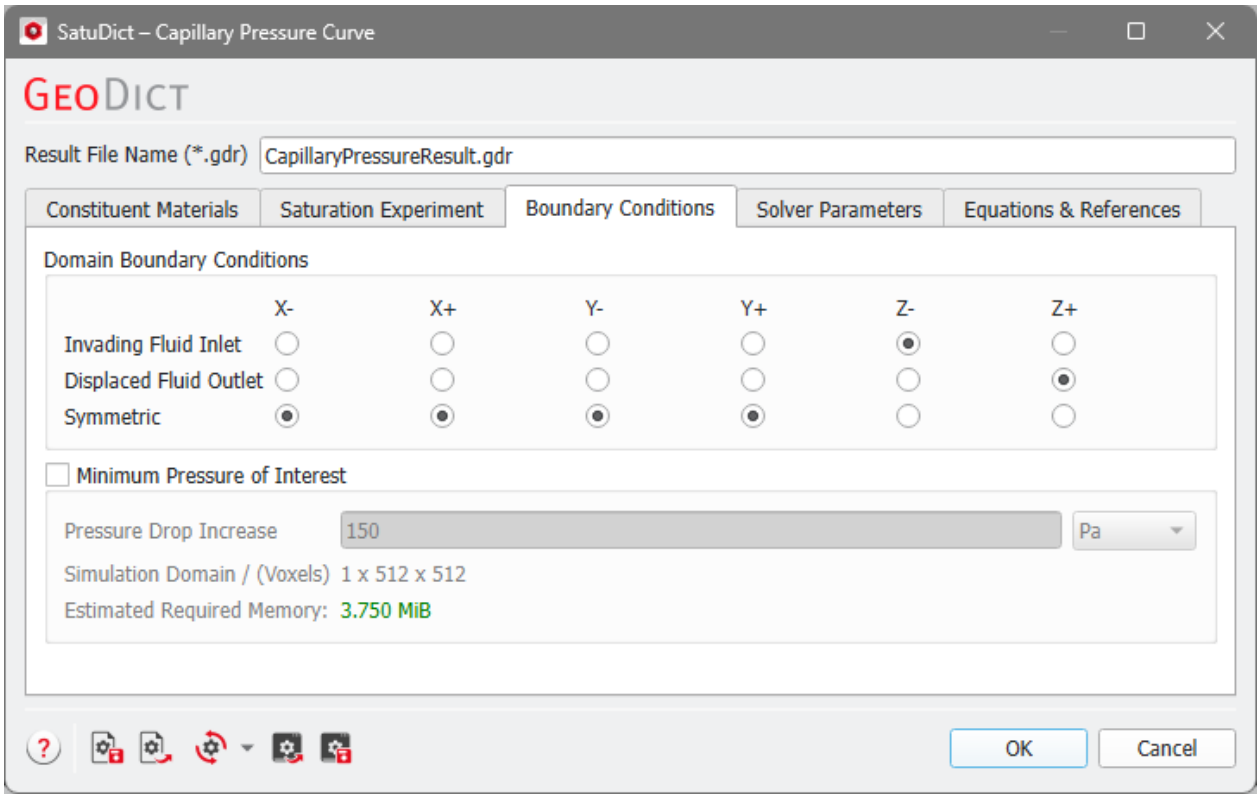
The option to define a **Transition Radius** is only available for mixed-wet cases, where there is a transition from imbibition to drainage algorithm. With the **Non-Monotonic Capillary Pressure** option, it is possible to switch dynamically between the two algorithms several times (automatically done 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.

Check **Use Dynamic Contact Angles** allow for the entered contact angles to change dynamically. See Dynamic Contact Angles 9 for more details. Below, choose the one of the **Dynamic Contact Angle Models**, **Kistler** (for liquid/gas systems) or **Cox** (for liquid/liquid systems), depending on the aggregate state of the fluids in the structure. For both models, the **Flow Rate** of the invading fluid on a **Flow Area** must be given. These settings can be based on the experimental conditions you are trying to recreate, i.e., based on the **Flow Rate** of an injection pump for the specific fluid and the **Flow Area** of the injection piston (commonly 1 – 1.5 inch^2). This will ensure that the simulations are nearing the experimental setups the most.

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.

Boundary Conditions

The **Boundary Conditions** tab is divided into two groups: **Domain Boundary Conditions** and **Minimum Pressure of Interest**.



Domain Boundary Conditions

Define if a side of the sample (X-, X+, Y-, Y+, Z-, and Z+) is the **Invading Fluid Inlet** or the **Displaced Fluid Outlet**. The **Invading Fluid Inlet** are the domain sides where the invading fluid can enter the domain from a reservoir, while the **Displaced Fluid Outlet** are the domain sides where the displaced fluid can leave the domain.

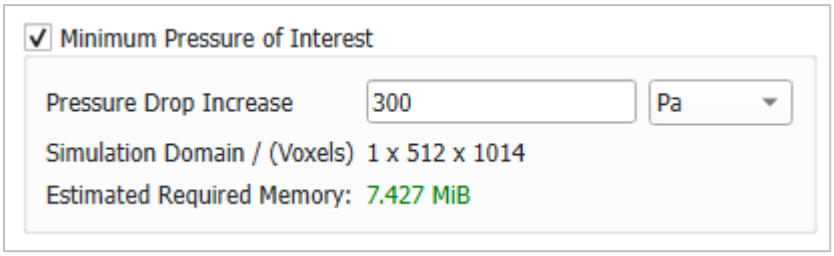
If a side is not connected to a reservoir, e.g., if the porous medium continues in that direction, select **Symmetric** boundary conditions in these directions, i.e. the pore structure is mirrored at this side.

In some cases, depending on the choices in the **Saturation Experiment** tab, the boundary conditions are grayed out and cannot be edited, e.g., if there is no invading fluid reservoir. Then, symmetric boundary conditions are used.

Minimum Pressure of Interest

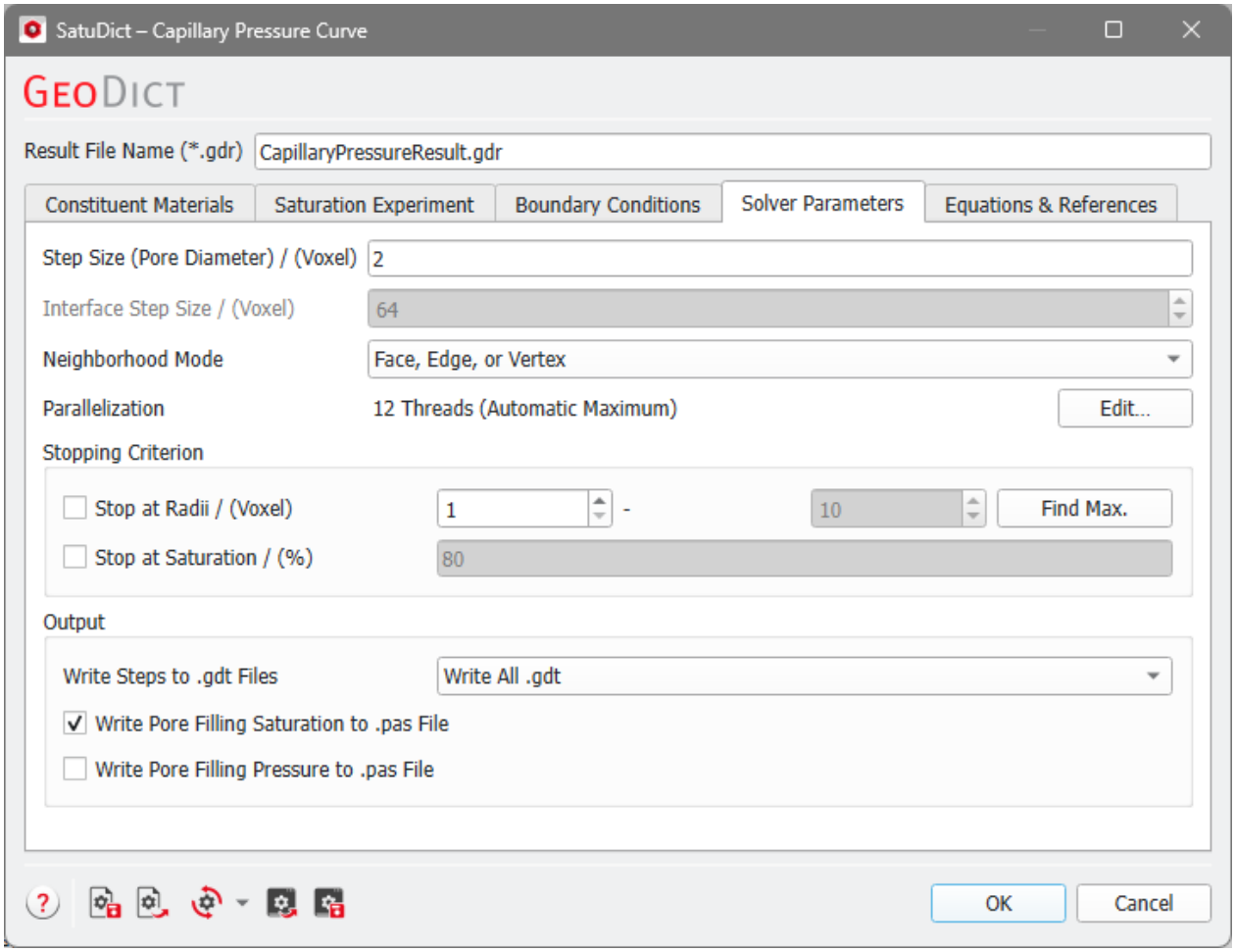
By checking **Minimum Pressure of Interest**, the size of the original simulation domain (voxels) is artificially increased in the direction(s) of the flow (here Z). The effect is to improve the capillary pressure results at least down to the desired value, by increasing the structure size such that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

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



Solver Parameters

The **Solver Parameters** define the settings for the solver run and the output files.



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.

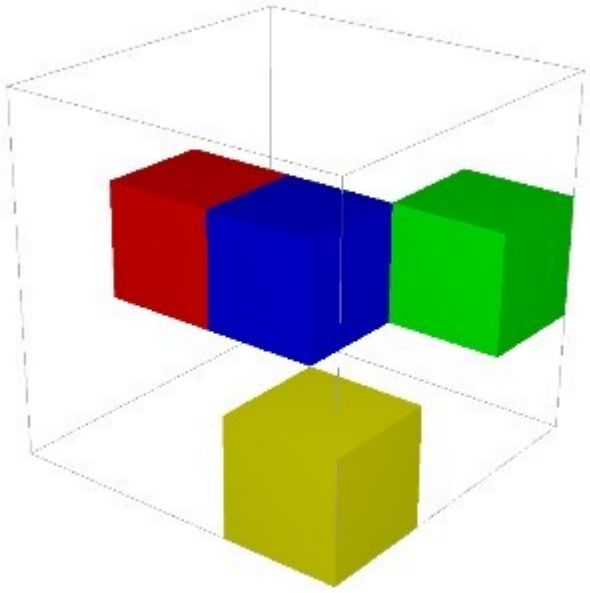
Interface Step Size

This feature is only available if the **Dynamic Pore Morphology Method** 23 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.

The different **Neighborhood Modes** are explained using this example.



Two voxels can be connected through faces, edges, and vertices (corners). Voxels that share a face, do also share edges and corners, as you can observe for the red and the blue voxel. The blue and the green voxel share an edge and the corner points of this edge. Finally, the blue and the yellow voxel share only one vertex (corner point).

Thus, checking **Face** is more restrictive than choosing **Face or Edge**, and this is more limiting than selecting **Face, Edge, or Vertex**.

When choosing the Neighborhood Mode **Face** only the red and the blue voxel are connected.

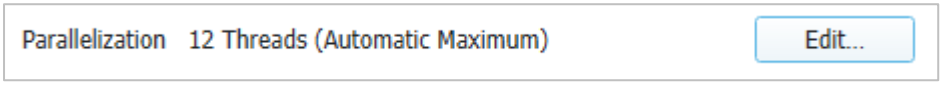
When choosing **Face or Edge** the red and the blue voxel and the blue and the green voxel are connected.

Finally, if **Face, Edge, or Vertex** is chosen, the red and the blue voxel, the blue and the green voxel and the blue and the yellow voxel are connected.

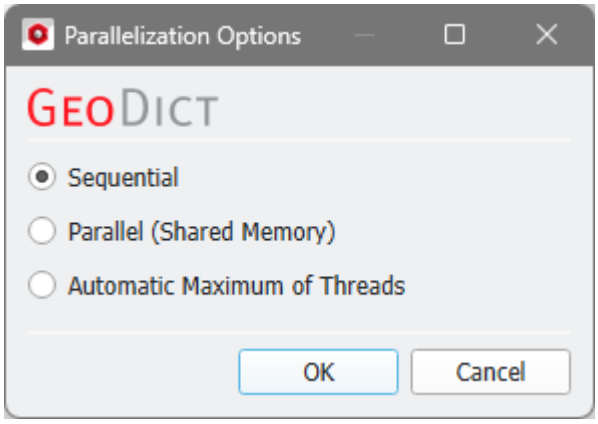
Parallelization

Control how many threads are used for the computation. Parallelization is possible if your license and hardware allow it.

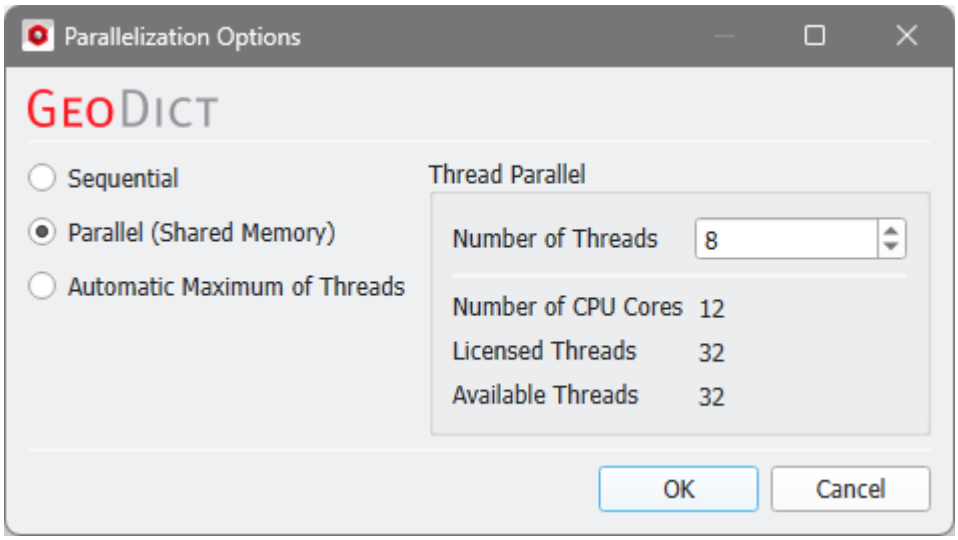
The **Parallelization Options** dialog opens when clicking the **Edit** button and you can choose between **Sequential**, **Parallel (Shared Memory)**, or **Automatic Maximum of Threads**.



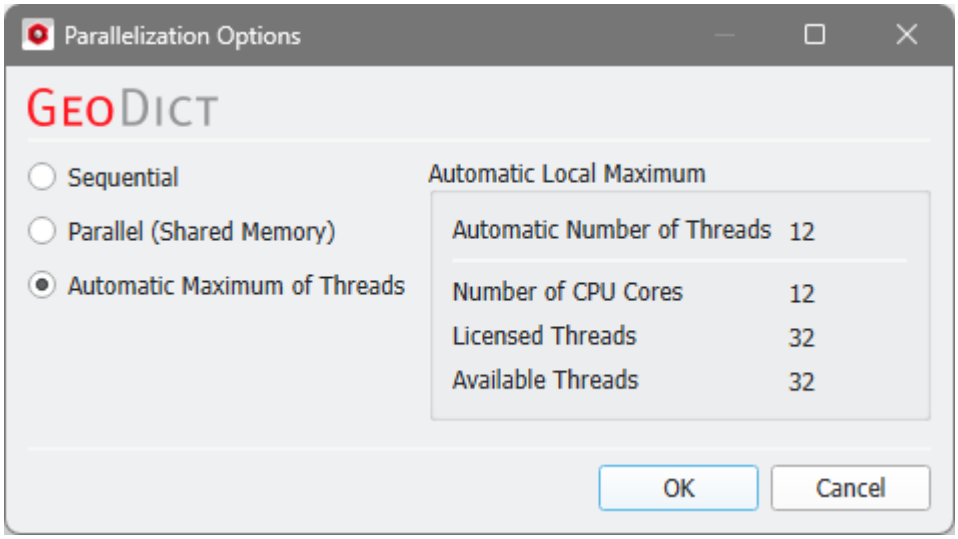
Selecting **Sequential** will not apply parallelization and only one thread is used for the computation.



When **Parallel (Shared Memory)** is selected, the **Number of Threads** can be entered. Below, the **Number of CPU Cores** that the current machine has, the maximum number of **Licensed Threads** and the number of those licensed threads that are available (**Available Threads**) are shown in the dialog. Of course, the maximal number of parallel processes you can use, is the smallest of those three numbers.



If **Automatic Maximum of Threads** is selected, the number of parallel processes is automatically selected for optimal speed, based on the CPU cores and licensed parallel processes.



The **Automatic Local Maximum** of processes is automatically selected, which is the minimum of **Number of CPU Cores**, **Licensed Threads**, and **Available Threads**.

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.

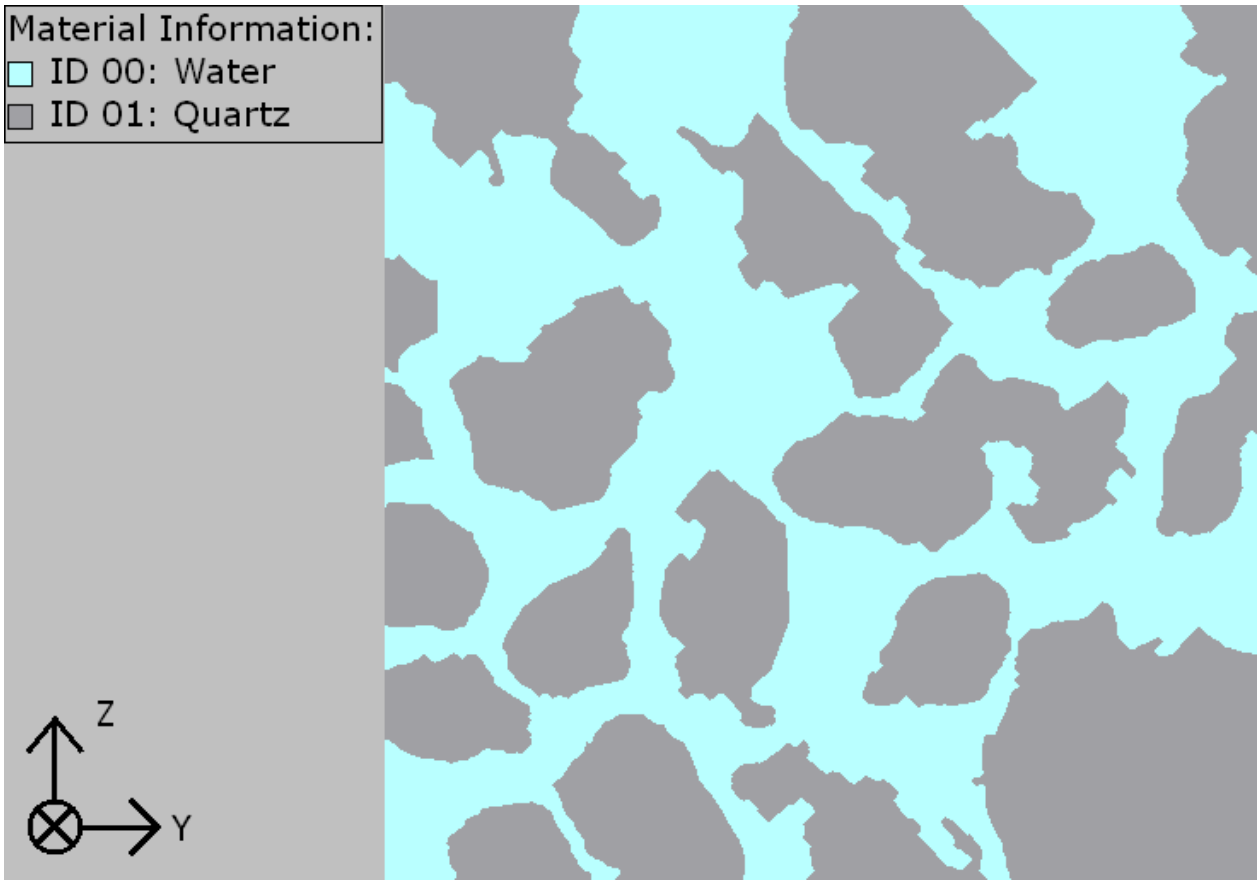
Select **Write No Files** if no intermediate .gdt files should be saved.

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 **a**nd **s**aturation) file is written and saved in the result folder. This is a volume file and can be loaded from the result viewer in the Data Visualization 38 tab. 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.

1.2.2 Results

The result file (*.gdr) is opened in the Result Viewer after the computation is finished. Only the tabs listed below are described in detail, for the other tabs look into the Result Viewer chapter.

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.



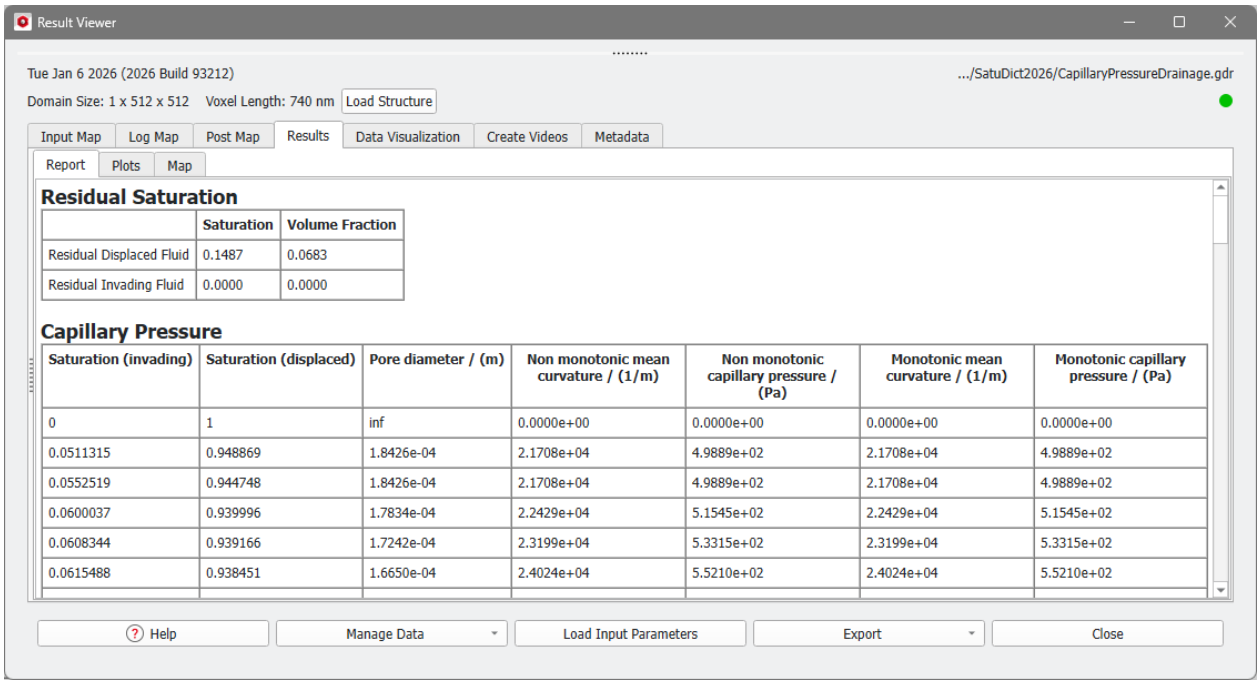
Capillary Pressure Curve Results

- Results Tab 32
  Learn about the resulting reports and plots.
- Data Visualization 37
  Load results for a graphical visualization.
- Create Videos 43
  Use a predefined macro to generate a video.

Results Tab

The **Results** tab is the central point analysis of the results. It is grouped in three subtabs: **Report**, **Plots**, and **Map**. The Report tab shows the residual saturation and the diameters, curvatures and capillary pressure values for each saturation step. The Plots tab contains plot options for the analysis of the results. The Map tab contains all resulting data from the Capillary Pressure run. This data is the basis for the tables in the Report tab and for the plots in the Plots tab.

Report



First, the **Residual Saturation** of invading and displaced fluid at the end of the simulation is given. Both the **Saturation** (using the pore space as reference volume) and **Volume Fraction** (relating to the total sample volume) are displayed.

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.

Note! If the Contact Angle Method **Multiple Contact Angle** 18 was used for the computation of the saturation pressure curve, a warning may appear in the result file created.

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

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

Two main 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 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

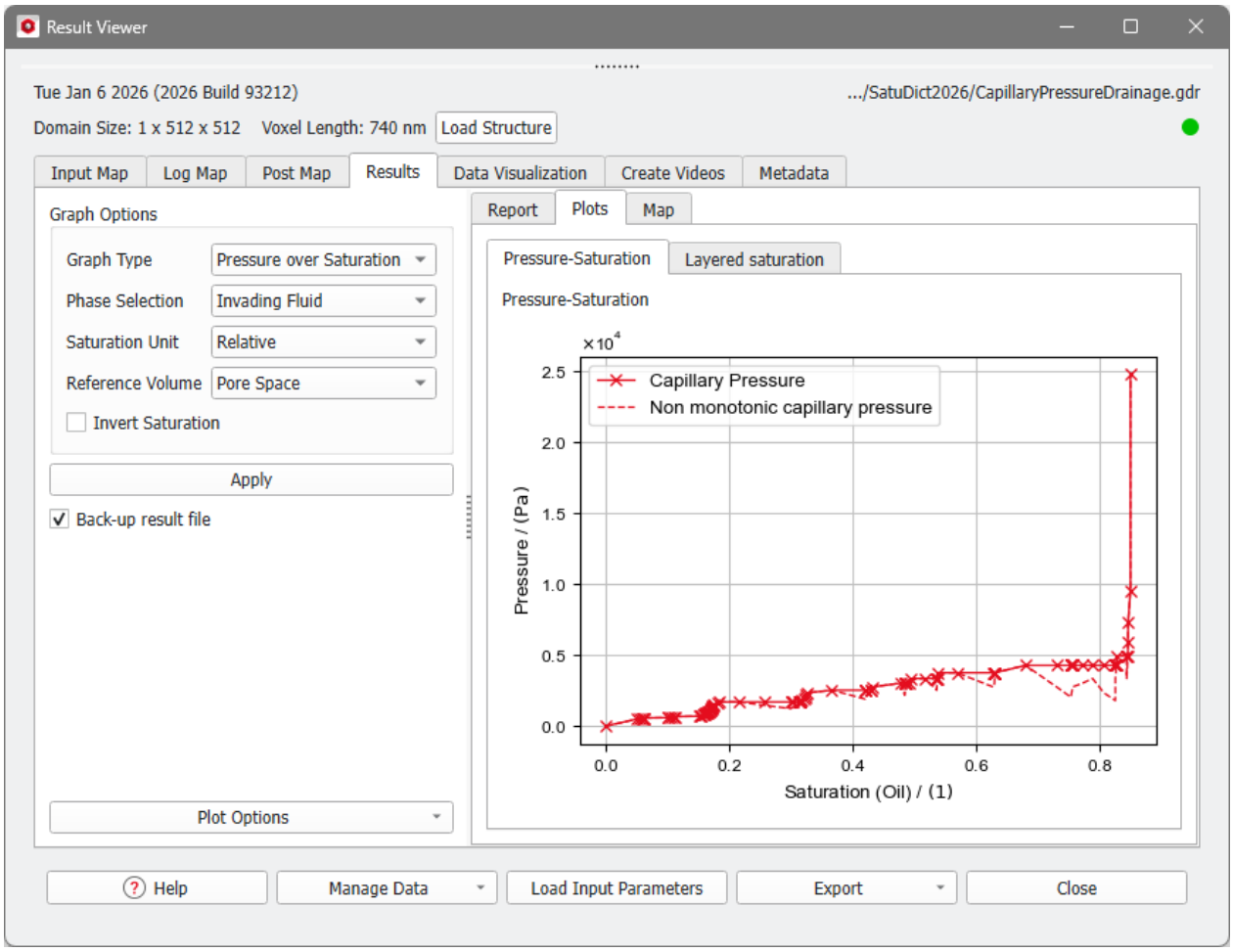
Pressure-Saturation

Observe the tabular results of the Report subtab as a diagram in the **Pressure-Saturation** subtab.

On the left, the Post-Processing Widget allows you to fine-tune this graph. Collapse the Post-Processing Widget by pulling it to the left.

Select the **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 or Total Sample Volume). Check **Invert Saturation** to show the values of the saturation in decreasing instead of increasing order.

Click **Apply** to modify the plot according to the chosen settings.

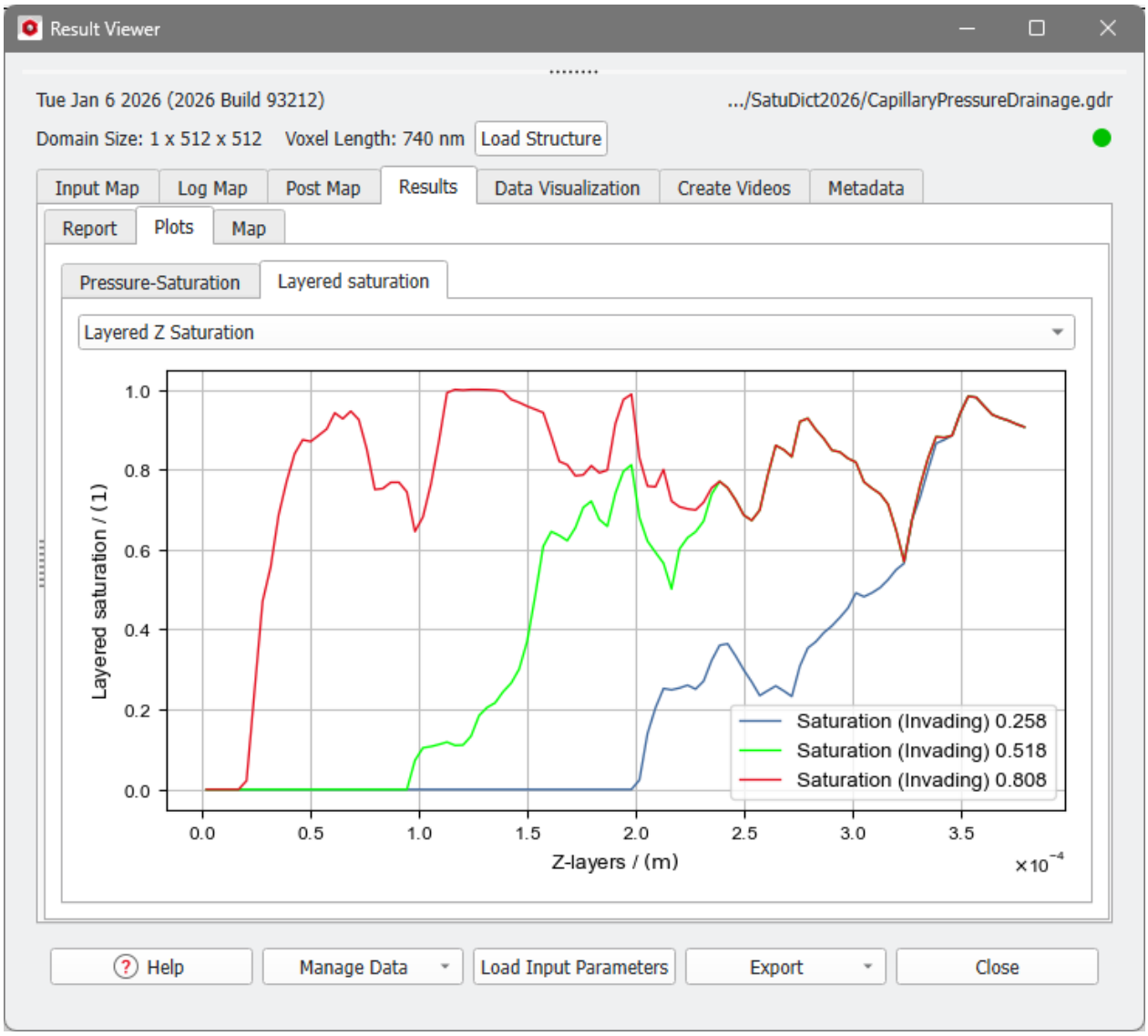


In the example, at the beginning of the drainage process, the porous structure does not contain the invading fluid Oil. It is saturated (100%) with Water. As the pressure increases, the Oil starts invading the structure and forces the Water out of it. Thus, the saturation of the Oil is increasing. By the end of the drainage process, where the pressure is at its highest level, the structure is 85% saturated with Oil and 15% 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%.

Layered saturation

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

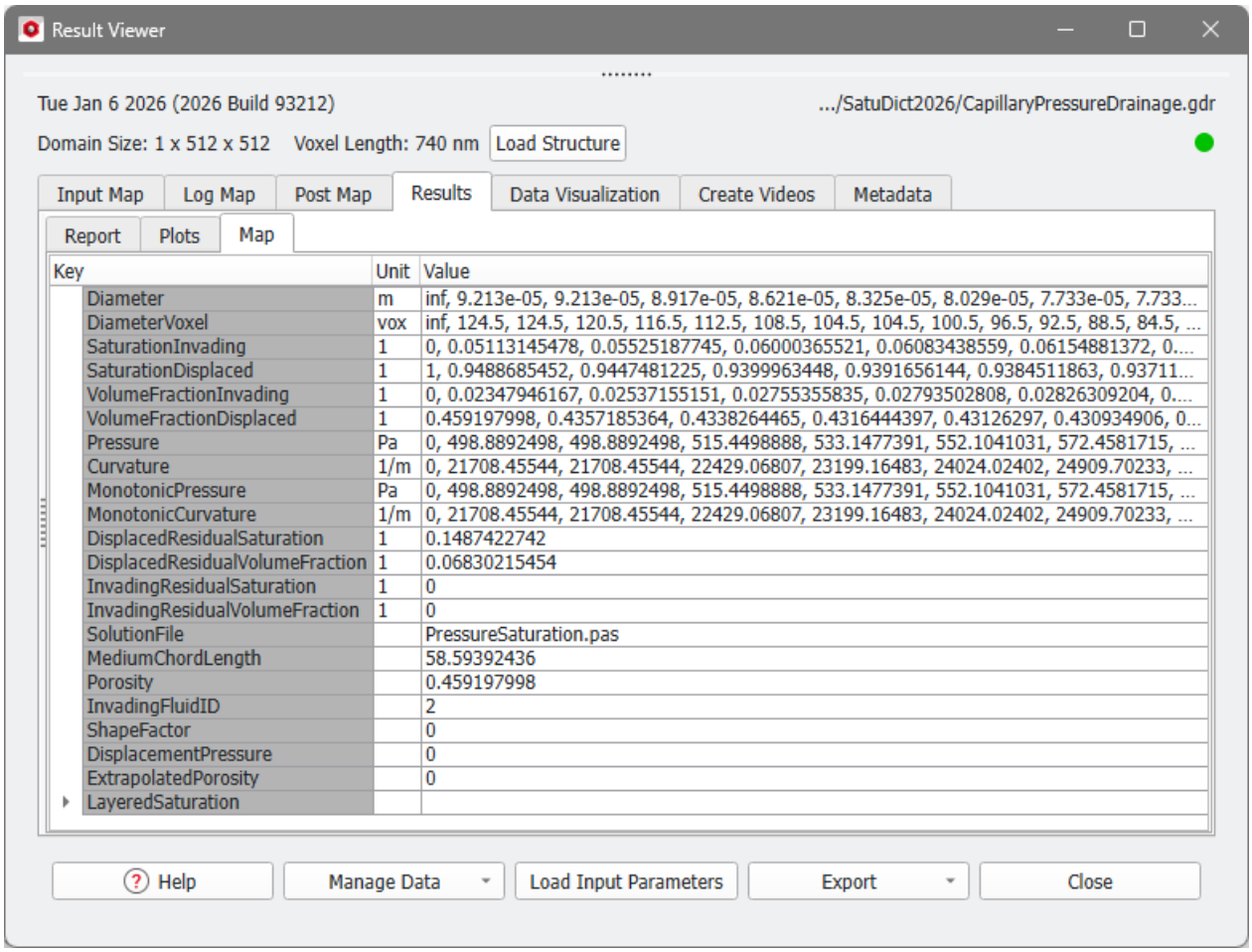
From the drop-down menu choose the direction to observe. For each layer, the occupied space of the invading fluid relative to the pore volume of this layer is plotted. This can be done for several steps of the calculation, which corresponds to different saturations of the whole structure. By right-clicking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



Map

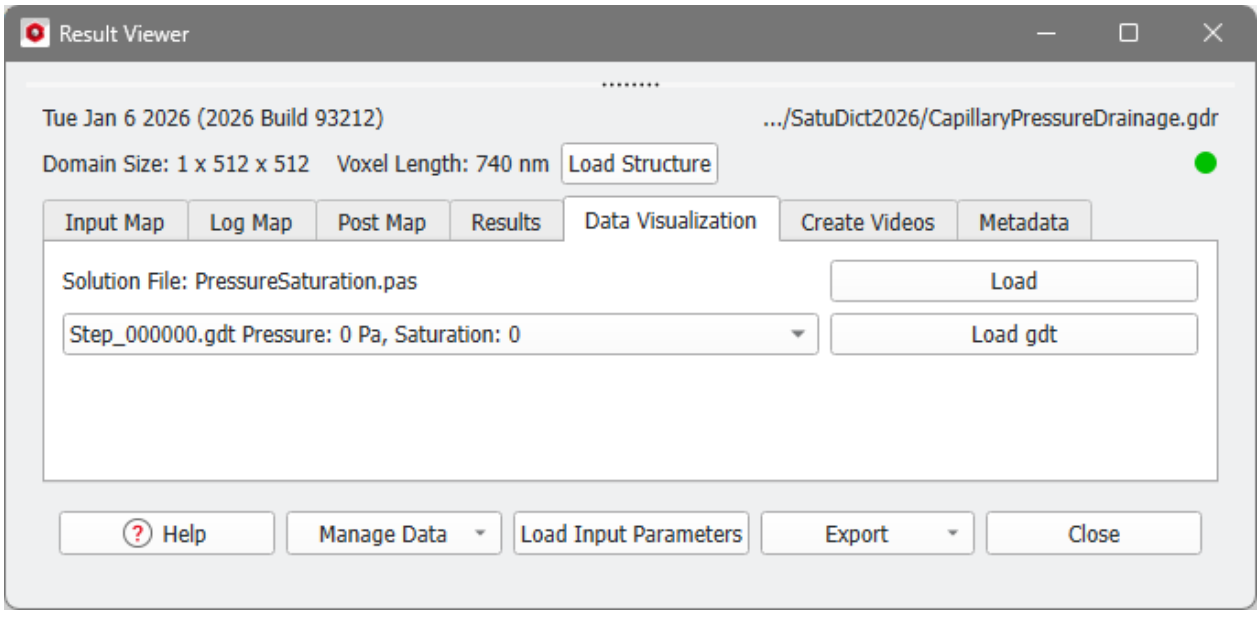
The **Results - Map** subtab gives access to the computed values. It contains also the values from the Report and Plots subtabs.

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

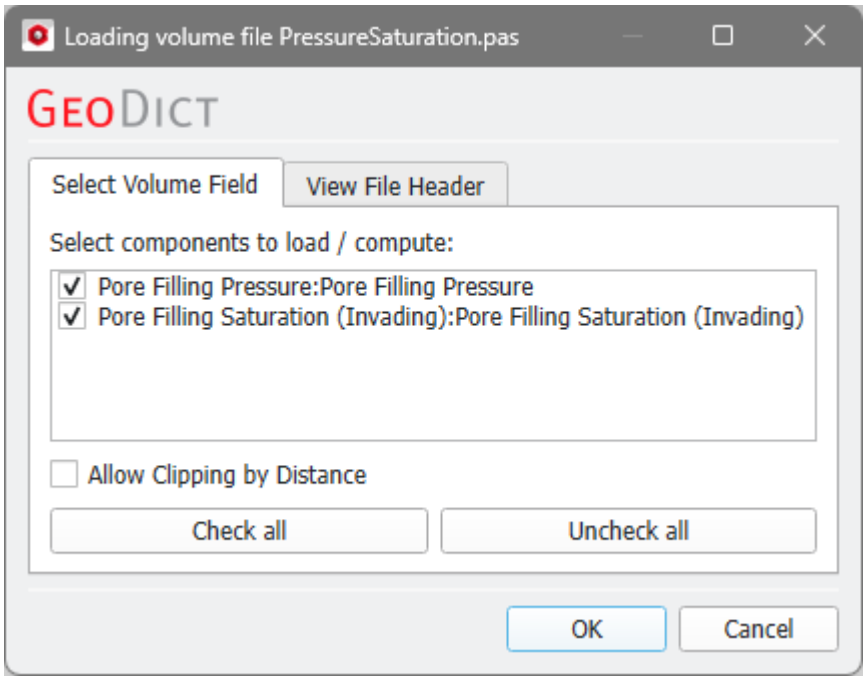
In the **Data Visualization** tab, you can load the *.pas file and the step-by-step images of the computed process.



Visualization of Pressure and Saturation (pas file)

Click **Load** to access the pressure and saturation field data saved in the **PressureSaturation.pas** file.

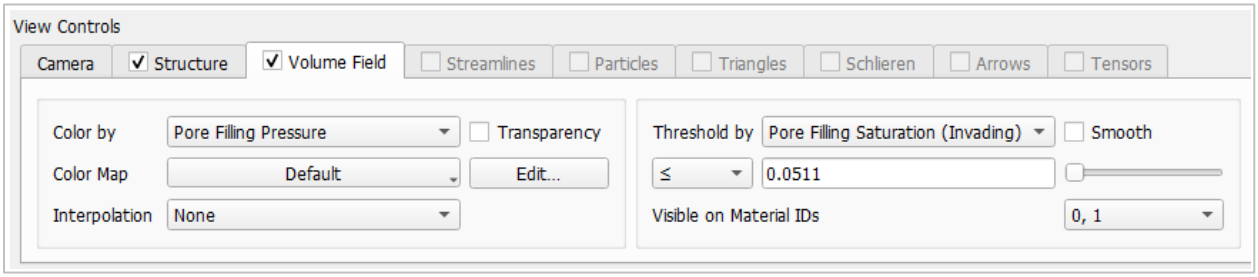
Depending on the choice made in the Solver Parameters tab under the output options[31] the **Pore Filling Pressure** and the **Pore Filling Saturation (Invading)** can be selected for the visualization. Click **OK** to load the selected fields.



The initial visualization, in 2D view or 3D rendering, is done using default settings which you 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 chapter.

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.

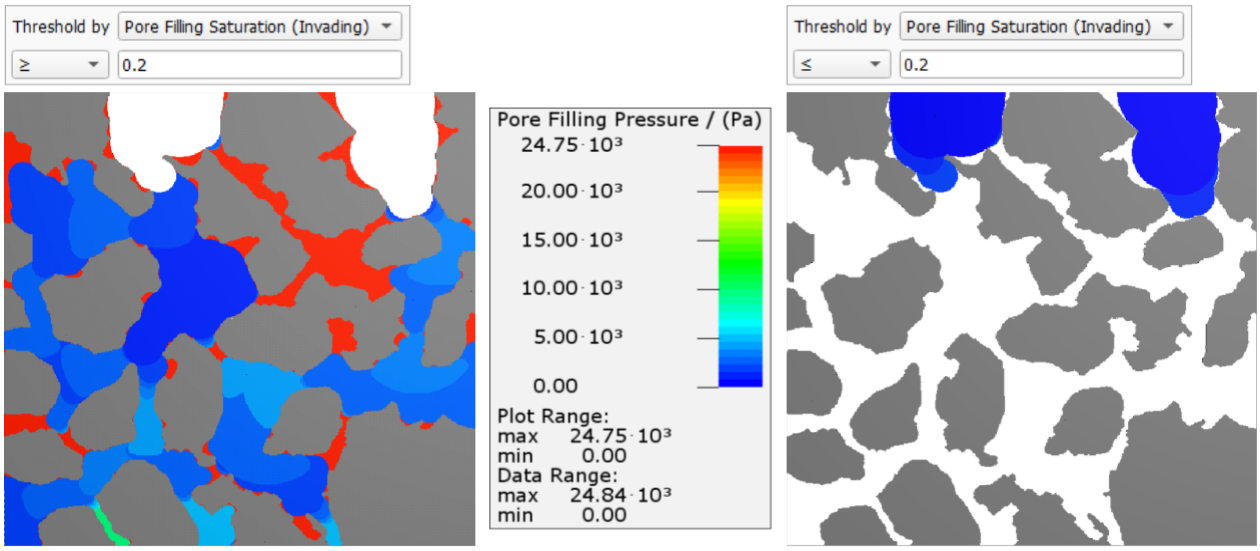
Select **Pore Filling Pressure** from the **Color by** and **Pore Filling Saturation (Invading)** from the **Threshold by** pull down menus.

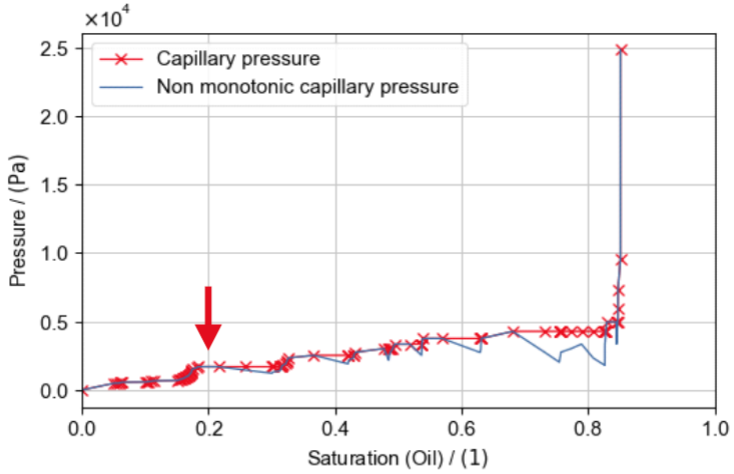
With these settings, the voxels are displayed in the color corresponding to the pressure at which this voxel was filled. The volume field legend shows which color represents which pressure value. The pressure values are shown dependent on the saturation level of the invading fluid, because Threshold 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 85%.
- **Clip Mode**: This makes the dual visualization of pressure values and distribution of phases possible because it links them based on the capillary pressure saturation curve 34.
  - By selecting ≥, color is shown in the pore space where the invading fluid occupies the structure only at a higher saturation than the Pore Filling Saturation (Invading) set in the threshold slider. This shows the locations where the displaced fluid is still in the structure at this saturation or below.
  - By selecting ≤, color is shown in the pore space where the invading fluid is already present for a saturation below the value for Pore Filling Saturation (Invading) set in the threshold slider. This shows the locations where the invading fluid has already entered the structure and replaced the displaced fluid.

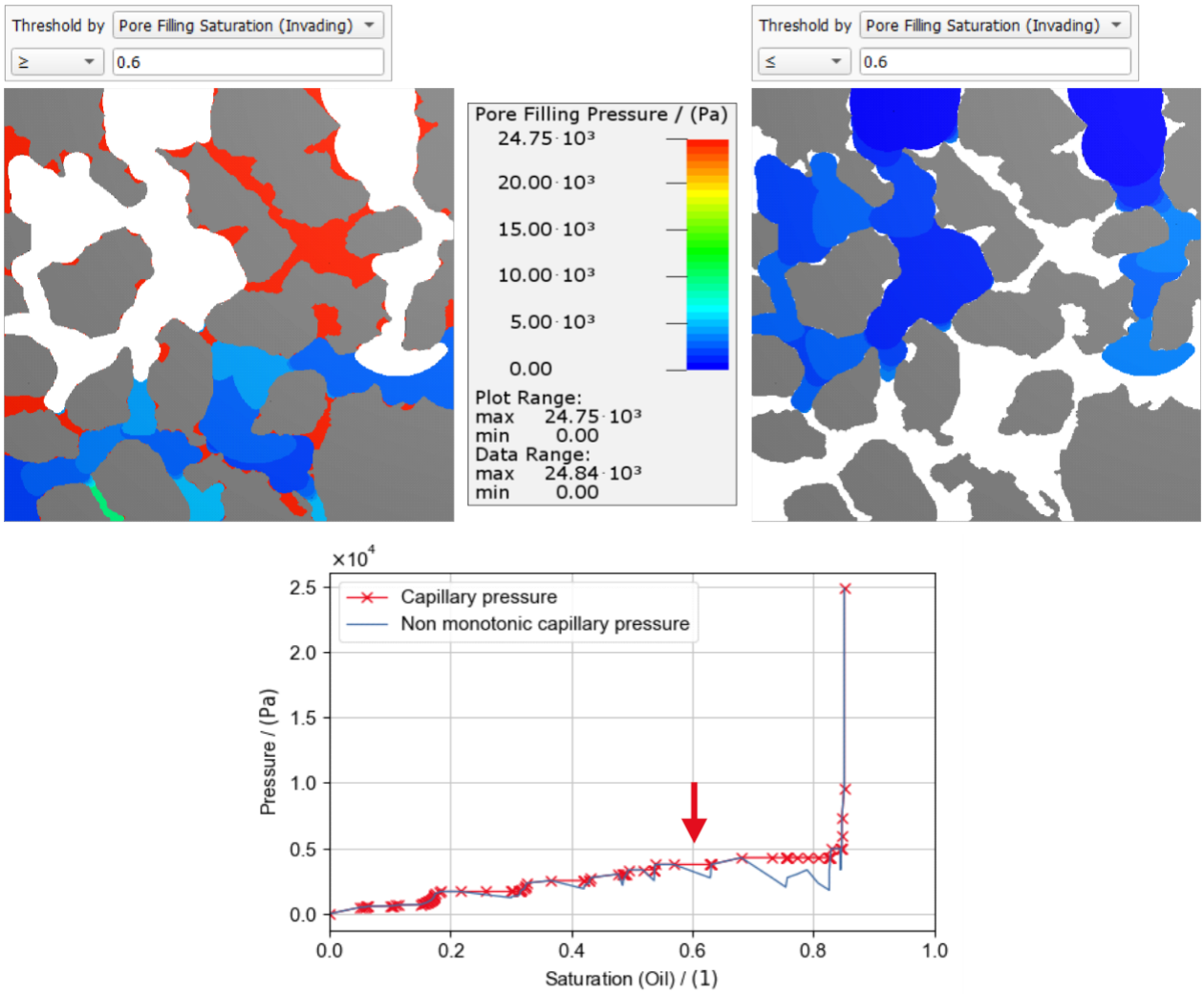
This leads to a twofold visualization, since for a given invading fluid saturation level (threshold value), the capillary pressure at particular locations in the structure is shown, together with the distribution of the two phases. While the color gradation refers to the capillary pressure values as 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**.





20% saturation of invading fluid

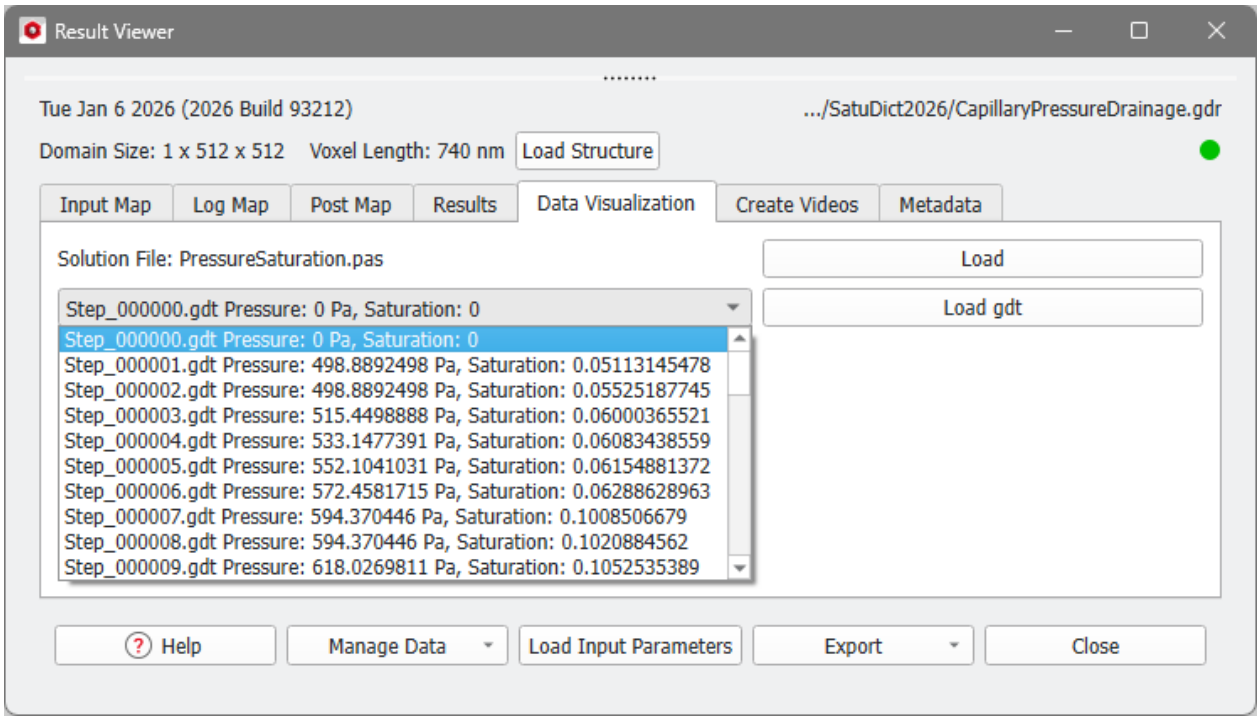


60% saturation of invading fluid

Visualization of intermediate states (gdt files)

Finally, the computed process can be visualized step-by-step with GDT files saved during the capillary pressure curve calculation. This is only possible if **Write All .gdt** or **Write Only Changed .gdt** was selected in the Solver Parameters tab. The GDT files corresponding to the computational steps (Step_000000.gdt, etc.) are stored in the automatically created result folder.

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

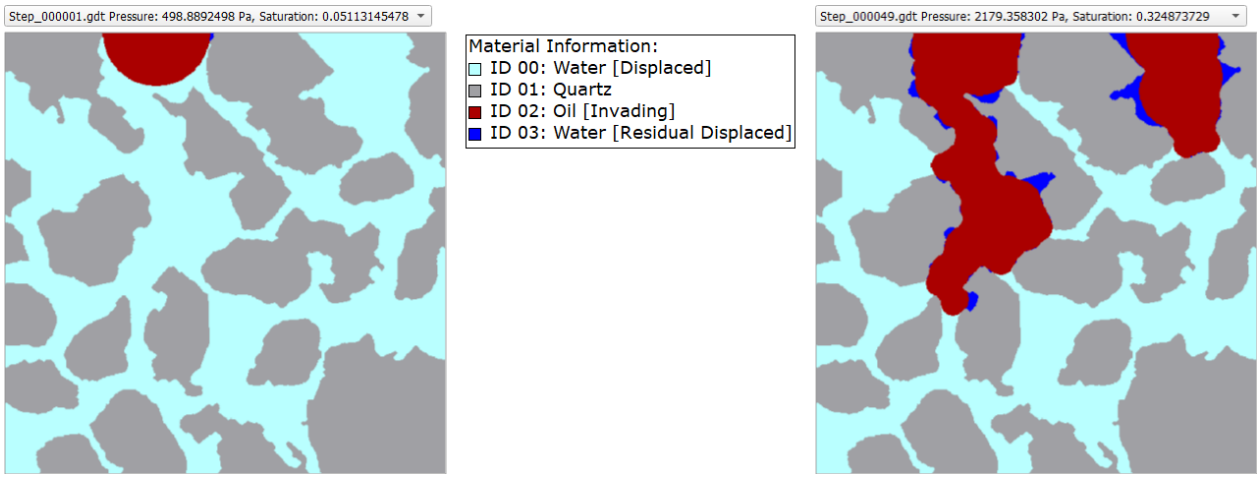


Select one of the GDT files, where the file names correspond to the simulation step in which the GDT file was saved. Also, the pressure und saturation of the invading fluid in this step are shown, which is the same as in the corresponding row of the table in the Results-Report tab.

Click **Load gdt** to open the desired file 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.



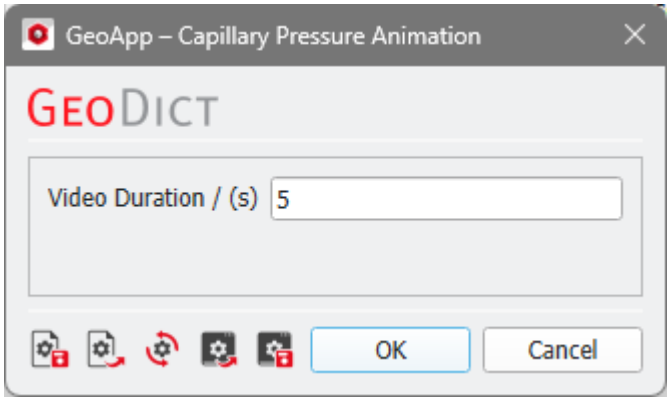
Create Videos

Generate a video showing an animation of the drainage or imbibition process from the **Create Videos** tab. The exemplary video shows which information will be contained in the video. On the left the changing distribution of invading and displaced fluid during the saturation simulation is animated, and on the right, the corresponding capillary pressure curve is shown. For a better visualization, only a part of the structure is set to visible.

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:

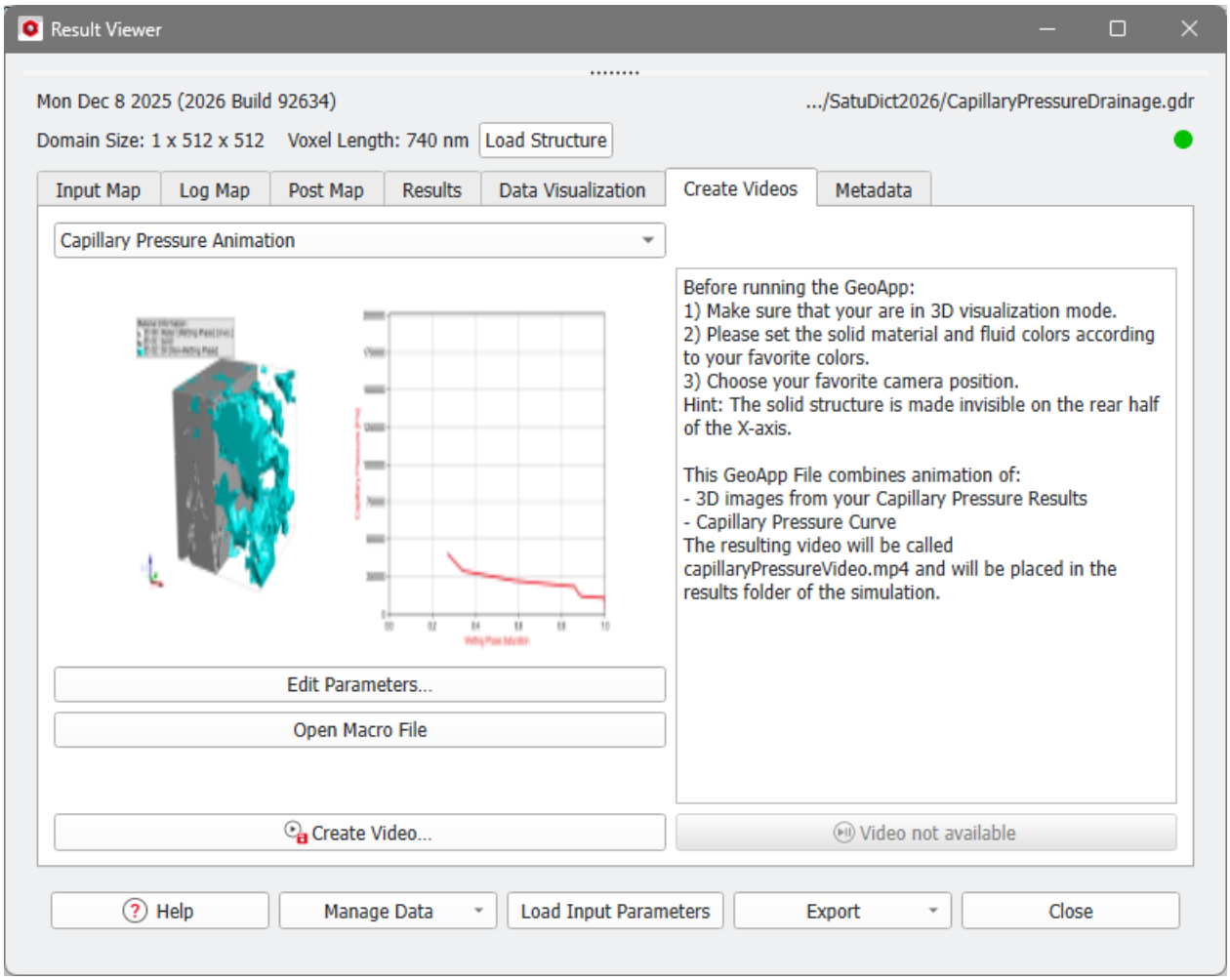
1. Make sure that you are in 3D mode,
2. Set the colors of solid and fluid materials to your preferred ones,
3. Choose your favorite camera position.

Select **Edit Parameters** to change the duration of the video.



With **Open Macro File** it is possible to open a text editor with the python file used for the video creation in order to modify it.

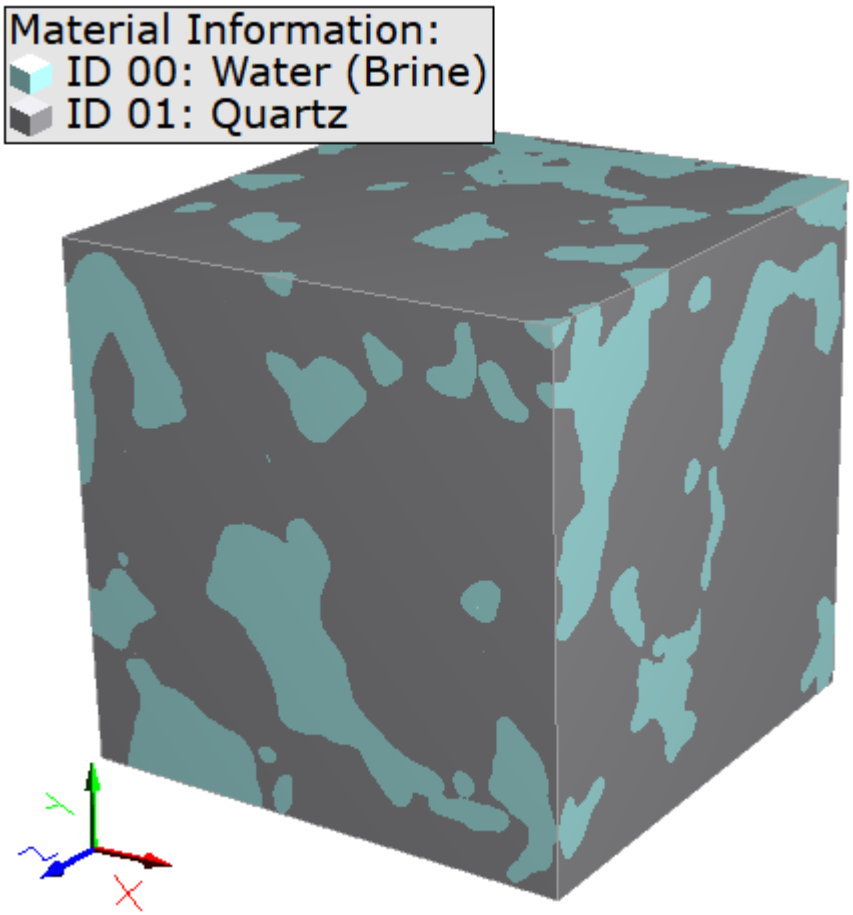
Click **Create Video**, to create and save the video capillaryPressureVideo.mp4 in the result file folder.



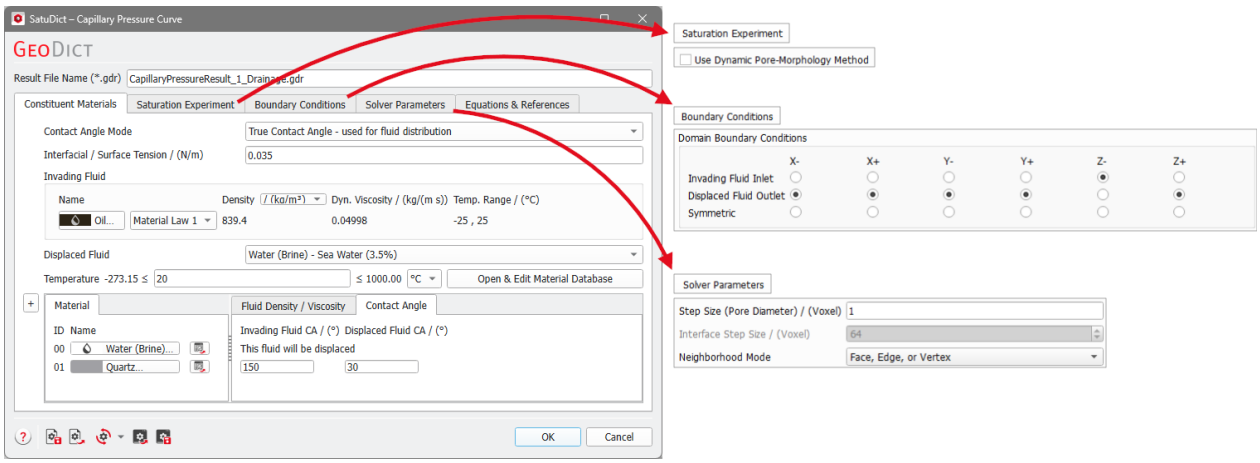
If the video was created successfully, the grayed-out **Video not available** button, is enabled and changes to a **Play Video** button. Click **Play Video** on the bottom right opens the video file in the default video player.

1.2.3 Capillary Pressure with Hysteresis Effect

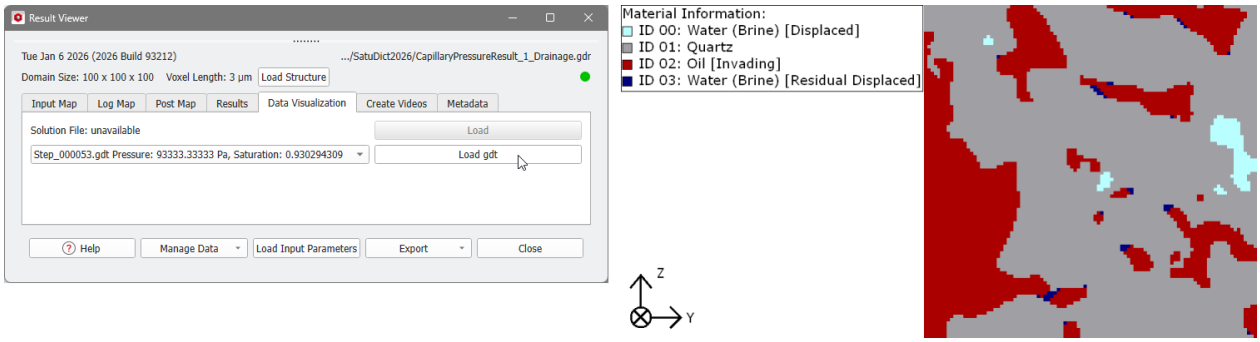
A generalization of the pore morphology method allows considering structures in which the invading fluid is already present in the structure. This makes the simulation of primary and secondary drainage experiments possible, as well as primary and secondary imbibition experiments. We illustrate this **Hysteresis** effect on the structure shown below, which has 17% porosity and is saturated with Water at the beginning.



First, a primary drainage simulation is done with the following settings.



To perform a follow-up imbibition simulation, the final state of the previous drainage simulation (Step_000053.gdt with 93333 Pa) is loaded from the Data Visualization tab in the result viewer as starting state for the imbibition simulation.

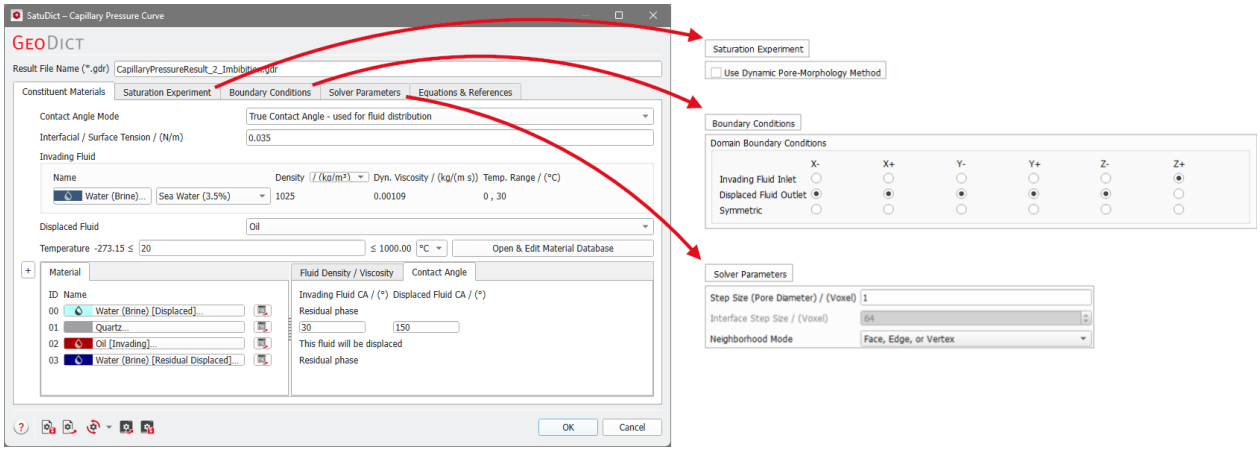


Then, open the **Capillary Pressure Curve Options** dialog to change the parameters for the imbibition simulation. Change the name for the result file from **CapillaryPressureResult_1_Drainage.gdr** to **CapillaryPressureResult_2_Imbibition.gdr**.

In the **Constituent Materials** 18 tab, select the **Invading Fluid** to be Water (Brine) and the **Displaced Fluid** to be Oil. Set the **Invading Fluid CA** to 30°, 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** is selected. In this example we leave the Dynamic Pore Morphology Method unchecked.

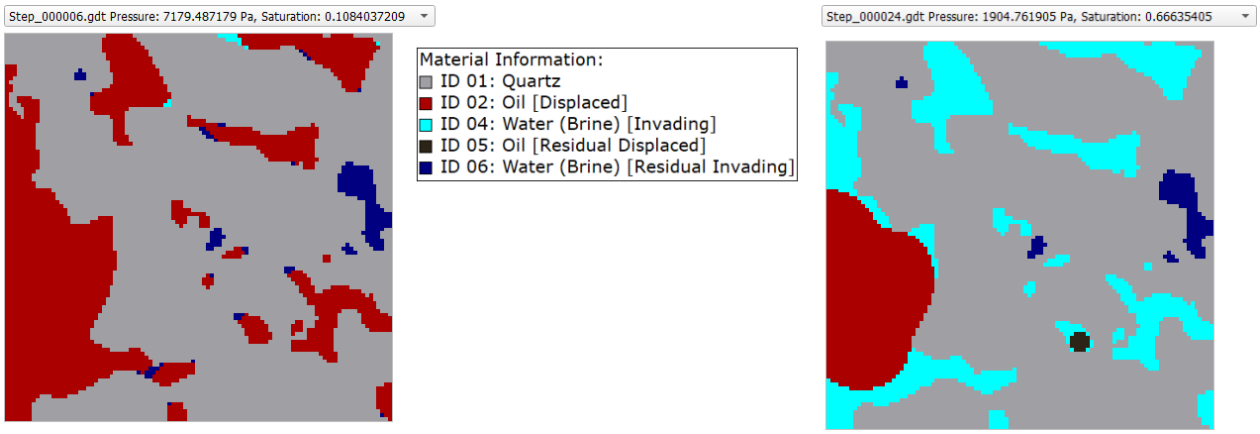
In the **Boundary Conditions** tab, switch the reservoirs boundary conditions of invading and displaced fluid in Z-direction.



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 Data Visualization 41 to observe the imbibition process.

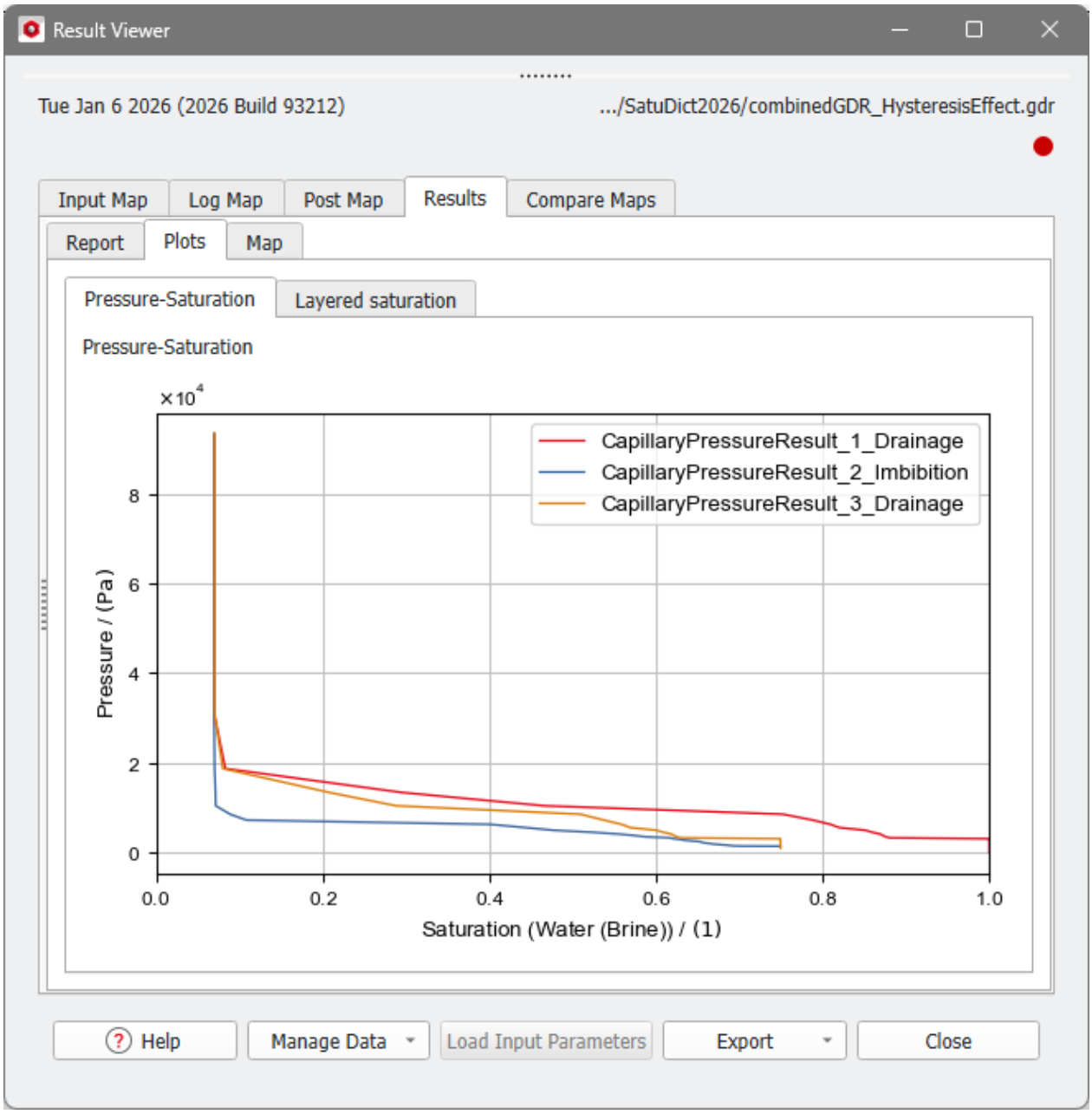
Observe that, step-by-step, the oil is displaced by the invading water, which reconnects with the water previously trapped in the structure (Residual Invading Phase in dark blue) from the earlier drainage simulation.



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

You can repeat the process of loading the final state of the imbibition simulation and setting up a secondary drainage simulation with the same settings as for the first drainage.

Then, combine the three result files and observe the combined capillary pressure curves, that show a typical hysteresis effect.



As this process of loading files, changing simulation parameters and combining result files requires a lot of manual work and is prone to errors, we developed the **Hysteresis for Oil-Water Setups** 174 GeoApp (for special setups in the oil&gas industry) and the **Hysteresis** 170 GeoApp (more general version for other industry areas) to help you setting up the whole simulation easily.

1.3 Mercury Porosimetry & Capillary Pressure

This command is similar to the Capillary Pressure Curve 15 command, but especially designed to simulate mercury invading a structure within a vacuum. This method is often called **Mercury Porosimetry** and is used to derive pore size from measured pressure values.

In GeoDict you can simulate **Mercury Intrusion Capillary Pressure** (MICP), where mercury is invading the structure, and (optional) **Mercury Extrusion Capillary Pressure** (MECP), where mercury leaves the structure. In the both cases the Pore Morphology Method 5 and the Young-Laplace equation 5 are used.

The MICP simulation results provide information about the pore throats sizes, while the MECP measures the size of the pore bodies. Additionally, the residual mercury remaining in the pore space is determined. For mercury intrusion it is possible to apply the Thomeer model 12 to predict the non-resolved porosity.

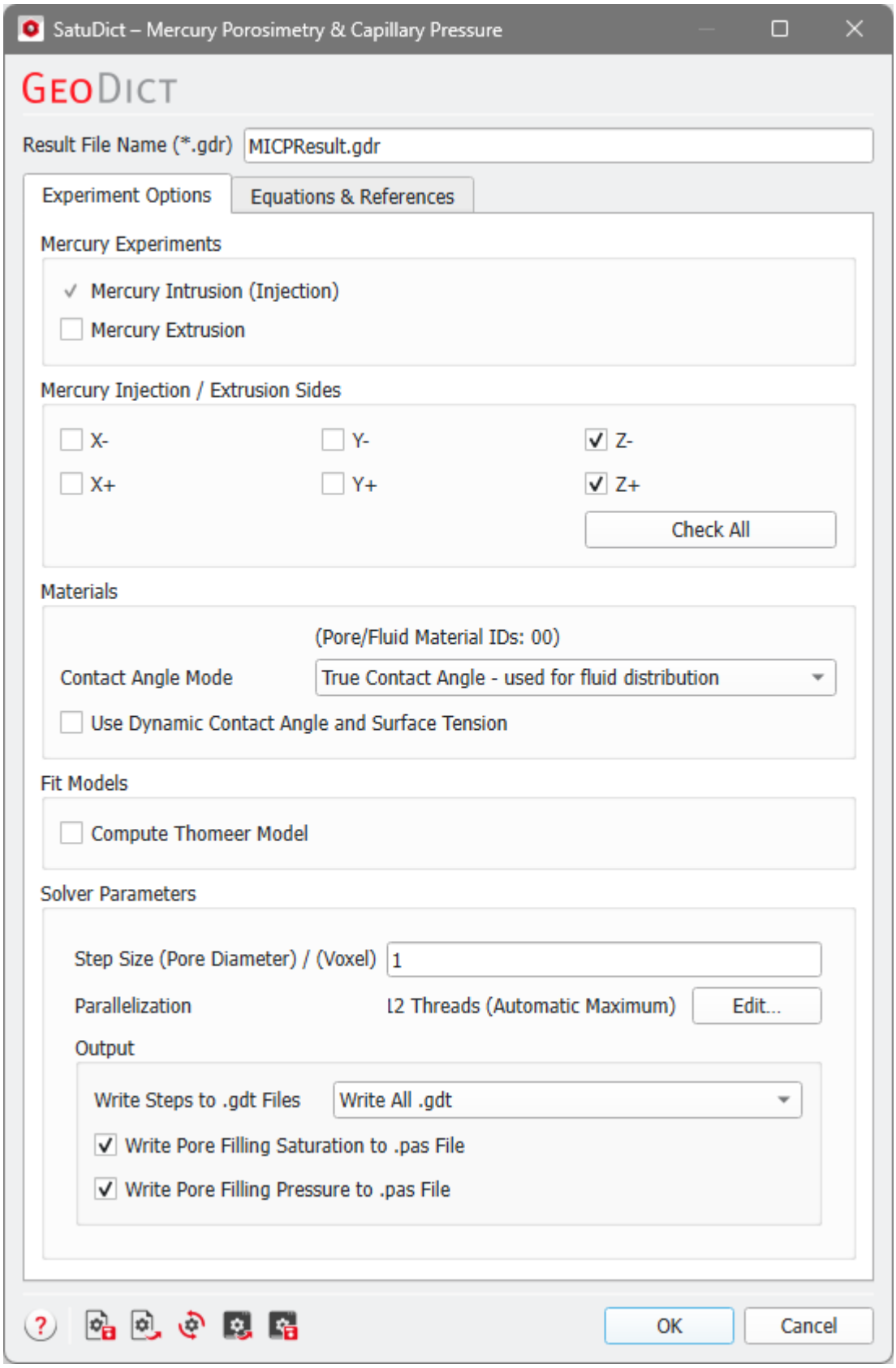
The Mercury Porosimetry & Capillary Pressure command

- Options 49
  Set the parameters for the calculation.
- Results 53
  View the computed results.

1.3.1 Options

The **Mercury Porosimetry & Capillary Pressure** dialog opens when clicking the **Edit...** button and includes the **Experiment Options** tab and the **Equations & References** tab, which cites several references 185.

At the top of the dialog, enter the **Result File Name**. The result file is saved in the chosen project folder (**File → Choose Project Folder** in the menu bar).



Mercury Experiments

The option **Mercury Injection** is always selected and cannot be unchecked. You can additionally choose to compute also the **Mercury Extrusion**.

Mercury Injection / Extrusion Sides

Similar to the Boundary Conditions[25] in Capillary Pressure Curve, you have to choose from which domain sides the mercury can enter the structure and leave the structure if **Mercury Extrusion** is computed.

For ease of use you can click on the button **Check All** if the mercury can intrude from all sides.

Note! In Contrast to the Capillary Pressure Curve command, you cannot chose a domain side to be the displaced fluid outlet because no residual remains in the structure.

Materials

The shown Material IDs are the pores that will be filled with mercury during the simulation.

Below, you choose the **Contact Angle Mode** used for the distribution of the mercury and the computation of the capillary pressure. The same options as for the Capillary Pressure Curve[18] are available, but an angle of 140° for the invading fluid is assumed for all solid materials.

With **Use Dynamic Contact Angle and Surface Tension** the assumed contact angle is not fixed anymore. Based on Rigby and Edler (2002)[186] it is assumed that contact angle and surface tension vary with pore size and the contact angle additionally depends on whether mercury is advancing or retreating.

According to Kloubek[185], the product $\gamma \cdot \cos\theta$ in the Young-Laplace equation[5] is replaced by:

$$\gamma \cos\theta_A = -302.533 + \frac{-0.739}{r} \quad (21)$$

For advancing mercury

$$\gamma \cos\theta_R = -68.366 + \frac{-235.561}{r} \quad (22)$$

For receding mercury

Note! This is only valid for pore radii between 4 nm and 100 nm.

Fit Models

Select if you want to compute the Thomeer Model 12 based on the computed capillary pressure curves. The Thomeer Model can also be computed afterwards as post-processing step 56 in the Result Viewer.

Solver Parameters

Step Size (Pore Diameter / Voxel)

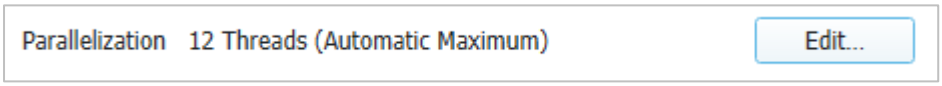
The algorithm increases or decreases the sphere diameter (and thus changes the capillary pressure) from step to step by this amount. Small values increase the accuracy of the result but lead to longer calculation times. The same option is also available in the Capillary Pressure Curve 27 command.

Note! The value for the step size is allowed to be smaller than 1.

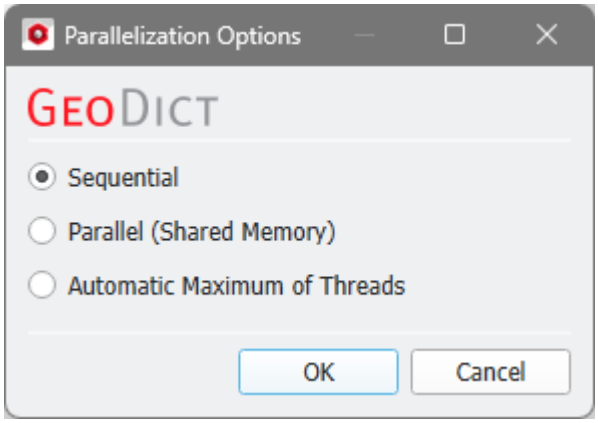
Parallelization

Control how many threads are used for the computation. Parallelization is possible if your license and hardware allow it.

The **Parallelization Options** dialog opens when clicking the **Edit** button and you can choose between **Sequential**, **Parallel (Shared Memory)**, or **Automatic Maximum of Threads**.

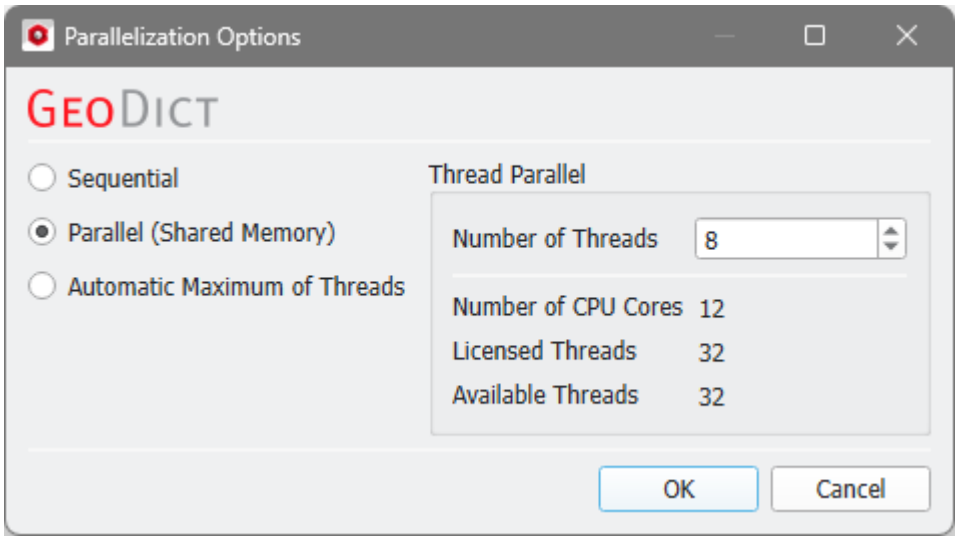


Selecting **Sequential** will not apply parallelization and only one thread is used for the computation.

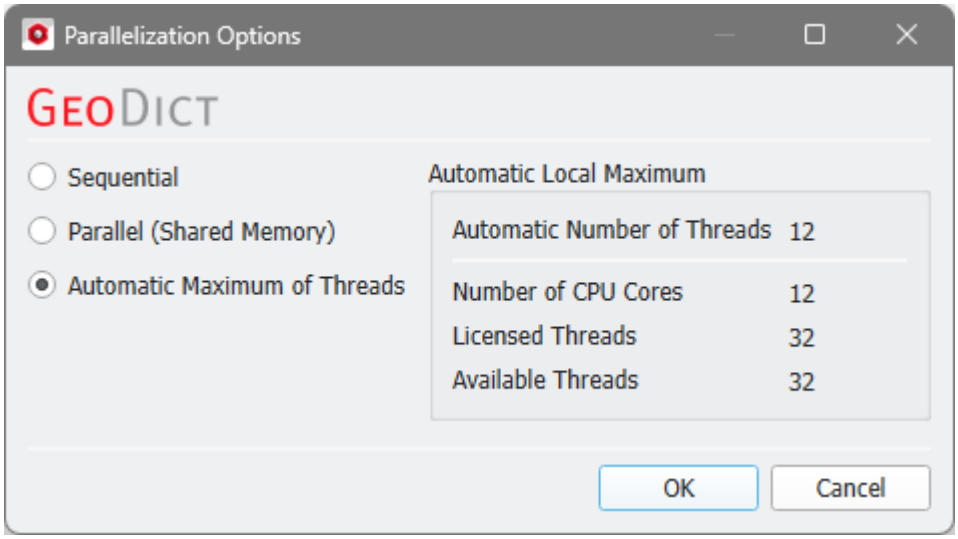


When **Parallel (Shared Memory)** is selected, the **Number of Threads** can be entered. Below, the **Number of CPU Cores** that the current machine has, the maximum number of **Licensed Threads** and the number of those licensed threads that are available (**Available Threads**) are shown in the dialog. Of course, the maximal number of parallel processes you can use, is the

smallest of those three numbers.



If **Automatic Maximum of Threads** is selected, the number of parallel processes is automatically selected for optimal speed, based on the CPU cores and licensed parallel processes.



The **Automatic Local Maximum** of processes is automatically selected, which is the minimum of **Number of CPU Cores**, **Licensed Threads**, and **Available Threads**.

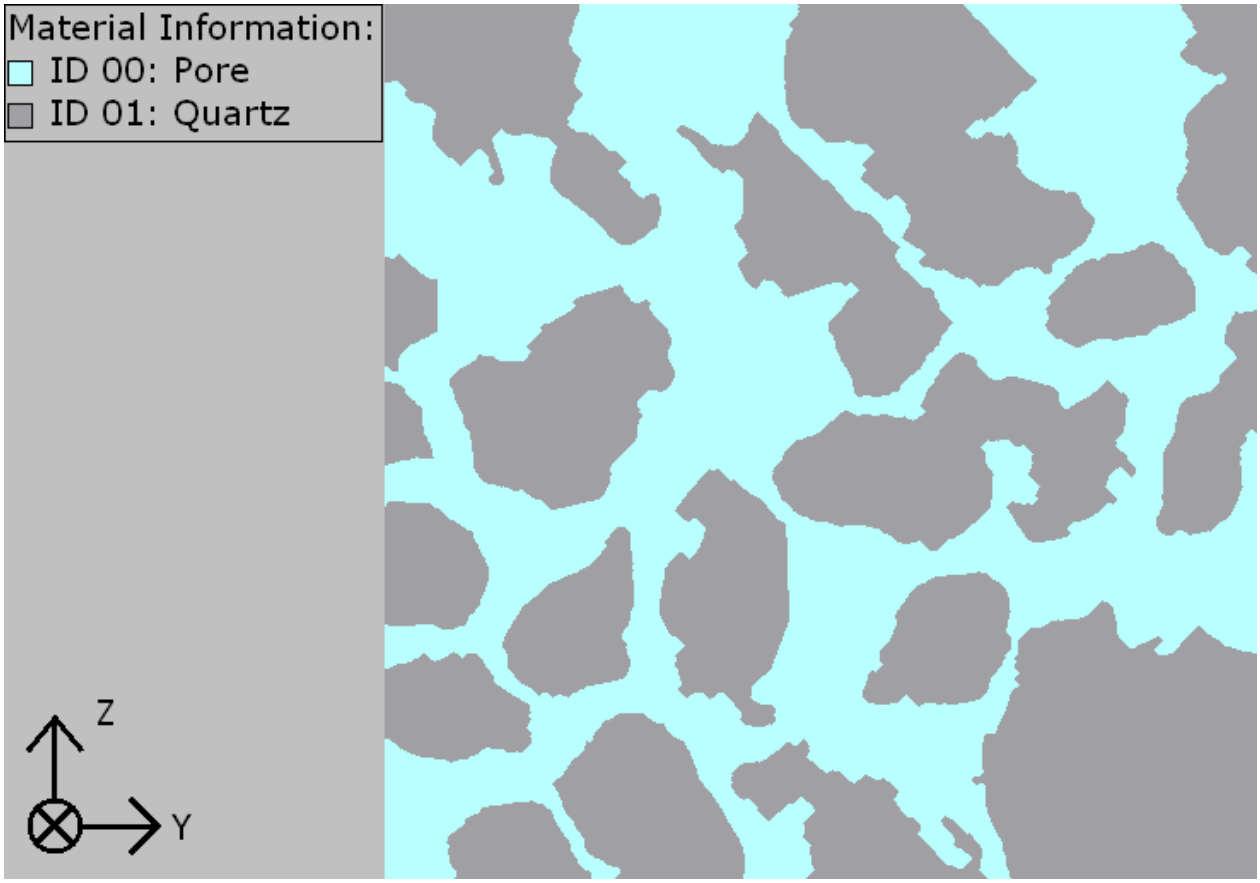
Output

The same options as for the Solver Parameters[31] in Capillary Pressure Curve are available. The saved result files can be loaded from the Data Visualization[60] tab in the result viewer.

1.3.2 Results

After the solver run has finished, the Result Viewer opens immediately. The results are similar as seen for the Capillary Pressure Curve[31], but some more options are additionally available which are special for the MICP, such as the pore throat size distribution.

In the example, the calculations of Mercury Porosimetry & Capillary Pressure 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 **Results** tab is the central point analysis of the results. It is grouped in three subtabs: **Report**, **Plots**, and **Map**. The Report tab shows diameters, curvatures and capillary pressure values for each saturation step. The Plots tab contains plot options for the analysis of the results. The Map tab contains all resulting data from the run. This data is the basis for the tables in the Report tab and for the plots in the Plots tab.

Mercury Porosimetry & Capillary Pressure Results

- Results Tab 54
  Learn about the resulting reports and plots.
- Data Visualization 60
  Load results for a graphical visualization.

Results Tab

Report

In the Report tab, if **Compute Thomeer Model** was checked in the options tab, the results are shown at the top of the Reports tab. This can also be computed as a post-processing step.

Thomeer Model

	Thomeer model	Original image
Porosity S_d / %	45.98 (hidden 0.06)	45.92
Displacement pressure P_d / Pa	1.7300e+05	-
Pore geometrical factor G	0.0029	-

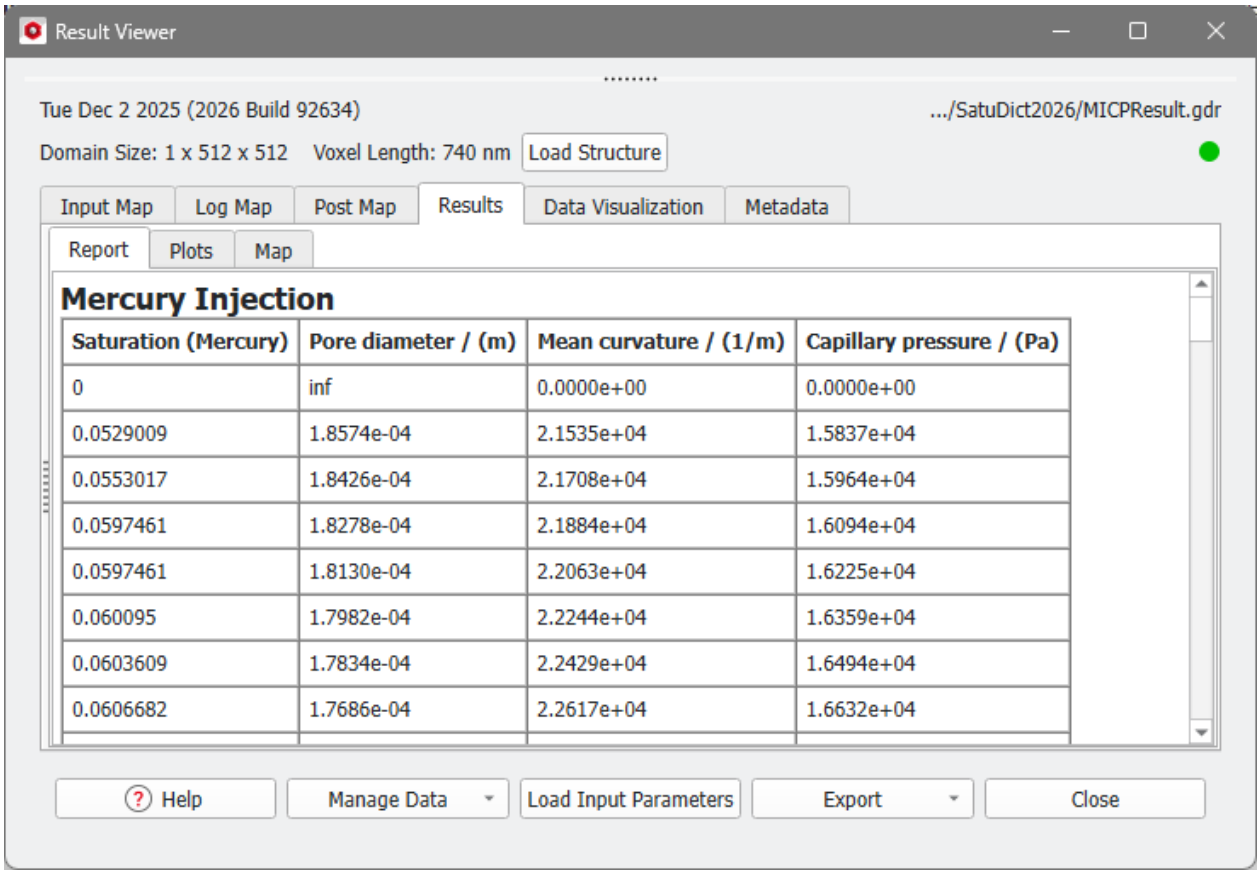
Thomeer model equation: $S_{NWP} = S_d * \exp(-G / \log(P_c / P_d))$
According to: Thomeer J.H.M., Introduction of a Pore Geometrical Factor defined by the Capillary Pressure Curve, 1960, J Pet Technol 12 (3): 73-77. SPE-1324-G.

If an additional **Mercury Extrusion** was computed, the **Residual Saturation** of the mercury at the end of the extrusion simulation is given. Both the **Saturation** (using the pore space as reference volume) and **Volume Fraction** (relating to the total sample volume) are displayed.

Residual Saturation

	Saturation	Volume Fraction
Residual Mercury	0.6434	0.2955

Then, for the **Mercury Injection** and, if selected, the **Mercury Extrusion** a table shows the saturation of the mercury (**Saturation (Mercury)**), the **Mean curvature / (1/m)**, and the calculated corresponding **Capillary pressure / (Pa)** for every step (pore size). The mean curvature approximates the fluid-fluid interface curvature.



Saturation (Mercury)	Pore diameter / (m)	Mean curvature / (1/m)	Capillary pressure / (Pa)
0	inf	0.0000e+00	0.0000e+00
0.0529009	1.8574e-04	2.1535e+04	1.5837e+04
0.0553017	1.8426e-04	2.1708e+04	1.5964e+04
0.0597461	1.8278e-04	2.1884e+04	1.6094e+04
0.0597461	1.8130e-04	2.2063e+04	1.6225e+04
0.060095	1.7982e-04	2.2244e+04	1.6359e+04
0.0603609	1.7834e-04	2.2429e+04	1.6494e+04
0.0606682	1.7686e-04	2.2617e+04	1.6632e+04

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

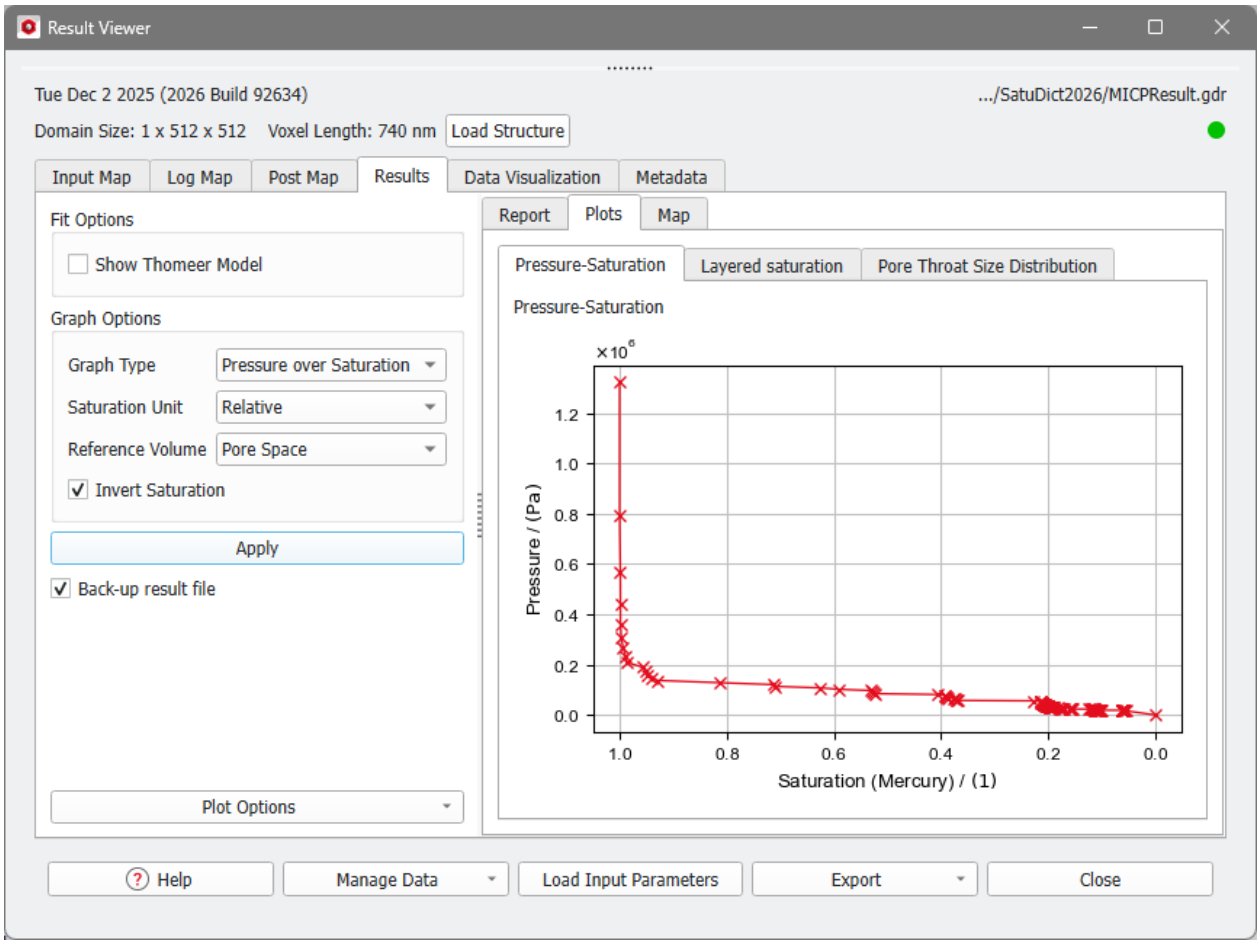
Plots

Pressure-Saturation

Observe the tabular results of the Report subtab as a diagram in the **Pressure-Saturation** subtab.

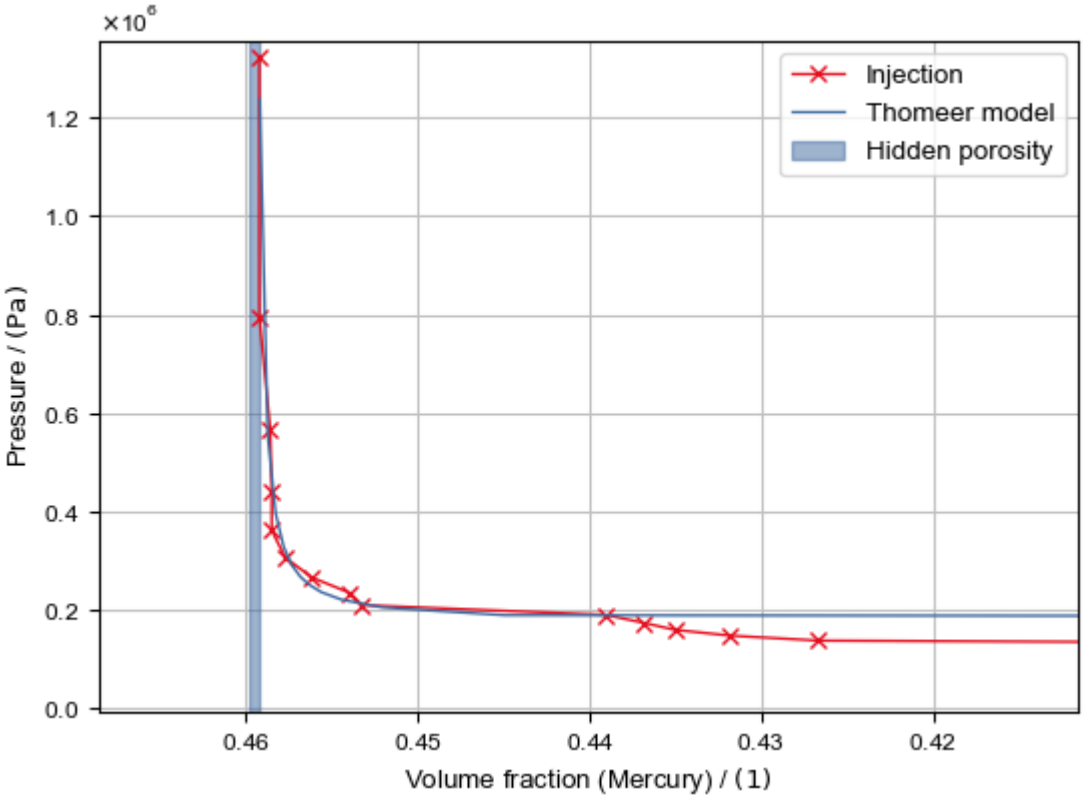
On the left, the **Post-Processing Widget** allows you to fine-tune this graph. Collapse the Post-Processing Widget by pulling it to the left.

Select the **Graph Type** (Pressure over Saturation or Saturation over Pressure), the **Saturation Unit** (Relative or Absolute) and **Reference Volume** (Pore Space or Total Sample Volume). Check **Invert Saturation** to show the values of the saturation in decreasing order instead of increasing order.



In the example, at the beginning of the injection process, the porous structure does not contain the invading fluid Mercury. As the pressure increases, the Mercury starts invading the structure and the saturation of the Mercury is increasing. By the end of the injection process, where the pressure is at its highest level, the pore space of the structure is 100% saturated with Mercury.

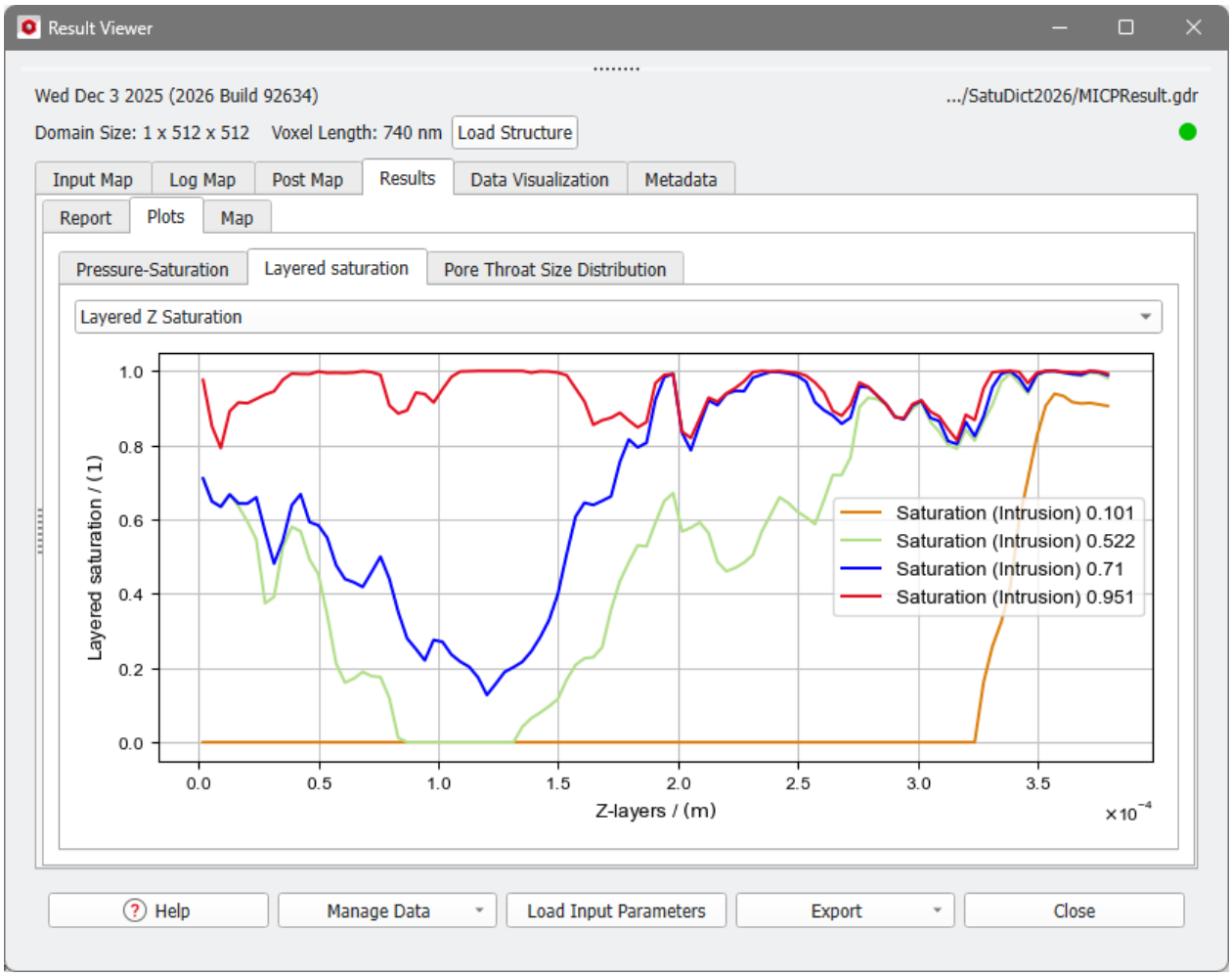
If a Thomeer Model 12 is fitted, this model can be shown by checking **Show Thomeer Model** under **Fit Options**. In this case, the **Reference Volume** is automatically set to **Total Sample Volume** and Pore Space can not be selected.



Layered saturation

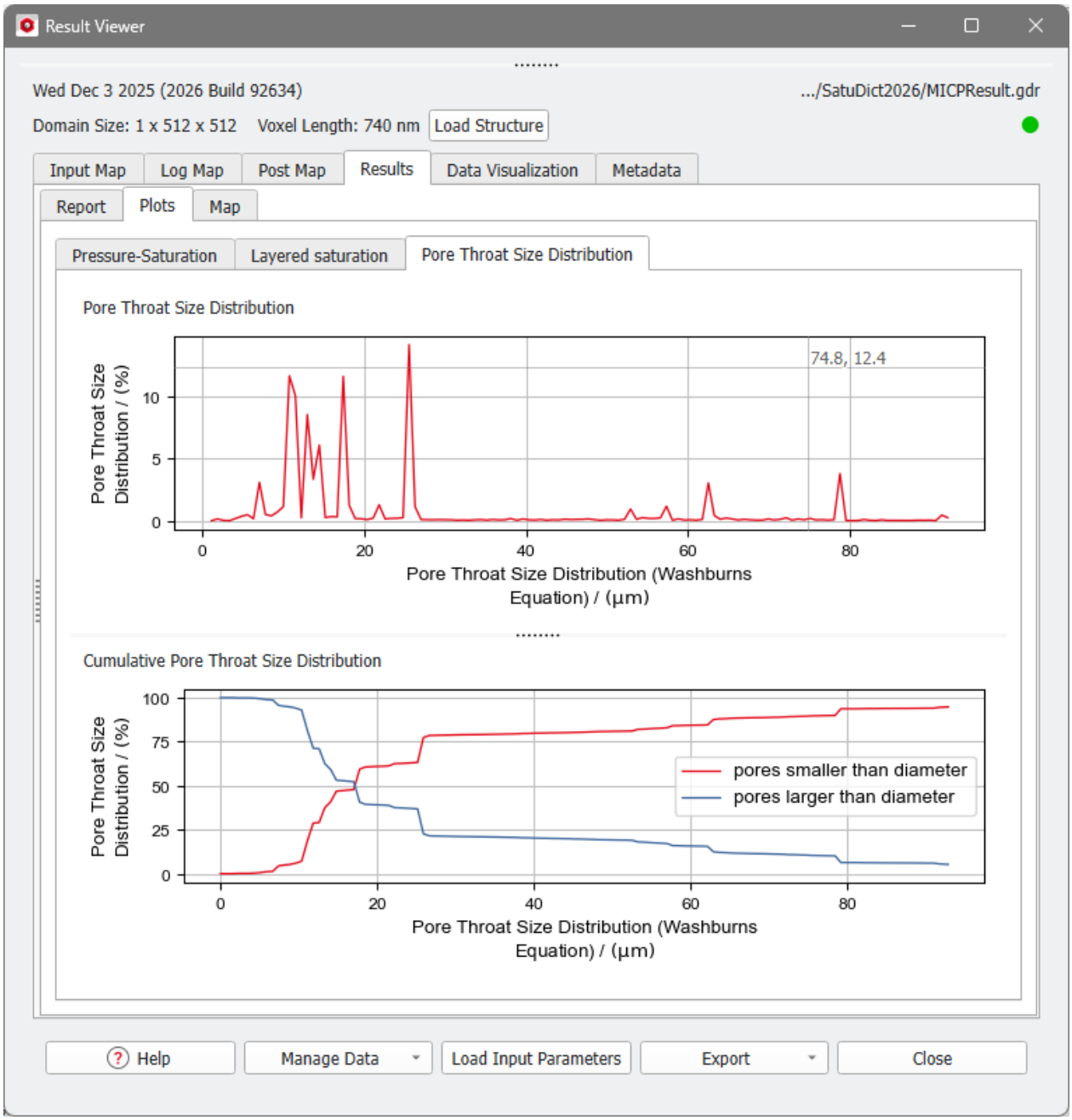
In the subtab **Layered saturation**, the saturation along each of the three axes (X-, Y-, and Z-axis) is shown.

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.



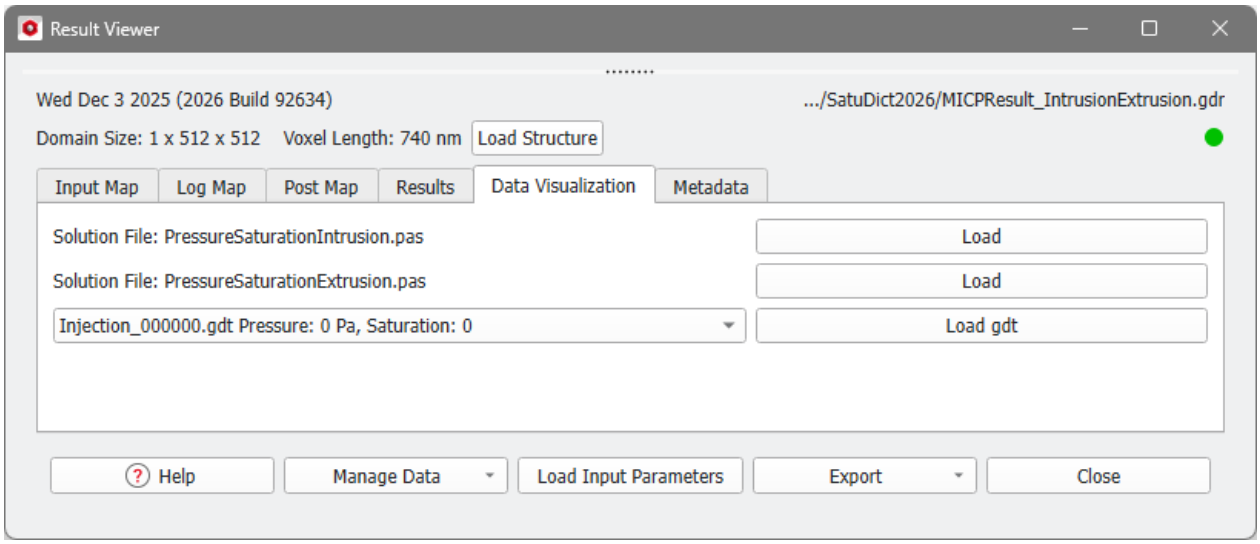
Pore Throat Size Distribution

Using the Washburn / Young-Laplace Equation[5] the resulting capillary pressure values are related to a **Pore Throat Diameter**. The resulting distribution is shown in two plots, which are very similar to the plots of PoroDict-Porosimetry.



Data Visualization

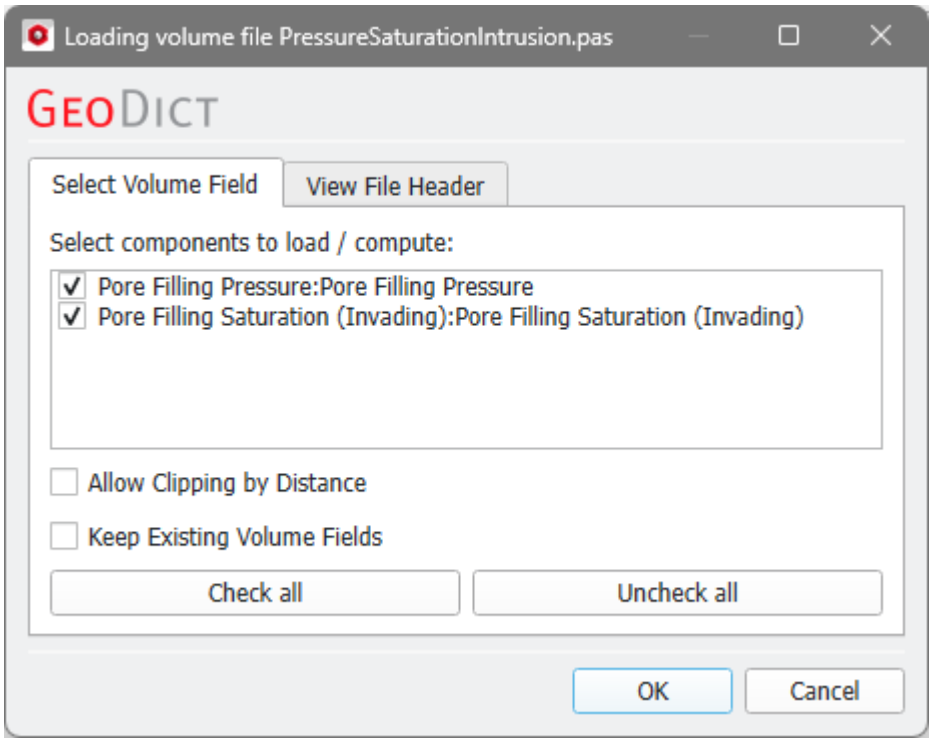
In the **Data Visualization** tab, you can load the *.pas files for the intrusion and, if selected, the extrusion, and the step-by-step images of the computed process.



Visualization of Pressure and Saturation (pas file)

Click **Load** to access the pressure and saturation field data saved in the **PressureSaturation.pas** file.

Depending on the choice made under the output options 49 the **Pore Filling Pressure** and the **Pore Filling Saturation (Invading)** can be selected for the visualization. Click **OK** to load the selected fields.



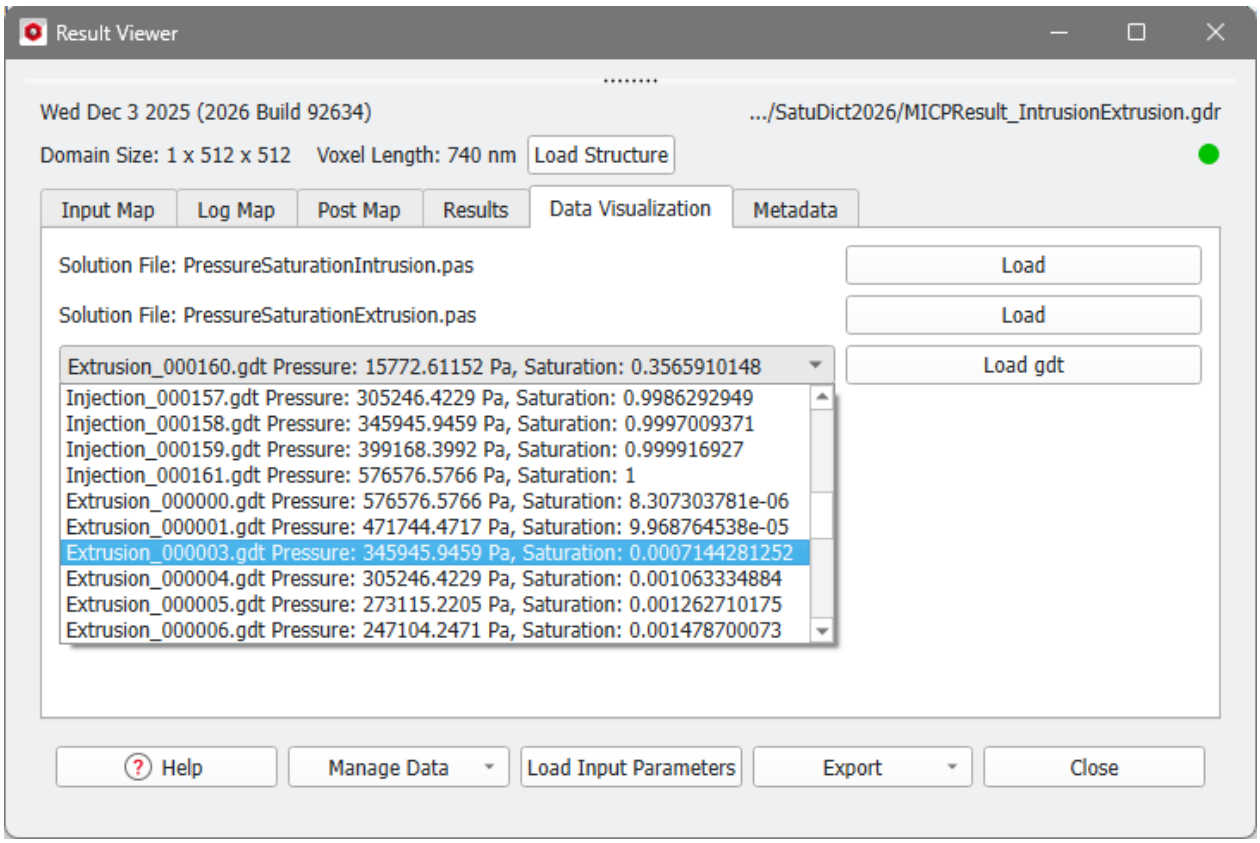
The initial visualization, in 2D view or 3D rendering, is done using default settings which you can modify (see the Data Visualization in Capillary Pressure Curve 38 for an example). These parameters can be found under the **Volume Field** tab in the **Visualization Panel**, above the

Visualization Area. For more information on a particular visualization setting, see the Visualization chapter.

Visualization of intermediate states (gdt files)

Finally, the computed process can be visualized step-by-step with GDT files saved during the MICP calculation. This is only possible if **Write All .gdt** or **Write Only Changed .gdt** was selected in the Output Options 49 section. The GDT files corresponding to the computational steps (Injection_000000.gdt, Extrusion_000000.gdt etc.) are stored in the automatically created result folder.

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



Select one of the GDT files, where the file names correspond to the simulation step in which the GDT file was saved. Also, the pressure and saturation of the invading fluid in this step are shown to easier identify a specific step.

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

1.4 Relative Permeability

Determine **Relative** and **Saturation-dependent (Effective) Permeability** for different fluid saturations. The pore morphology method[5] 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.

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

The **Effective Permeability** can be calculated for the invading fluid or the displaced fluid. In both cases, the unconsidered fluid is treated as an unmovable obstacle and the flow calculation treats it as a solid. Thus, flow only takes place in the pores filled with the corresponding fluid, while the other pores are ignored. Specifically, no movement of bubbles is simulated. To determine the whole effective permeability curve, it is necessary to select several different saturations and both invading and displaced fluid for the computation. After the computation, in a post-processing step, you can calculate an LET fit[12] or a Corey fit[13] for the effective permeability curves.

The permeability values are then determined as described in the Flow permeability section of the FlowDict chapter. Similar as in FlowDict, a volume field containing velocity and pressure values at each voxel is saved for each saturation step.

The **Relative Permeability** is a dimensionless measure, defined as the ratio of the **Saturation-dependent Permeability** (K_s) to the **Absolute Permeability** (K_1). The relative permeability thus lies between zero and one:

$$\frac{K_s}{K_1} \in [0,1] \qquad \text{(23) Relative Permeability}$$

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

The Relative Permeability command

- Options[64]
  Set the parameters for the calculation.
- Results[90]
  View the computed results.

1.4.1 Options

The **Relative Permeability** dialog opens when clicking the **Edit...** button and includes the **Wetting Parameters** tab, the **Constituent Materials** tab, the **Boundary Conditions** tab, the **Solver** tab, and the **Equations & References** tab, which cites several references 185.

At the top of the dialog, enter the **Result File Name**. The result file is saved in the chosen project folder (**File → Choose Project Folder** in the menu bar).

The **Equations & References** tab shows the formulas that are used for the solver which are described in the FlowDict chapter:

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

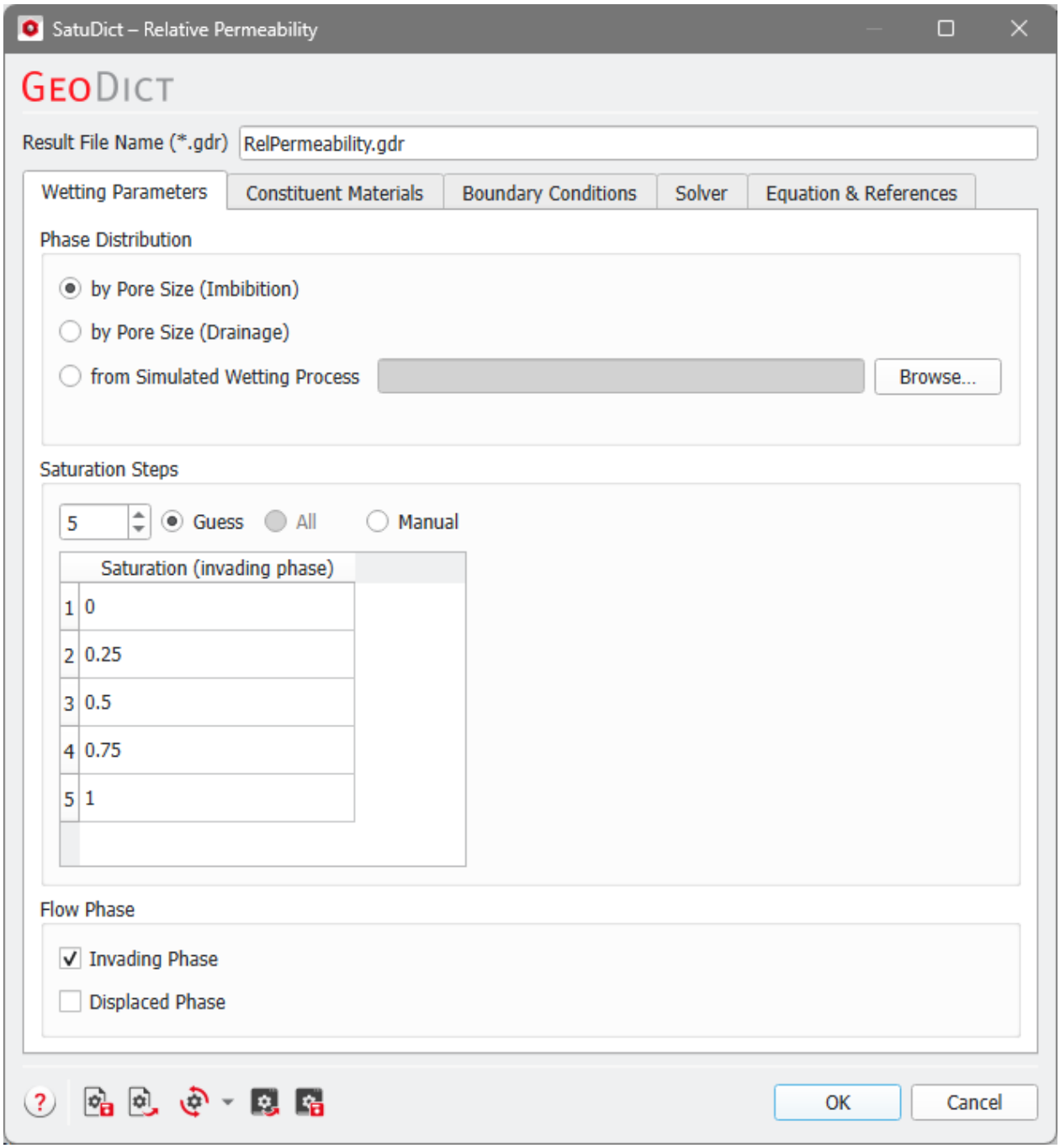
No parameters can be edited on this tab.

Tabs of the Relative Permeability dialog

- Wetting Parameters 64
  Select how the fluid distribution is determined and choose the saturation steps for the permeability calculations.
- Constituent Materials 68
  Select the materials in the structure and their properties, including the selection of invading and displaced fluid.
- Boundary Conditions 68
  Set the boundary conditions for the flow calculations.
- Solver 77
  Select a flow solver and its settings.

Wetting Parameters

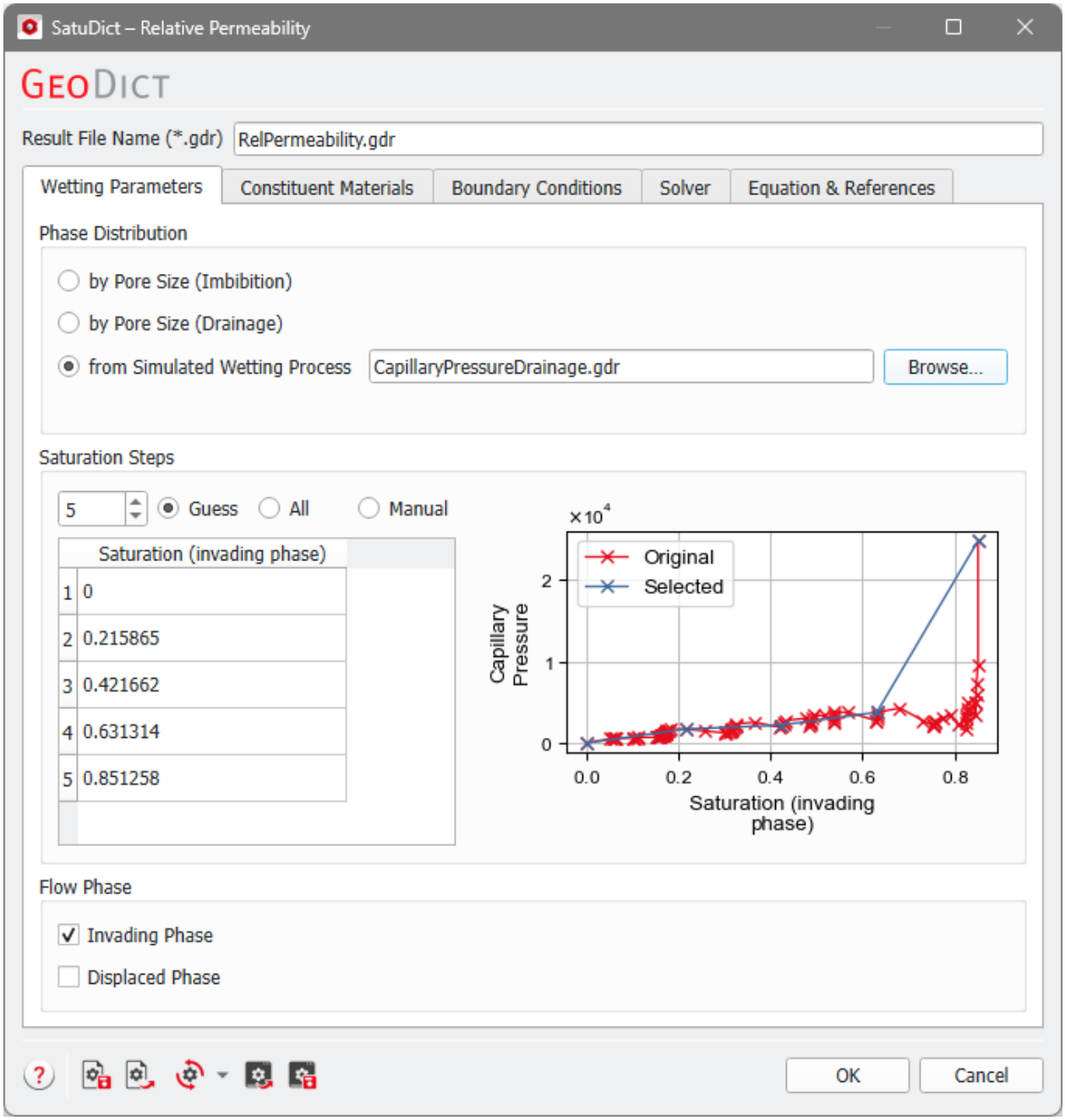
The **Wetting Parameters** tab is divided into three panels: **Phase Distribution**, **Saturation Steps**, and **Flow Phase**.



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° for the invading fluid is assumed. When choosing **by Pore Size (Drainage)**, the invading fluid contact angle is assumed to be 180°.

However, the phase or fluid distribution at different saturation points can be taken from a previously simulated imbibition or drainage process. Select **from Simulated Wetting Process** and click **Browse...** to choose a result file (GDR file) of a Capillary Pressure Curve computation on the same structure.



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. The plot to the right 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 chapter). This way you can control if the guessed saturation points are indeed representative.

All

This option 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.

Important! This can lead to very long computation times, depending on the number of saturation steps contained in the capillary pressure result file.

Manual

In manual mode, you can modify the table at will and enter your desired saturation steps.

Flow Phase

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

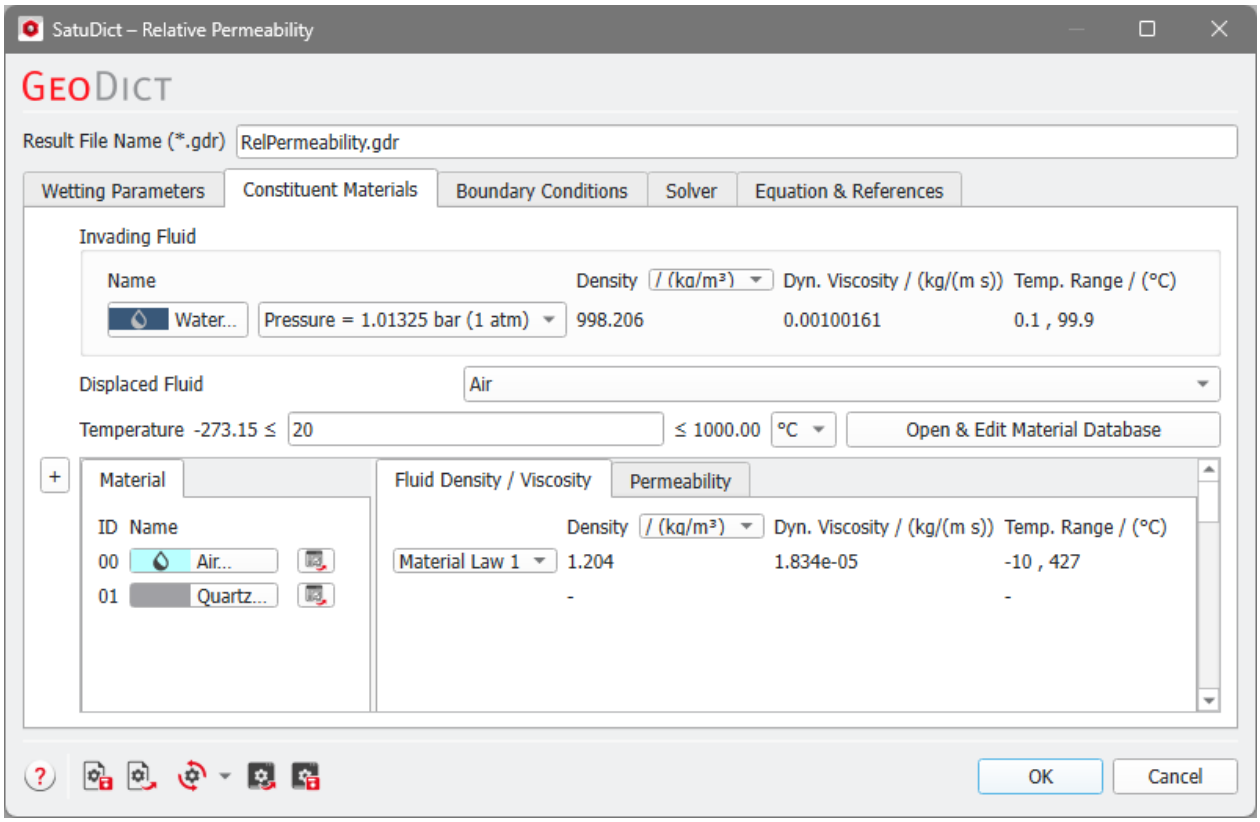
- If you select **Invading Phase**, the displaced fluid will be treated as solid and flow only takes place in the invading fluid.
- If you select **Displaced Phase**, the invading fluid will be treated as solid and flow only takes place in the displaced fluid.

You can also select both phases, then, for each saturation step, two flow calculations will be made: one for each phase as described above.

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 Curve 18 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 and can be chosen from the drop-down menu. If the phase distribution is taken **from Simulated Wetting Process**, then both fluids are defined by the capillary pressure curve result file.



In the **Permeability** panel define the permeability for porous materials in the structure.

Boundary Conditions

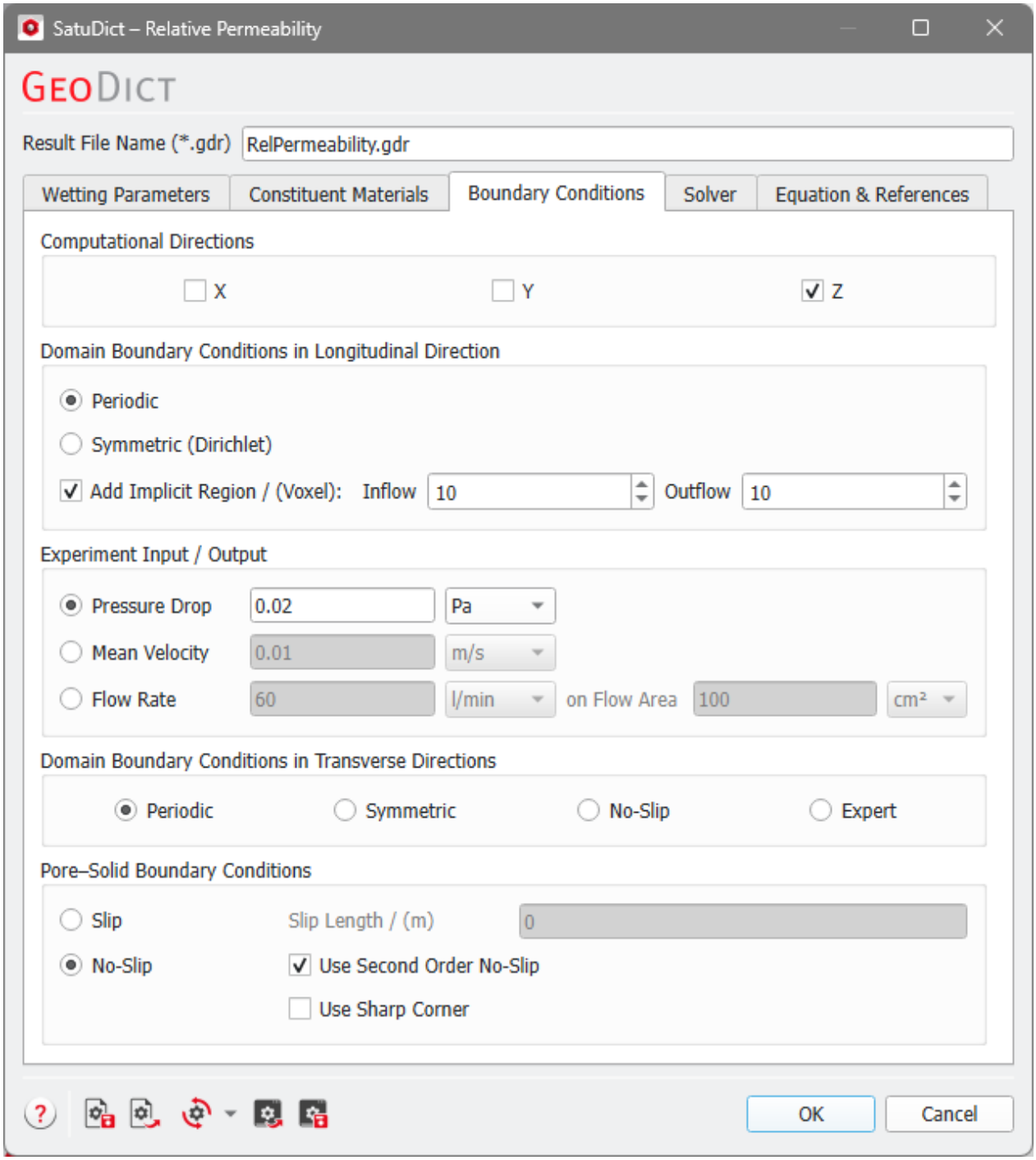
The **Boundary Conditions** tab is divided into five panels: **Computational Directions**, **Domain Boundary Conditions in Longitudinal Direction**, **Experiment Input / Output**, **Domain Boundary Conditions in Transverse Direction**, and **Pore-Solid Boundary Conditions**.

Note! The parameters are very similar to the parameters in the FlowDict Stokes(-Brinkman) command.

To simulate the flow through the domain, GeoDict solves a boundary-value problem. In the fluid-filled part of the domain, the flow is governed by a differential equation. The boundary values describe what happens at the boundaries, and are a necessary and important part of the problem description. Boundaries are the six faces of the cuboid (X-, X+, Y-, Y+, Z-, Z+), and the

pore-solid walls within the structure.

For the six cuboid faces, FlowDict distinguishes between the domain faces in the computational direction (also called flow direction or longitudinal direction) and the domain faces in the two other space directions (called transversal or tangential directions). The computational direction is the direction in which pressure drop and flow rates are measured.



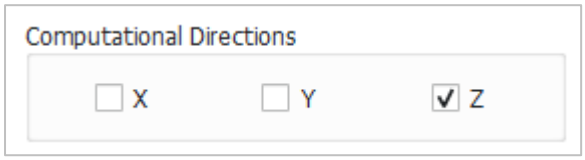
Computational Direction

As **Computational Directions**, select the directions for which you want to calculate the flow.

To obtain the full 3x3 permeability matrix and a pressure drop value for each direction in the results file, select all three directions.

For every selected direction, a boundary value problem is solved in which the **Domain Boundary Conditions in Longitudinal Direction** and the corresponding **Experiment Input/Output** are applied in the computational direction, and the **Domain Boundary Conditions in Transverse Directions** are applied on the other two space directions.

Any directions not selected will not be calculated and will be marked as 'unknown' in the permeability matrix in the **Report** tab of the result file.

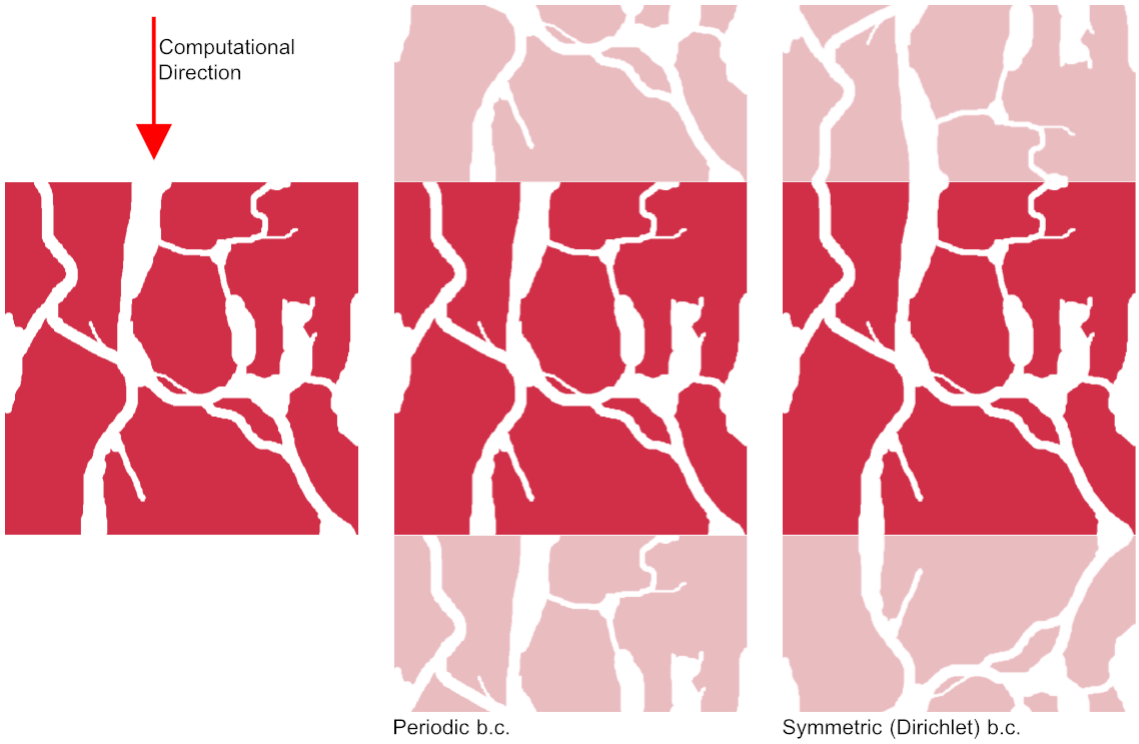


Domain Boundary Conditions in Longitudinal Direction

The **Domain Boundary Conditions in Longitudinal Direction** can be checked to be **Periodic** or **Symmetric (Dirichlet)**.

Use **Periodic** boundary conditions for periodically generated structure models and for non-periodic structures with high porosity. The structure is internally repeated periodically at the domain boundaries in the computational directions.

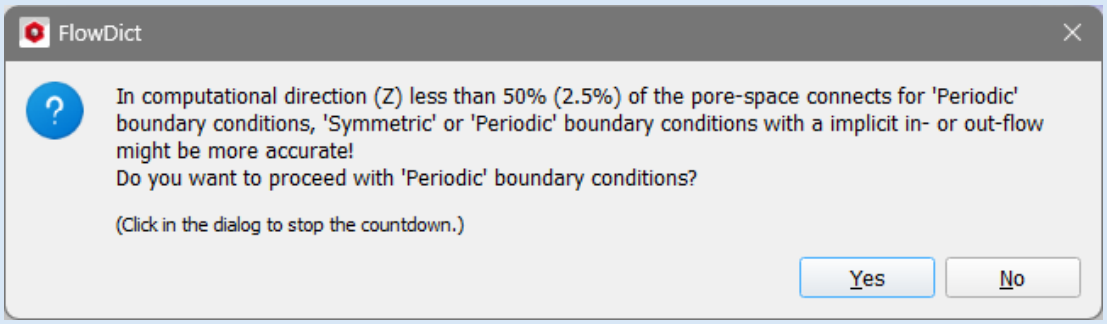
Use **Symmetric** boundary conditions for non-periodic structures if the percentage of solid voxels is high at the inlet. The solver treats the structure as mirrored at the domain boundaries in the computational directions.



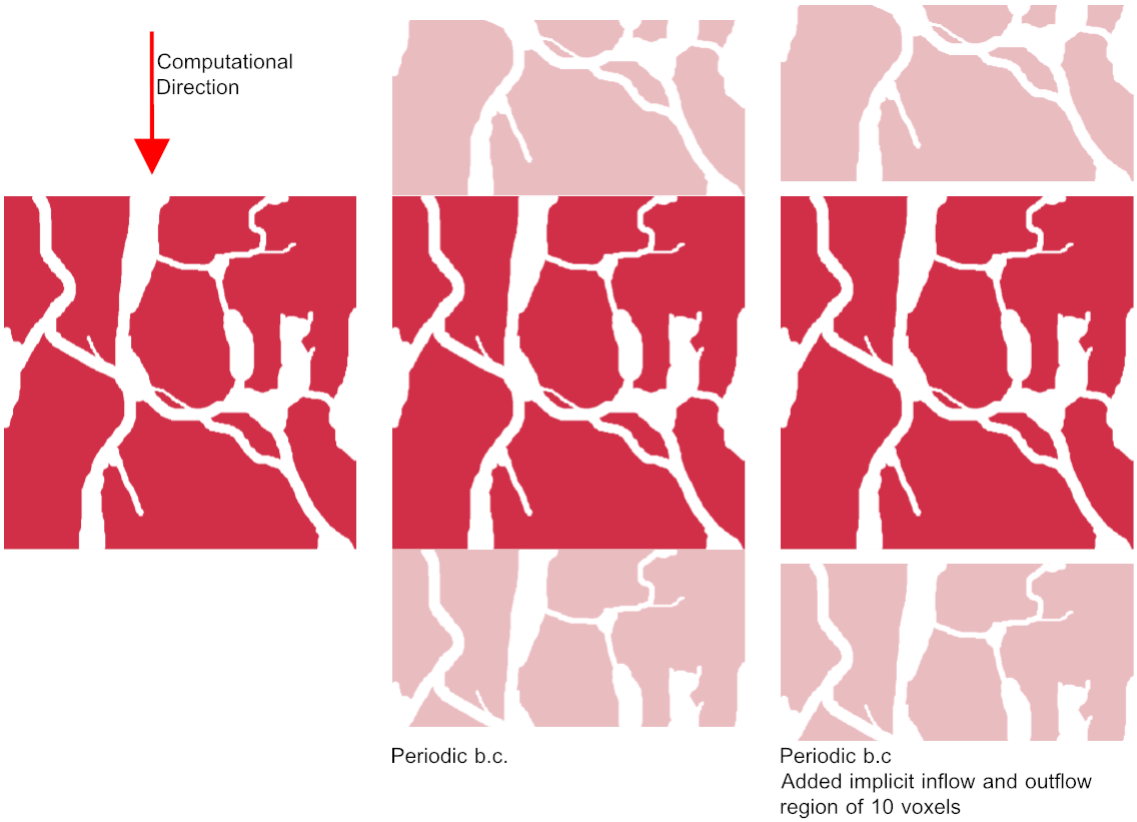
The option to **Add** an **Implicit Region** is not available for **Symmetric** boundary conditions. The size of the implicit region in the computational directions is given in voxel, where the default added implicit inflow and outflow are 10 voxels, respectively.

Know how! The term implicit means that the region is only added by the solver internally. Thus, these regions do not contribute to the computed permeability and flow resistivity.

Note! A warning may appear when trying to run flow computations without adding an inflow region when the pore space at the domain boundaries in the computational directions is less than 50%.



The inlet and outlet are essential to avoid the possibility of closing the flow channels when the structure is periodically repeated. In the example shown below choosing periodic boundary conditions in the direction of the flow without adding an implicit region results in the flow channels being artificially closed.



To open the channels and enable flow, you can either add an inflow and/or outflow region, or select symmetric boundary conditions. However, when possible, we recommend using periodic boundary conditions, as these require less computational memory and take less time to run.

Experiment Input / Output

In the **Experiment Input / Output** panel select which property is prescribed in the computational direction. This will also define the property that will be computed. You can prescribe the **Pressure Drop** and obtain the **Mean Velocity** as result. Alternatively, you can prescribe the **Mean Velocity** or the **Flow Rate** and obtain the **Pressure Drop** as result.

This selection corresponds to the typical experimental setup, where you either apply a constant pressure drop over the media and measure the through flow rate or you apply a fixed pump flow rate and measure the resulting pressure drop over the media.

The **Pressure Drop** is the difference between the inflow and outflow pressures.

The **Mean Velocity** is the average speed of the flow in the positive direction, i.e., from Z- to Z+ if the Z-direction is the computational direction.

The **Flow Rate on Flow Area** is a volumetric flow rate. It is the fluid volume which passes per unit time through a given area.

For each property, the desired unit can be selected from the pull-down menu.

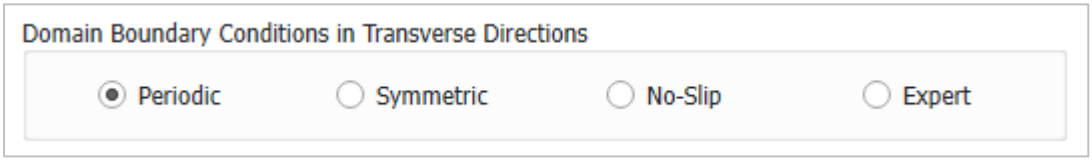
It is possible to use the **Mean Velocity** or the **Flow Rate** as input because the Stokes(-Brinkman) equation is linear. Thus, the solver can prescribe a pressure drop (sp) and compute a mean velocity (sv). This mean velocity is not the desired mean velocity (ds) entered in the **Experiment Input / Output** panel. Therefore, the velocity and pressure field are rescaled by $^{dv}/_{sv}$. Then, the pressure drop (dp) is calculated by

$$dp = sp \cdot \frac{dv}{sv} \tag{24}$$

For example, if the desired velocity is twice the mean velocity used by the solver, the computed pressure drop is doubled to obtain the pressure drop corresponding to the desired mean velocity.

Domain Boundary Conditions in Transverse Direction

The **Domain Boundary Conditions in Transverse Directions** can be **Periodic**, **Symmetric**, **No-Slip**, or **Expert**.

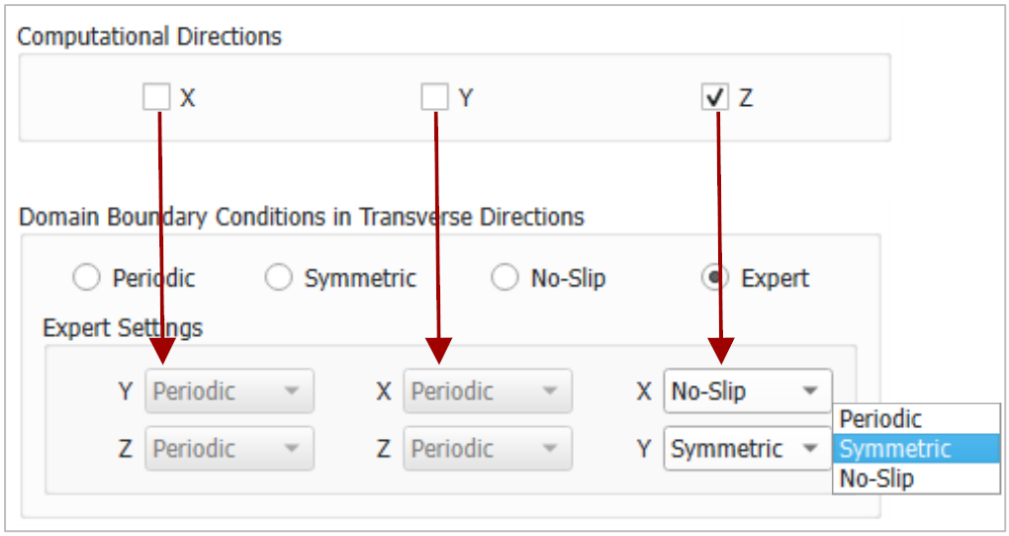


With **Periodic** boundary conditions, the structure is repeated in the transverse directions.

With **Symmetric** boundary conditions, the structure is mirrored at the domain boundary. The LIR and EJ solver solve the symmetric boundary condition by using Neumann (or zero flux) condition at the domain boundary.

With **No-Slip** (or Encase) boundary conditions, the domain boundary is treated as closed by solid material. When **No-Slip** is used, the solver internally adds a one-voxel layer in the required direction and solves with periodic boundary conditions. This is effectively equivalent to solving the structure with casing at both sides in the transverse direction. So, the structure size in the corresponding transverse direction becomes enlarged by one voxel internally.

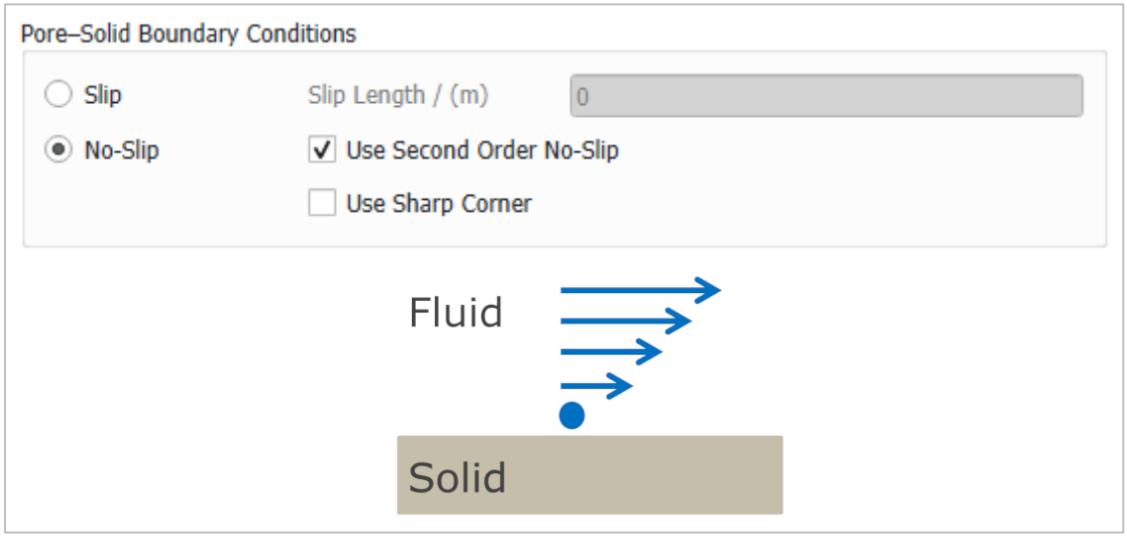
With **Expert**, it is possible to define different boundary conditions for each side in each computation. The boundary conditions in the two directions transverse to the flow can also be different by checking **Expert** boundary conditions. For example, when the fluid is chosen to flow in the Z-direction, the boundary conditions could be chosen to be **No-slip** in X-direction and **Symmetric** in the Y-direction.



Pore-Solid Boundary Conditions

The **Slip Length** allows to include sliding effects in the flow simulation. Sometimes the permeability of gases can be somewhat different from the permeability of liquids in the same media. One difference is attributable to "slippage" of gas at the interface with the solid when the gas mean free path is comparable to the pore size.

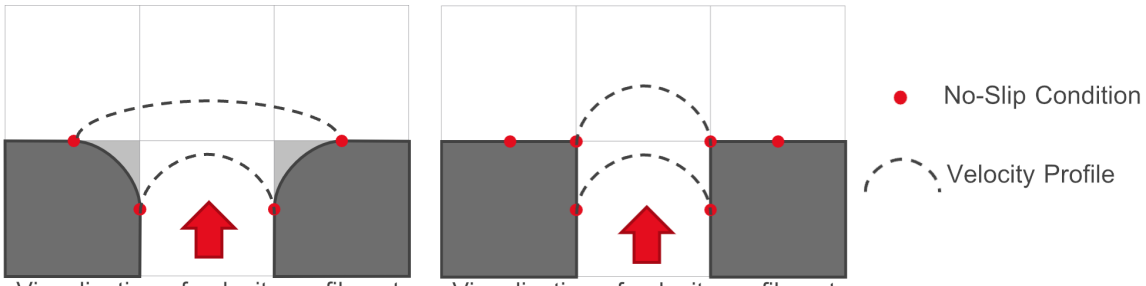
The default setting **No-Slip** corresponds to a flow velocity of zero along the structure.



Two settings are available for the **No-Slip** boundary condition. **Use Second Order No-Slip** is activated by default. This sets the tangential velocity to zero at the center of the voxel surfaces and uses a second order approximation of the velocity field. The first order setting, which is used when the box is left unchecked uses a linear approximation (Harlow-Welch, 1965).

Use Sharp Corner can be used for digital rocks where permeability is usually overestimated or cases where voxels represent exact geometry. Activating it sets the tangential velocity to zero at the voxel corners. When the box is unchecked the default

Round Corner is applied, which should be used for structures with round obstacles like fibers or grains.

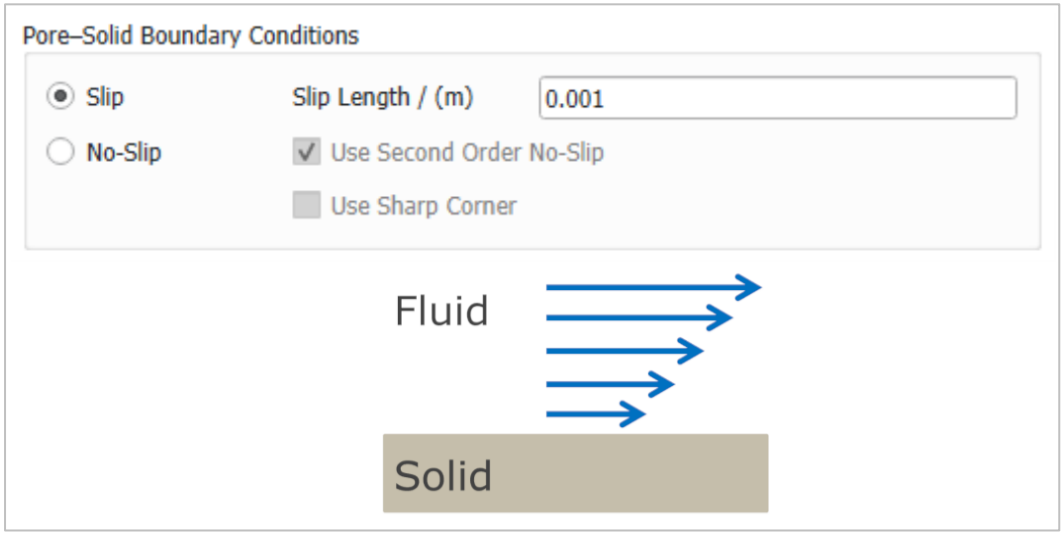


Visualization of velocity profiles at round corners

Visualization of velocity profiles at sharp corners

Slip with a non-zero **Slip Length** simulates the sliding of the fluid along the solid, increasing the fluid mean flux and thus, the permeability of the structure. This option might be used when it is realistic for a given physical material. Currently, the same slip length value must be set for all materials in the structure.

In earlier releases, this feature worked correctly for axis aligned walls only, but since GeoDict 2020 the expression of the slip velocity, which assumes the slip velocity proportional to the shear stress at the surface, is reformulated for different velocity components when the angle of fiber surface is known, and reimplemented in the flow solver. Thus, direct simulation of the slip flow is possible.



$$\vec{n} \cdot \vec{u} = 0 \text{ on } \Gamma$$

(25) No flow into solid

$$\vec{t} \cdot \vec{u} = -\lambda \vec{n} \cdot \nabla(\vec{u} \cdot \vec{t}) \text{ on } \Gamma$$

(26) Slip flow along solid

Here, $\vec{u}$ is the fluid flow velocity as it was introduced in Darcy's law and the Stokes

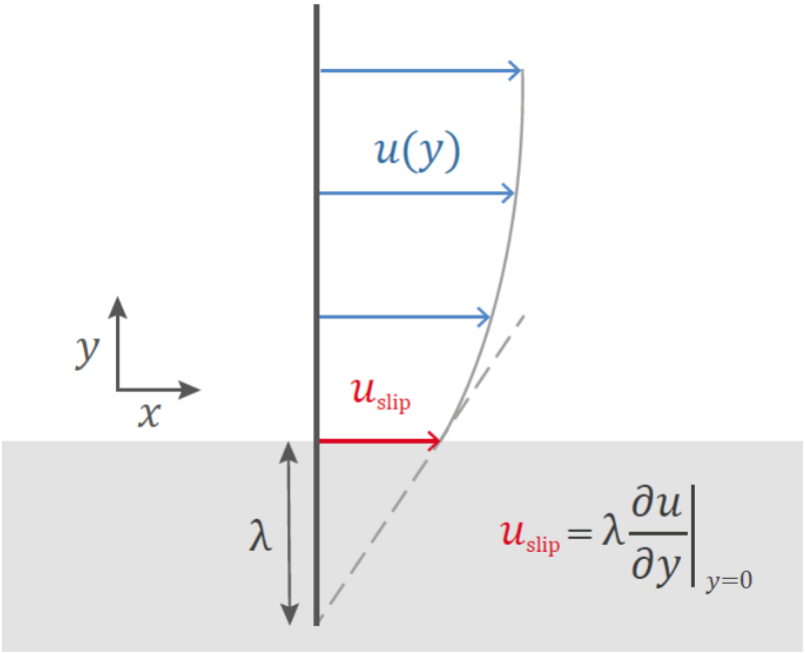
equation, $\vec{n}$ is the normal direction to the solid surface, Γ is the fiber surface, λ is the **Slip Length** and $\vec{t}$ is any tangential direction with $\vec{t} \cdot \vec{n} = 0$. For the same pressure drop, the computed velocities for slip boundary conditions are higher than for no-slip boundary conditions. Conversely, for a given velocity or equivalently, a given mass flux, the pressure drop is lower when computed with slip boundary conditions.

For a straight channel structure, the two slip flow equations above become:

$$u = \lambda \frac{\partial u}{\partial y}$$

(27) Slip flow in straight channels

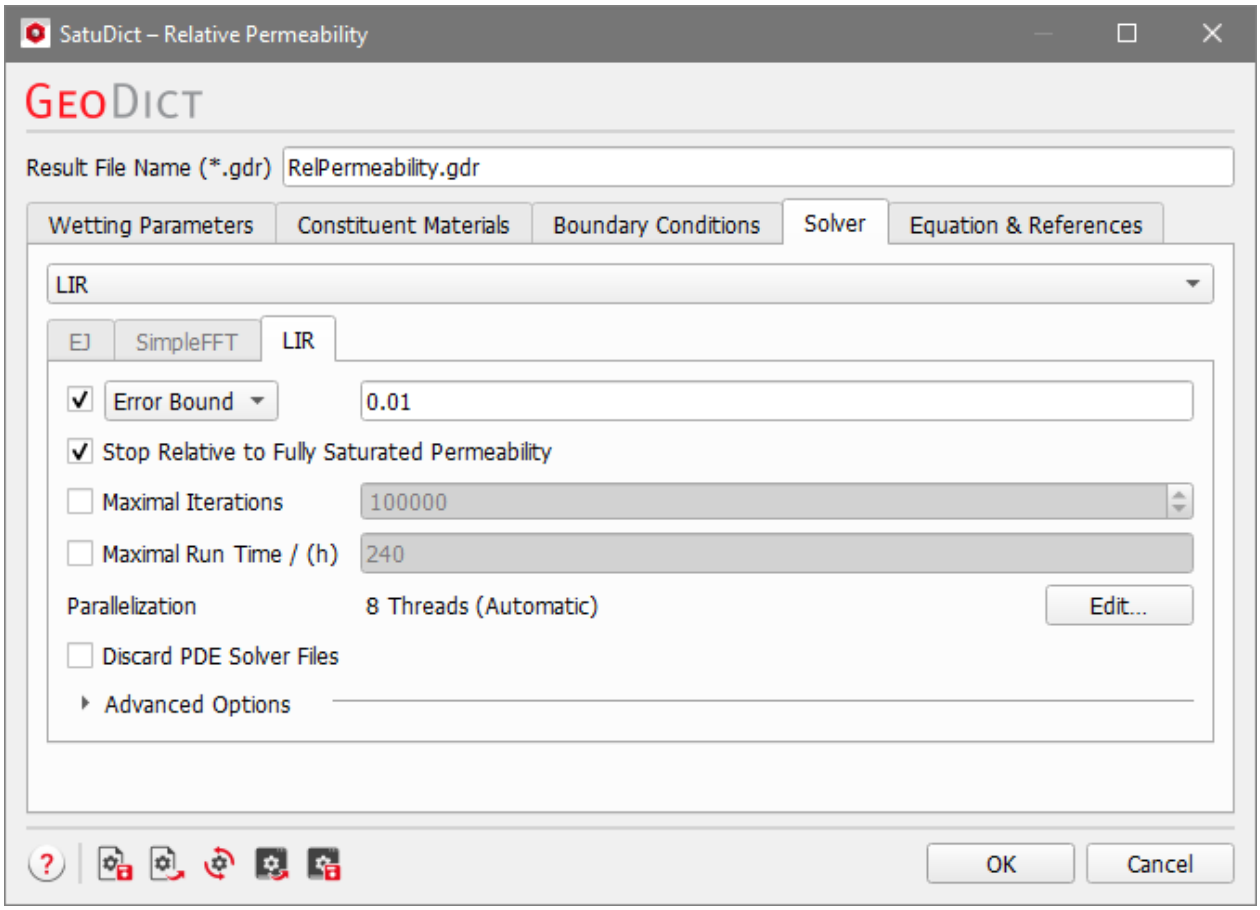
In this following example figure, the gray solid serves as a wall for a straight channel. To obtain the flow velocity along the solid (u_{slip}) a coordinate system is defined by the solid orientation.



For a **Slip Length** of zero ($\lambda = 0$), the graph that describes the flow velocity in dependence of the distance to the solid surface, would start at the surface of the solid. However, for a positive **Slip Length** ($\lambda > 0$) it is shifted into the solid by λ . Thus, the flow velocity u_{slip} is defined.

Solver

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.



Parameters for all solvers

Stopping Criteria

The equations are solved by an iterative approach.

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
3. Repeat the iterative process until one of the stopping criteria is reached.

The iterative process is controlled by setting the values and activation for **Error Bound, Tolerance, Residual, Stop Relative to Fully Saturated Permeability**, **Maximal Iterations**, and **Maximal Run Time (h**). The stopping criteria apply for each computational direction individually.

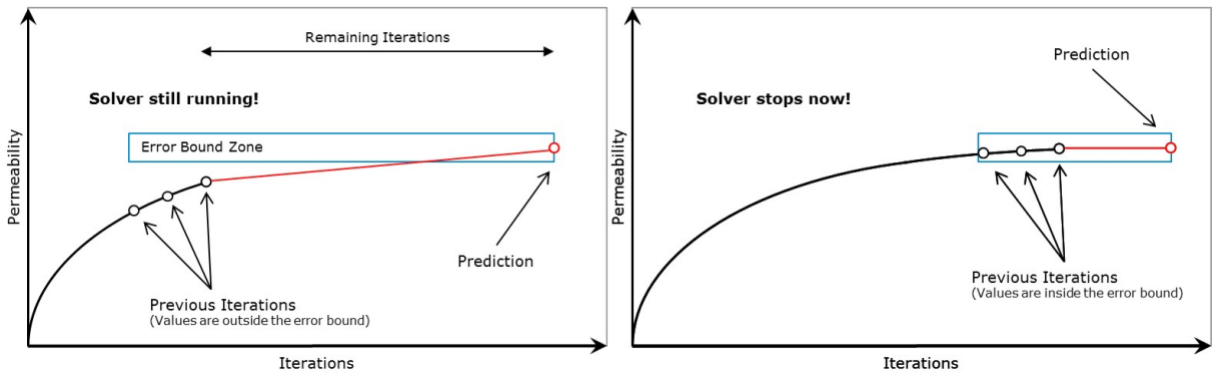
If multiple stopping criteria are selected, the first criterion that is reached causes the solver to stop.

The stopping criterion that has been reached can be viewed in the Result Viewer of the GeoDict result file (*.gdr) under the **Results Report** tab.

The available stopping criteria apply to each single permeability calculation run, not to the whole relative permeability prediction run. For each calculation, a different stopping criterion may occur and cause the solver to stop. Thus, for **Relative Permeability**, the reached stopping criterion is not printed in the result file.

Error Bound (LIR and SimpleFFT)

The stopping criterion **Error Bound** uses the result of previous iterations, and predicts the final solution based on linear and quadratic extrapolation. The solver stops if the relative difference between computed and predicted solution is smaller than the specified error bound. The stopping criterion recognizes oscillations in the convergence behavior and prevents premature stopping at local minima or maxima. A damped convergence curve is fit through the oscillating curve and the solver stops then regarding the damped convergence curve.



If the Krylov method (under LIR - Advanced Options) is activated, the definition of **Error Bound** is somewhat different. Here, no prediction is made, instead the continuity between neighboring cells and the conservation of mass is checked. The maximal value is normalized by the mean flow and if this value is smaller than the **Error Bound** the simulation stops.

Tolerance

The **Tolerance** stopping criterion looks for stagnation of the method when the process becomes stationary, i.e., the improvement in the permeability value becomes extremely small from iteration to iteration.

In each iteration, the solver checks for the current computed value x_c against the values x_{c-i} of the last 100 iterations if there are any changes.

$$\max_{i\in[1,100]} \frac{x_c - x_{c-i}}{x_{c-i}} < \text{tolerance} \tag{28}$$

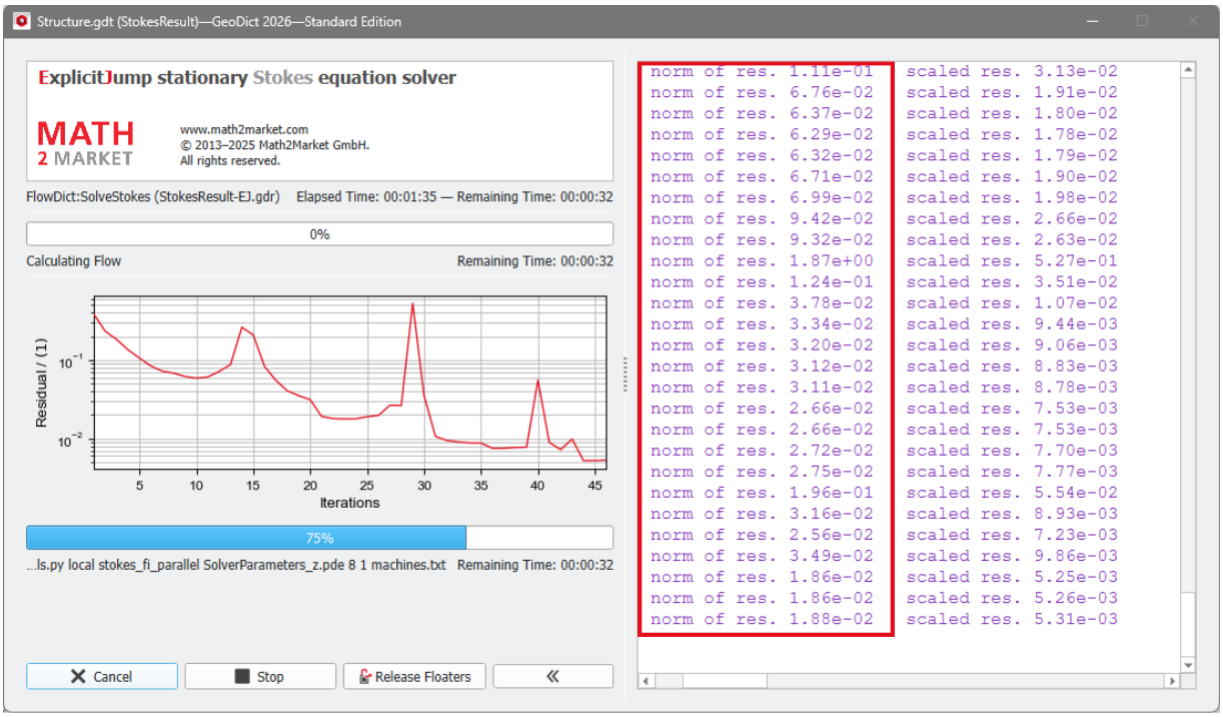
The computation is stopped if the maximal relative change is smaller than the value entered

for **Tolerance**. When there is doubt about the quality of the solution, decrease the **Tolerance** value by a factor of ten. The drawback of this criterion is that the solver sometimes might stop too early in case of slow convergence rate or at local extrema of oscillatory convergence curves.

Residual (EJ and SimpleFFT)

When the **Residual** stopping criterion is used, the iteration is stopped if the solution satisfies the equation up to the required accuracy.

By setting the stopping criterion to **Residual**, the computations terminate as soon as the relative norm drops below the selected residual threshold. The relative norm of the Schur Complement residual is computed and displayed in the console window during the calculations. The console is visible by clicking the double arrow button on the lower right corner in the progress dialog.



The recommendation to choose **Tolerance** or **Residual** for the **EJ** solver is based on the structure's porosity. Both give similar results for highly porous structures. For dense structures, if using the Schur Complement **Residual**, the relative norm of the residual may be small even though the correct permeability has not been reached. So, when in doubt, use the **Tolerance** criteria – the default option.

Stop Relative to Fully Saturated Permeability

The option to **Stop Relative to Fully Saturated Permeability** is only available in the Relative Permeability command of SatuDict and relaxes the chosen stopping criterion for the computation of each partially saturated state.

First, the absolute permeability for the structure is computed, this yields the highest permeability value. For states with two fluids inside, the permeability of the selected flow phase[67] will be smaller than the absolute permeability.

For the computation not the entered stopping criterion will be used, but it will be adapted to the absolute permeability. It is important to know how the stopping criteria work to understand how this option works.

E.g., if **Error Bound** is chosen as stopping criterion, the solver estimates the final solution and checks if the current solution is inside the error bound zone. An Error Bound of 0.01 means that the difference between current solution and predicted solution relative to the predicted solution must be smaller than 1% for the solver to stop. With Stop Relative to Fully Saturated Permeability activated the error bound will not be 1% of the predicted relative permeability in each run, but the error bound is a bit higher. For the exact value of the error bound, the absolute value of 1% of the absolute permeability is taken into account.

$$max_{1 \le i \le k} \frac{|v_i - p|}{\sqrt{p * r}}$$

(29) adapted error bound stopping criterion

$$max_{1 \le i \le k} \frac{|v_i - v|}{\sqrt{v * r}}$$

(30) adapted tolerance stopping criterion

p	current predicted permeability
v	current computed permeability
$\{v_1, ..., v_k\}$	last computed permeabilities
r	reference value (absolute permeability)

The effect becomes most visible for low saturations. Here, the permeability is near zero and the computation is much more expensive. With this option activated, the computation is stopped earlier, because the stopping criterion is more relaxed and thus earlier fulfilled.

Maximal Iterations & Maximal Run Time

Use the **Maximum Iterations** value or the **Maximum Run Time (h)** stopping criteria

causes the solver to stop if the maximal number of iterations and/or the maximal runtime (in hours) is exceeded.

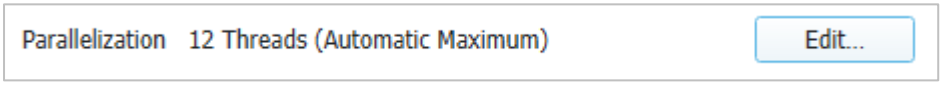
When the solver stops because one of these criteria has been reached, no guarantee on the quality of solution can be given. In this case, a warning is printed into the report. The following possibilities might help:

- Check the corresponding .log file to see how large the residual values and the permeability values are. If the permeability values are in reasonable range and they do not have changed during the last iterations, you may decide to use the current result.
- Double-check the structure and parameter values. Unphysical parameters or too rough resolution of the structure (leading, e.g., to artificial unconnected components) can cause an iterative solver to fail.

Parallelization

Control how many threads are used for the computation. Parallelization is possible if your license and hardware allow it.

The **Parallelization Options** dialog opens when clicking the **Edit** button and you can choose between **Sequential**, **Parallel (Shared Memory)**, **Automatic Maximum of Threads**, or **Cluster** (only available if EJ, SimpleFFT, or FeelMath were selected as solver).



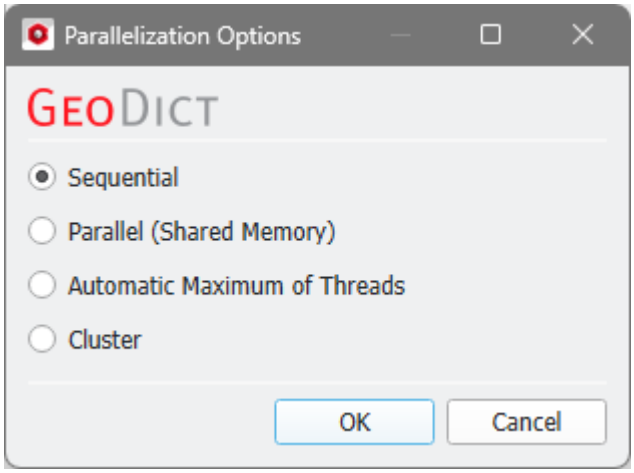
The parallelization of the solvers is done with two technical methods: **MPI Parallelization** or **Thread parallelization**. The following table shows the support of both parallelization methods:

Solver	Parallelization method	
	MPI Parallel	Thread Parallel
EJ	✔	✘
SimpleFFT	✔	✘
LIR	✘	✔
FeelMath	✔	✔
BEST	✘	✔

Depending on the used parallelization method, the **Number of Processes** (MPI parallel) or the **Number of Threads** (thread parallel) can be entered.

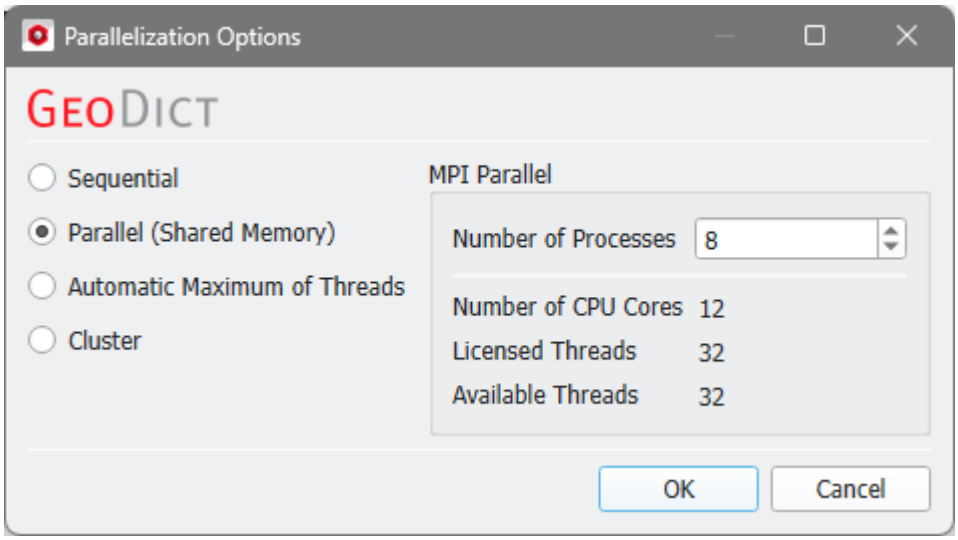
Sequential

Selecting **Sequential** will not apply parallelization and only one thread is used for the computation.



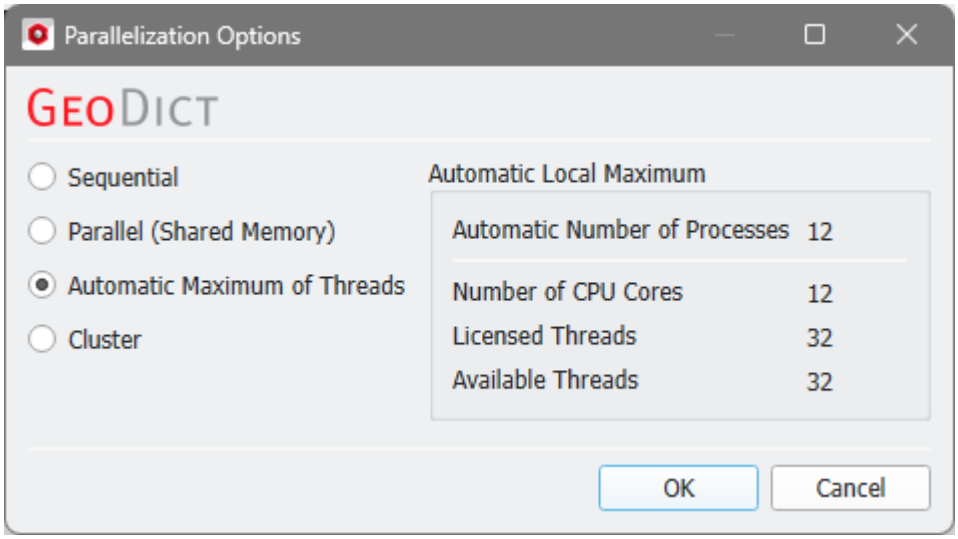
Parallel (Shared Memory)

When **Parallel (Shared Memory)** is selected, the **Number of Processes** or **Number of Threads** can be entered. Below, the **Number of CPU Cores** that the current machine has, the maximum number of **Licensed Threads** and the number of those licensed threads that are available (**Available Threads**) are shown in the dialog. Of course, the maximal number of parallel processes you can use, is the smallest of those three numbers.



Automatic Maximum of Threads

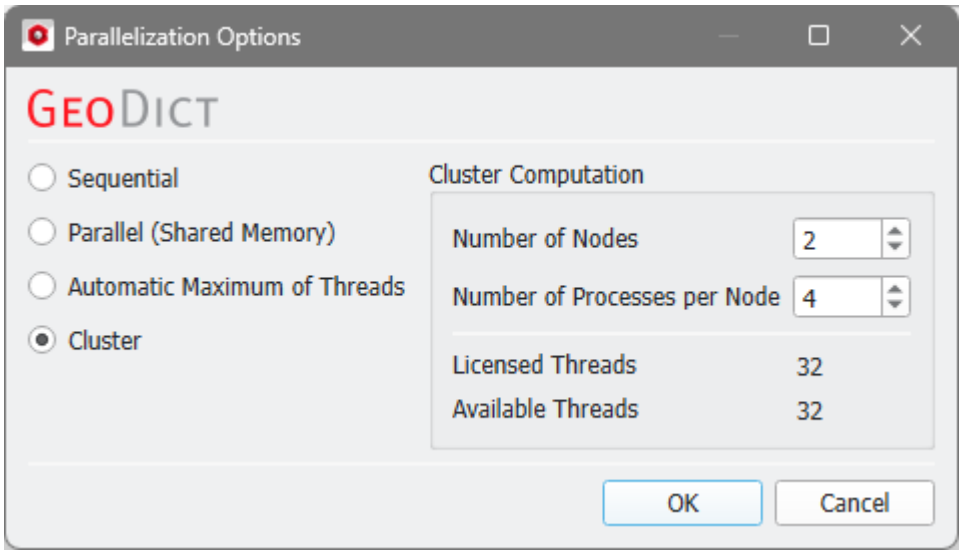
If **Automatic Maximum of Threads** is selected, the number of parallel processes is automatically selected for optimal speed, based on the CPU cores and licensed parallel processes.



The **Automatic Local Maximum** of processes is automatically selected, which is the minimum of **Number of CPU Cores**, **Licensed Threads**, and **Available Threads**.

Cluster

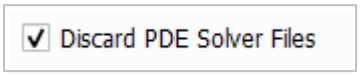
The **Cluster** parallelization requires that the solver supports the **MPI Parallelization** method. Moreover, the choice of **Cluster** is for users of Linux systems only.



For details on how to set up and run parallel computations, consult the High Performance Computing chapter.

Discard PDE Solver Files

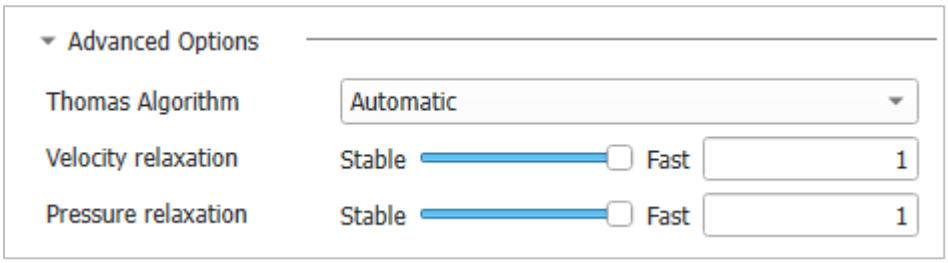
Checking **Discard PDE Solver Files** causes the deletion of all intermediate computation files, such as log files and flow field files.



Only the content of the final GeoDict result file (*.gdr) is stored.

While having the benefit of saving hard disk storage place, discarding intermediate solver files has also the effect of disabling the 3D visualization of the results.

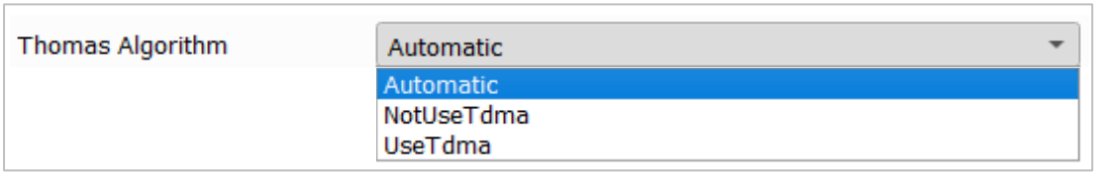
SimpleFFT specific parameters (Advanced Options)



Thomas Algorithm

The tridiagonal matrix algorithm (Tdma), also known as the **Thomas Algorithm**, may help to improve the convergence for high porosity structure, especially for Navier-Stokes. The algorithm transforms the 3D flow problem to 2D. Thus, it leads to a shorter runtime and increases the convergence speed.

Three options can be chosen from the pull-down menu: **Automatic**, **NotUse Tdma** or **Use Tdma**.



If **Automatic** is selected, the SimpleFFT solver decides if **Tdma** will be used, regarding the porosity of the structure. Thus, **Tdma** is used if the porosity is high. For most cases it is recommended to choose **Automatic**.

If a message dialog appears, displaying that NaN is detected in iterations, **NotUse Tdma** should be tried.

If the structures porosity is very high, it might decrease the runtime a little bit to explicitly choose **Use Tdma**. But for most cases **Automatic** will work well.

For more information about the Thomas algorithm see here.

Velocity and Pressure Relaxation

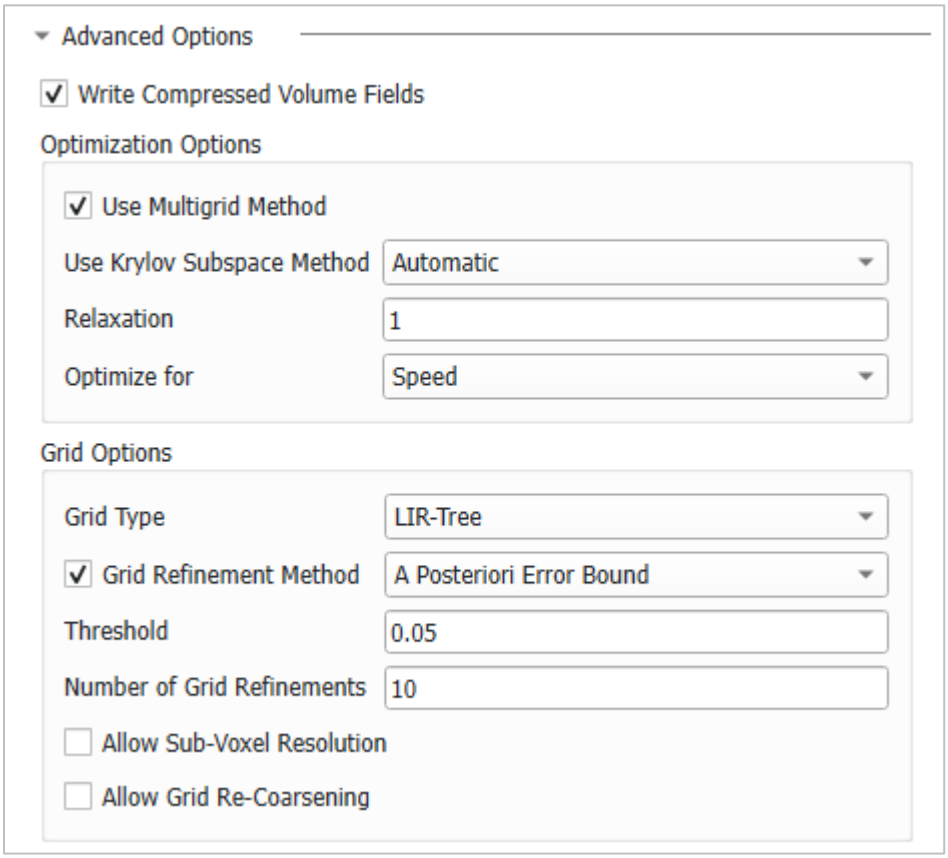
Depending on the material parameters and geometrical structure of the structure, the

underlying mathematical problem can vary in complexity, thus influencing the behavior of the solver. This is directly related to the Reynolds number, an indication of the complexity of the flow solver computations. The higher the Reynolds number, the more **Stable** the flow solver settings should be, resulting in higher number of iterations, slower time stepping, and longer flow solver run times. However, making the solver run less iterations and, thus, faster (**Fast**), implies the risk that the solver does not converge.

For the SimpleFFT solver, the management of this balance is done through the **Velocity relaxation: Stable ↔ Fast** and **Pressure relaxation: Stable ↔ Fast** slide bars.

Setting the balance of **Stable** versus **Fast** is a trial-and-error process. Although there is no general rule to optimize it, the log files and the visualization of the structure might help finding the balance. Non-sense structure visualization results indicate that a more stable, slower solver is needed.

LIR specific parameters (Advanced Options)



Write Compressed Volume Fields

The LIR solver uses a very memory efficient adaptive grid structure for the simulations.

If the option **Write Compressed Volume Fields** is checked, then the adaptive grid is used as compression method for writing out *.vap files. This option allows to save 80-90% space on hard drive. The runtime for writing *.vap files is also reduced significantly. But the runtime for loading and uncompressing of compressed *.vap 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 a usual regular grid is used for writing out *.vap files.

Use Multigrid Method

The **Multigrid Method** (see, e.g., Wesseling, 2004) was introduced to speed-up the computation and reduce the runtime significantly. The main idea of **Multigrid** is the usage of multiple coarser adaptive grids to speed up convergence behavior but requires only little more memory.

The method is available to solve the Stokes and Stokes–Brinkman equations as well as for solving mechanics, diffusion, thermal, and electrical conduction and is enabled by default.

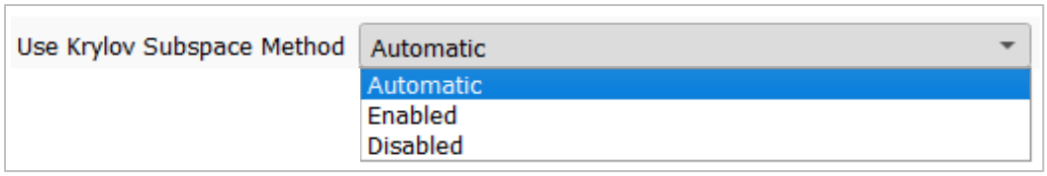
Use Krylov Subspace Method

Another speed-up option to accelerate the convergence behavior of the LIR solver is called **Krylov Subspace Method**.

The runtime of the LIR solver depends on many different properties of the structure and the simulation parameters. The BiCGStab algorithm is used, which can reduce the runtime for challenging simulation very drastically.

> **Note!** Using the BiCGStab method approximately doubles the amount of RAM needed for the computation.

Unfortunately, the Krylov method is not always faster than a simulation without the Krylov method and therefore we introduced an **Automatic** mode which uses some heuristics to choose the most efficient method based on structure, material parameters, and boundary conditions automatically. Of course, it is possible to explicitly enable (**Enabled**) or disable (**Disabled**) the method.



Note! In case that the Krylov subspace method (BICGStab) is used, the **Relaxation** may also be adapted automatically.

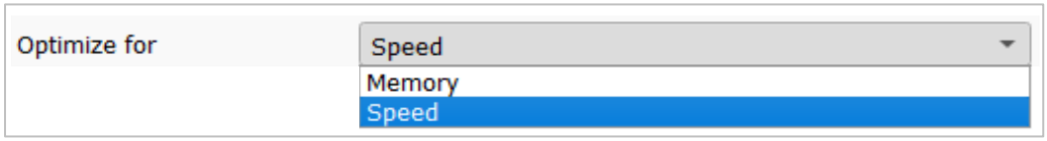
Relaxation

Depending on the material parameters and geometry of the structure, the underlying mathematical problem can vary in complexity, thus influencing the behavior of the solver. The more complex the problem is, the more stable the solver settings should be.

With the **Relaxation** number, the solver is adjusted from **Stable** (which results in higher number of iterations, slower time stepping, and longer solver run times), to **Fast**, which makes the solver run less iterations but implies the risk that the solver does not converge. The **Relaxation** is a parameter of the SOR method and must be between 0 and 2 to ensure convergence. For relaxation values smaller than one (<1.0), the simulation is more stable. For relaxation values larger than one (>1.0), the simulation converges faster.

Optimize For

The **LIR** solver can **Optimize for Speed** or **Memory**.



- If **Speed** is chosen, the solver constructs additional optimization structures. The runtime is decreased by up to 30% but requires up to 50% more memory compared to the other option.
- If **Memory** is chosen, the runtime is increased by up to 40% but the solver requires up to 50% less memory.

Grid Type

The **Grid Type** decides what kind of tree structure is used for the simulation.

The default option is **LIR-Tree** and should always be used. The solver uses an adaptive grid structure called LIR-tree and needs up to 10 times less runtime and memory compared to the **Regular Grid** option.

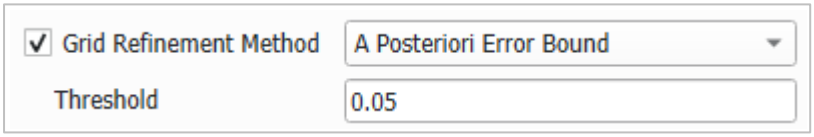
The solver can analyze the result field during the computation and improves the adaptive grid in places where more accuracy is needed. The LIR solver splits cells where a high gradient occurs.

Grid Refinement Method

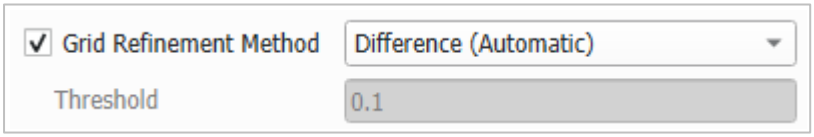
The solver can analyze the computed field and refines the adaptive grid during the computation at locations where more accuracy is needed. The LIR solver splits cells where a high gradients occur when the **Grid Refinement Method** is enabled. In this case, the additional parameters **Number of Grid Refinements**, **Allow Sub-Voxel Resolution**, and **Allow Grid Re-Coarsening** become available.

Select one of the three available refinement methods from the drop-down menu.

When **A Posteriori Error Bound** is selected, the solver targets the specified accuracy **Threshold**. While the **Error Bound** (set as Simulation Stopping Criterion) determines the relative error in the solution of the linear system, **A Posteriori Error Bound** refers to the relative error estimated by comparing high-order and low-order discrete solutions. The accuracy **Threshold** refers to the relative error to the analytical solution and the value must be between 0.0 and 1.0.

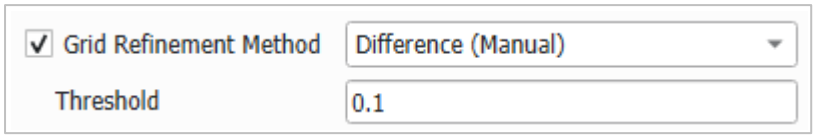


Choosing **Difference (Automatic)** leads to computational cells being split when the difference in values between neighboring cells exceeds a certain **Threshold**. The solver automatically chooses all internal parameters based on the structure and simulation settings. For this option, cells are split where the current gradient is greater than the **Threshold** multiplied by the maximum gradient, where the threshold is determined automatically.



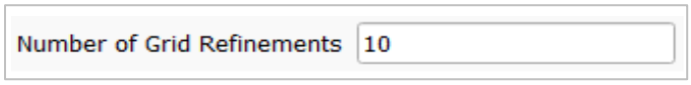
Selecting **Difference (Manual)** also causes the computational cells to be split when the difference in values between neighboring cells exceeds the specified **Threshold**. You can specify all parameters (Threshold and Number of Grid Refinements) for the grid refinement manually. For this option, cells are split where the current gradient is

greater than the **Threshold** multiplied by the maximum gradient. The **Threshold** value must be between 0.0 and 1.0. The recommended value range is between 0.05 and 0.1.



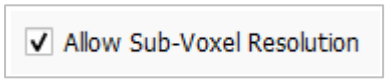
Number Of Grid Refinements

The **Number of Grid Refinements** controls the maximum number of grid refinements that the solver can perform during the simulation. The value should be set between 0 and 10, where a value of 0 means that no grid refinements will be made. Grid refinements may increase the number of iterations, runtime, and memory requirements.



Allow Sub-Voxel Resolution

When **Allow Sub-Voxel Resolution** is enabled, the solver is allowed to split computational cells to sizes smaller than the voxel length.



This feature is beneficial for low-porosity structures for which the pore throats require finer resolution or for modeling fast Navier-Stokes flows with strong vortices.

Enabling this feature may increase the number of iterations, runtime, and memory requirements.

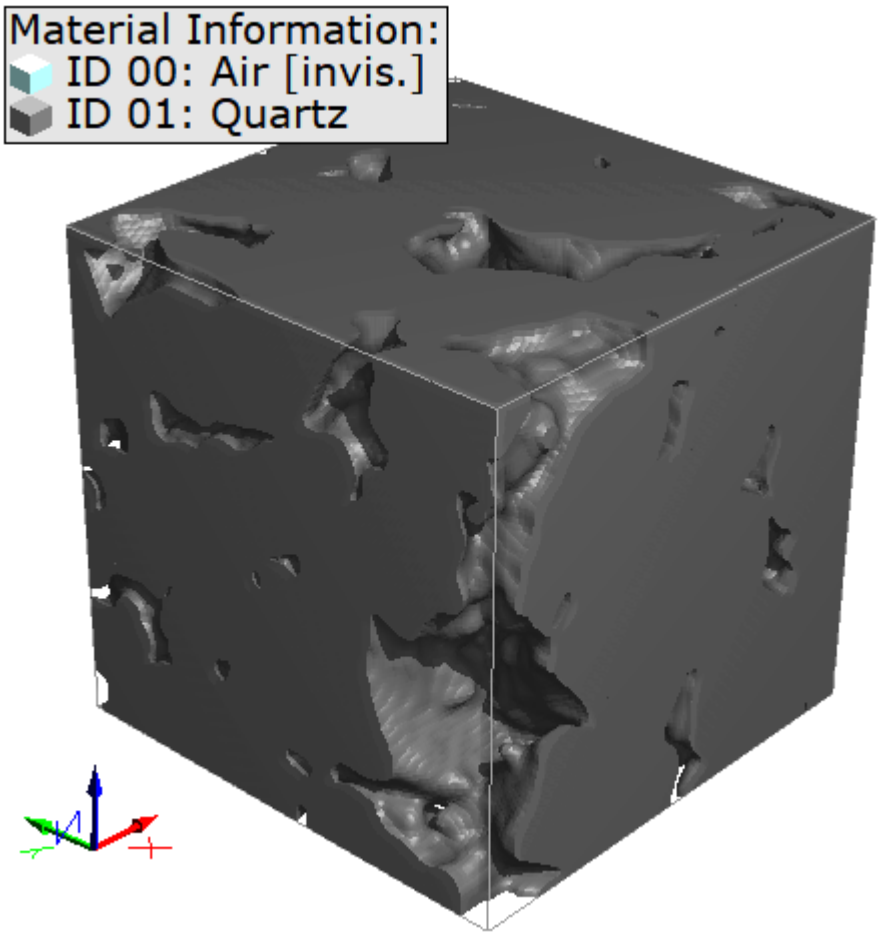
Allow Grid Re-Coarsening

Check **Allow Grid Re-Coarsening** to allow the solver to automatically revert the grid refinement and coarsen the computational cells.

This means, grid refinement is done temporarily. Afterwards, the cells are merged as soon as accuracy is not needed anymore. This reduces the memory and runtime requirements.

1.4.2 Results

The result file (*.gdr) is opened in the Result Viewer after the computation is finished. Only the tabs listed below are described in detail, for the other tabs look into the Result Viewer chapter.



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

Relative Permeability Results

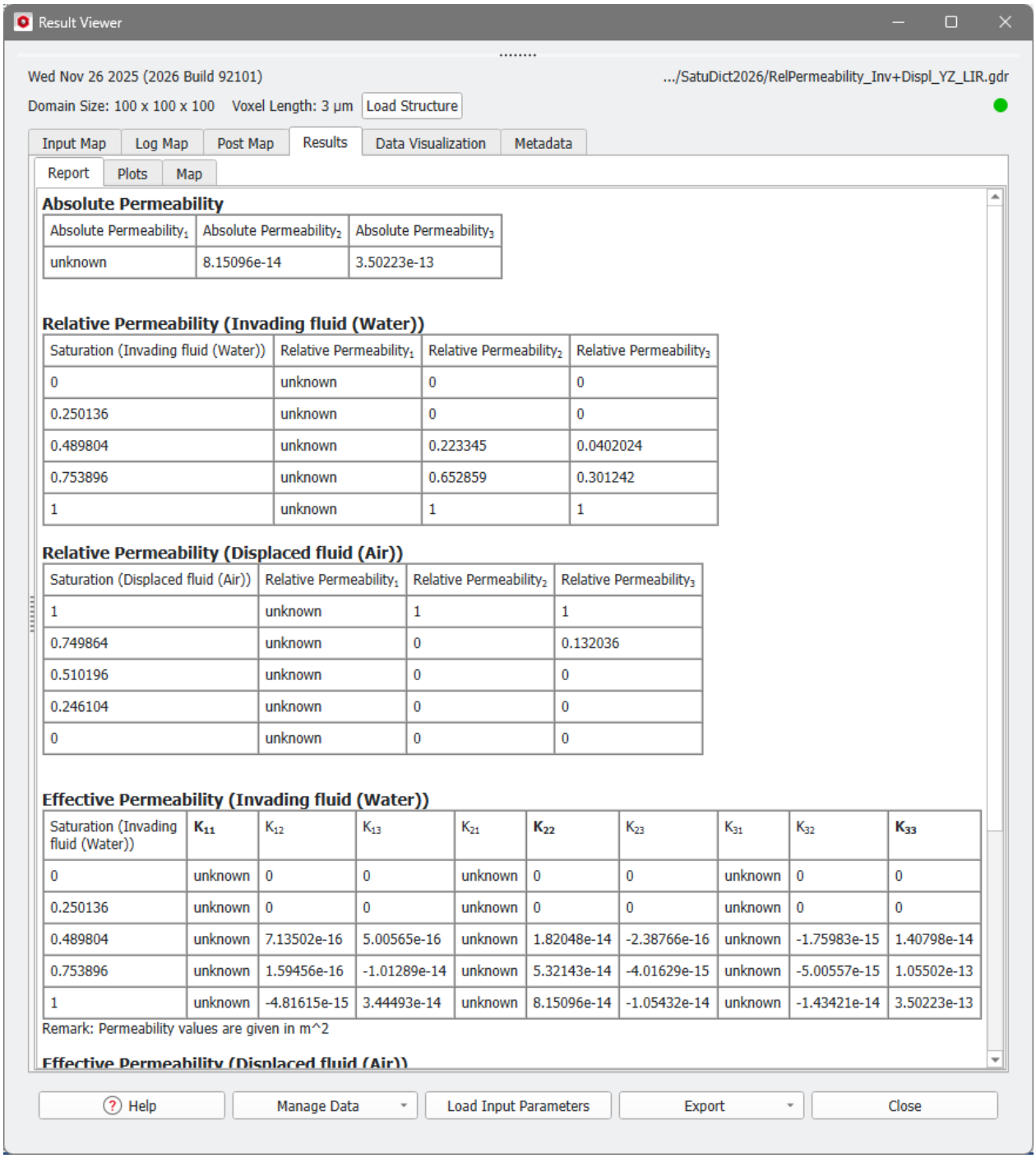
- Results Tab 91
  Learn about the resulting reports and plots.
- Data Visualization Tab 97
  Load results for a graphical visualization.

Results Tab

Report tab

Under the **Results-Report** sub-tab, the **Relative Permeability** (dimensionless relative permeability) and **Effective Permeability** (saturation-dependent permeability) tables are

shown for the chosen saturation rates[66] (here, 0, 0.25, 0.50, 0.75, and 1), which are approximated as best as possible (here, 0, 0.250136, 0.489804, 0.753896, and 1).



Absolute Permeability

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.

Relative Permeability

For each selected Flow Phase[67] the saturation-dependent relative permeability of the fluid is shown in the tables, where each row stands for one saturation level. The relative permeability values of each direction are given in the corresponding column (1 corresponds to the X-direction, 2 to Y-direction, and 3 to Z-direction). For directions which were not selected as Computational Direction[68] the permeability value is unknown.

Know how! In the example above, 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 flow path for the invading fluid.

Effective Permeability

For each selected Flow Phase[67] the saturation-dependent effective permeability of the fluid is shown in the tables, where each row stands for one saturation level. The values of the whole permeability tensor at each saturation step are given in the columns.

In the example above, the entries K_{13}, K_{23}, K_{33} for the computation in Z-direction and K_{12}, K_{22}, K_{32} for the computation in Y-direction are given, the other values are unknown as the computations were not carried out.

If **Show LET Model** or **Show Corey Model** was checked under Fit Options[95] in the Post-Processing Widget, the corresponding tables are shown in the Report tab. There are individual tables for invading and displaced fluid.

LET Model

For the **LET Model**, the parameters L, E, and T for each Computational Direction[68] are given.

LET Model (Invading fluid (Water))

L_1	L_2	L_3
unknown	4.409637451	5.077262878
E_1	E_2	E_3
unknown	0.152053833	0.7291030884
T_1	T_2	T_3
unknown	7.629394531e-06	0.197593689

$k(S) = k_{max} (S^L / (S^L - E (1 - S)^T))$ (LET model)
L: describes the lower part of the curve
E: describes the position of the slope
T: describes the upper part of the curve

Corey Model

For the **Corey Model** the Corey exponent for each Computational Direction[68] is shown.

Corey Model (Invading fluid (Water))

$Exponent_1$	$Exponent_2$	$Exponent_3$
unknown	2.100219727	4.502738953

$k(S) = k_{max} ((S - S_{min}) / (S_{max} - S_{max}))^n$ (Corey model)
S: Saturation
n: Corey exponent

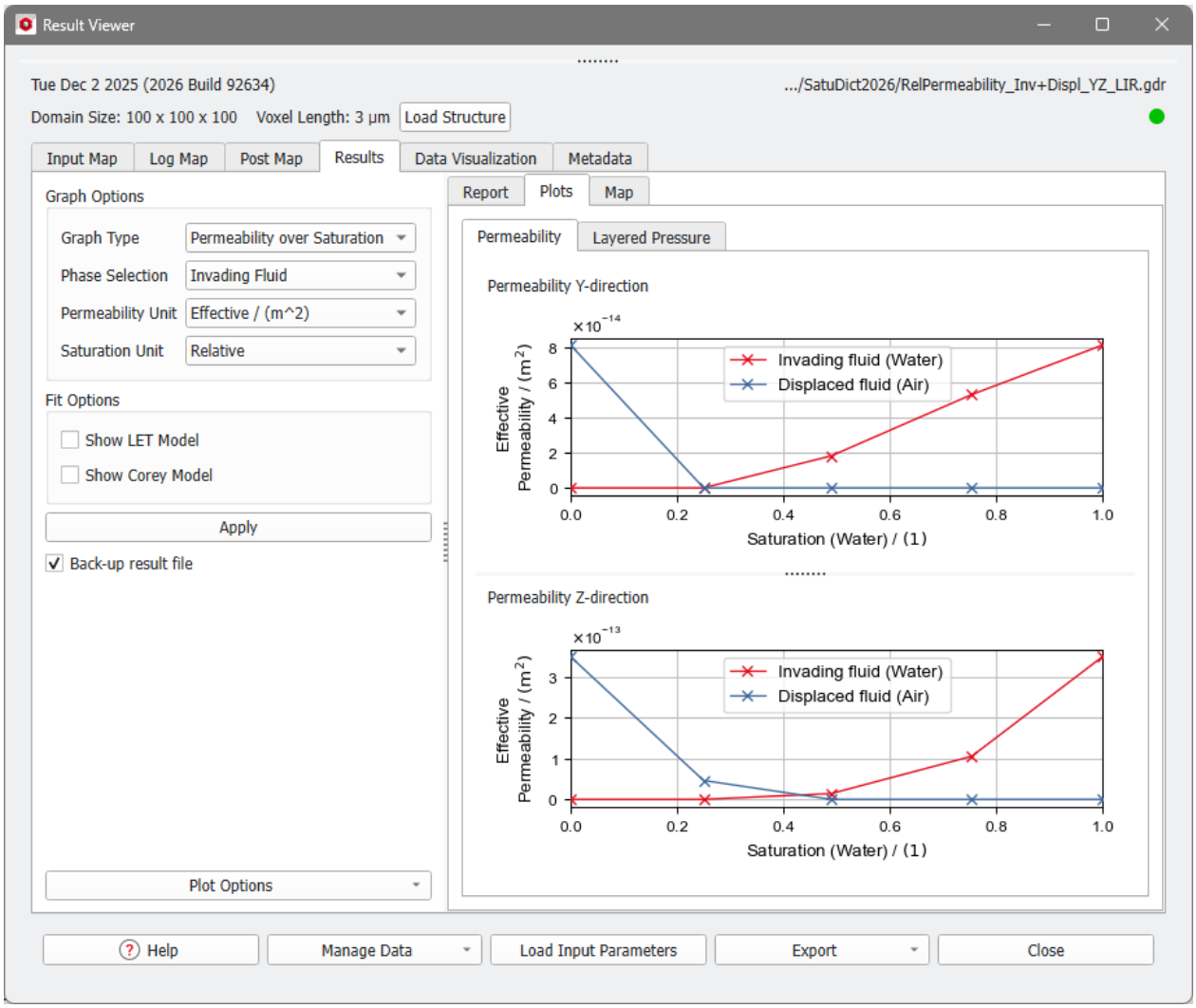
Plots tab

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.

Permeability Plot

The values of the permeability in all selected Computational Directions[68] and for the selected Flow Phases[67] at the different saturation levels are shown in a graph.

On the left, the **Post-Processing Widget** allows you to fine-tune the **Permeability** plot. Collapse the Post-Processing Widget by pulling it to the left.



Graph Options

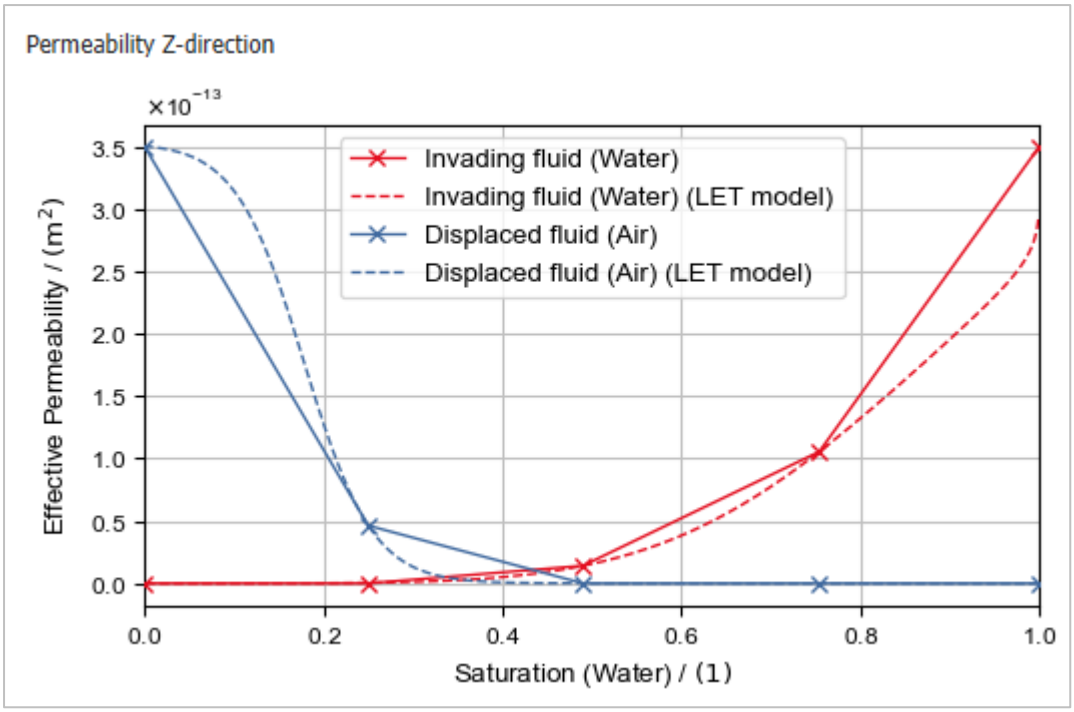
On the left side in the expandable **Graph Options**, you can modify the way the permeability graph is displayed by selecting

- 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^2 or Relative permeability between 0 and 1),
- and the **Saturation Unit** (Relative or Absolute).

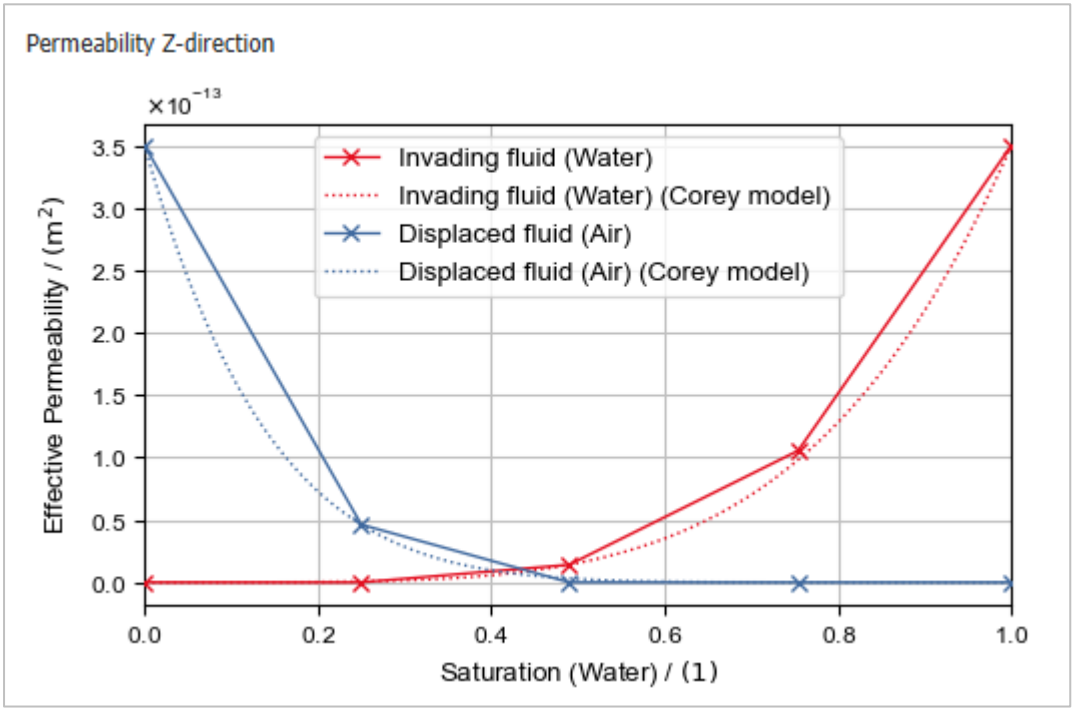
Click **Apply** to change the graph shown according to the options selected.

Fit Options

Check **Show LET Model** to additionally show an LET fit in the permeability plot. After clicking **Apply**, the parameters are computed and displayed in the Report tab.

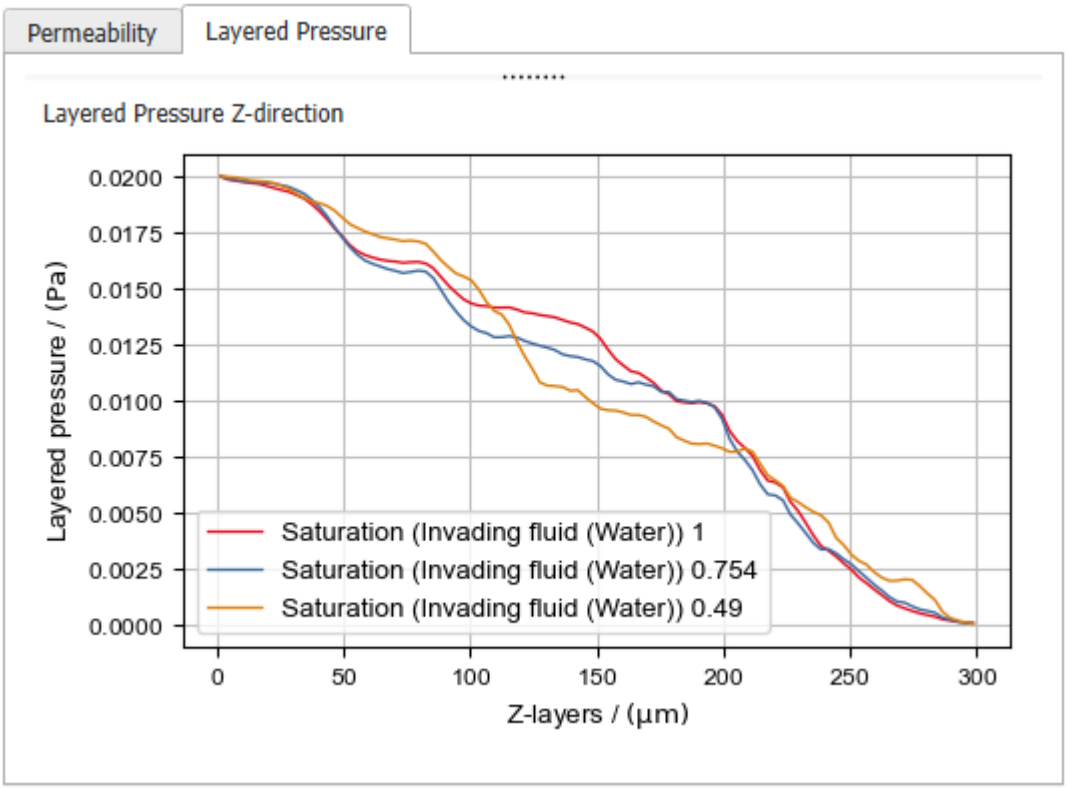


Check **Show Corey Model** to to additionally show a Corey fit[13] in the permeability plot. The Corey exponent is computed and can be found in the Report tab.



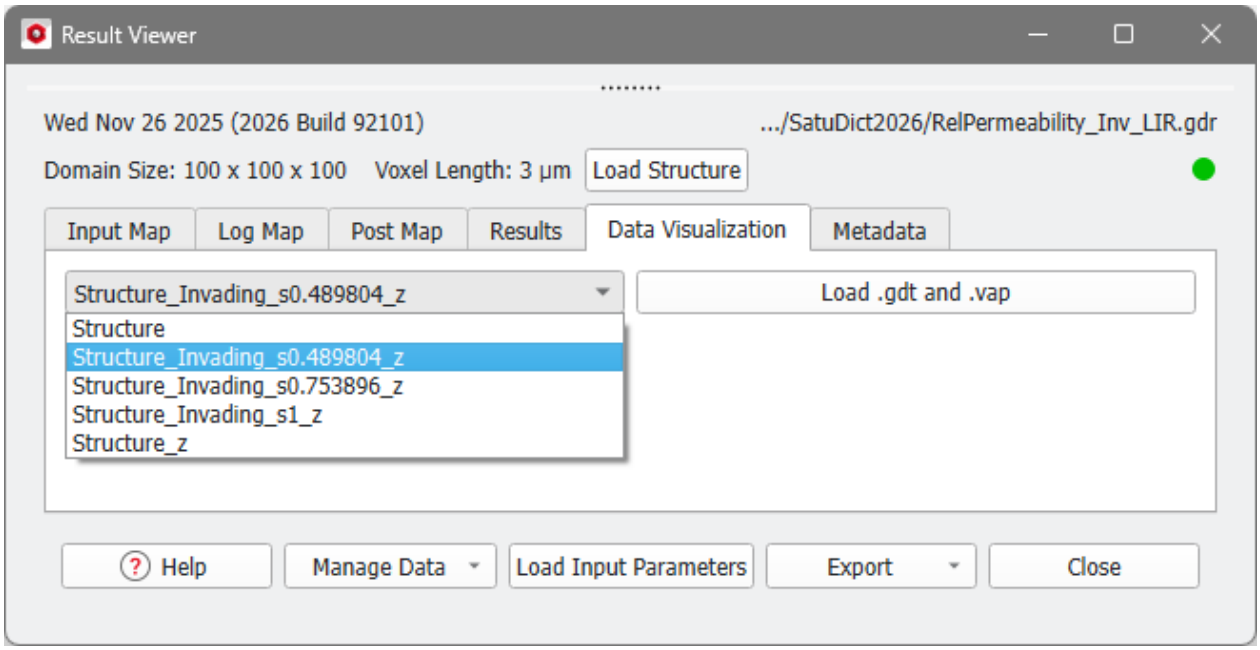
Layered Pressure

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



Data Visualization Tab

Under the **Data Visualization** tab, the .gdt and .vap files, corresponding to the saturation levels computed, can be opened, as explained in the FlowDict chapter. No files are available if **Discard PDE Solver Files** was checked in the **Solver** settings tab.



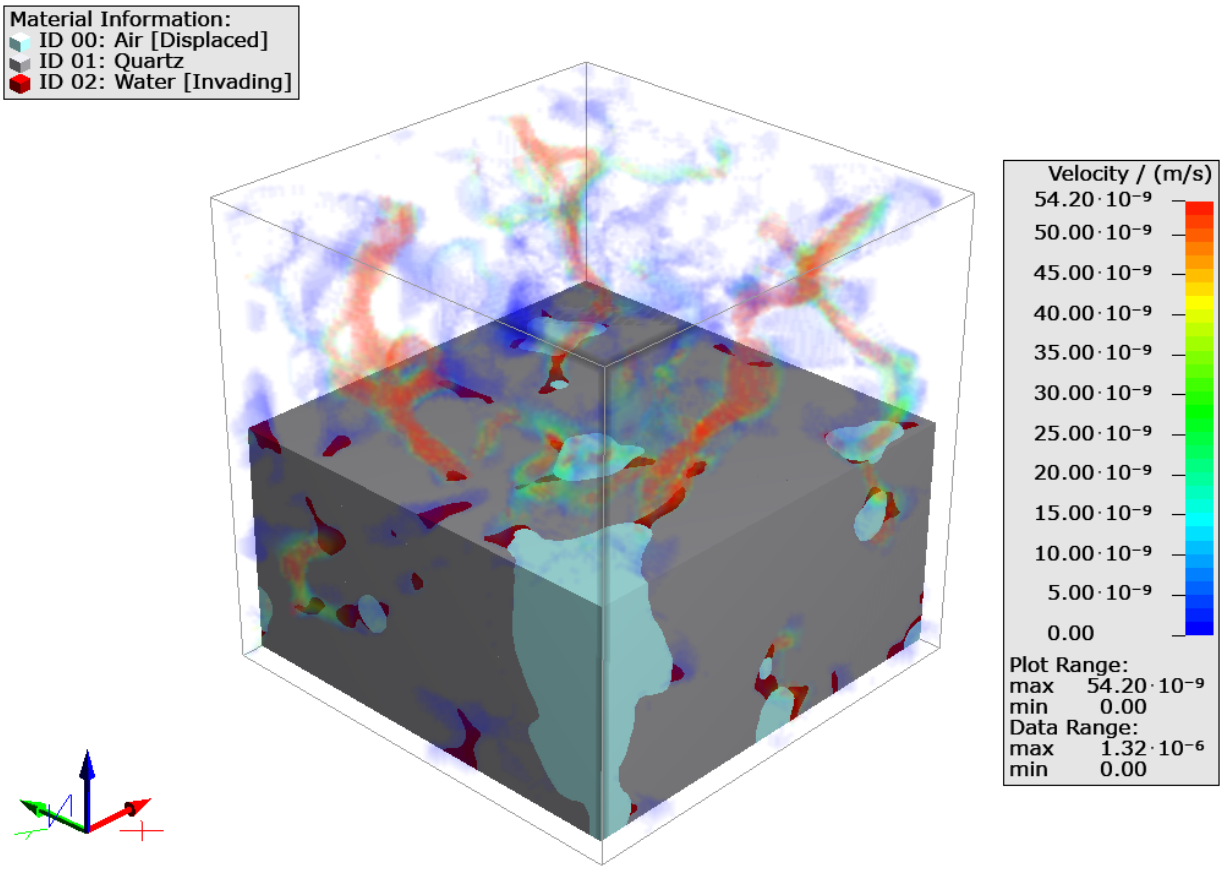
For each selected Flow Phase[67] and Computational Direction[69] the solution files for the saturation steps with non-zero permeability are saved and can be loaded by clicking on the **Load .gdt and .vap** button.

In the structure file (.gdt) you can observe the fluid distribution, while the .vap file contains the velocity and pressure values at each voxel.

Select **Structure** to load the original structure which is saturated with the displaced fluid. No additional .vap file will be loaded.

Select **Structure_z** (z can be replaced by x or y, depending on the chosen computational directions) to view the results of the absolute permeability computation.

Shown below 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.



More information about the visualization parameters is available in the Visualization chapter.

1.5 Relative Gas Diffusivity

Calculate **Saturation-dependent (Relative) Gas Diffusivity** for different fluid saturations. The pore morphology method 5 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.

SatuDict calculates the saturation-dependent diffusivity as in DiffuDict. 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.

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

The Relative Gas Diffusivity command

- Options 99
  Set the parameters for the calculation.
- Results 114
  View the computed results.

1.5.1 Options

The **Relative Gas Diffusivity** dialog opens when clicking the **Edit...** button and includes the **Wetting Parameters** tab, the **Constituent Materials** tab, the **Boundary Conditions** tab, the **Solver** tab, and the **Equations & References** tab, which cites several references 185.

At the top of the dialog, enter the **Result File Name**. The result file is saved in the chosen project folder (**File → Choose Project Folder** in the menu bar).

The **Equations & References** tab shows the formulas that are used for the solver which are described in the DiffuDict chapter:

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

No parameters can be edited on this tab.

Tabs of the Relative Gas Diffusivity dialog

- Wetting Parameters 100
  Select how the fluid distribution is determined and choose the saturation steps for the diffusivity calculations.
- Constituent Materials 101

Tabs of the Relative Gas Diffusivity dialog

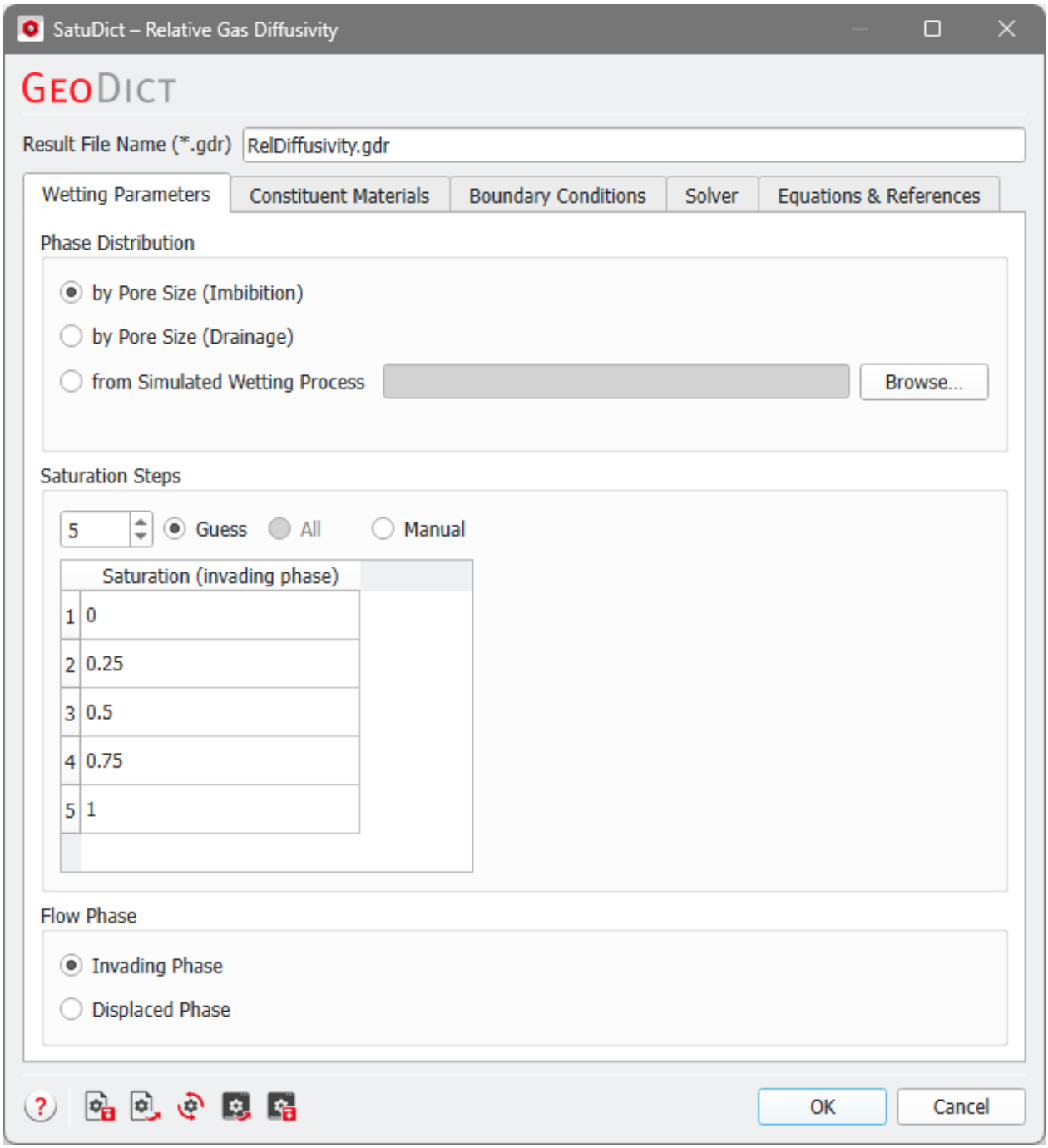
Select the materials in the structure and their properties, including the selection of invading and displaced fluid.

- Boundary Conditions 102
  Set the boundary conditions for the diffusivity calculations.
- Solver 103
  Select a diffusivity solver and its settings.

Wetting Parameters

The wetting parameters for the calculation of the **Relative Diffusivity** are the same as seen for the Relative Permeability 64.

The diffusivity can only be calculated for one of the phases (set under **Flow Phase**).

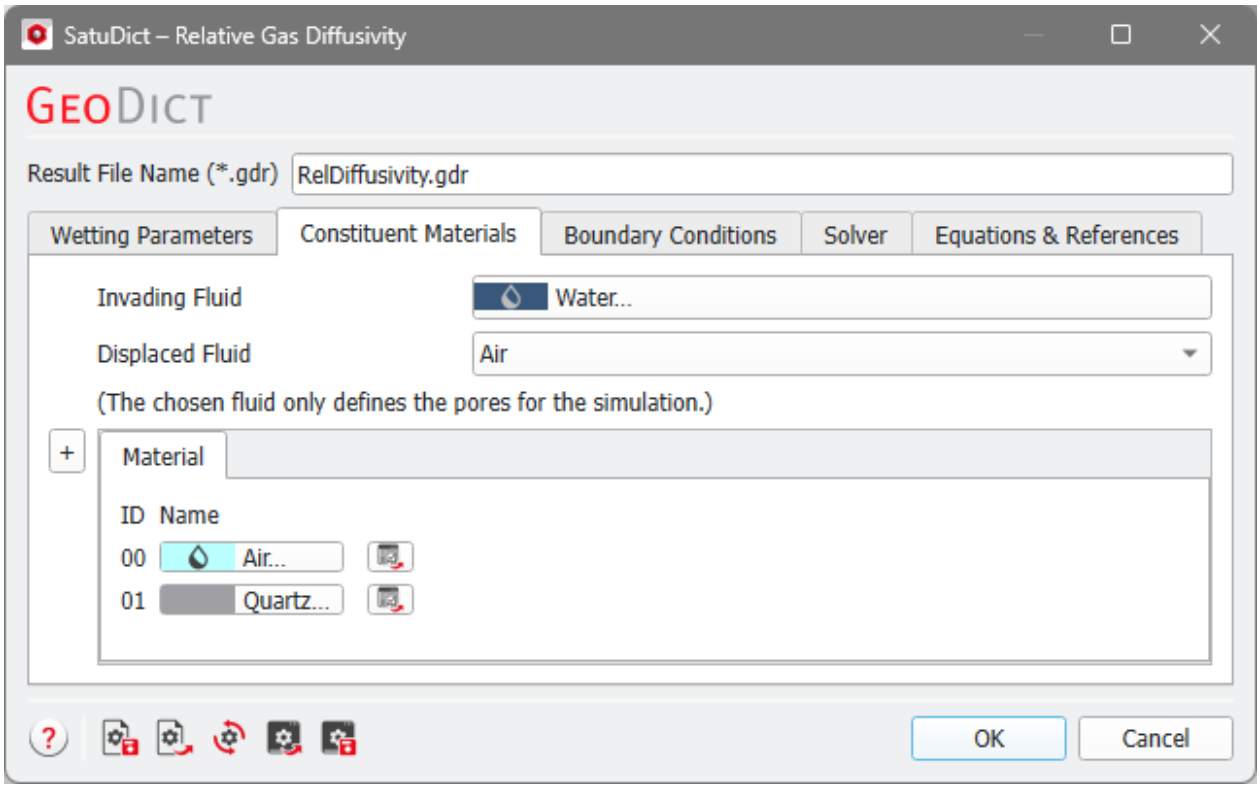


Constituent Materials

In the **Constituent Materials** tab, the **Invading Fluid** and the **Displaced Fluid** can be entered.

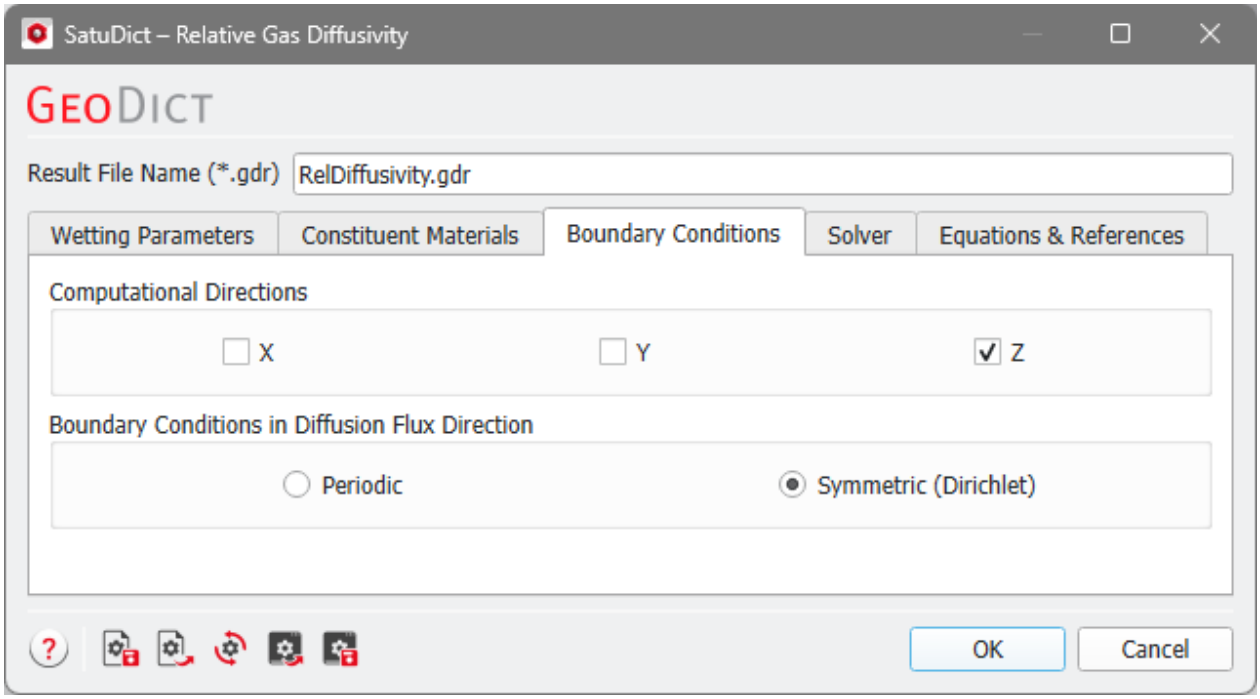
If the phase distribution under the Wetting Parameters tab is chosen **by Pore Size**, the displaced fluid must be present in the structure and can be chosen from the drop-down menu. If the phase distribution is taken **from Simulated Wetting Process**, then both fluids are defined by the capillary pressure curve result file.

No more settings need to be done as the diffusivity is always set to 1.



Boundary Conditions

The **Boundary Conditions** tab has two panels, **Computational Directions** and **Boundary Conditions in Diffusion Flux Direction**. They are the same as in Simulate Diffusion in DiffuDict.



For the **Computation Directions**, choose the directions for which the diffusivity should be calculated. To obtain the whole 3x3 diffusivity matrix in the result file, it is necessary to choose

all three directions. The directions that are not checked will not be calculated and will appear as unknown in the diffusivity matrix in the result file.

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

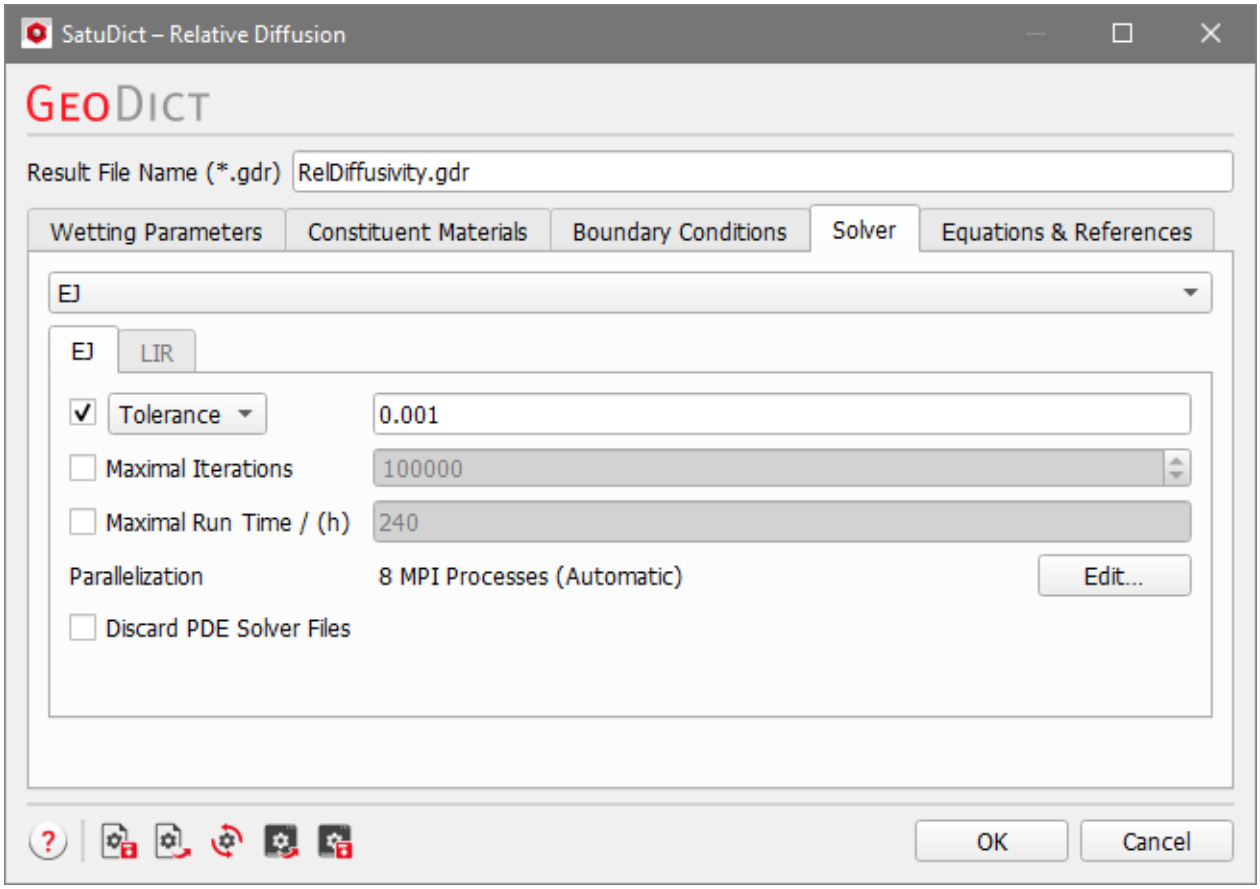
If **Periodic** is selected, the solution is computed assuming that the structure is periodically repeated in the diffusion direction(s).

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 solvers **EJ** and **LIR** are available and can be chosen from the pull-down menu. The solver settings are similar to those available in the DiffuDict module.



Parameters for all solvers

Stopping Criteria

The equations are solved by an iterative approach.

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
3. Repeat the iterative process until one of the stopping criteria is reached.

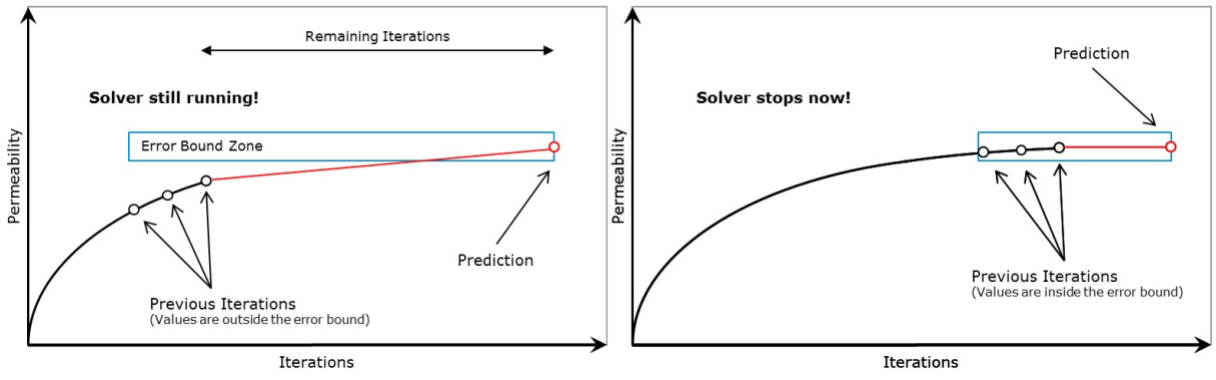
The iterative process is controlled by setting the values and activation for **Error Bound, Tolerance, Residual**, **Maximal Iterations**, and **Maximal Run Time (h**). The stopping criteria apply for each computational direction individually.

If multiple stopping criteria are selected, the first criterion that is reached causes the solver to stop.

The stopping criterion that has been reached can be viewed in the Result Viewer of the GeoDict result file (*.gdr) under the **Results Report** tab.

Error Bound (LIR)

The stopping criterion **Error Bound** uses the result of previous iterations, and predicts the final solution based on linear and quadratic extrapolation. The solver stops if the relative difference between computed and predicted solution is smaller than the specified error bound. The stopping criterion recognizes oscillations in the convergence behavior and prevents premature stopping at local minima or maxima. A damped convergence curve is fit through the oscillating curve and the solver stops then regarding the damped convergence curve.



If the Krylov method (under LIR - Advanced Options) is activated, the definition of **Error Bound** is somewhat different. Here, no prediction is made, instead the continuity between neighboring cells and the conservation of mass is checked. The maximal value is normalized by the mean flow and if this value is smaller than the **Error Bound** the simulation stops.

Tolerance

The **Tolerance** stopping criterion looks for stagnation of the method when the process becomes stationary, i.e., the improvement in the diffusivity value becomes extremely small from iteration to iteration.

In each iteration, the solver checks for the current computed value x_c against the values x_{c-i} of the last 100 iterations if there are any changes.

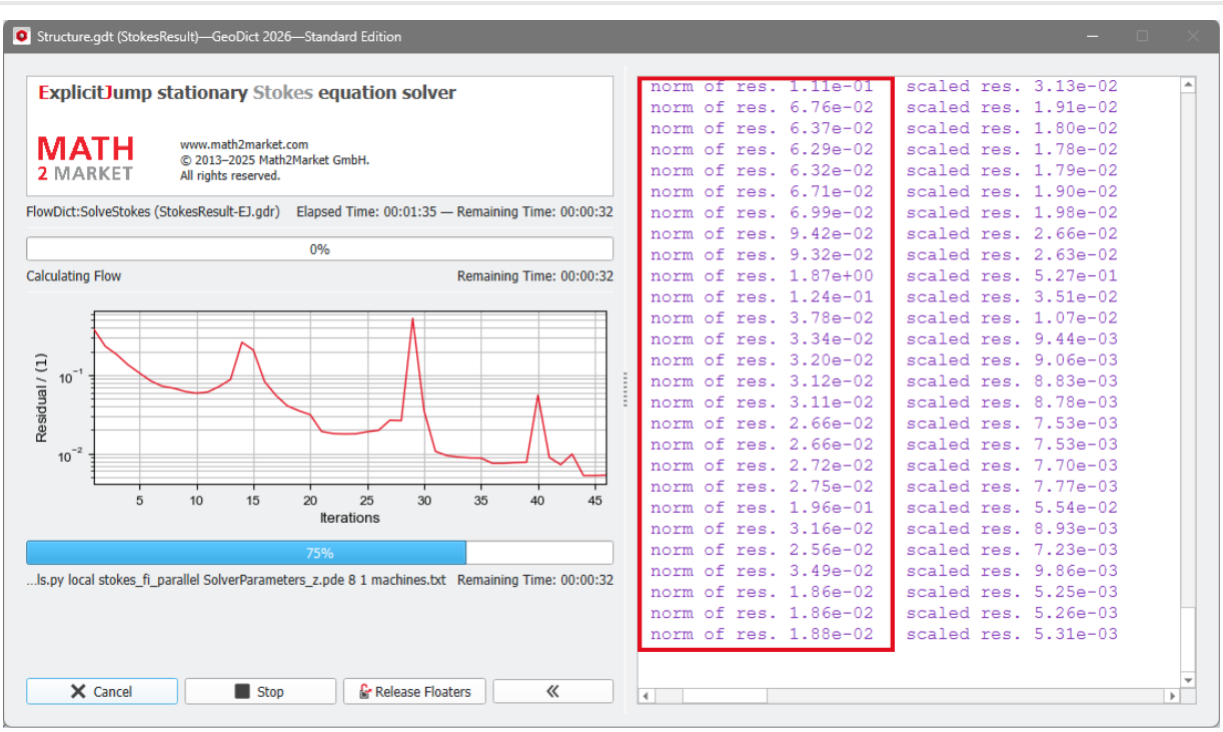
$$\max_{i\in[1,100]} \frac{x_c - x_{c-i}}{x_{c-i}} < \text{tolerance} \tag{31}$$

The computation is stopped if the maximal relative change is smaller than the value entered for **Tolerance**. When there is doubt about the quality of the solution, decrease the **Tolerance** value by a factor of ten. The drawback of this criterion is that the solver sometimes might stop too early in case of slow convergence rate or at local extrema of oscillatory convergence curves.

Residual (EJ)

When the **Residual** stopping criterion is used, the iteration is stopped if the solution satisfies the equation up to the required accuracy.

By setting the stopping criterion to **Residual**, the computations terminate as soon as the relative norm drops below the selected residual threshold. The relative norm of the Schur Complement residual is computed and displayed in the console window during the calculations. The console is visible by clicking the double arrow button on the lower right corner in the progress dialog.



The recommendation to choose **Tolerance** or **Residual** for the **EJ** solver is based on the structure's porosity. Both give similar results for highly porous structures. For dense structures, if using the Schur Complement **Residual**, the relative norm of the residual may be small even though the correct diffusivity has not been reached. So, when in doubt, use the **Tolerance** criteria – the default option.

Maximal Iterations & Maximal Run Time

Use the **Maximum Iterations** value or the **Maximum Run Time (h)** stopping criteria causes the solver to stop if the maximal number of iterations and/or the maximal runtime (in hours) is exceeded.

When the solver stops because one of these criteria has been reached, no guarantee on the quality of solution can be given. In this case, a warning is printed into the report. The following possibilities might help:

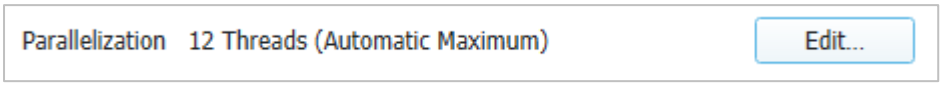
- Check the corresponding .log file to see how large the residual values and the diffusivity values are. If the diffusivity values are in reasonable range and they do not have changed during the last iterations, you may decide to use the current result.
- Double-check the structure and parameter values. Unphysical parameters or too rough resolution of the structure (leading, e.g., to artificial unconnected components) can cause an iterative solver to fail.

Parallelization

Control how many threads are used for the computation. Parallelization is possible if your

license and hardware allow it.

The **Parallelization Options** dialog opens when clicking the **Edit** button and you can choose between **Sequential**, **Parallel (Shared Memory)**, **Automatic Maximum of Threads**, or **Cluster** (only available if EJ, SimpleFFT, or FeelMath were selected as solver).



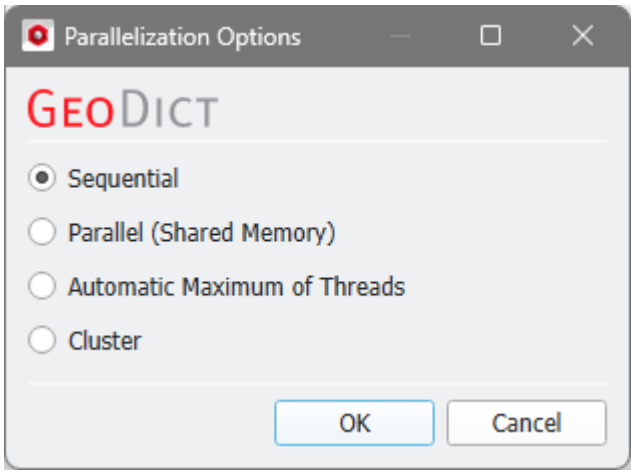
The parallelization of the solvers is done with two technical methods: **MPI Parallelization** or **Thread parallelization**. The following table shows the support of both parallelization methods:

Solver	Parallelization method	
	MPI Parallel	Thread Parallel
EJ	✔	✘
SimpleFFT	✔	✘
LIR	✘	✔
FeelMath	✔	✔
BEST	✘	✔

Depending on the used parallelization method, the **Number of Processes** (MPI parallel) or the **Number of Threads** (thread parallel) can be entered.

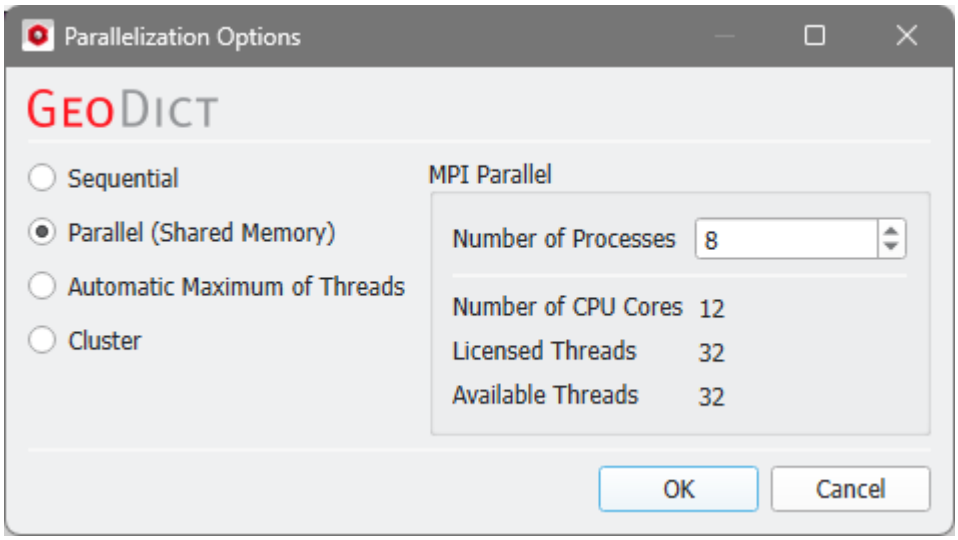
Sequential

Selecting **Sequential** will not apply parallelization and only one thread is used for the computation.



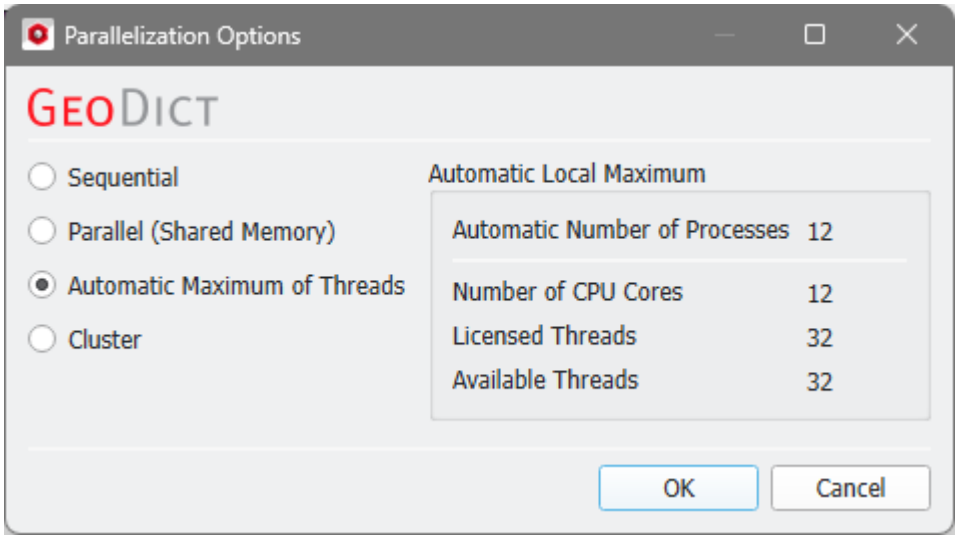
Parallel (Shared Memory)

When **Parallel (Shared Memory)** is selected, the **Number of Processes** or **Number of Threads** can be entered. Below, the **Number of CPU Cores** that the current machine has, the maximum number of **Licensed Threads** and the number of those licensed threads that are available (**Available Threads**) are shown in the dialog. Of course, the maximal number of parallel processes you can use, is the smallest of those three numbers.



Automatic Maximum of Threads

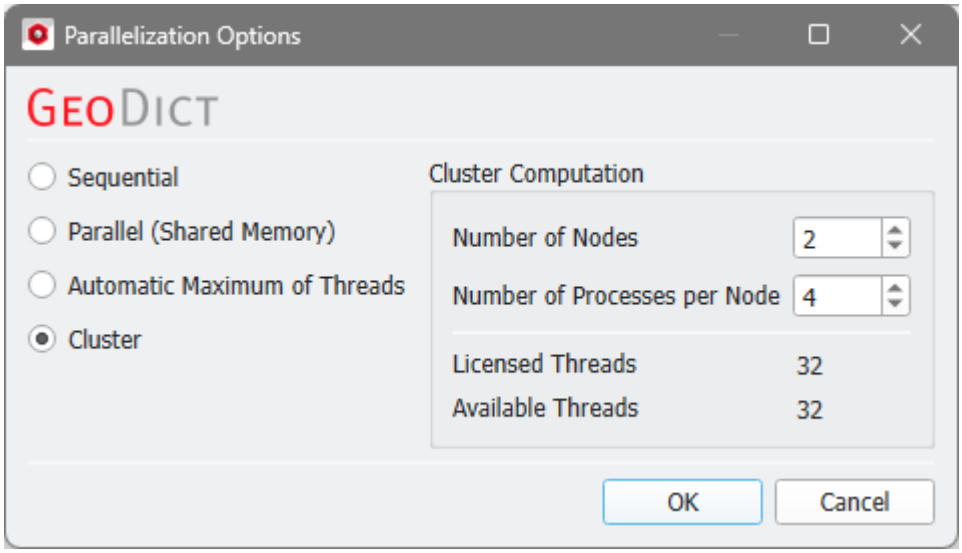
If **Automatic Maximum of Threads** is selected, the number of parallel processes is automatically selected for optimal speed, based on the CPU cores and licensed parallel processes.



The **Automatic Local Maximum** of processes is automatically selected, which is the minimum of **Number of CPU Cores**, **Licensed Threads**, and **Available Threads**.

Cluster

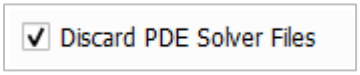
The **Cluster** parallelization requires that the solver supports the **MPI Parallelization** method. Moreover, the choice of **Cluster** is for users of Linux systems only.



For details on how to set up and run parallel computations, consult the High Performance Computing chapter.

Discard PDE Solver Files

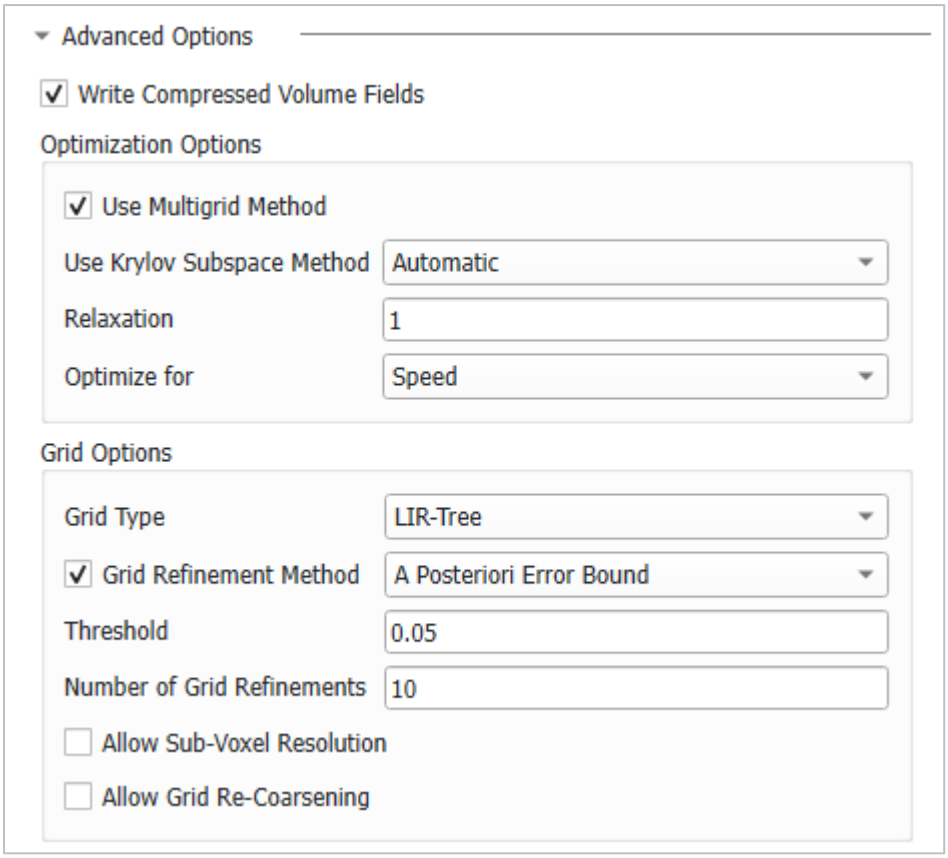
Checking **Discard PDE Solver Files** causes the deletion of all intermediate computation files, such as log files and flow field files.



Only the content of the final GeoDict result file (*.gdr) is stored.

While having the benefit of saving hard disk storage place, discarding intermediate solver files has also the effect of disabling the 3D visualization of the results.

LIR specific parameters (Advanced Options)



Write Compressed Volume Fields

The LIR solver uses a very memory efficient adaptive grid structure for the simulations.

If the option **Write Compressed Volume Fields** is checked, then the adaptive grid is used as compression method for writing out *.hht files. This option allows to save 80-90% space on hard drive. The runtime for writing *.hht files is also reduced significantly. But the runtime for loading and uncompressing of compressed *.hht is increased by the amount of runtime that was saved for writing out compressed *.hht files.

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

Use Multigrid Method

The **Multigrid Method** (see, e.g., Wesseling, 2004) was introduced to speed-up the computation and reduce the runtime significantly. The main idea of **Multigrid** is the usage of multiple coarser adaptive grids to speed up convergence behavior but requires only little more memory.

The method is available to solve the Stokes and Stokes–Brinkman equations as well as

for solving mechanics, diffusion, thermal, and electrical conduction and is enabled by default.

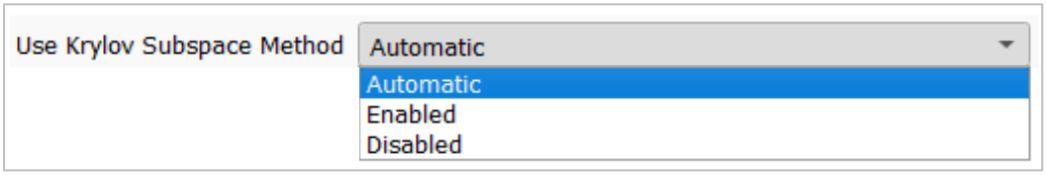
Use Krylov Subspace Method

Another speed-up option to accelerate the convergence behavior of the LIR solver is called **Krylov Subspace Method**.

The runtime of the LIR solver depends on many different properties of the structure and the simulation parameters. The BiCGStab algorithm is used, which can reduce the runtime for challenging simulation very drastically.

Note! Using the BiCGStab method approximately doubles the amount of RAM needed for the computation.

Unfortunately, the Krylov method is not always faster than a simulation without the Krylov method and therefore we introduced an **Automatic** mode which uses some heuristics to choose the most efficient method based on structure, material parameters, and boundary conditions automatically. Of course, it is possible to explicitly enable (**Enabled**) or disable (**Disabled**) the method.



Note! In case that the Krylov subspace method (BICGStab) is used, the **Relaxation** may also be adapted automatically.

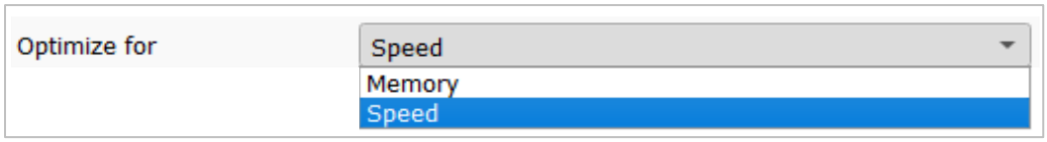
Relaxation

Depending on the material parameters and geometry of the structure, the underlying mathematical problem can vary in complexity, thus influencing the behavior of the solver. The more complex the problem is, the more stable the solver settings should be.

With the **Relaxation** number, the solver is adjusted from **Stable** (which results in higher number of iterations, slower time stepping, and longer solver run times), to **Fast**, which makes the solver run less iterations but implies the risk that the solver does not converge. The **Relaxation** is a parameter of the SOR method and must be between 0 and 2 to ensure convergence. For relaxation values smaller than one (<1.0), the simulation is more stable. For relaxation values larger than one (>1.0), the simulation converges faster.

Optimize For

The **LIR** solver can **Optimize for Speed** or **Memory**.



- If **Speed** is chosen, the solver constructs additional optimization structures. The runtime is decreased by up to 30% but requires up to 50% more memory compared to the other option.
- If **Memory** is chosen, the runtime is increased by up to 40% but the solver requires up to 50% less memory.

Grid Type

The **Grid Type** decides what kind of tree structure is used for the simulation.

The default option is **LIR-Tree** and should always be used. The solver uses an adaptive grid structure called LIR-tree and needs up to 10 times less runtime and memory compared to the **Regular Grid** option.

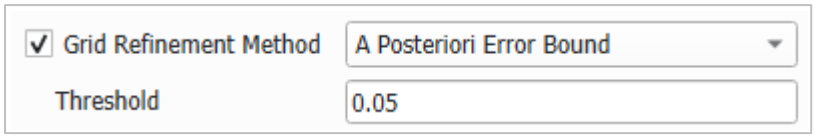
The solver can analyze the result field during the computation and improves the adaptive grid in places where more accuracy is needed. The LIR solver splits cells where a high gradient occurs.

Grid Refinement Method

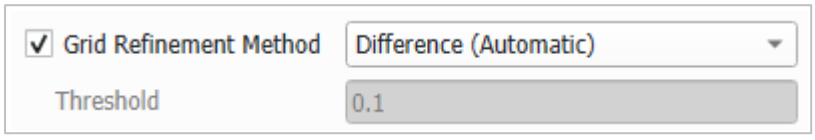
The solver can analyze the computed field and refines the adaptive grid during the computation at locations where more accuracy is needed. The LIR solver splits cells where a high gradients occur when the **Grid Refinement Method** is enabled. In this case, the additional parameters **Number of Grid Refinements**, **Allow Sub-Voxel Resolution**, and **Allow Grid Re-Coarsening** become available.

Select one of the three available refinement methods from the drop-down menu.

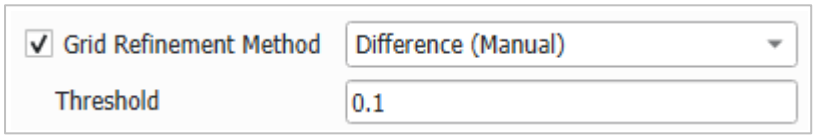
When **A Posteriori Error Bound** is selected, the solver targets the specified accuracy **Threshold**. While the **Error Bound** (set as Simulation Stopping Criterion) determines the relative error in the solution of the linear system, **A Posteriori Error Bound** refers to the relative error estimated by comparing high-order and low-order discrete solutions. The accuracy **Threshold** refers to the relative error to the analytical solution and the value must be between 0.0 and 1.0.



Choosing **Difference (Automatic)** leads to computational cells being split when the difference in values between neighboring cells exceeds a certain **Threshold**. The solver automatically chooses all internal parameters based on the structure and simulation settings. For this option, cells are split where the current gradient is greater than the **Threshold** multiplied by the maximum gradient, where the threshold is determined automatically.

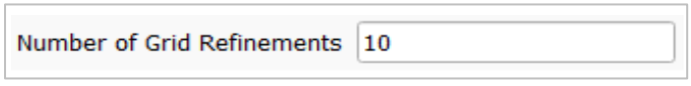


Selecting **Difference (Manual)** also causes the computational cells to be split when the difference in values between neighboring cells exceeds the specified **Threshold**. You can specify all parameters (Threshold and Number of Grid Refinements) for the grid refinement manually. For this option, cells are split where the current gradient is greater than the **Threshold** multiplied by the maximum gradient. The **Threshold** value must be between 0.0 and 1.0. The recommended value range is between 0.05 and 0.1.



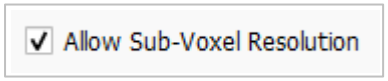
Number Of Grid Refinements

The **Number of Grid Refinements** controls the maximum number of grid refinements that the solver can perform during the simulation. The value should be set between 0 and 10, where a value of 0 means that no grid refinements will be made. Grid refinements may increase the number of iterations, runtime, and memory requirements.



Allow Sub-Voxel Resolution

When **Allow Sub-Voxel Resolution** is enabled, the solver is allowed to split computational cells to sizes smaller than the voxel length.



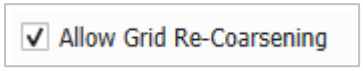
This feature is beneficial for low-porosity structures for which the pore throats require finer resolution or for modeling fast Navier-Stokes flows with strong vortices.

Enabling this feature may increase the number of iterations, runtime, and memory

requirements.

Allow Grid Re-Coarsening

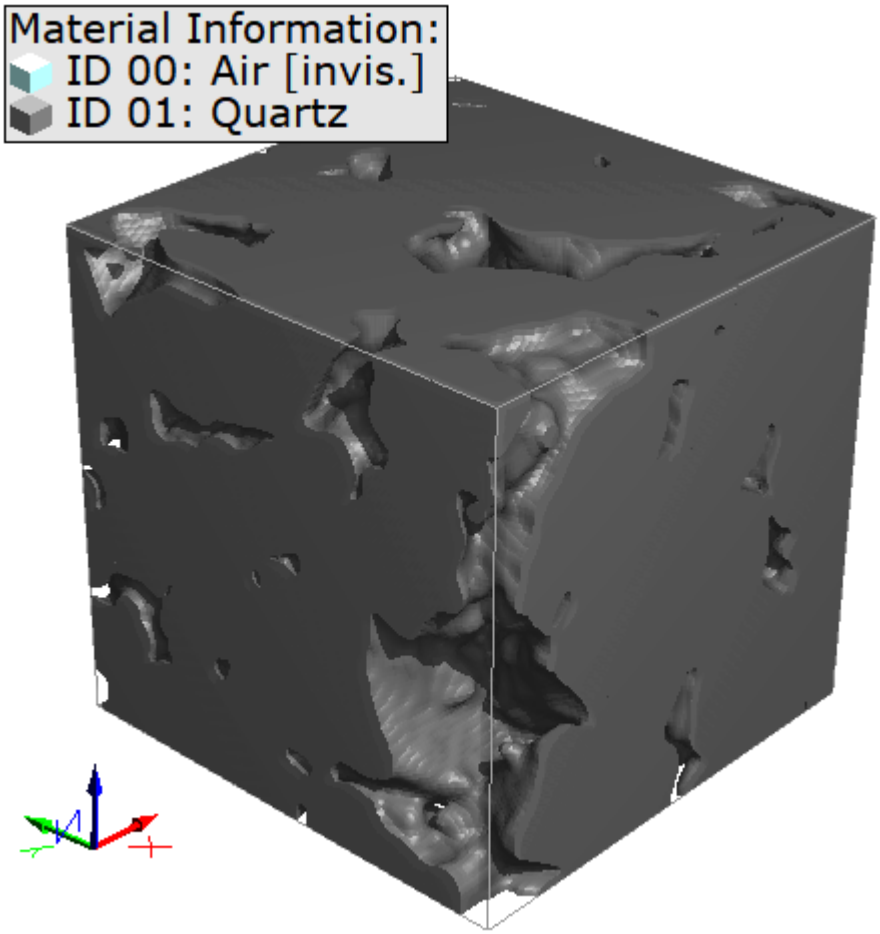
Check **Allow Grid Re-Coarsening** to allow the solver to automatically revert the grid refinement and coarsen the computational cells.



This means, grid refinement is done temporarily. Afterwards, the cells are merged as soon as accuracy is not needed anymore. This reduces the memory and runtime requirements.

1.5.2 Results

The result file (*.gdr) is opened in the Result Viewer after the computation is finished. Only the tabs listed below are described in detail, for the other tabs look into the Result Viewer chapter.



The results of the relative diffusivity 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 diffusivity was calculated in Z-direction with Dirichlet boundary conditions (Boundary Conditions tab). Computations were run using the LIR solver.

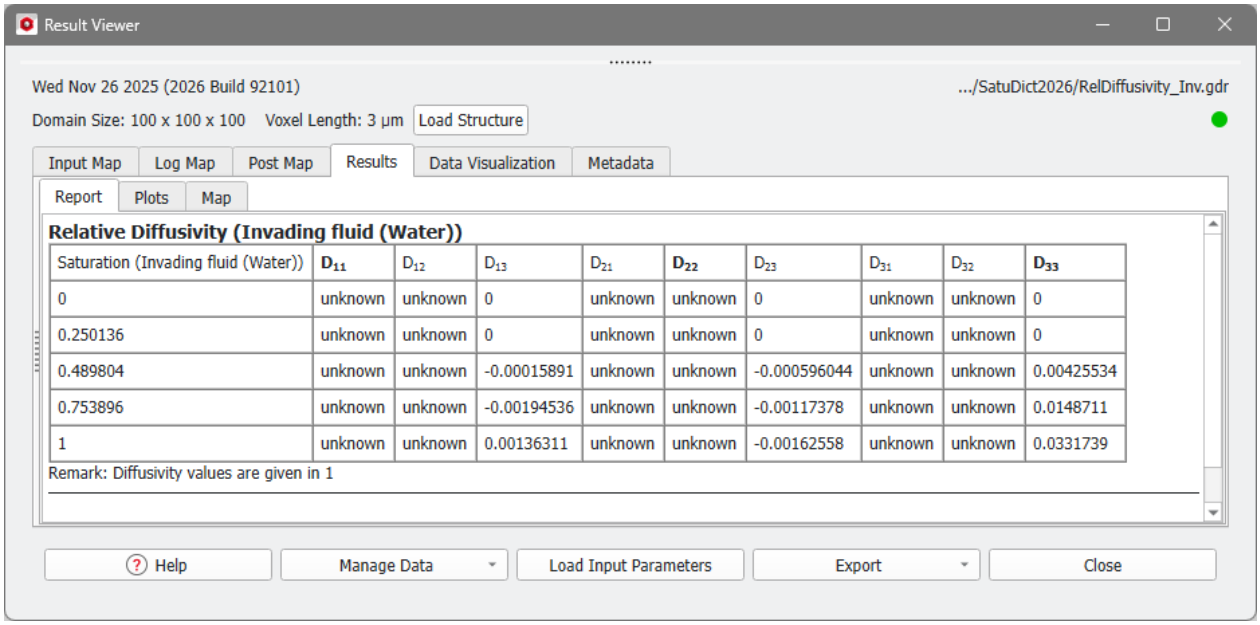
Relative Gas Diffusivity Results

- Results Tab 115
  Learn about the resulting reports and plots.
- Data Visualization 117
  Load results for a graphical visualization.

Results Tab

Report tab

Under the **Results-Report** sub-tab, the **Relative Diffusivity** (dimensionless saturation-dependent diffusivity) table is shown for the chosen saturation rates 100 (here, 0, 0.25, 0.50, 0.75, and 1), which are approximated as best as possible (here, 0, 0.250136, 0.489804, 0.753896, and 1).



For the selected Flow Phase 100 the saturation-dependent relative diffusivity of the fluid is shown in the table, where each row stands for one saturation level. The values of the whole diffusivity tensor at each saturation step are given in the columns. For directions which were not selected as Computational Direction 102 the diffusivity value is unknown.

In the example above, the entries D_{13}, D_{23}, D_{33} for the computation in Z-direction are given, the other values are unknown as the computations were not carried out.

Know how! In the example above, the relative diffusivity 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 invading fluid.

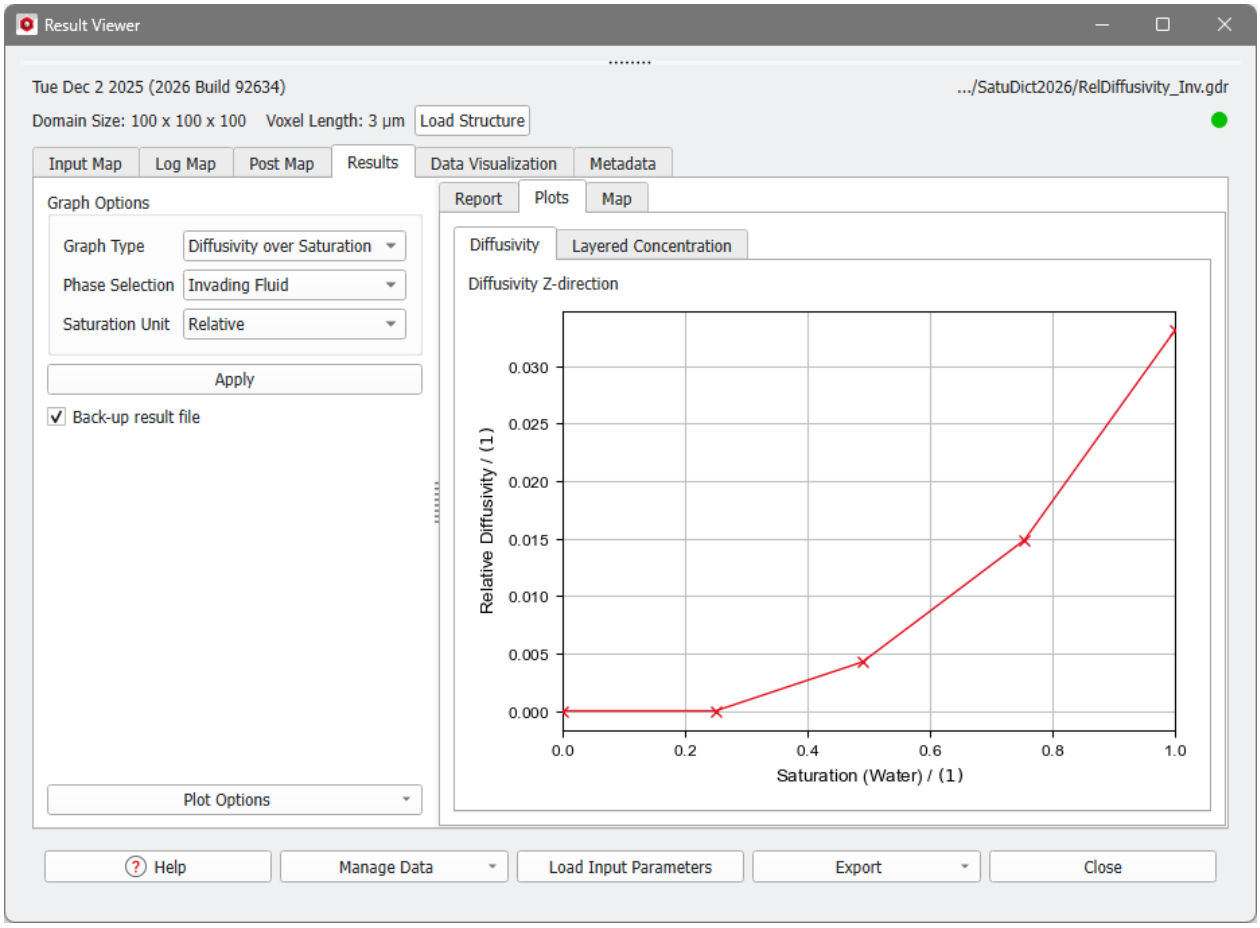
Plots tab

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

Diffusivity Plot

The values of the diffusivity in all selected Computational Directions and for the selected Flow Phase at the different saturation levels are shown in a graph.

On the left, the **Post-Processing Widget** allows you to fine-tune the **Diffusivity** plot. Collapse the Post-Processing Widget by pulling it to the left.



Graph Options

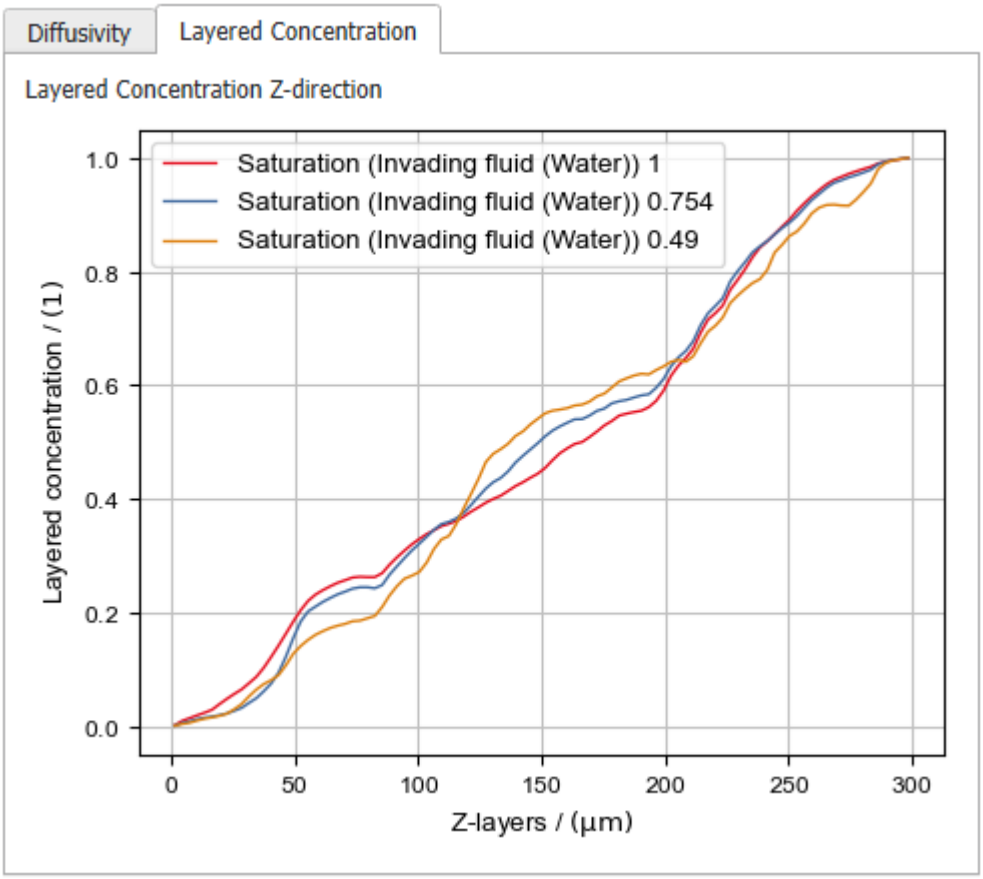
On the left side in the expandable **Graph Options**, you can modify the way the diffusivity graph is displayed by selecting

- the **Graph Type** (Diffusivity over Saturation or Saturation over Diffusivity),
- the **Phase Selection** (Invading Fluid or Displaced Fluid),
- and the **Saturation Unit** (Relative or Absolute).

Click **Apply** to change the graph shown according to the options selected.

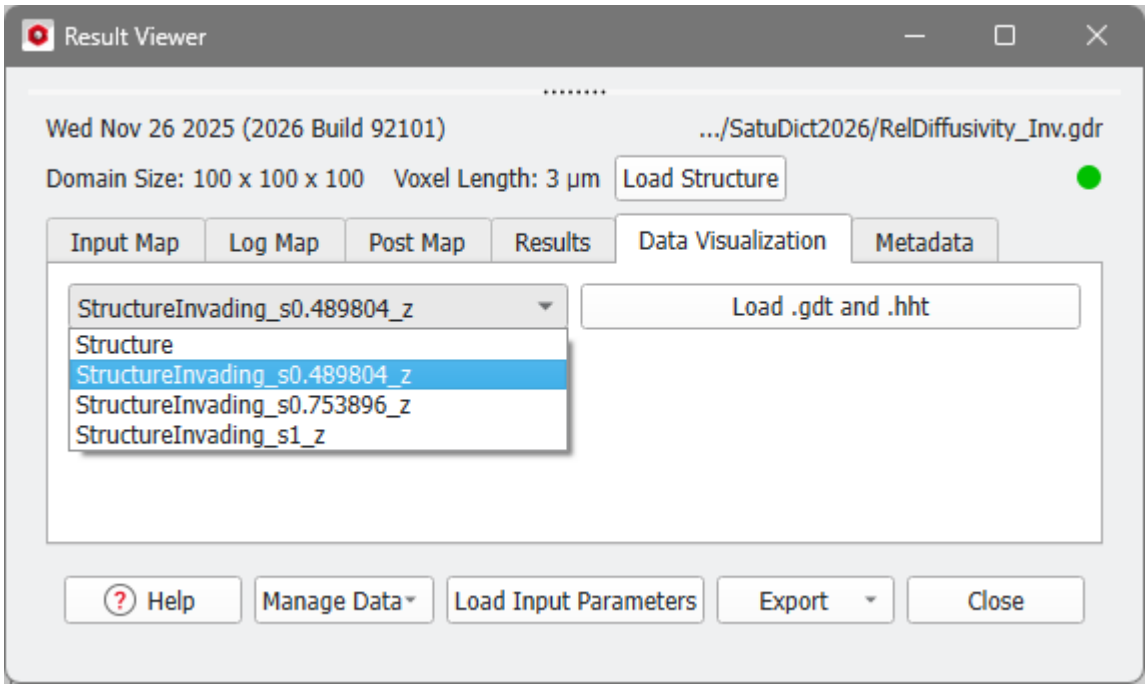
Layered Concentration

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



Data Visualization

Under the **Data Visualization** tab, the .gdt and .hht files, corresponding to the saturation levels computed, can be opened, as explained in the DiffuDict chapter. No files are available if **Discard PDE Solver Files** [109] was checked in the **Solver** settings tab.

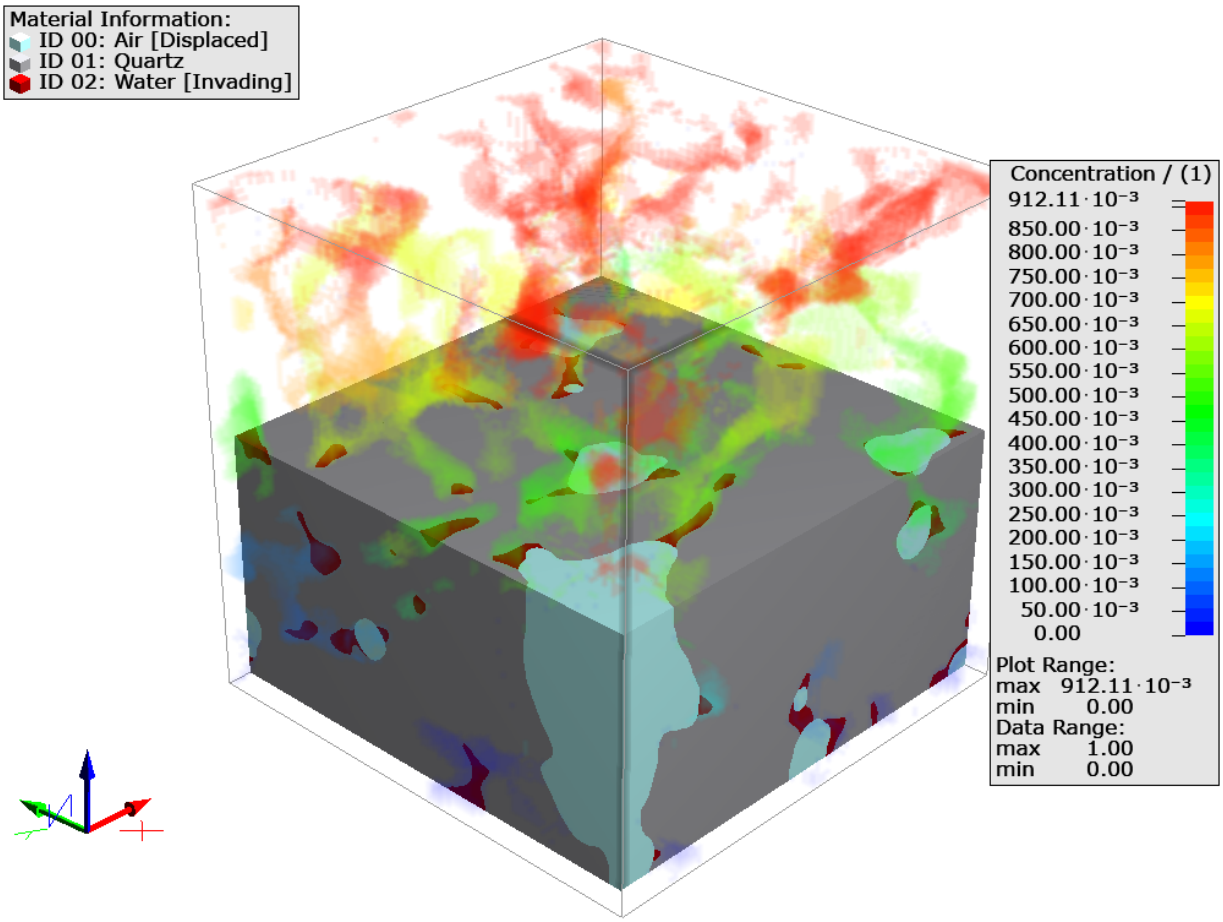


For the selected Flow Phase and Computational Directions the solution files for the saturation steps with non-zero diffusivity are saved and can be loaded by clicking on the **Load .gdt and .hht** button.

In the structure file (.gdt) you can observe the fluid distribution, while the .hht (homogenized heat) file contains the concentration values at each voxel.

Select **Structure** to load the original structure which is saturated with the displaced fluid. No additional .hht file will be loaded.

Shown below 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 concentration field of the Water with transparent effect on the clipped structure model.



More information about the visualization parameters is available in the Visualization chapter.

1.6 Relative Thermal Conductivity

Determine **Saturation-dependent (Relative) Thermal Conductivity** as in ConductoDict (see also Pfrang et. al.[186]). The pore morphology method[5] 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.

The thermal 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.

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

The Relative Thermal Conductivity command

- Options[120]
  Set the parameters for the calculation.
- Results[134]
  View the computed results.

1.6.1 Options

The **Relative Thermal Conductivity** dialog opens when clicking the **Edit...** button and includes the **Wetting Parameters** tab, the **Constituent Materials** tab, the **Boundary Conditions** tab, the **Solver** tab, and the **Equations & References** tab, which cites several references[185].

At the top of the dialog, enter the **Result File Name**. The result file is saved in the chosen project folder (**File → Choose Project Folder** in the menu bar).

The **Equations & References** tab shows the formulas that are used for the solver which are described in the ConductoDict chapter:

- Poisson equation,
- Fourier's law.

No parameters can be edited on this tab.

Tabs of the Relative Thermal Conductivity dialog

- Wetting Parameters[121]
  Select how the fluid distribution is determined and choose the saturation steps for the conductivity calculations.
- Constituent Materials[121]
  Select the materials in the structure and their properties, including the selection of invading and displaced fluid.
- Boundary Conditions[122]

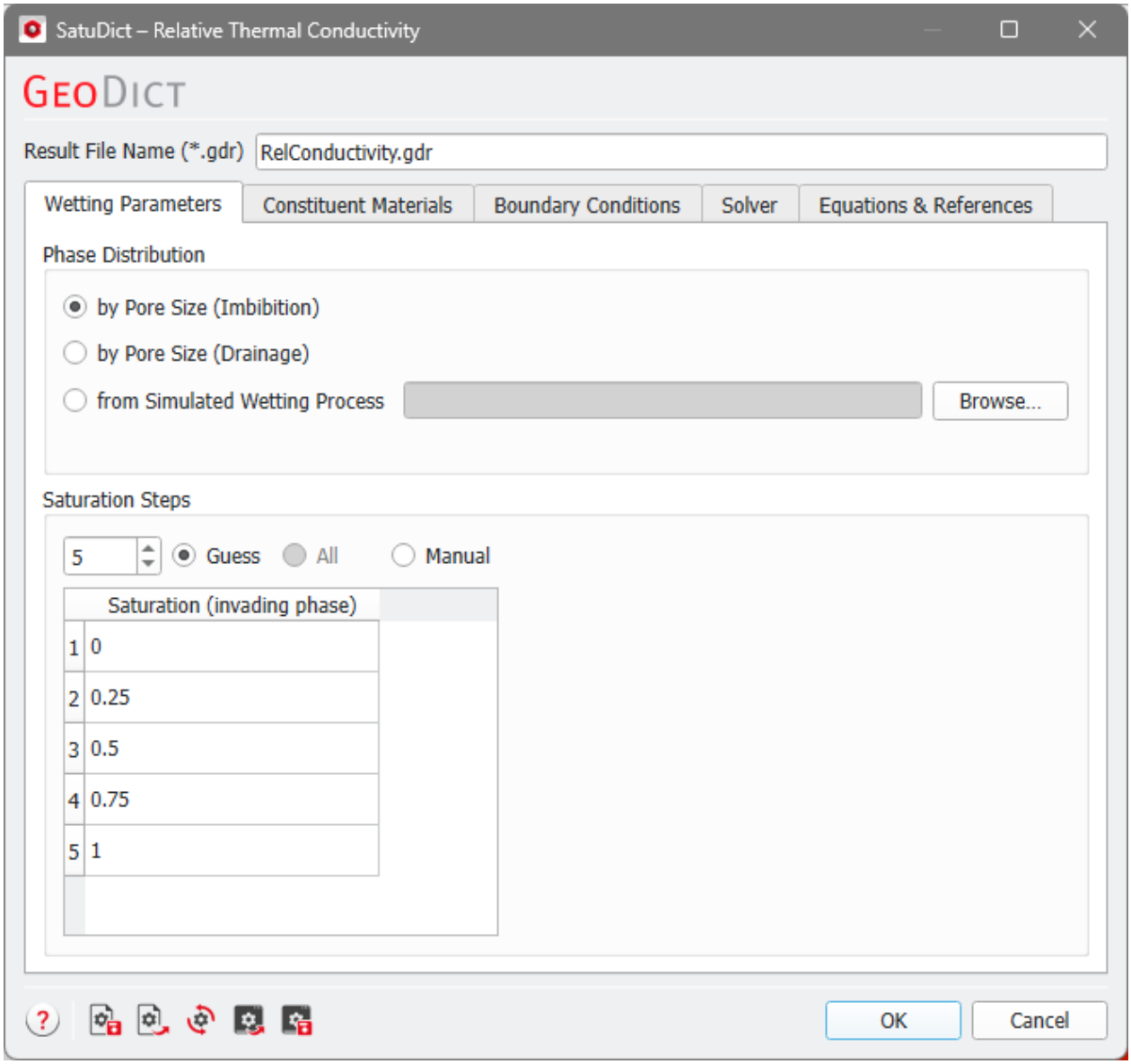
Tabs of the Relative Thermal Conductivity dialog

Set the boundary conditions for the conductivity calculations.

- Solver
  Select a conductivity solver and its settings.

Wetting Parameters

The wetting parameters for the calculation of the **Relative Thermal Conductivity** are the same as seen for the Relative Permeability, except that no Flow Phase needs to be selected.

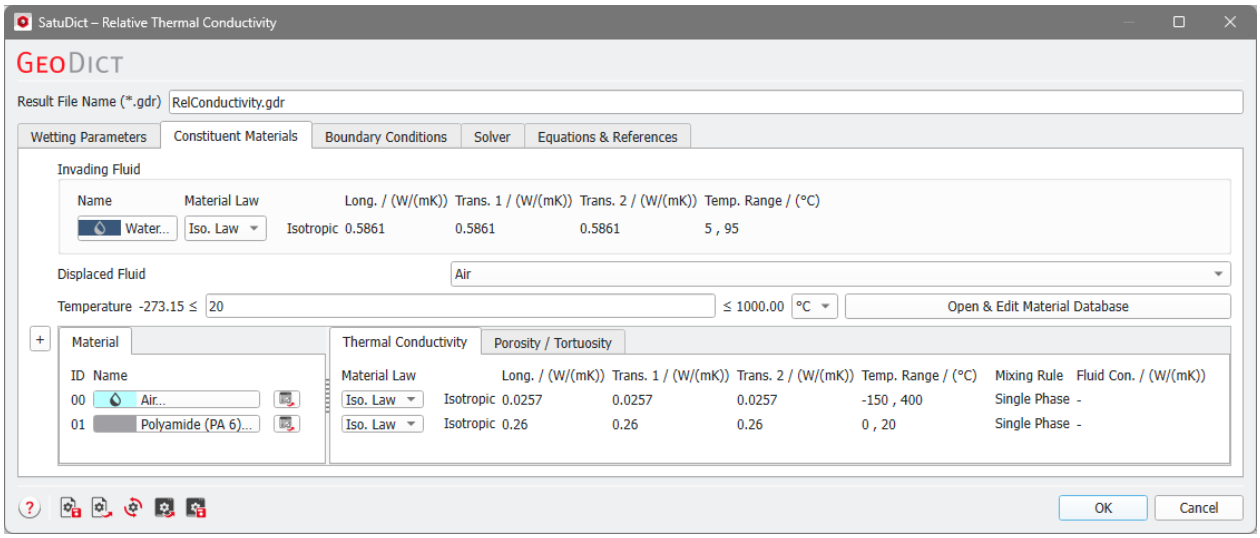


Constituent Materials

Under the **Constituent Materials** tab, the **Invading Fluid** and **Displaced Fluid** can be entered and their thermal conductivity (W/(mK)) can be defined. The tab is similar to the one for

Capillary Pressure Curve 18 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 and can be chosen from the drop-down menu. If the phase distribution is taken **from Simulated Wetting Process**, then both fluids are defined by the capillary pressure curve result file.

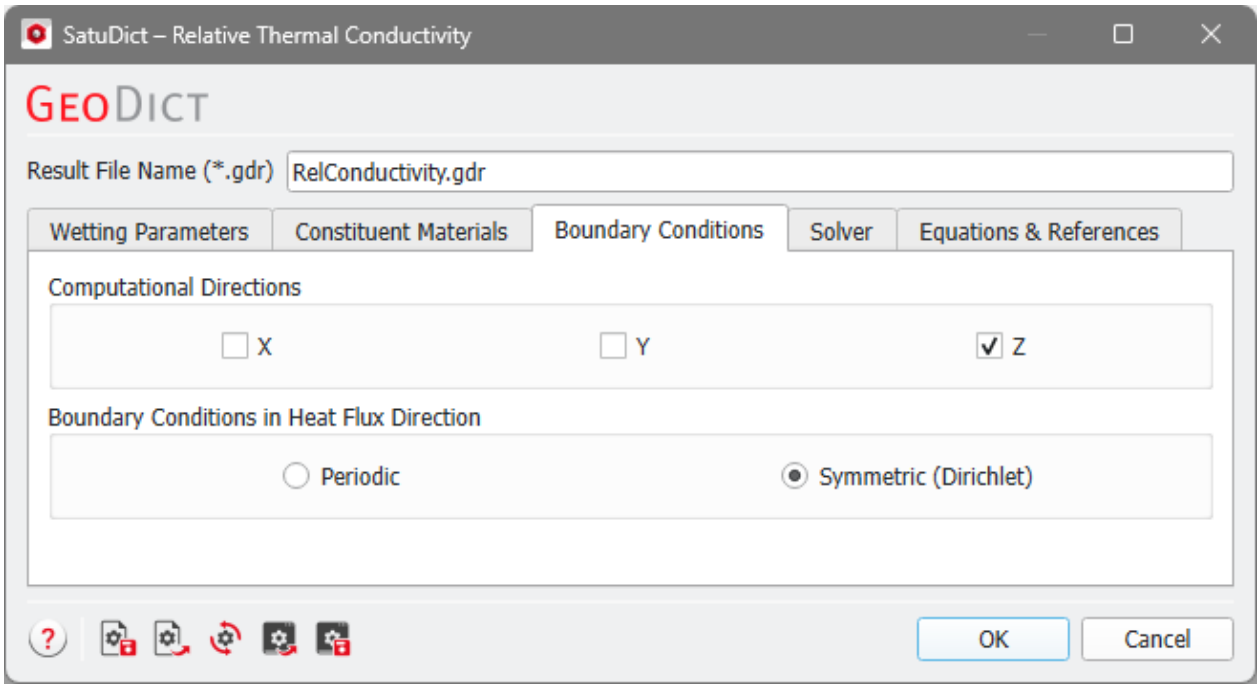


Set the **Temperature** applied for the calculation in the selected units below. Click **Open & Edit Material Database** to edit the materials properties in the material database if needed.

The table with the materials contained in the structure has the same entries and tabs as the table in the Constituent Materials tab in ConductoDict (except for the Specific Thermal Contact Resistivity tab).

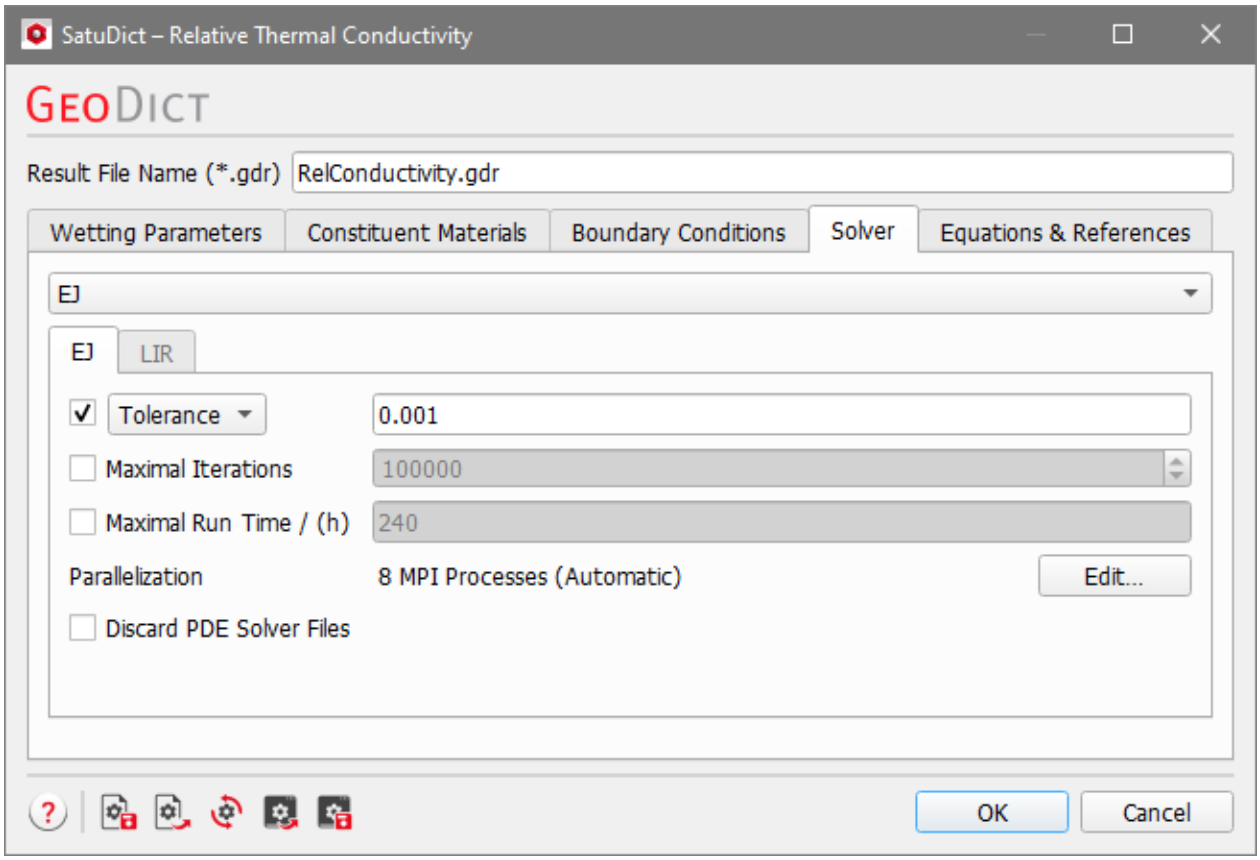
Boundary Conditions

The choice of **Boundary Conditions** and the selection of **Computation Directions** for the calculation of the Relative Thermal Conductivity are the same as seen for the Relative Diffusivity 102.



Solver

For **Relative Thermal Conductivity**, the two solvers **EJ** and **LIR** are available and can be chosen from the pull-down menu. The solver settings are similar to those available in the ConductoDict module.



Parameters for all solvers

Stopping Criteria

The equations are solved by an iterative approach.

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
3. Repeat the iterative process until one of the stopping criteria is reached.

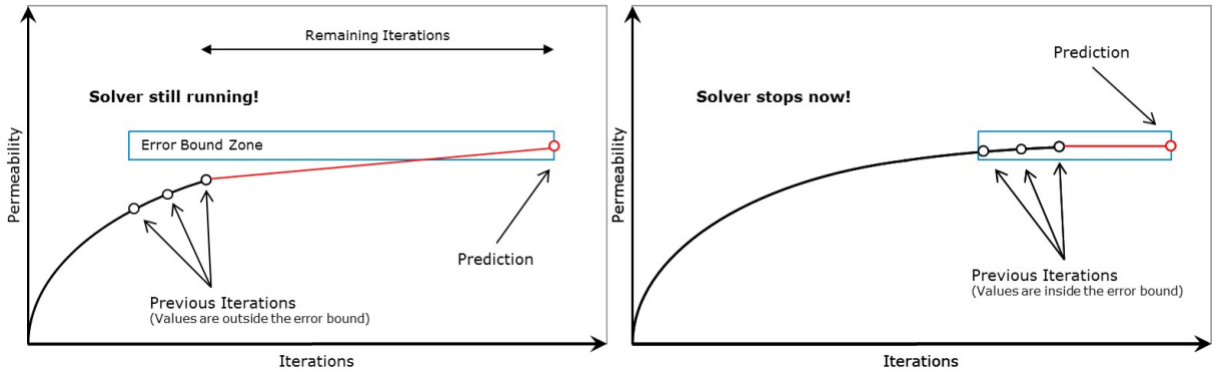
The iterative process is controlled by setting the values and activation for **Error Bound, Tolerance, Residual**, **Maximal Iterations**, and **Maximal Run Time (h**). The stopping criteria apply for each computational direction individually.

If multiple stopping criteria are selected, the first criterion that is reached causes the solver to stop.

The stopping criterion that has been reached can be viewed in the Result Viewer of the GeoDict result file (*.gdr) under the **Results Report** tab.

Error Bound (LIR)

The stopping criterion **Error Bound** uses the result of previous iterations, and predicts the final solution based on linear and quadratic extrapolation. The solver stops if the relative difference between computed and predicted solution is smaller than the specified error bound. The stopping criterion recognizes oscillations in the convergence behavior and prevents premature stopping at local minima or maxima. A damped convergence curve is fit through the oscillating curve and the solver stops then regarding the damped convergence curve.



If the Krylov method (under LIR - Advanced Options) is activated, the definition of **Error**

Bound is somewhat different. Here, no prediction is made, instead the continuity between neighboring cells and the conservation of mass is checked. The maximal value is normalized by the mean flow and if this value is smaller than the **Error Bound** the simulation stops.

Tolerance

The **Tolerance** stopping criterion looks for stagnation of the method when the process becomes stationary, i.e., the improvement in the conductivity value becomes extremely small from iteration to iteration.

In each iteration, the solver checks for the current computed value x_c against the values x_{c-i} of the last 100 iterations if there are any changes.

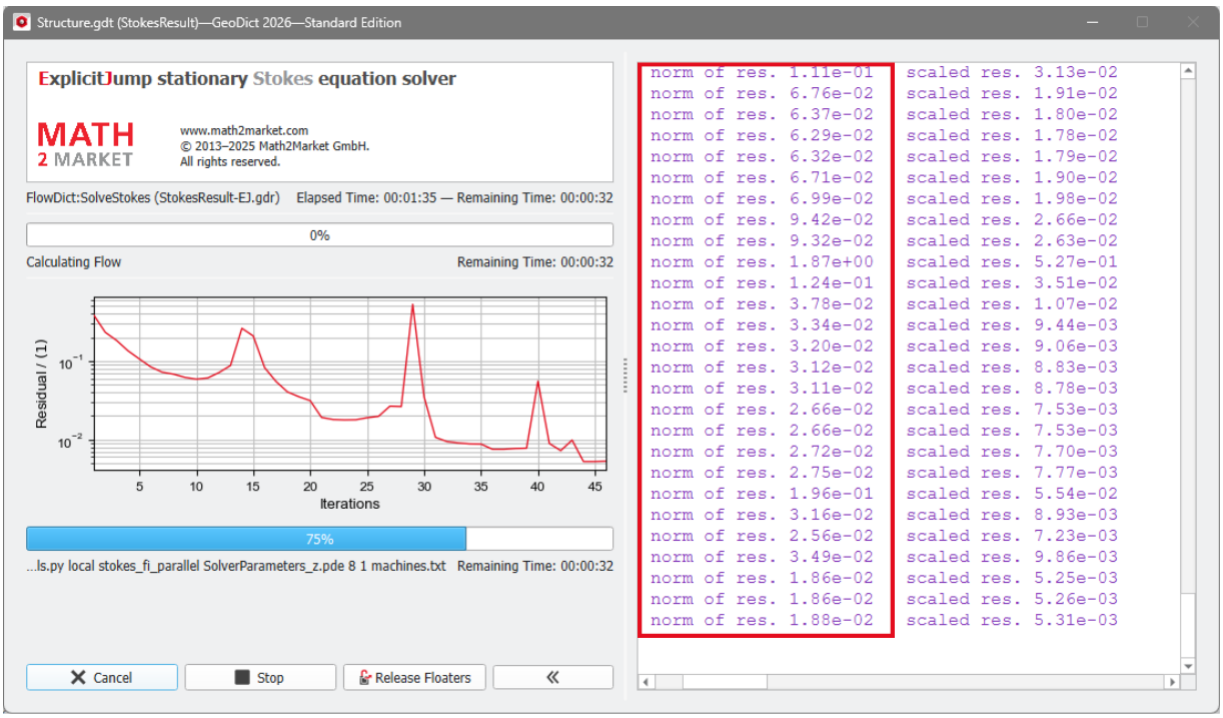
$$\max_{i\in[1,100]} \frac{x_c - x_{c-i}}{x_{c-i}} < \text{tolerance} \tag{32}$$

The computation is stopped if the maximal relative change is smaller than the value entered for **Tolerance**. When there is doubt about the quality of the solution, decrease the **Tolerance** value by a factor of ten. The drawback of this criterion is that the solver sometimes might stop too early in case of slow convergence rate or at local extrema of oscillatory convergence curves.

Residual (EJ)

When the **Residual** stopping criterion is used, the iteration is stopped if the solution satisfies the equation up to the required accuracy.

By setting the stopping criterion to **Residual**, the computations terminate as soon as the relative norm drops below the selected residual threshold. The relative norm of the Schur Complement residual is computed and displayed in the console window during the calculations. The console is visible by clicking the double arrow button on the lower right corner in the progress dialog.



The recommendation to choose **Tolerance** or **Residual** for the **EJ** solver is based on the structure's porosity. Both give similar results for highly porous structures. For dense structures, if using the Schur Complement **Residual**, the relative norm of the residual may be small even though the correct conductivity has not been reached. So, when in doubt, use the **Tolerance** criteria – the default option.

Maximal Iterations & Maximal Run Time

Use the **Maximum Iterations** value or the **Maximum Run Time (h)** stopping criteria causes the solver to stop if the maximal number of iterations and/or the maximal runtime (in hours) is exceeded.

When the solver stops because one of these criteria has been reached, no guarantee on the quality of solution can be given. In this case, a warning is printed into the report. The following possibilities might help:

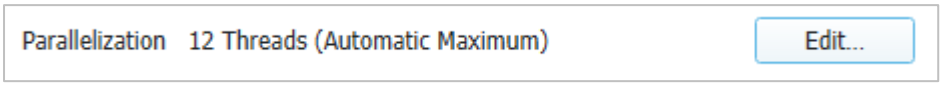
- Check the corresponding .log file to see how large the residual values and the conductivity values are. If the conductivity values are in reasonable range and they do not have changed during the last iterations, you may decide to use the current result.
- Double-check the structure and parameter values. Unphysical parameters or too rough resolution of the structure (leading, e.g., to artificial unconnected components) can cause an iterative solver to fail.

Parallelization

Control how many threads are used for the computation. Parallelization is possible if your

license and hardware allow it.

The **Parallelization Options** dialog opens when clicking the **Edit** button and you can choose between **Sequential**, **Parallel (Shared Memory)**, **Automatic Maximum of Threads**, or **Cluster** (only available if EJ, SimpleFFT, or FeelMath were selected as solver).



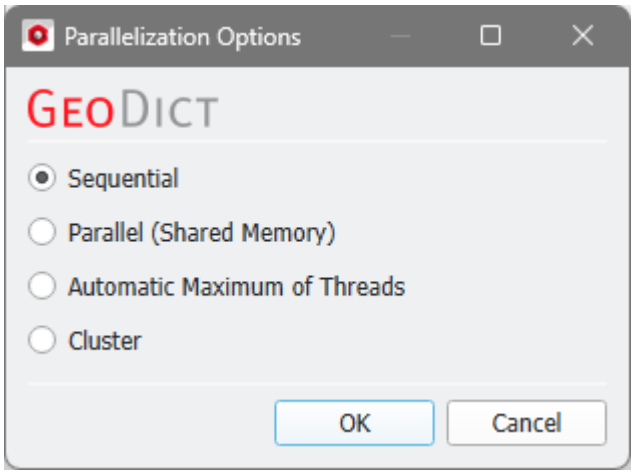
The parallelization of the solvers is done with two technical methods: **MPI Parallelization** or **Thread parallelization**. The following table shows the support of both parallelization methods:

Solver	Parallelization method	
	MPI Parallel	Thread Parallel
EJ	✔	✘
SimpleFFT	✔	✘
LIR	✘	✔
FeelMath	✔	✔
BEST	✘	✔

Depending on the used parallelization method, the **Number of Processes** (MPI parallel) or the **Number of Threads** (thread parallel) can be entered.

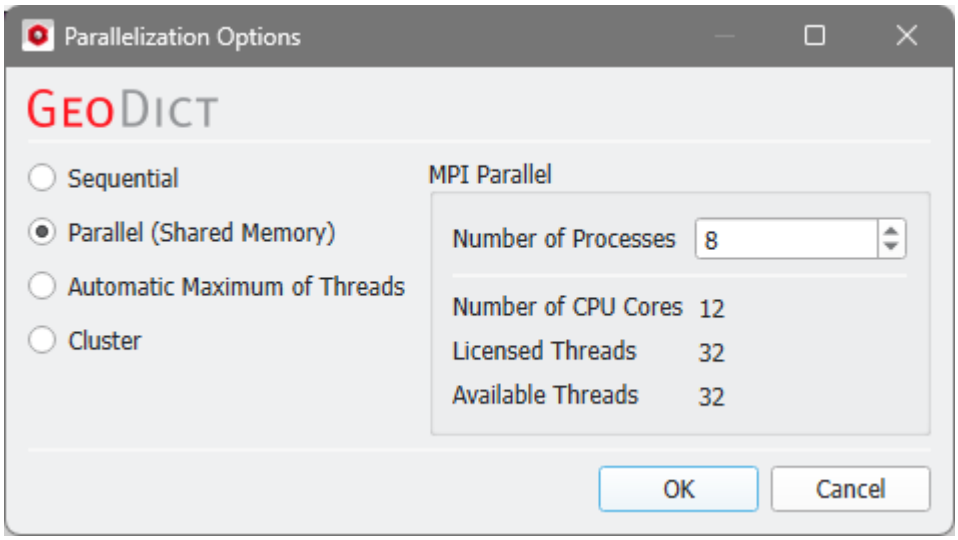
Sequential

Selecting **Sequential** will not apply parallelization and only one thread is used for the computation.



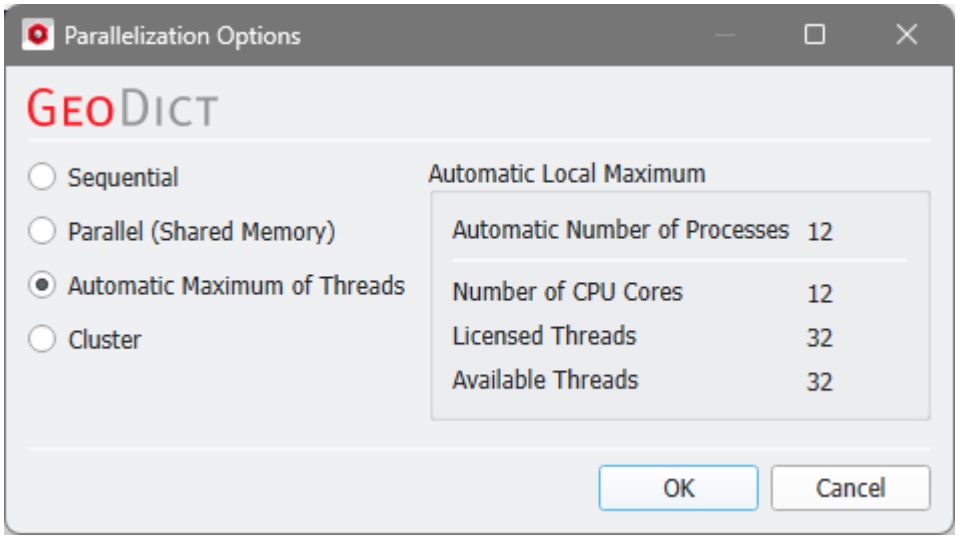
Parallel (Shared Memory)

When **Parallel (Shared Memory)** is selected, the **Number of Processes** or **Number of Threads** can be entered. Below, the **Number of CPU Cores** that the current machine has, the maximum number of **Licensed Threads** and the number of those licensed threads that are available (**Available Threads**) are shown in the dialog. Of course, the maximal number of parallel processes you can use, is the smallest of those three numbers.



Automatic Maximum of Threads

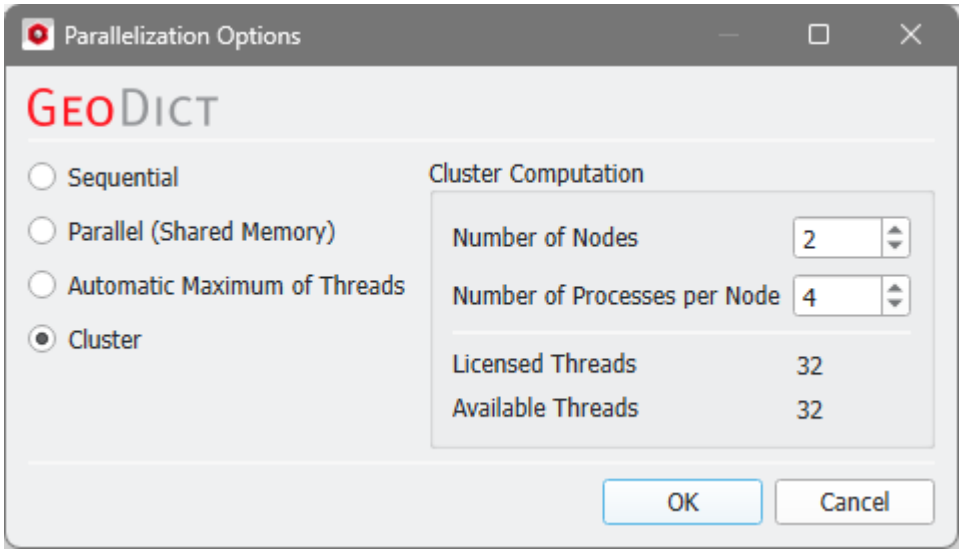
If **Automatic Maximum of Threads** is selected, the number of parallel processes is automatically selected for optimal speed, based on the CPU cores and licensed parallel processes.



The **Automatic Local Maximum** of processes is automatically selected, which is the minimum of **Number of CPU Cores**, **Licensed Threads**, and **Available Threads**.

Cluster

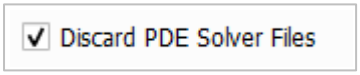
The **Cluster** parallelization requires that the solver supports the **MPI Parallelization** method. Moreover, the choice of **Cluster** is for users of Linux systems only.



For details on how to set up and run parallel computations, consult the High Performance Computing chapter.

Discard PDE Solver Files

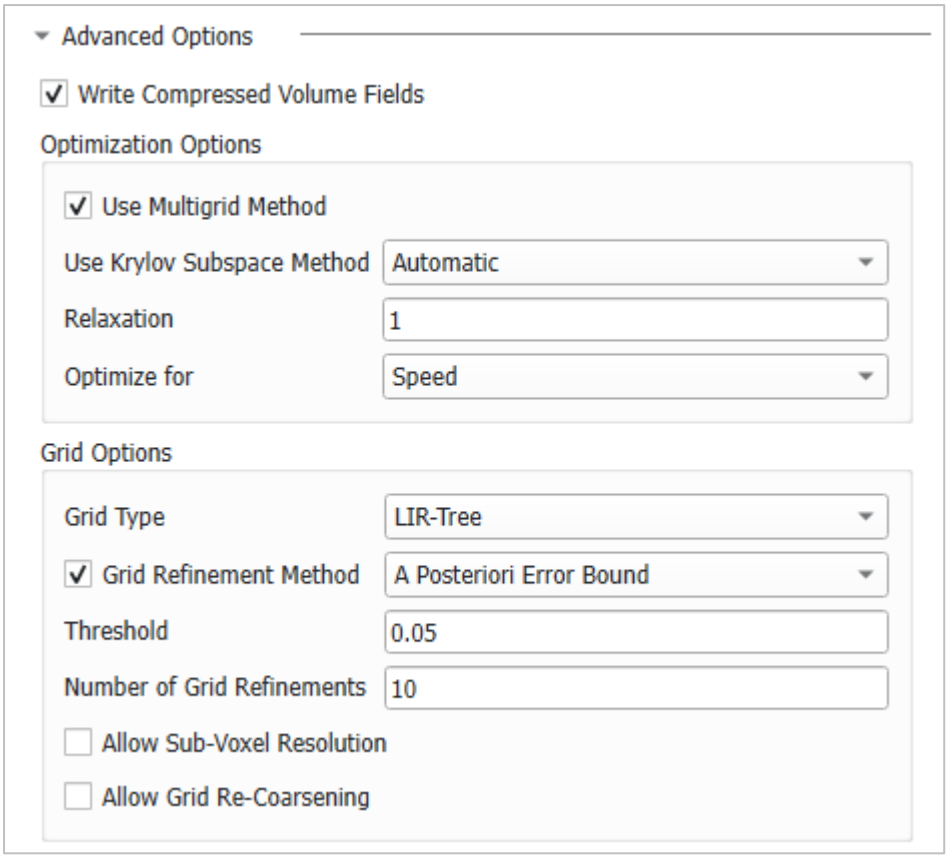
Checking **Discard PDE Solver Files** causes the deletion of all intermediate computation files, such as log files and flow field files.



Only the content of the final GeoDict result file (*.gdr) is stored.

While having the benefit of saving hard disk storage place, discarding intermediate solver files has also the effect of disabling the 3D visualization of the results.

LIR specific parameters (Advanced Options)



Write Compressed Volume Fields

The LIR solver uses a very memory efficient adaptive grid structure for the simulations.

If the option **Write Compressed Volume Fields** is checked, then the adaptive grid is used as compression method for writing out *.hht files. This option allows to save 80-90% space on hard drive. The runtime for writing *.hht files is also reduced significantly. But the runtime for loading and uncompressing of compressed *.hht is increased by the amount of runtime that was saved for writing out compressed *.hht files.

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

Use Multigrid Method

The **Multigrid Method** (see, e.g., Wesseling, 2004) was introduced to speed-up the computation and reduce the runtime significantly. The main idea of **Multigrid** is the usage of multiple coarser adaptive grids to speed up convergence behavior but requires only little more memory.

The method is available to solve the Stokes and Stokes–Brinkman equations as well as

for solving mechanics, diffusion, thermal, and electrical conduction and is enabled by default.

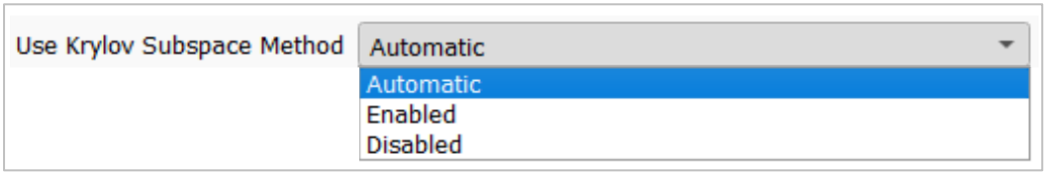
Use Krylov Subspace Method

Another speed-up option to accelerate the convergence behavior of the LIR solver is called **Krylov Subspace Method**.

The runtime of the LIR solver depends on many different properties of the structure and the simulation parameters. The BiCGStab algorithm is used, which can reduce the runtime for challenging simulation very drastically.

Note! Using the BiCGStab method approximately doubles the amount of RAM needed for the computation.

Unfortunately, the Krylov method is not always faster than a simulation without the Krylov method and therefore we introduced an **Automatic** mode which uses some heuristics to choose the most efficient method based on structure, material parameters, and boundary conditions automatically. Of course, it is possible to explicitly enable (**Enabled**) or disable (**Disabled**) the method.



Note! In case that the Krylov subspace method (BICGStab) is used, the **Relaxation** may also be adapted automatically.

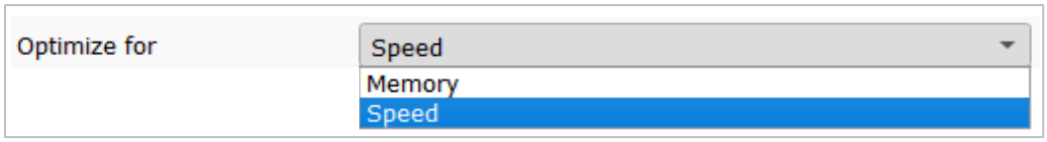
Relaxation

Depending on the material parameters and geometry of the structure, the underlying mathematical problem can vary in complexity, thus influencing the behavior of the solver. The more complex the problem is, the more stable the solver settings should be.

With the **Relaxation** number, the solver is adjusted from **Stable** (which results in higher number of iterations, slower time stepping, and longer solver run times), to **Fast**, which makes the solver run less iterations but implies the risk that the solver does not converge. The **Relaxation** is a parameter of the SOR method and must be between 0 and 2 to ensure convergence. For relaxation values smaller than one (<1.0), the simulation is more stable. For relaxation values larger than one (>1.0), the simulation converges faster.

Optimize For

The **LIR** solver can **Optimize for Speed** or **Memory**.



- If **Speed** is chosen, the solver constructs additional optimization structures. The runtime is decreased by up to 30% but requires up to 50% more memory compared to the other option.
- If **Memory** is chosen, the runtime is increased by up to 40% but the solver requires up to 50% less memory.

Grid Type

The **Grid Type** decides what kind of tree structure is used for the simulation.

The default option is **LIR-Tree** and should always be used. The solver uses an adaptive grid structure called LIR-tree and needs up to 10 times less runtime and memory compared to the **Regular Grid** option.

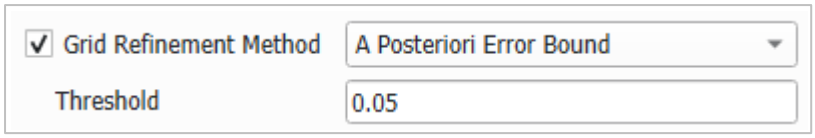
The solver can analyze the result field during the computation and improves the adaptive grid in places where more accuracy is needed. The LIR solver splits cells where a high gradient occurs.

Grid Refinement Method

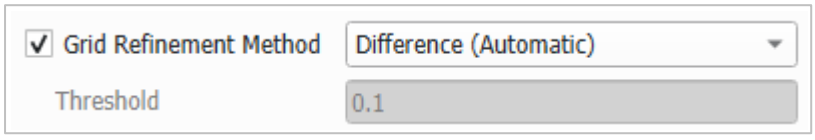
The solver can analyze the computed field and refines the adaptive grid during the computation at locations where more accuracy is needed. The LIR solver splits cells where a high gradients occur when the **Grid Refinement Method** is enabled. In this case, the additional parameters **Number of Grid Refinements**, **Allow Sub-Voxel Resolution**, and **Allow Grid Re-Coarsening** become available.

Select one of the three available refinement methods from the drop-down menu.

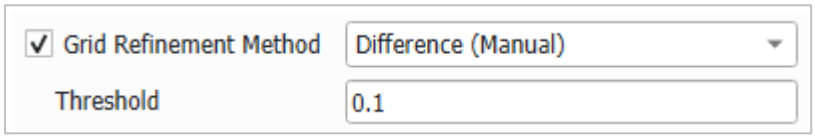
When **A Posteriori Error Bound** is selected, the solver targets the specified accuracy **Threshold**. While the **Error Bound** (set as Simulation Stopping Criterion) determines the relative error in the solution of the linear system, **A Posteriori Error Bound** refers to the relative error estimated by comparing high-order and low-order discrete solutions. The accuracy **Threshold** refers to the relative error to the analytical solution and the value must be between 0.0 and 1.0.



Choosing **Difference (Automatic)** leads to computational cells being split when the difference in values between neighboring cells exceeds a certain **Threshold**. The solver automatically chooses all internal parameters based on the structure and simulation settings. For this option, cells are split where the current gradient is greater than the **Threshold** multiplied by the maximum gradient, where the threshold is determined automatically.

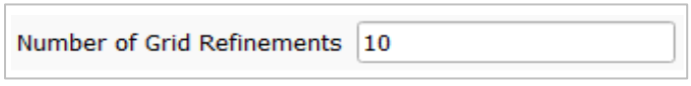


Selecting **Difference (Manual)** also causes the computational cells to be split when the difference in values between neighboring cells exceeds the specified **Threshold**. You can specify all parameters (Threshold and Number of Grid Refinements) for the grid refinement manually. For this option, cells are split where the current gradient is greater than the **Threshold** multiplied by the maximum gradient. The **Threshold** value must be between 0.0 and 1.0. The recommended value range is between 0.05 and 0.1.



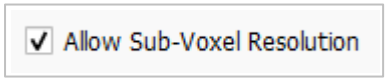
Number Of Grid Refinements

The **Number of Grid Refinements** controls the maximum number of grid refinements that the solver can perform during the simulation. The value should be set between 0 and 10, where a value of 0 means that no grid refinements will be made. Grid refinements may increase the number of iterations, runtime, and memory requirements.



Allow Sub-Voxel Resolution

When **Allow Sub-Voxel Resolution** is enabled, the solver is allowed to split computational cells to sizes smaller than the voxel length.



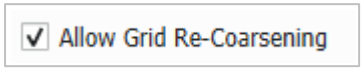
This feature is beneficial for low-porosity structures for which the pore throats require finer resolution or for modeling fast Navier-Stokes flows with strong vortices.

Enabling this feature may increase the number of iterations, runtime, and memory

requirements.

Allow Grid Re-Coarsening

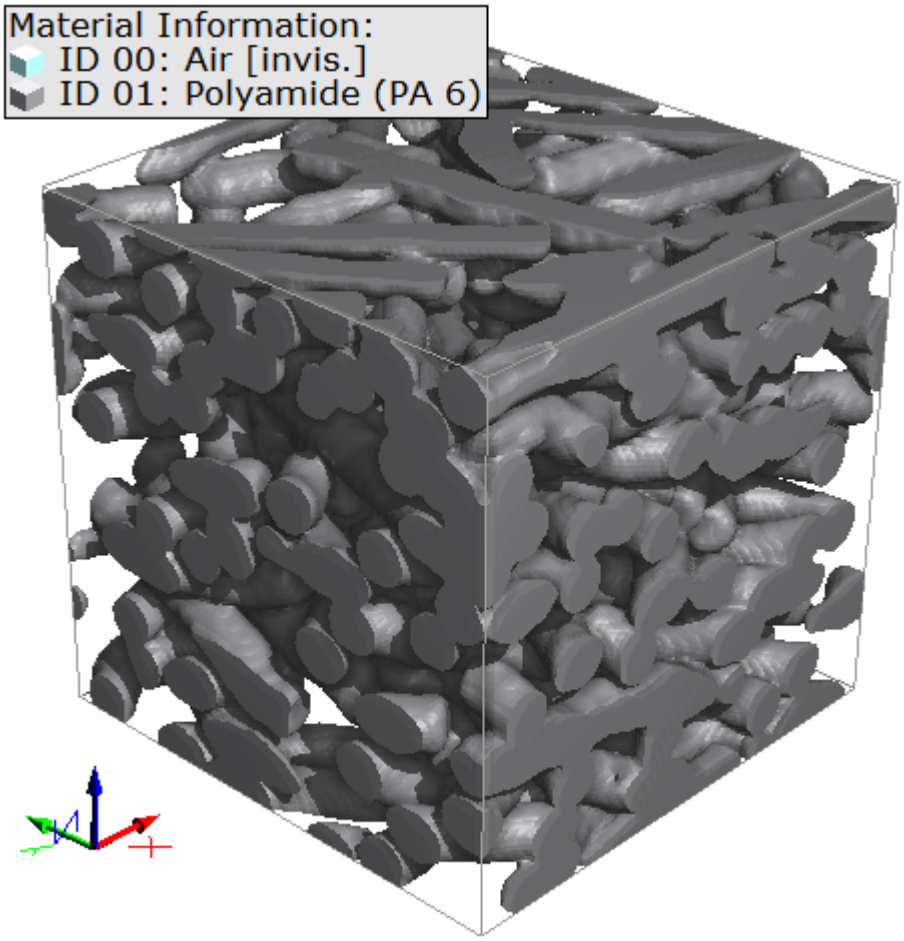
Check **Allow Grid Re-Coarsening** to allow the solver to automatically revert the grid refinement and coarsen the computational cells.



This means, grid refinement is done temporarily. Afterwards, the cells are merged as soon as accuracy is not needed anymore. This reduces the memory and runtime requirements.

1.6.2 Results

The result file (*.gdr) is opened in the Result Viewer after the computation is finished. Only the tabs listed below are described in detail, for the other tabs look into the Result Viewer chapter.



The results of the relative thermal conductivity calculated on a partially saturated fiber material (with 70% porosity) made of polyamide PA6 are shown. The invading phase Water

displaces Air and conductivity was calculated in Z-direction with Dirichlet boundary conditions (Boundary Conditions tab). Computations were run using the EJ solver.

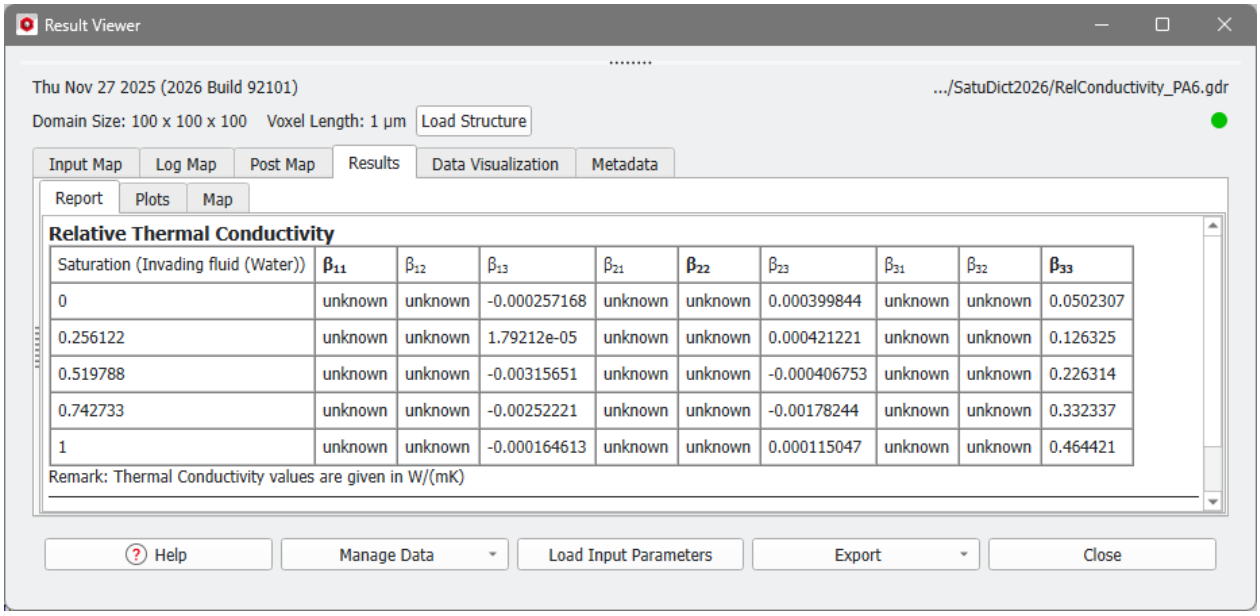
Relative Thermal Conductivity Results

- Results Tab 135
  Learn about the resulting reports and plots.
- Data Visualization 137
  Load results for a graphical visualization.

Results Tab

Report tab

Under the **Results-Report** sub-tab, the saturation-dependent **Relative Thermal Conductivity** table is shown for the chosen saturation rates 121 (here, 0, 0.25, 0.50, 0.75, and 1), which are approximated as best as possible (here, 0, 0.256122, 0.519788, 0.742733, and 1).



The saturation-dependent **Relative Thermal Conductivity** is shown in the tables, where each row stands for one saturation level. The values of the whole thermal conductivity tensor at each saturation step are given in the columns. For directions which were not selected as Computational Direction 122 the conductivity value is unknown.

In the example above, the entries β_{13}, β_{23}, β_{33} for the computation in Z-direction are given, the other values are unknown as the computations were not carried out.

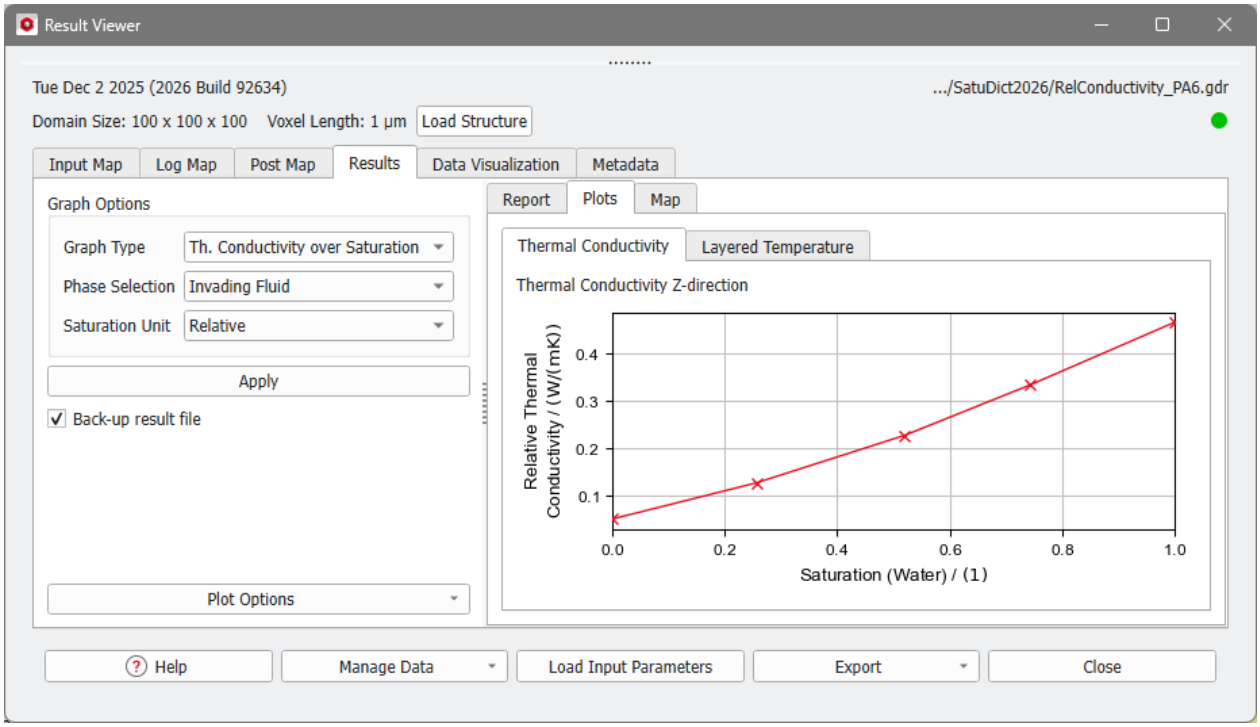
Plots tab

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

Thermal Conductivity Plot

The values of the conductivity in all selected Computational Directions 122 at the different saturation levels are shown in a graph.

On the left, the **Post-Processing Widget** allows you to fine-tune the **Thermal Conductivity** plot. Collapse the Post-Processing Widget by pulling it to the left.



Graph Options

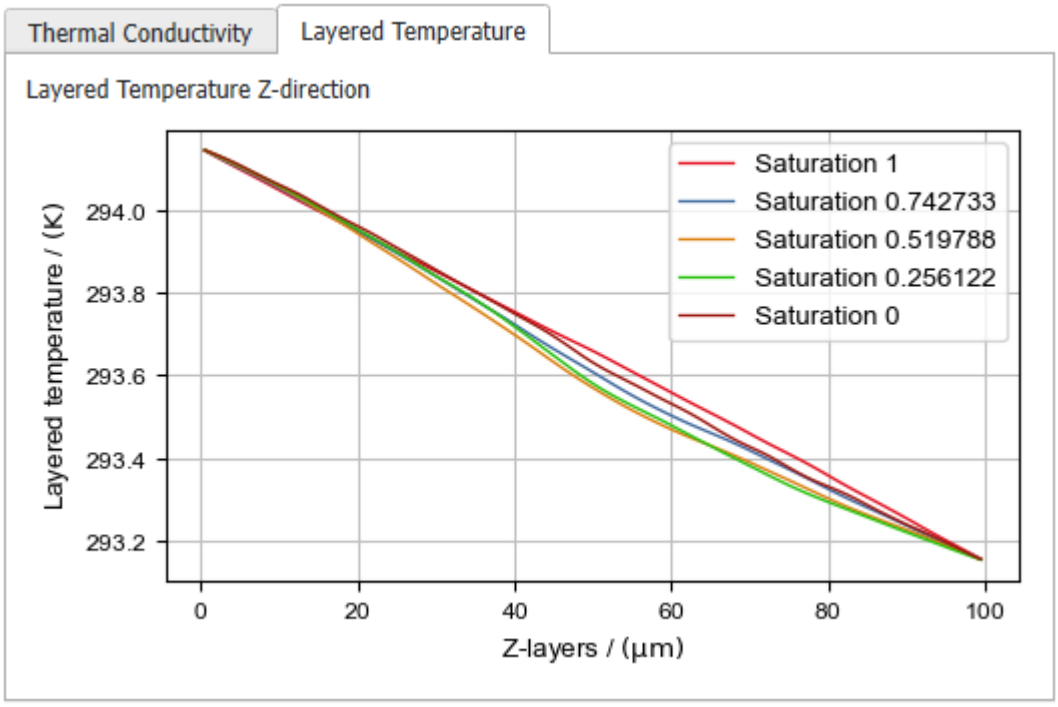
On the left side in the expandable **Graph Options**, you can modify the way the thermal conductivity graph is displayed by selecting

- the **Graph Type** (Th. Conductivity over Saturation or Saturation over Th. Conductivity),
- the **Phase Selection** (Invading Fluid or Displaced Fluid),
- and the **Saturation Unit** (Relative or Absolute).

Click **Apply** to change the graph shown according to the options selected.

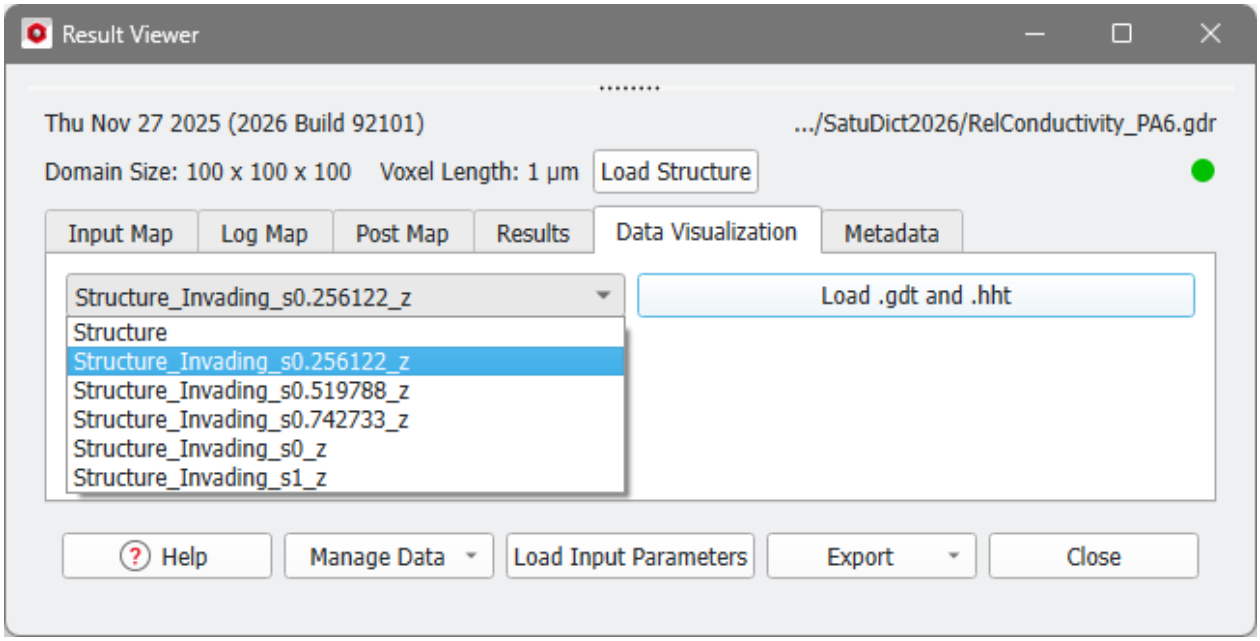
Layered Temperature

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



Data Visualization

Under the **Data Visualization** tab, the .gdt and .hht files, corresponding to the saturation levels computed, can be opened, as explained in the ConductoDict chapter. No files are available if **Discard PDE Solver Files** was checked in the **Solver** settings tab.

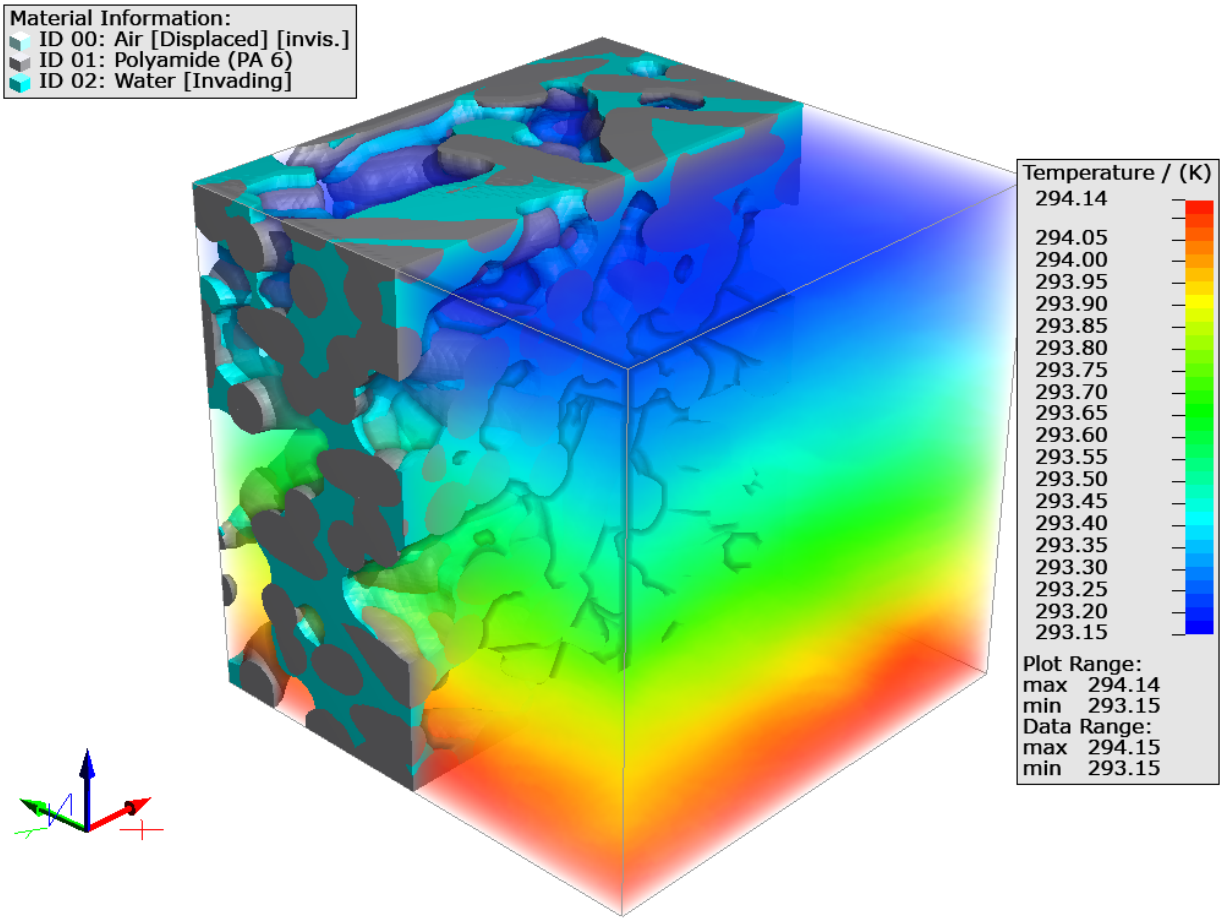


For each selected Computational Direction 122 the solution files for the saturation steps with non-zero conductivity are saved and can be loaded by clicking on the **Load .gdt and .hht** button.

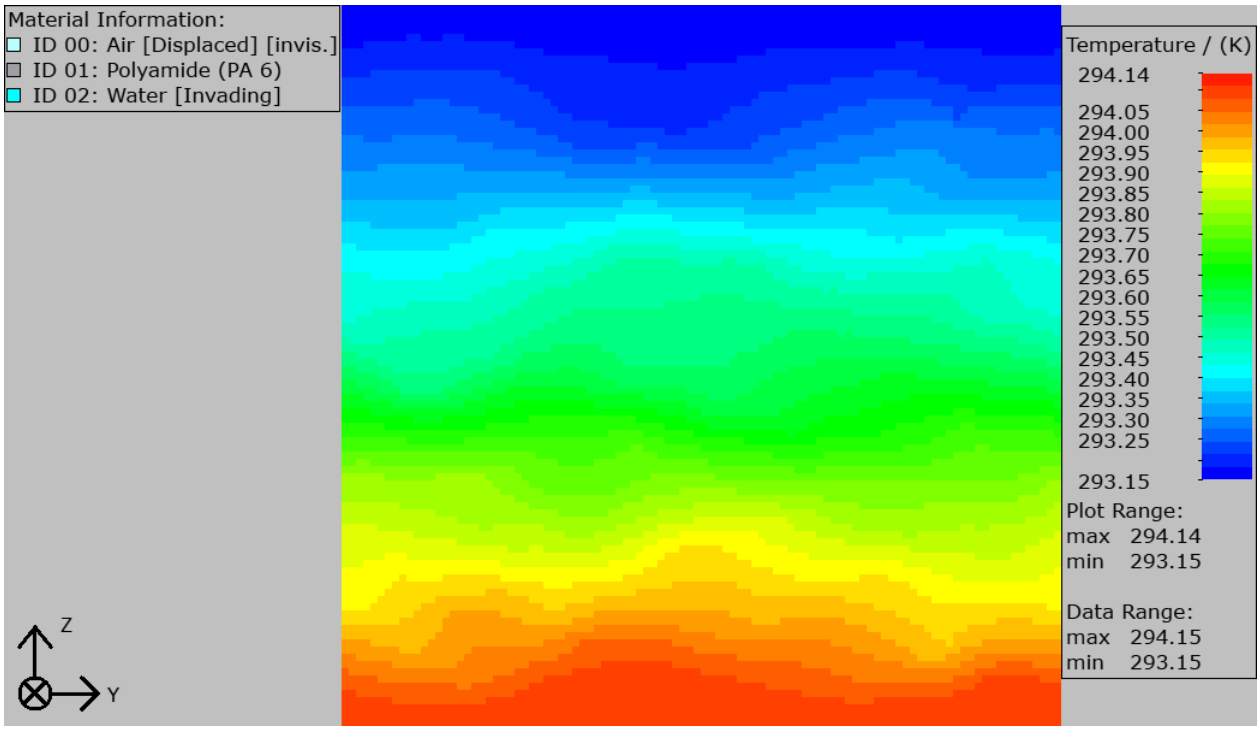
In the structure file (.gdt) you can observe the fluid distribution, while the .hht (homogenized heat) file contains the temperature values at each voxel.

Select **Structure** to load the original structure which is saturated with the displaced fluid. No additional .hht file will be loaded.

Shown below is the .gdt file for a 25% invading fluid saturation level. The right part of the image shows the temperature field with transparent effect on the clipped structure model.



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 and the transparent effect for the volume field. Observe how the heat is distributed in the structure.



More information about the visualization parameters is available in the Visualization chapter.

1.7 Resistivity Index (Relative Electrical Conductivity)

Determine **Saturation-dependent (Relative) Electrical Conductivity (Resistivity Index)** as in ConductoDict (see also Pfrang et.al. 186). The pore morphology method 5 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.

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, the Poisson equations is solved. Advection or radiation is not considered.

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

The Resistivity Index command

- Options 140
  Set the parameters for the calculation.
- Results 154
  View the computed results.

1.7.1 Options

The **Resistivity Index (Relative Electrical Conductivity)** dialog opens when clicking the **Edit...** button and includes the **Wetting Parameters** tab, the **Constituent Materials** tab, the **Boundary Conditions** tab, the **Solver** tab, and the **Equations & References** tab, which cites several references 185.

At the top of the dialog, enter the **Result File Name**. The result file is saved in the chosen project folder (**File → Choose Project Folder** in the menu bar).

The **Equations & References** tab shows the formulas that are used for the solver which are described in the ConductoDict chapter:

- Poisson equation,
- Ohm's law.

No parameters can be edited on this tab.

Tabs of the Resistivity Index (Relative Electrical Conductivity) dialog

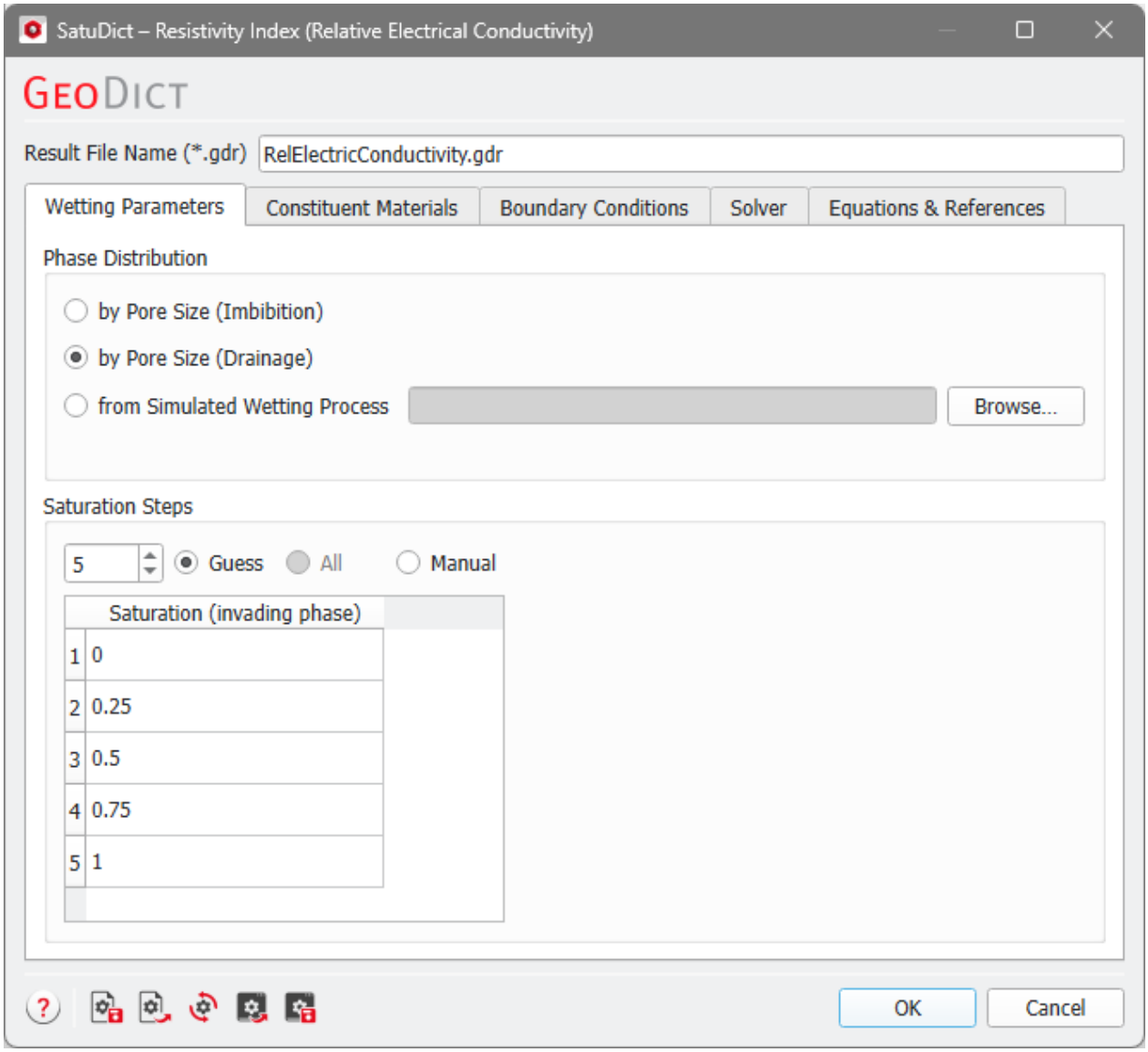
- Wetting Parameters 141
  Select how the fluid distribution is determined and choose the saturation steps for the conductivity calculations.
- Constituent Materials 141
  Select the materials in the structure and their properties, including the selection of invading and displaced fluid.

Tabs of the Resistivity Index (Relative Electrical Conductivity) dialog

- Boundary Conditions 142
  Set the boundary conditions for the conductivity calculations.
- Solver 143
  Select a conductivity solver and its settings.

Wetting Parameters

The wetting parameters for the calculation of the **Resistivity Index** are the same as seen for the Relative Permeability 64, except that no Flow Phase needs to be selected.

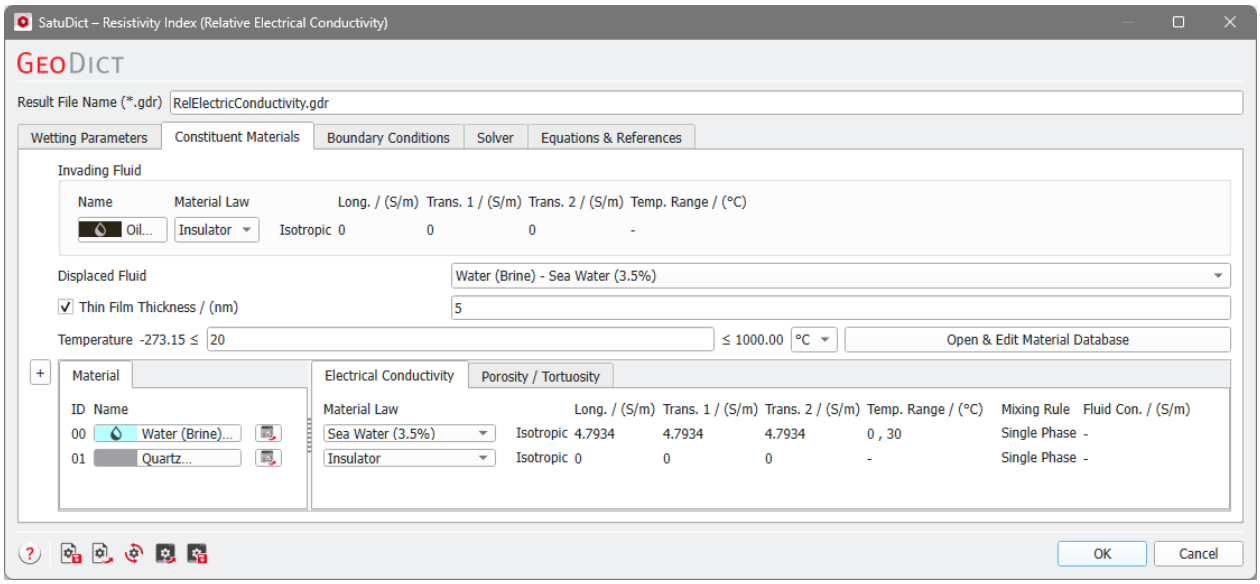


Constituent Materials

Under the **Constituent Materials** tab, the **Invading Fluid** and **Displaced Fluid** can be entered and their electrical conductivity (S/m) can be defined. The tab is similar to the one for Capillary

Pressure Curve 18 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 and can be chosen from the drop-down menu. If the phase distribution is taken **from Simulated Wetting Process**, then both fluids are defined by the capillary pressure curve result file.

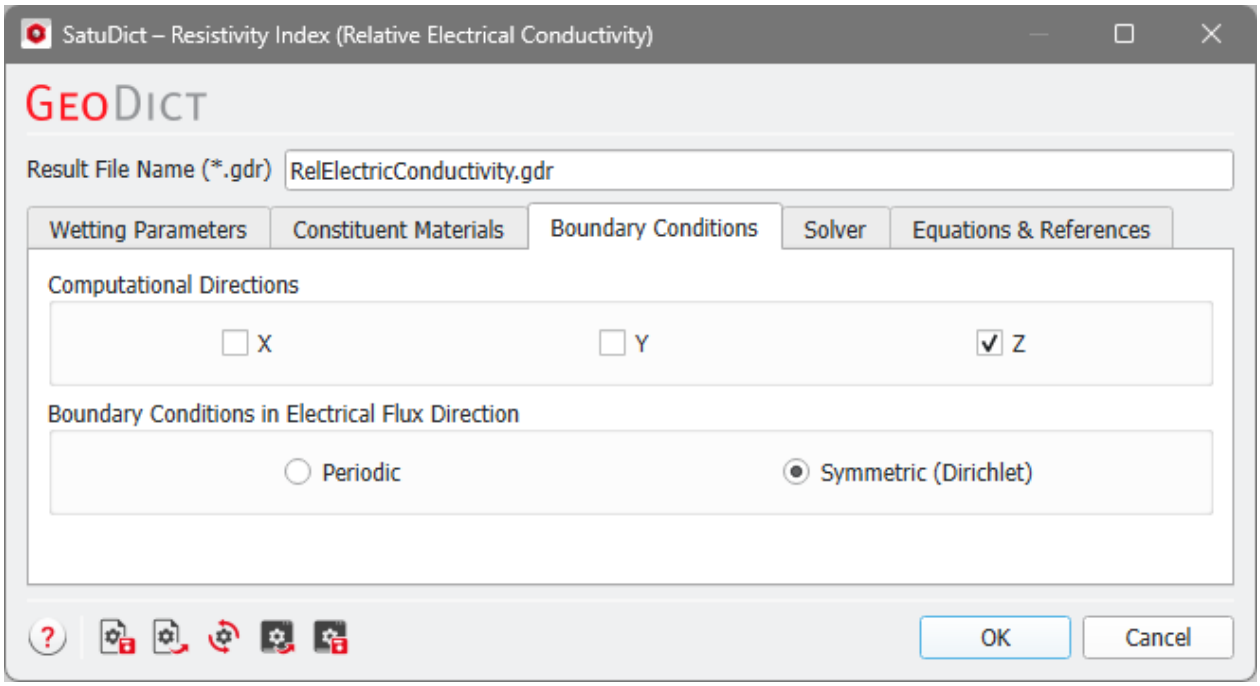


The table with the materials contained in the structure has the same entries and tabs as the table in the Constituent Materials tab in ConductoDict (except for the Specific Electrical Contact Resistivity tab).

Additionally, by checking **Thin Film Thickness**, the Thin Film Model 13 can be used. The thickness of the thin film must be smaller than the current voxel length.

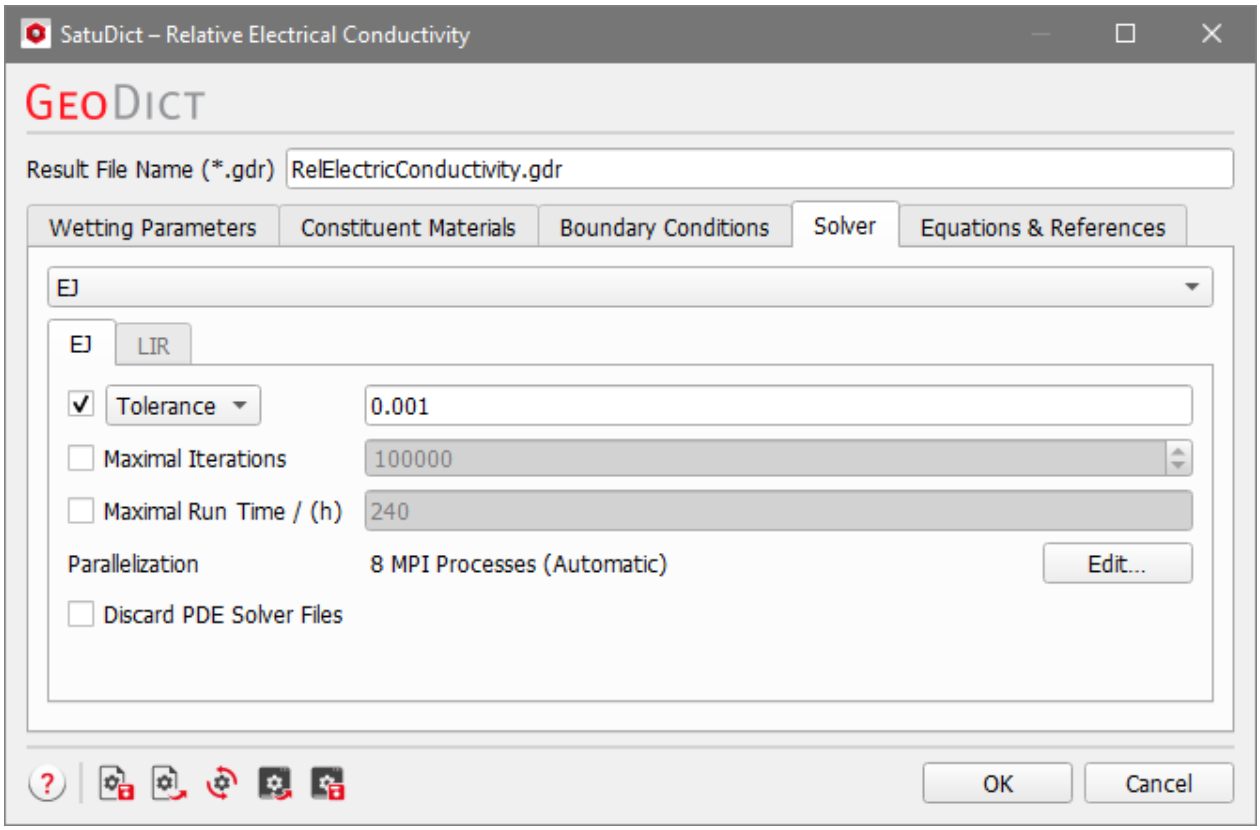
Boundary Conditions

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 102 and the Relative Thermal Conductivity.



Solver

For **Relative Electrical Conductivity**, the two solvers **EJ** and **LIR** are available and can be chosen from the pull-down menu. The solver settings are similar to those available in the ConductoDict module.



Parameters for all solvers

Stopping Criteria

The equations are solved by an iterative approach.

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
3. Repeat the iterative process until one of the stopping criteria is reached.

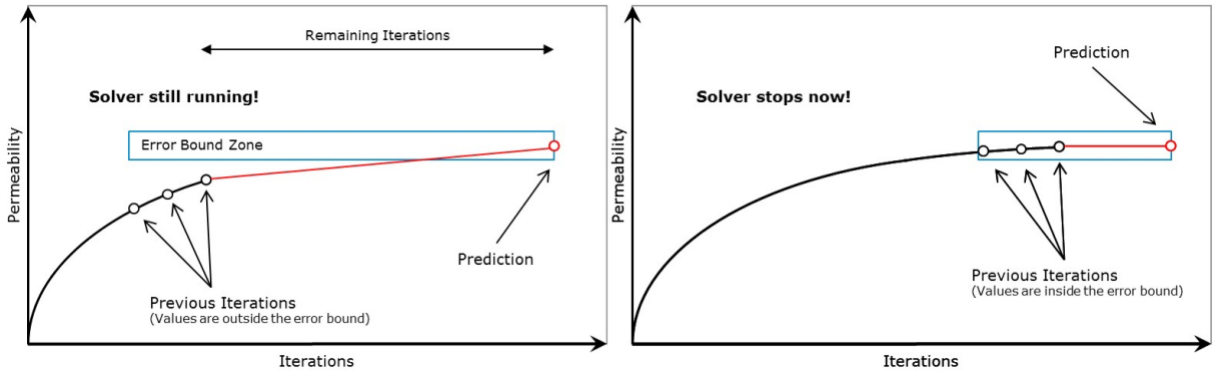
The iterative process is controlled by setting the values and activation for **Error Bound, Tolerance, Residual**, **Maximal Iterations**, and **Maximal Run Time (h**). The stopping criteria apply for each computational direction individually.

If multiple stopping criteria are selected, the first criterion that is reached causes the solver to stop.

The stopping criterion that has been reached can be viewed in the Result Viewer of the GeoDict result file (*.gdr) under the **Results Report** tab.

Error Bound (LIR)

The stopping criterion **Error Bound** uses the result of previous iterations, and predicts the final solution based on linear and quadratic extrapolation. The solver stops if the relative difference between computed and predicted solution is smaller than the specified error bound. The stopping criterion recognizes oscillations in the convergence behavior and prevents premature stopping at local minima or maxima. A damped convergence curve is fit through the oscillating curve and the solver stops then regarding the damped convergence curve.



If the Krylov method (under LIR - Advanced Options) is activated, the definition of **Error**

Bound is somewhat different. Here, no prediction is made, instead the continuity between neighboring cells and the conservation of mass is checked. The maximal value is normalized by the mean flow and if this value is smaller than the **Error Bound** the simulation stops.

Tolerance

The **Tolerance** stopping criterion looks for stagnation of the method when the process becomes stationary, i.e., the improvement in the conductivity value becomes extremely small from iteration to iteration.

In each iteration, the solver checks for the current computed value x_c against the values x_{c-i} of the last 100 iterations if there are any changes.

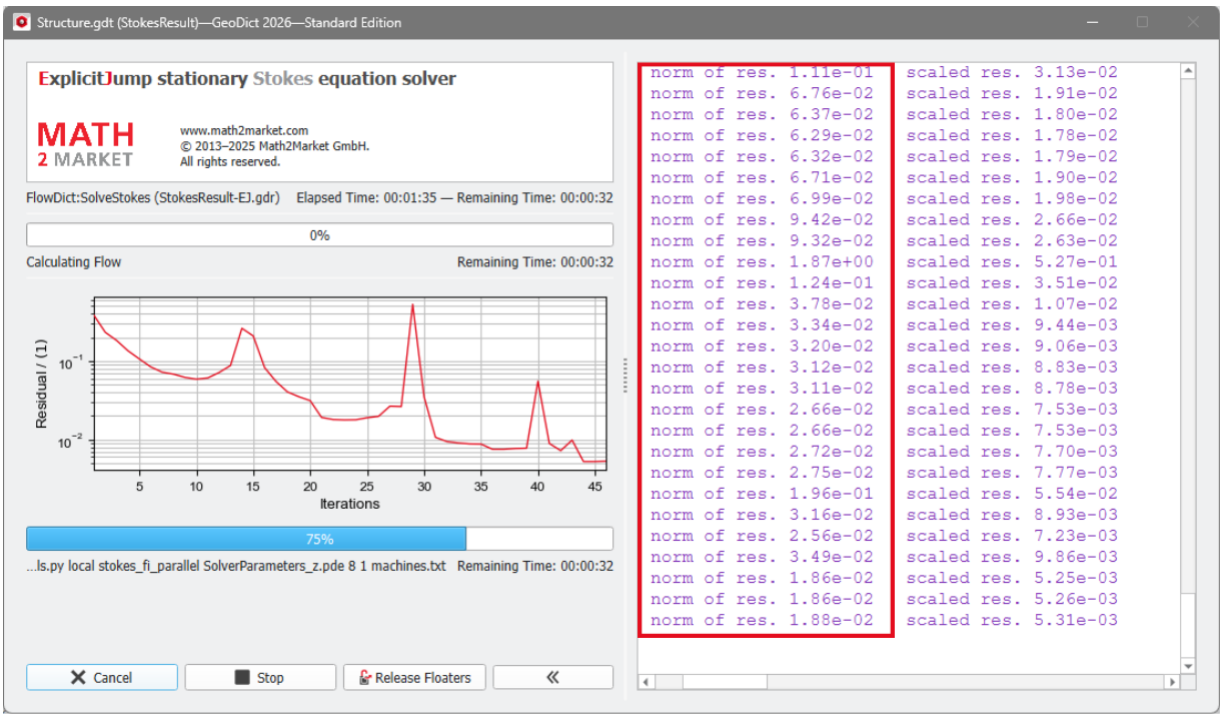
$$\max_{i\in[1,100]} \frac{x_c - x_{c-i}}{x_{c-i}} < \text{tolerance} \tag{33}$$

The computation is stopped if the maximal relative change is smaller than the value entered for **Tolerance**. When there is doubt about the quality of the solution, decrease the **Tolerance** value by a factor of ten. The drawback of this criterion is that the solver sometimes might stop too early in case of slow convergence rate or at local extrema of oscillatory convergence curves.

Residual (EJ)

When the **Residual** stopping criterion is used, the iteration is stopped if the solution satisfies the equation up to the required accuracy.

By setting the stopping criterion to **Residual**, the computations terminate as soon as the relative norm drops below the selected residual threshold. The relative norm of the Schur Complement residual is computed and displayed in the console window during the calculations. The console is visible by clicking the double arrow button on the lower right corner in the progress dialog.



The recommendation to choose **Tolerance** or **Residual** for the **EJ** solver is based on the structure's porosity. Both give similar results for highly porous structures. For dense structures, if using the Schur Complement **Residual**, the relative norm of the residual may be small even though the correct conductivity has not been reached. So, when in doubt, use the **Tolerance** criteria – the default option.

Maximal Iterations & Maximal Run Time

Use the **Maximum Iterations** value or the **Maximum Run Time (h)** stopping criteria causes the solver to stop if the maximal number of iterations and/or the maximal runtime (in hours) is exceeded.

When the solver stops because one of these criteria has been reached, no guarantee on the quality of solution can be given. In this case, a warning is printed into the report. The following possibilities might help:

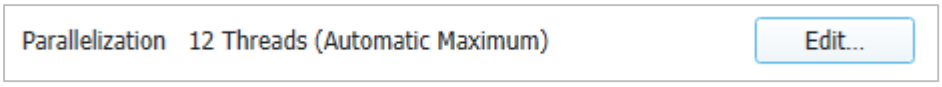
- Check the corresponding .log file to see how large the residual values and the conductivity values are. If the conductivity values are in reasonable range and they do not have changed during the last iterations, you may decide to use the current result.
- Double-check the structure and parameter values. Unphysical parameters or too rough resolution of the structure (leading, e.g., to artificial unconnected components) can cause an iterative solver to fail.

Parallelization

Control how many threads are used for the computation. Parallelization is possible if your

license and hardware allow it.

The **Parallelization Options** dialog opens when clicking the **Edit** button and you can choose between **Sequential**, **Parallel (Shared Memory)**, **Automatic Maximum of Threads**, or **Cluster** (only available if EJ, SimpleFFT, or FeelMath were selected as solver).



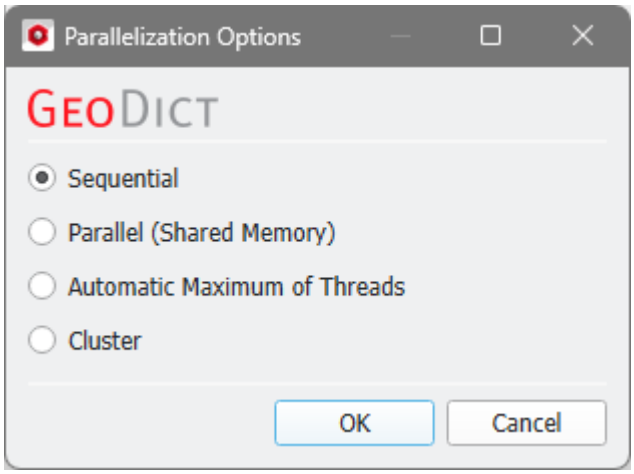
The parallelization of the solvers is done with two technical methods: **MPI Parallelization** or **Thread parallelization**. The following table shows the support of both parallelization methods:

Solver	Parallelization method	
	MPI Parallel	Thread Parallel
EJ	✔	✘
SimpleFFT	✔	✘
LIR	✘	✔
FeelMath	✔	✔
BEST	✘	✔

Depending on the used parallelization method, the **Number of Processes** (MPI parallel) or the **Number of Threads** (thread parallel) can be entered.

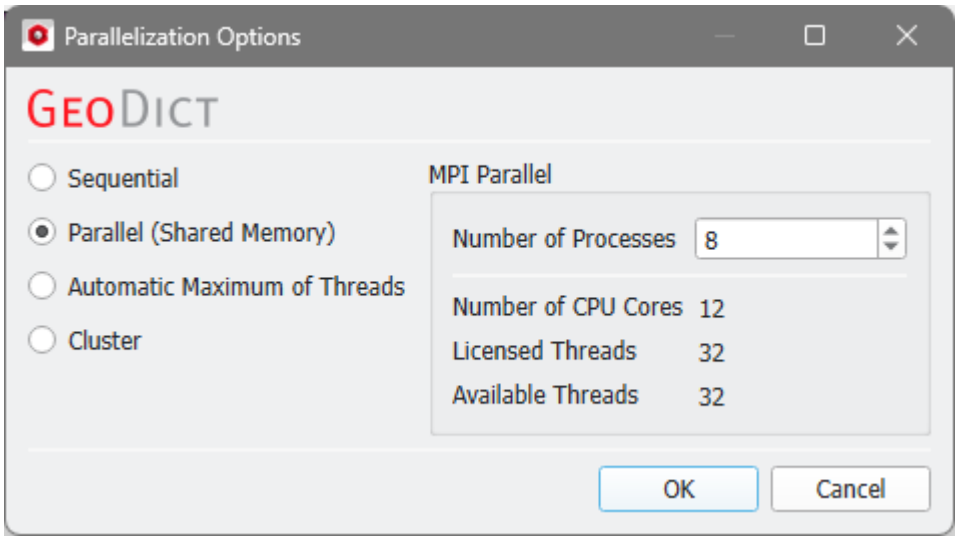
Sequential

Selecting **Sequential** will not apply parallelization and only one thread is used for the computation.



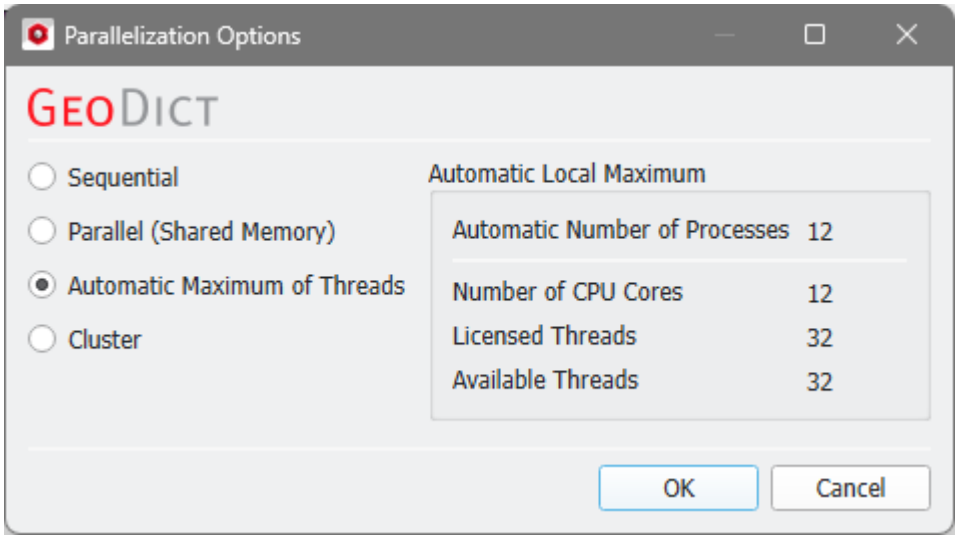
Parallel (Shared Memory)

When **Parallel (Shared Memory)** is selected, the **Number of Processes** or **Number of Threads** can be entered. Below, the **Number of CPU Cores** that the current machine has, the maximum number of **Licensed Threads** and the number of those licensed threads that are available (**Available Threads**) are shown in the dialog. Of course, the maximal number of parallel processes you can use, is the smallest of those three numbers.



Automatic Maximum of Threads

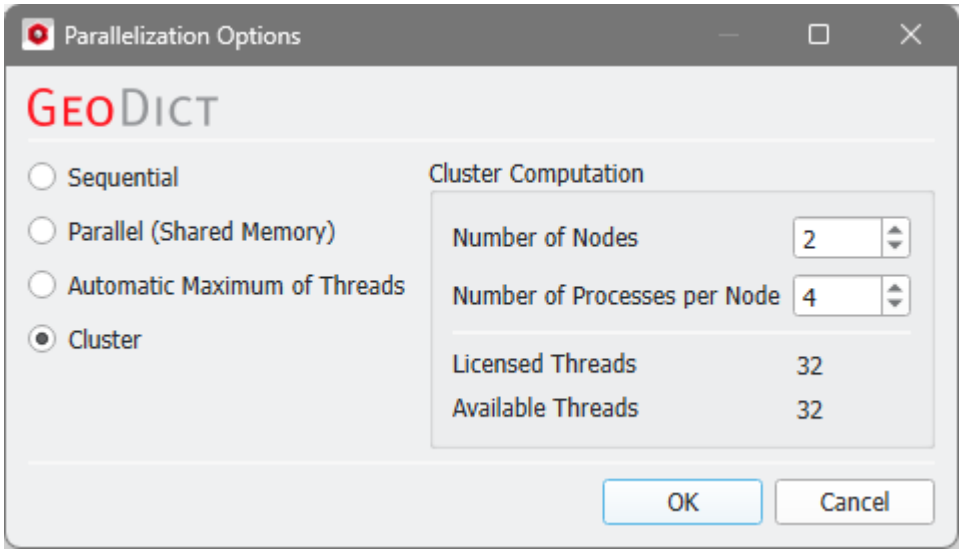
If **Automatic Maximum of Threads** is selected, the number of parallel processes is automatically selected for optimal speed, based on the CPU cores and licensed parallel processes.



The **Automatic Local Maximum** of processes is automatically selected, which is the minimum of **Number of CPU Cores**, **Licensed Threads**, and **Available Threads**.

Cluster

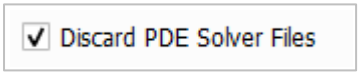
The **Cluster** parallelization requires that the solver supports the **MPI Parallelization** method. Moreover, the choice of **Cluster** is for users of Linux systems only.



For details on how to set up and run parallel computations, consult the High Performance Computing chapter.

Discard PDE Solver Files

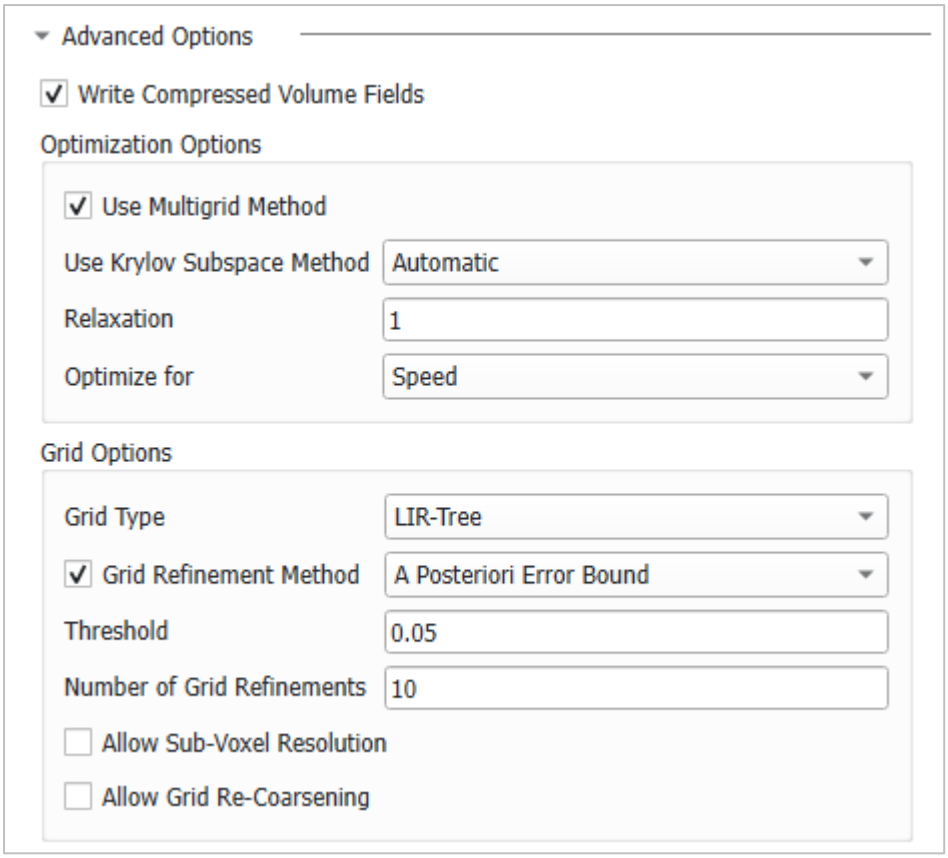
Checking **Discard PDE Solver Files** causes the deletion of all intermediate computation files, such as log files and flow field files.



Only the content of the final GeoDict result file (*.gdr) is stored.

While having the benefit of saving hard disk storage place, discarding intermediate solver files has also the effect of disabling the 3D visualization of the results.

LIR specific parameters (Advanced Options)



Write Compressed Volume Fields

The LIR solver uses a very memory efficient adaptive grid structure for the simulations.

If the option **Write Compressed Volume Fields** is checked, then the adaptive grid is used as compression method for writing out *.hht files. This option allows to save 80-90% space on hard drive. The runtime for writing *.hht files is also reduced significantly. But the runtime for loading and uncompressing of compressed *.hht is increased by the amount of runtime that was saved for writing out compressed *.hht files.

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

Use Multigrid Method

The **Multigrid Method** (see, e.g., Wesseling, 2004) was introduced to speed-up the computation and reduce the runtime significantly. The main idea of **Multigrid** is the usage of multiple coarser adaptive grids to speed up convergence behavior but requires only little more memory.

The method is available to solve the Stokes and Stokes–Brinkman equations as well as

for solving mechanics, diffusion, thermal, and electrical conduction and is enabled by default.

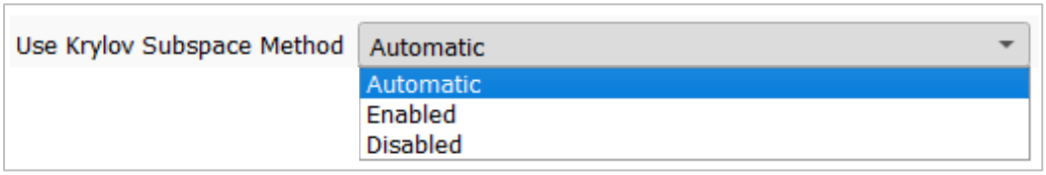
Use Krylov Subspace Method

Another speed-up option to accelerate the convergence behavior of the LIR solver is called **Krylov Subspace Method**.

The runtime of the LIR solver depends on many different properties of the structure and the simulation parameters. The BiCGStab algorithm is used, which can reduce the runtime for challenging simulation very drastically.

Note! Using the BiCGStab method approximately doubles the amount of RAM needed for the computation.

Unfortunately, the Krylov method is not always faster than a simulation without the Krylov method and therefore we introduced an **Automatic** mode which uses some heuristics to choose the most efficient method based on structure, material parameters, and boundary conditions automatically. Of course, it is possible to explicitly enable (**Enabled**) or disable (**Disabled**) the method.



Note! In case that the Krylov subspace method (BICGStab) is used, the **Relaxation** may also be adapted automatically.

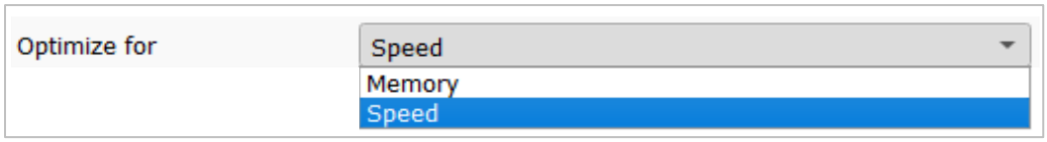
Relaxation

Depending on the material parameters and geometry of the structure, the underlying mathematical problem can vary in complexity, thus influencing the behavior of the solver. The more complex the problem is, the more stable the solver settings should be.

With the **Relaxation** number, the solver is adjusted from **Stable** (which results in higher number of iterations, slower time stepping, and longer solver run times), to **Fast**, which makes the solver run less iterations but implies the risk that the solver does not converge. The **Relaxation** is a parameter of the SOR method and must be between 0 and 2 to ensure convergence. For relaxation values smaller than one (<1.0), the simulation is more stable. For relaxation values larger than one (>1.0), the simulation converges faster.

Optimize For

The **LIR** solver can **Optimize for Speed** or **Memory**.



- If **Speed** is chosen, the solver constructs additional optimization structures. The runtime is decreased by up to 30% but requires up to 50% more memory compared to the other option.
- If **Memory** is chosen, the runtime is increased by up to 40% but the solver requires up to 50% less memory.

Grid Type

The **Grid Type** decides what kind of tree structure is used for the simulation.

The default option is **LIR-Tree** and should always be used. The solver uses an adaptive grid structure called LIR-tree and needs up to 10 times less runtime and memory compared to the **Regular Grid** option.

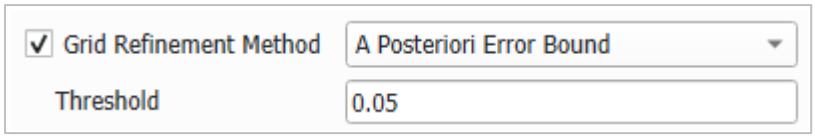
The solver can analyze the result field during the computation and improves the adaptive grid in places where more accuracy is needed. The LIR solver splits cells where a high gradient occurs.

Grid Refinement Method

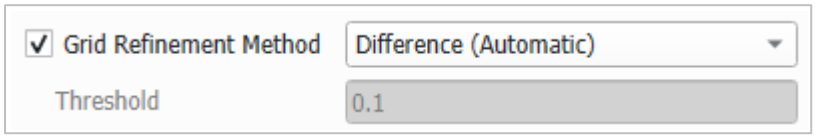
The solver can analyze the computed field and refines the adaptive grid during the computation at locations where more accuracy is needed. The LIR solver splits cells where a high gradients occur when the **Grid Refinement Method** is enabled. In this case, the additional parameters **Number of Grid Refinements**, **Allow Sub-Voxel Resolution**, and **Allow Grid Re-Coarsening** become available.

Select one of the three available refinement methods from the drop-down menu.

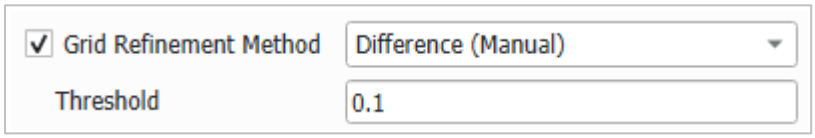
When **A Posteriori Error Bound** is selected, the solver targets the specified accuracy **Threshold**. While the **Error Bound** (set as Simulation Stopping Criterion) determines the relative error in the solution of the linear system, **A Posteriori Error Bound** refers to the relative error estimated by comparing high-order and low-order discrete solutions. The accuracy **Threshold** refers to the relative error to the analytical solution and the value must be between 0.0 and 1.0.



Choosing **Difference (Automatic)** leads to computational cells being split when the difference in values between neighboring cells exceeds a certain **Threshold**. The solver automatically chooses all internal parameters based on the structure and simulation settings. For this option, cells are split where the current gradient is greater than the **Threshold** multiplied by the maximum gradient, where the threshold is determined automatically.

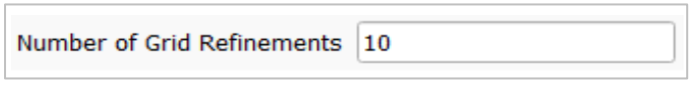


Selecting **Difference (Manual)** also causes the computational cells to be split when the difference in values between neighboring cells exceeds the specified **Threshold**. You can specify all parameters (Threshold and Number of Grid Refinements) for the grid refinement manually. For this option, cells are split where the current gradient is greater than the **Threshold** multiplied by the maximum gradient. The **Threshold** value must be between 0.0 and 1.0. The recommended value range is between 0.05 and 0.1.



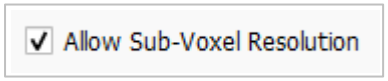
Number Of Grid Refinements

The **Number of Grid Refinements** controls the maximum number of grid refinements that the solver can perform during the simulation. The value should be set between 0 and 10, where a value of 0 means that no grid refinements will be made. Grid refinements may increase the number of iterations, runtime, and memory requirements.



Allow Sub-Voxel Resolution

When **Allow Sub-Voxel Resolution** is enabled, the solver is allowed to split computational cells to sizes smaller than the voxel length.



This feature is beneficial for low-porosity structures for which the pore throats require finer resolution or for modeling fast Navier-Stokes flows with strong vortices.

Enabling this feature may increase the number of iterations, runtime, and memory

requirements.

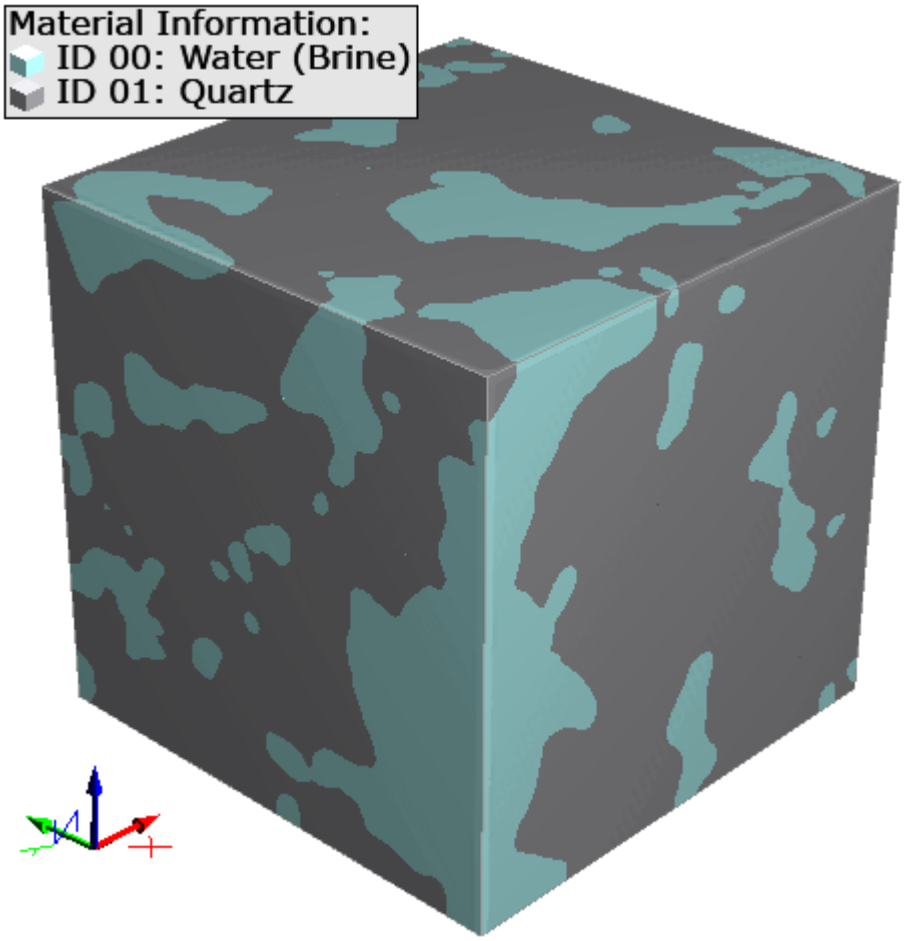
Allow Grid Re-Coarsening

Check **Allow Grid Re-Coarsening** to allow the solver to automatically revert the grid refinement and coarsen the computational cells.

This means, grid refinement is done temporarily. Afterwards, the cells are merged as soon as accuracy is not needed anymore. This reduces the memory and runtime requirements.

1.7.2 Results

The result file (*.gdr) is opened in the Result Viewer after the computation is finished. Only the tabs listed below are described in detail, for the other tabs look into the Result Viewer chapter.



The results of the resistivity index calculated on a partially saturated porous material with 17% porosity (83% SVF) are shown. The invading fluid is Oil (0 S/m) and the displaced fluid is Water (Brine) (5 S/m) while the only solid material in the structure is the non-conductive material

Quartz (Material ID 01) with 0 S/m. The relative electrical conductivity was calculated in Z-direction with Dirichlet boundary conditions (Boundary Conditions tab). Computations were run using the EJ solver.

Resistivity Index (Relative Electrical Conductivity) Results

- Results Tab 155
  Learn about the resulting reports and plots.
- Data Visualization 159
  Load results for a graphical visualization.

Results Tab

Report tab

Under the **Results-Report** sub-tab, the tables for **Saturation exponent**, **Cementation exponent**, **Resistivity index**, and **Relative Electrical Conductivity** are shown for the chosen saturation rates 141 (here, 0, 0.25, 0.50, 0.75, and 1), which are approximated as best as possible (here, 0, 0.246104, 0.510196, 0.749864, and 1).

Saturation Exponent

The resistivity index is empirically related to the water saturation by the **Saturation Exponent** using Archie's equation.

Saturation exponent

$Saturation\ exponent_1$	$Saturation\ exponent_2$	$Saturation\ exponent_3$
unknown	unknown	4.100708766

$I = S_w^{-n}$ (Archie's equation)
I: Resistivity index
S_w: Water saturation
n: Saturation exponent

Cementation Exponent

The **Cementation Exponent** is used to determine how porosity affects resistivity in fully water saturated conditions and it indirectly influences the interpretation of the resistivity index.

Cementation exponent

Cementation exponent$_1$	Cementation exponent$_2$	Cementation exponent$_3$
unknown	unknown	2.375

$F = R_o / R_w = a\ phi^{-m}$
F: Formation resistivity factor
R_o: Resistivity of the sample filled with water
R_w: Water resistivity
a: Tortuosity factor
phi: Porosity
m: Cementation exponent

Resistivity Index

The **Resistivity Index** compares the resistivity at a partial saturation to the resistivity at full water saturation.

Resistivity index

Saturation (Invading fluid (Oil))	Resistivity index$_1$	Resistivity index$_2$	Resistivity index$_3$
0	unknown	unknown	1
0.246104	unknown	unknown	2.27908
0.510196	unknown	unknown	8.12472
0.749864	unknown	unknown	482.646
1	unknown	unknown	inf

$I = R_t / R_o$
I: Resistivity index
R_t: True resistivity
R_o: Resistivity of sample only with water

Relative Electrical Conductivity

The saturation-dependent **Relative Electrical Conductivity** of the fluid is shown in the tables, where each row stands for one saturation level. The values of the whole electrical conductivity tensor at each saturation step are given in the columns.

Relative Electrical Conductivity

Saturation (Invading fluid (Oil))	**β_{11}**	β_{12}	β_{13}	β_{21}	**β_{22}**	β_{23}	β_{31}	β_{32}	**β_{33}**
0	unknown	unknown	0.00809212	unknown	unknown	-0.00808147	unknown	unknown	0.152879
0.246104	unknown	unknown	-0.00729038	unknown	unknown	-0.00487064	unknown	unknown	0.0670793
0.510196	unknown	unknown	7.27543e-05	unknown	unknown	-0.00193152	unknown	unknown	0.0188165
0.749864	unknown	unknown	-1.50913e-05	unknown	unknown	-1.20096e-05	unknown	unknown	0.000316751
1	unknown	unknown	0	unknown	unknown	0	unknown	unknown	0

Remark: Electrical Conductivity values are given in S/m

In the example above, the entries β_{13}, β_{23}, β_{33} for the computation in Z-direction are given, the other values are unknown as the computations were not carried out.

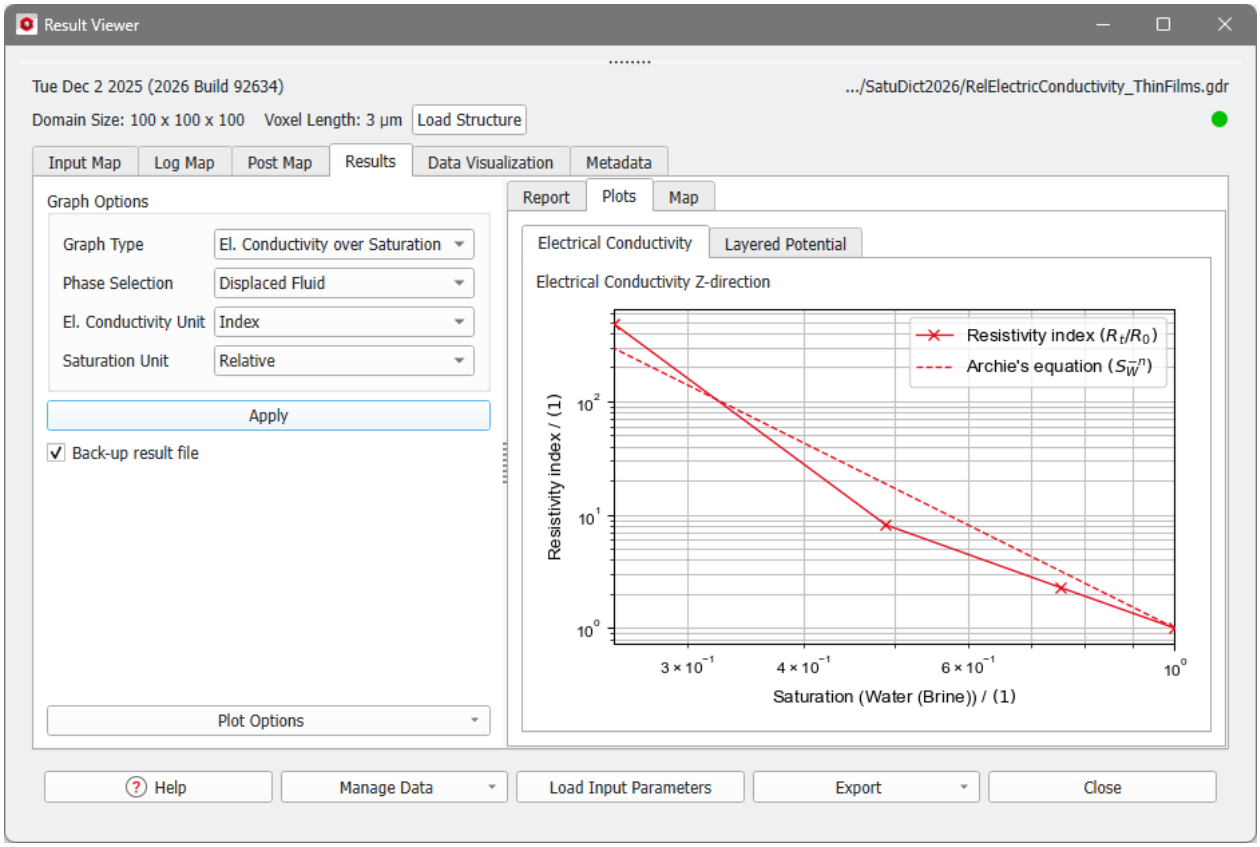
Plots tab

In the **Results-Plots** subtab, the values of the **Relative Electrical Conductivity** table are shown in a graph. Also, the **Layered Potential** in the computed directions is given.

Electrical Conductivity Plot

The values of the electrical conductivity in all selected Computational Directions[102] at the different saturation levels are shown in a graph.

On the left, the **Post-Processing Widget** allows you to fine-tune the **Electrical Conductivity** plot. Collapse the Post-Processing Widget by pulling it to the left.



Graph Options

On the left side in the expandable **Graph Options**, you can modify the way the diffusivity graph is displayed by selecting

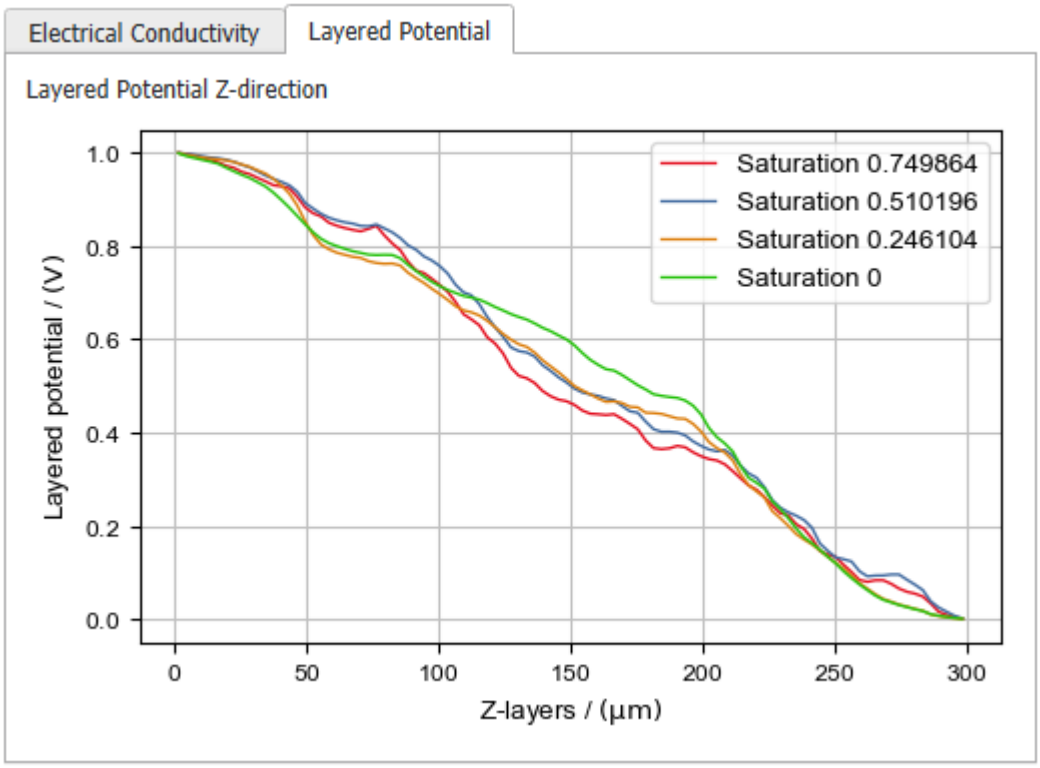
- the **Graph Type** (El. Conductivity over Saturation or Saturation over El. Conductivity),

- the **Phase Selection** (Invading Fluid or Displaced Fluid),
- the **El. Conductivity Unit** (Effective conductivity in S/m or Index),
- and the **Saturation Unit** (Relative or Absolute).

Click **Apply** to change the graph shown according to the options selected.

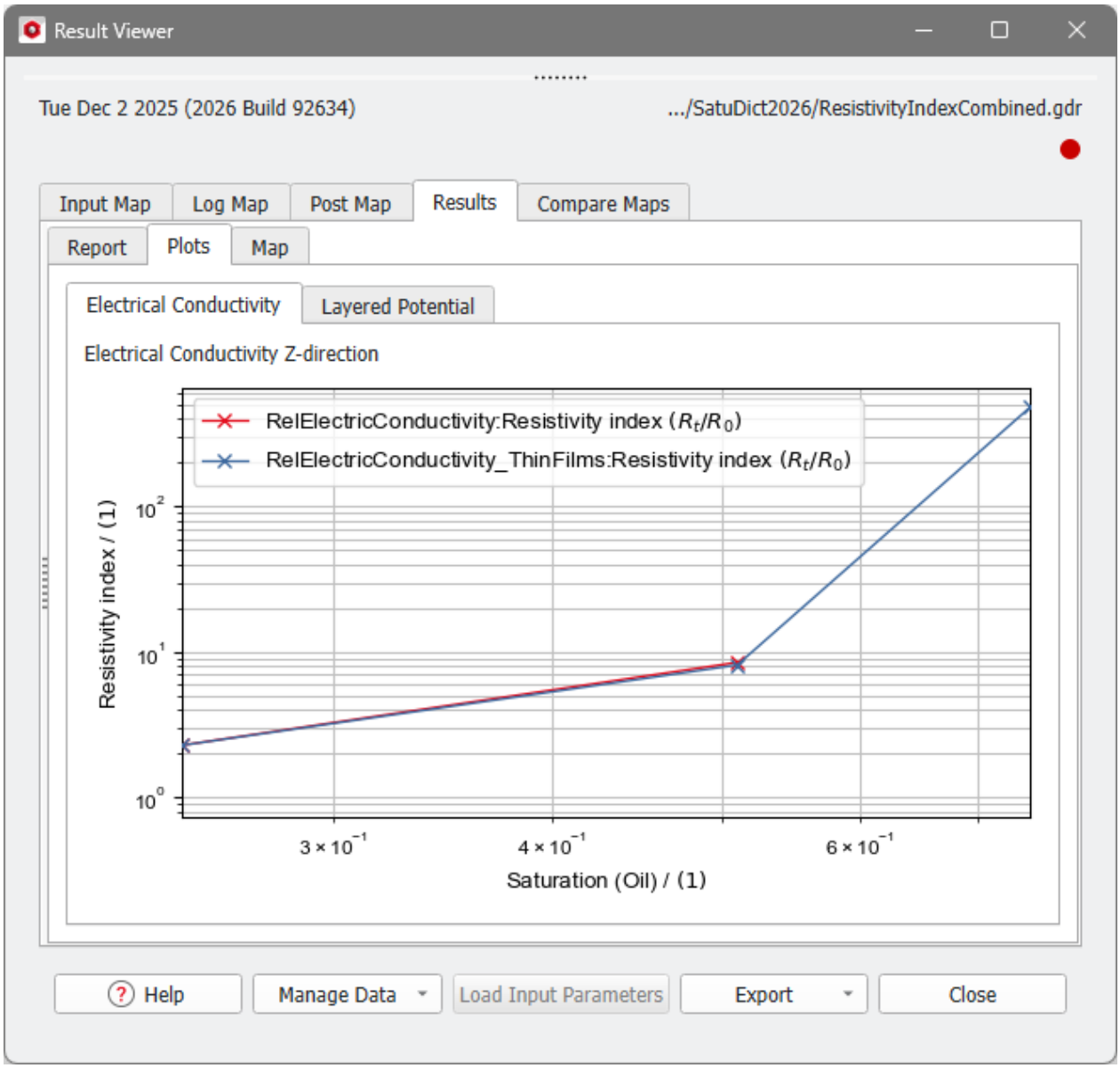
Layered Potential

In the **Layered Potential** tab for each computational direction the potential in each layer is shown in a graph. The saturation values for each graph correspond to the saturation of the invading fluid. 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**.



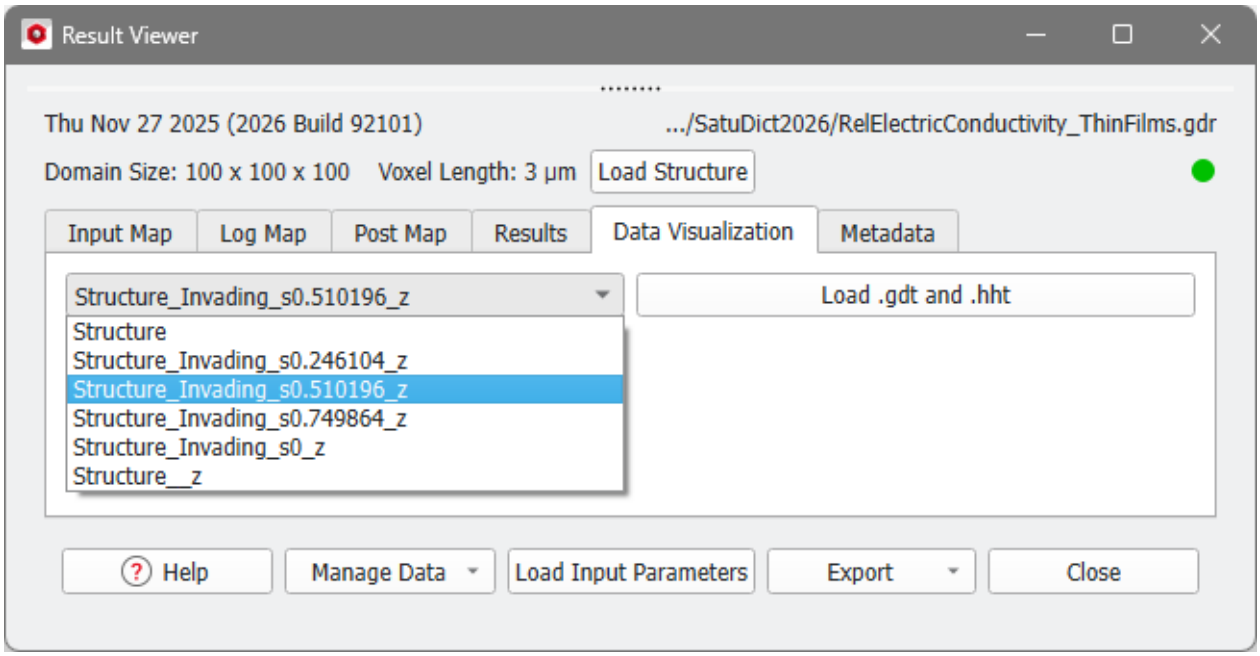
Influence of Thin Films

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%.



Data Visualization

Under the **Data Visualization** tab, the .gdt and .hht files, corresponding to the saturation levels computed, can be opened, as explained in the ConductoDict chapter. No files are available if **Discard PDE Solver Files** 143 was checked in the **Solver** settings tab.



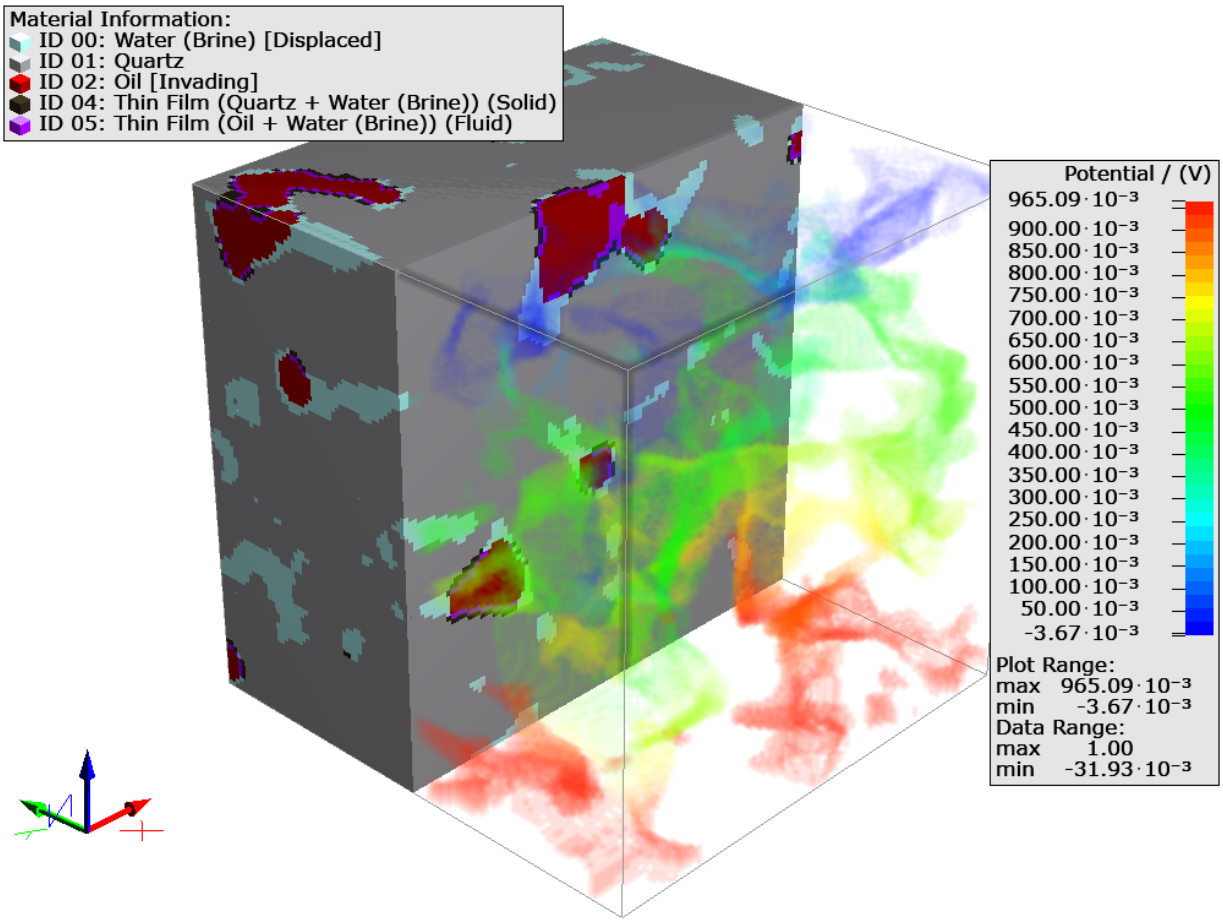
For each selected Computational Direction 142 the solution files for the saturation steps with non-zero conductivity are saved and can be loaded by clicking on the **Load .gdt and .hht** button.

In the structure file (.gdt) you can observe the fluid distribution, while the .hht (homogenized heat) file contains the potential values at each voxel.

Select **Structure** to load the original structure which is saturated with the displaced fluid. No additional .hht file will be loaded.

Select **Structure__z** to load the reference solution (needed to calculate the Resistivity Index), where the structure is fully saturated with Water (Brine).

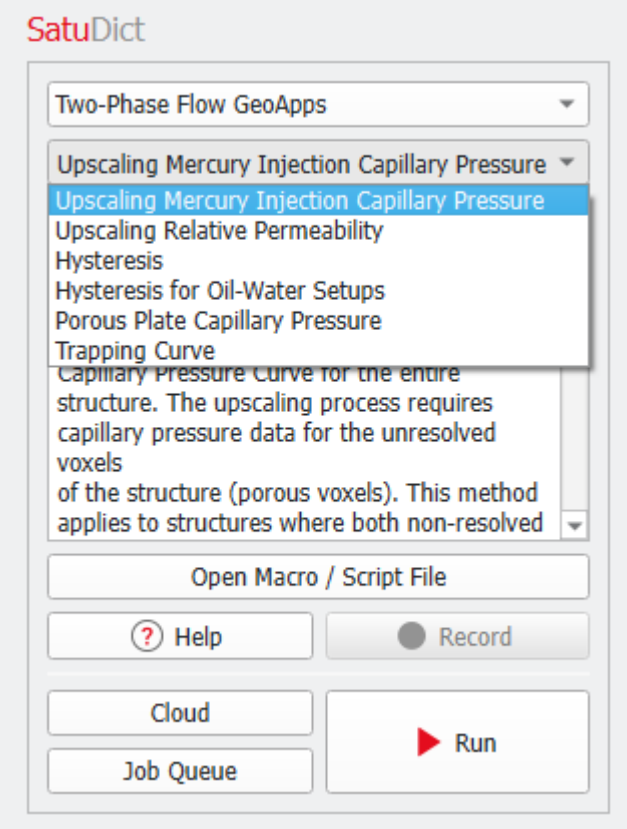
Shown below is the .gdt file for a 51% invading fluid saturation level. The solid phase (Quartz) is shown together with the Displaced fluid (Water) and the Invading Fluid (Oil). The right part of the image shows the potential field of the Water with transparent effect on the clipped structure model.



More information about the visualization parameters is available in the Visualization chapter.

1.8 Two-Phase Flow GeoApps

Under **Two-Phase Flow GeoApps**, predefined computation settings can be chosen from the pull-down menu. The SatuDict **Two-Phase Flow GeoApps** are GeoDict macros containing combinations of SatuDict commands with certain default parameters to mimic experiments or real observations.



By clicking the **Edit...** button, the corresponding parameter dialog box opens and the parameters defining the saturation experiments are displayed and can be modified. After choosing the options click **OK** to close the dialog, and then **Run** to execute the computation.

The Two-Phase Flow GeoApps

- Upscaling Mercury Injection Capillary Pressure 163
  Conduct a MICP experiment for structures containing both resolved and unresolved porous materials.
- Upscaling Relative Permeability 167
  Predict relative permeability and capillary pressure curves for structures containing both resolved and unresolved porous materials.
- Hysteresis 170
  This GeoApp executes the Drainage and Imbibition algorithms alternately.
- Hysteresis for Oil-Water Setups 174
  Predict a Capillary Pressure Hysteresis Cycle in an oil-water setup.
- Porous Plate Capillary Pressure 178

The Two-Phase Flow GeoApps

Run a Porous Plate Capillary Pressure (PPCP) simulation.

- Trapping Curve
  Creates a trapping curve for the currently loaded structure and given contact angle.

Add Predefined Computations

Click the **Open Macro / Script File** button, to open the macro file containing all steps for the predefined simulations with the default text editor. You can then check or edit the syntax of the computation steps. The modified scripts can be added as custom GeoApp as described in the GeoApps chapter.

1.8.1 Upscaling Mercury Injection Capillary Pressure

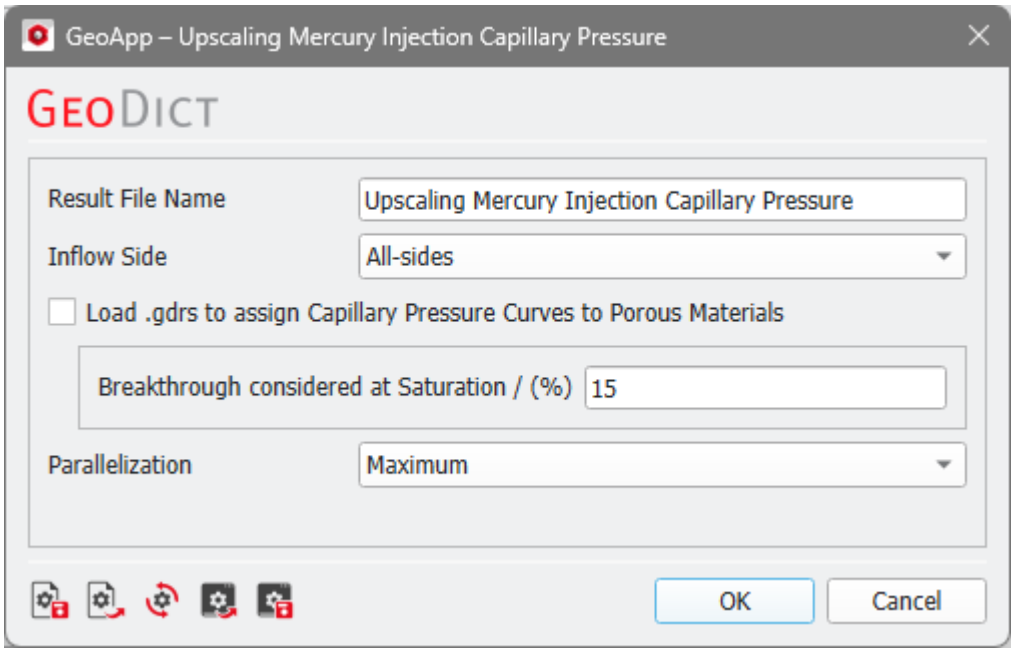
The **Upscaling MICP** GeoApp is a comprehensive solution for analyzing complex porous media, effectively bridging the gap between small-scale, detailed experiments and large-scale, practical applications. This capability is essential for improving the precision of simulations, enhancing material performance predictions, and making informed decisions in various industrial and research contexts.

This GeoApp computes the MICP on structures with unresolved porous materials. For those materials, no exact fluid distribution can be calculated as the location of the pores is unknown. However, you can determine or measure the capillary pressure curve of the porous material at a higher scale and use this information for the computations in the GeoApp.

Important! The structure you want to analyze must contain at least one porous material phase.

Modules needed to run this GeoApp:

SatuDict, GeoApp-Upscaling MICP

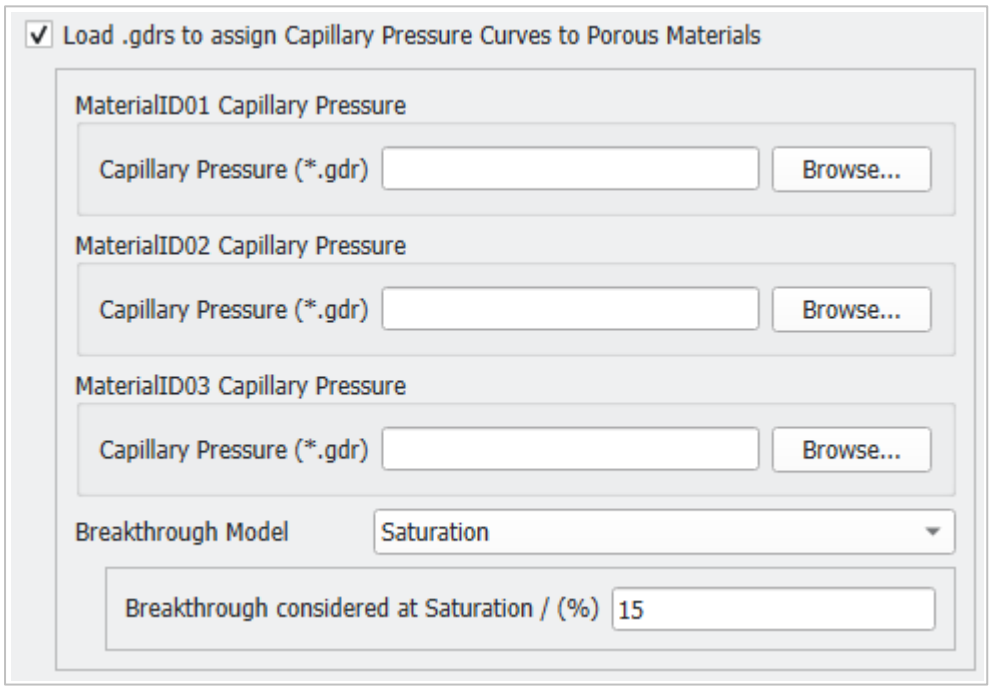


At the top of the dialog, enter the **Result File Name**. The result file is saved in the chosen project folder (**File → Choose Project Folder** in the menu bar).

Below, choose from which domain sides the mercury may intrude the structure. Either **All-sides** can be chosen, or one specific domain side (e.g., z+) is available.

Next, you have to define from which source the capillary pressure curve values are taken.

Load .gdrs to assign Capillary Pressure Curves to Porous Materials



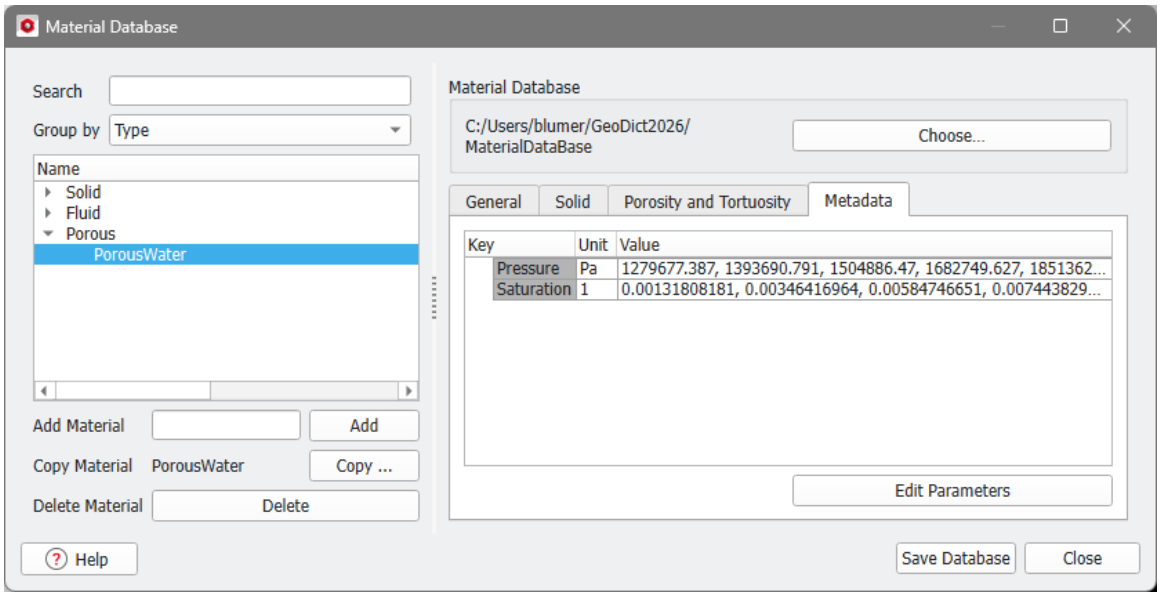
Load pre-computed result files of Capillary Pressure for all porous material phases according to the Material IDs. For the materials you have to specify at which saturation

the porous region is filled enough to establish a continuous pathway through the material securing capillary connectivity.

With the **Breakthrough Model** you decide to either use a fixed **Saturation** (enter the value under **Breakthrough considered at Saturation**), or the **Thomeer**[12] fit based on the Capillary Pressure Curve result files is used.

Define capillary pressure values in the material properties

With this option you have to add and edit the porous material in the Material Database. Enter the pressure and saturation values in the Metadata tab and use the keys **Pressure** and **Saturation**, respectively.

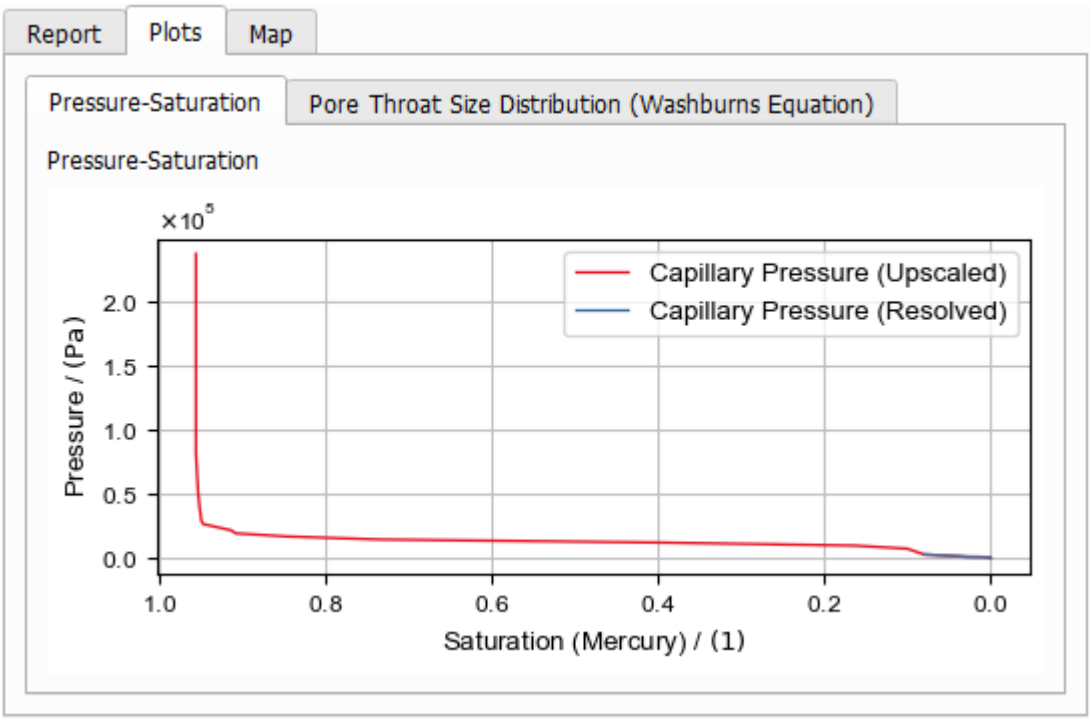


In this case, no choice of **Breakthrough Model** is available, you can only enter a value for **Breakthrough considered at Saturation**.

For the **Parallelization** of the execution either use the **Maximum** number of cores or enter a **Manual** value.

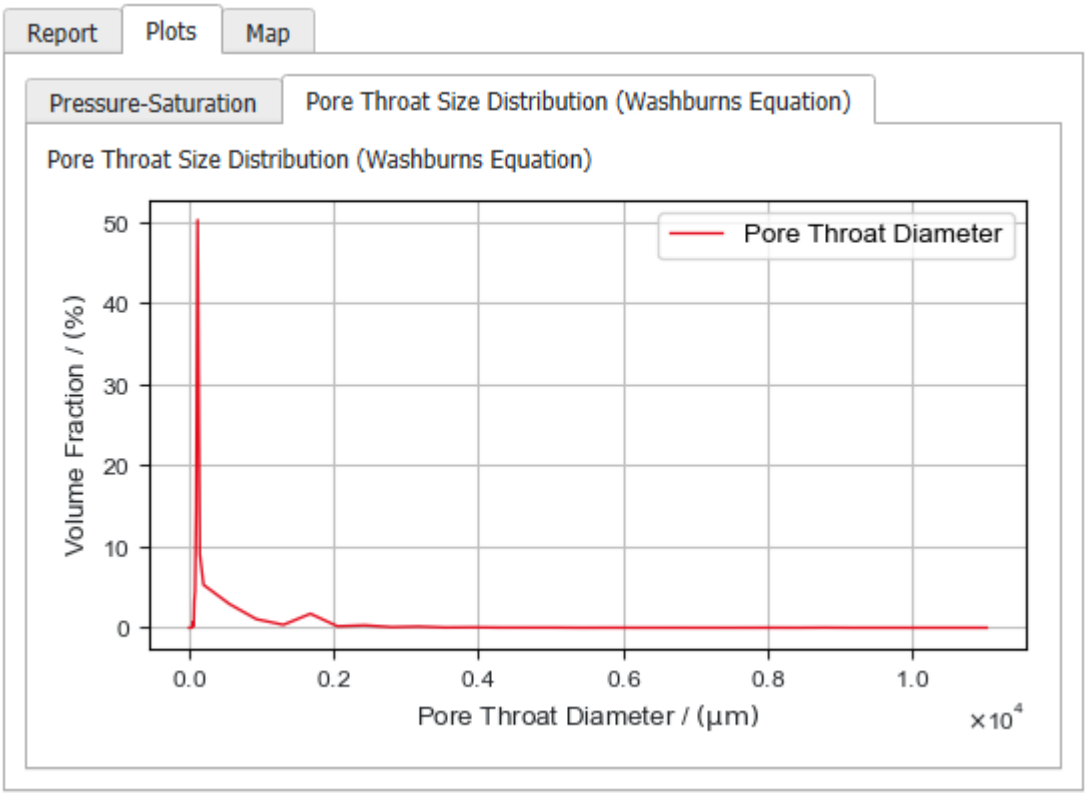
Results

The result file shows the capillary pressure curve, where the resolved part, which could be calculated with the Mercury Porosimetry & Capillary Pressure[49] command, and the upscaled (unresolved) part are marked.



Note! No residual is left in the structure, except the closed pores, which cannot be filled with mercury as they are not connected to any inflow side. Thus, the mercury saturation is not exactly 100%.

Additionally, the pore throat size distribution calculated with the Washburn equation[5] is given as in the result file[53] of the MICP command.

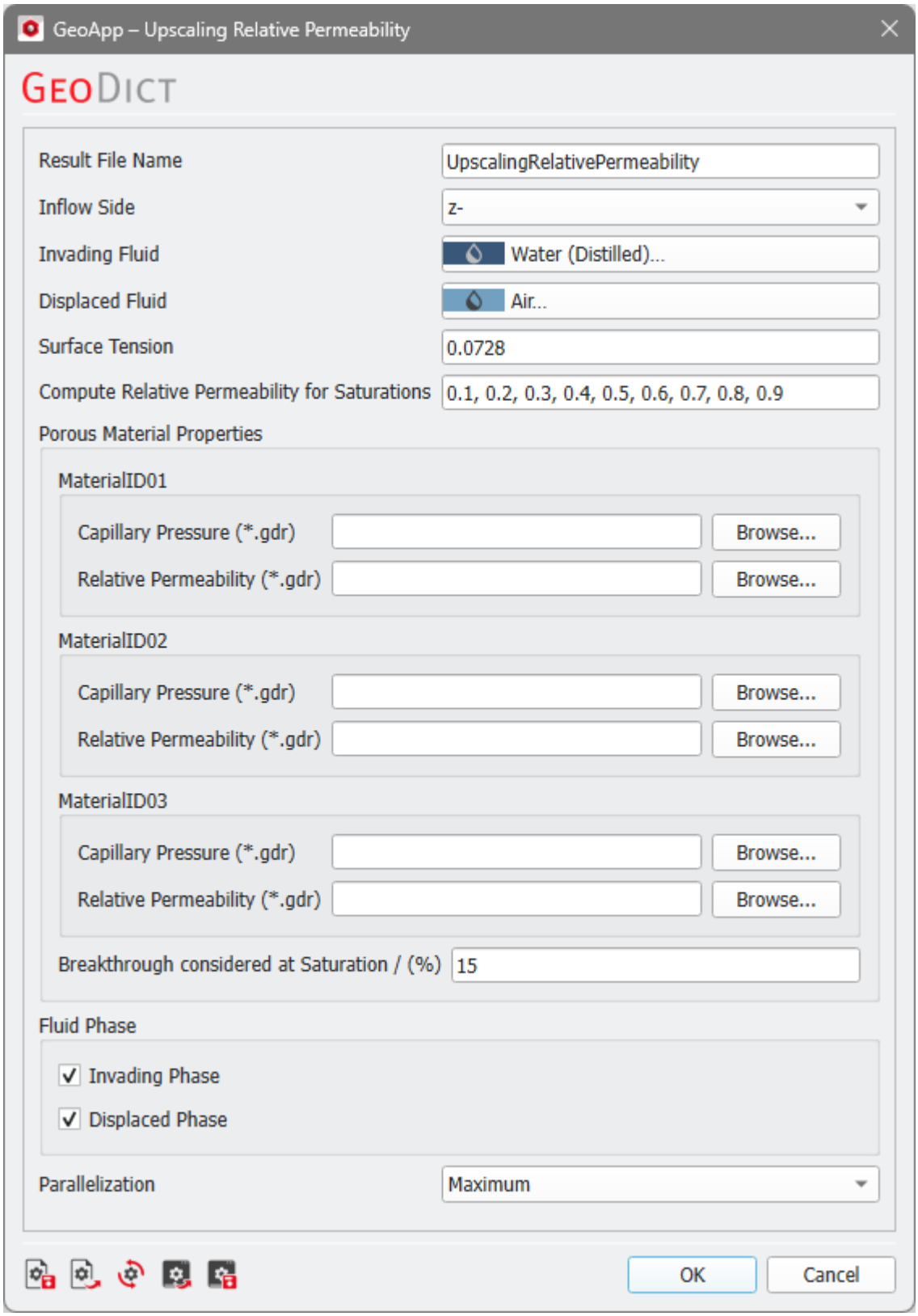


1.8.2 Upscaling Relative Permeability

The **Upscaling Relative Permeability** GeoApp allows you to compute relative permeability and capillary pressure curves for structures containing both resolved and unresolved porous materials. For the unresolved materials you need to pre-compute the capillary pressure curve and relative permeability on a higher resolution scale.

Modules needed to run this GeoApp:

SatuDict, GeoApp-Upscaling Relative Permeability



At the top of the dialog, enter the **Result File Name**. The result file is saved in the chosen project folder (**File → Choose Project Folder** in the menu bar).

Below, choose the **Inflow Side**, which defines from which domain side the invading fluid may enter the structure.

The **Invading Fluid** and the **Displaced Fluid** must be chosen from the Material Selector. Note, that the displaced fluid must be present in the loaded structure.

The **Surface Tension** between the fluids works as described for Capillary Pressure Curve 18.

To **Compute Relative Permeability for Saturations** you enter the saturations as comma separated list. They work in the same way as for the Relative Permeability 66 command.

For the **Porous Material Properties** you have to load a Capillary Pressure Curve and a Relative Permeability result file (*.gdr) for each of the porous material phases. Up to three porous materials can be present in the structure and they have to be assigned the Material IDs 01, 02, or 03.

Important! We strongly recommend, that the capillary pressure curve result files are computed with the same fluids and surface tension as entered in this dialog. Otherwise the phase distribution and thus the permeability may not be correct. The contact angles of the fluids are taken from the capillary pressure curve result files.

Important! For the relative permeability result files select the computational direction according to the Inflow Side you want to choose in this dialog. This means if you choose **z-** as inflow plane, you have to compute the relative permeability in **Z** direction.

The two parameters, **Breakthrough considered at Saturation** and **Parallelization** are explained in Upscaling Mercury Injection Capillary Pressure 163.

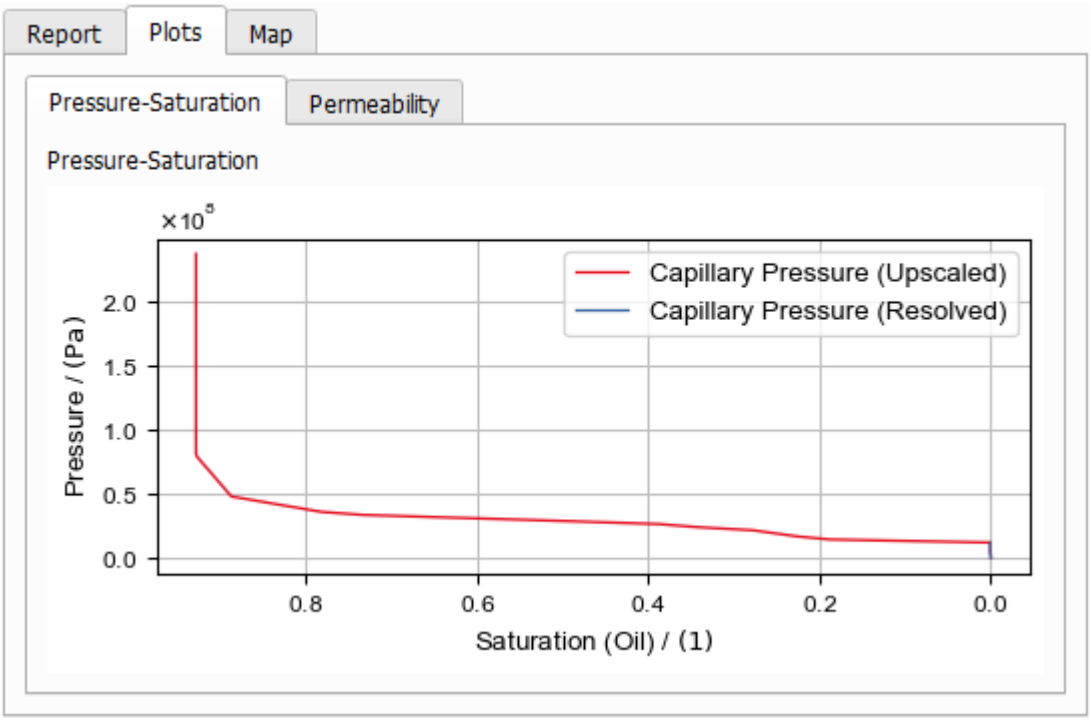
Additionally, you can check whether the Relative Permeability should be computed for the **Invading Phase** and/or the **Displaced Phase**.

During the calculation, first a capillary pressure curve is computed, where the displaced fluid can leave a residual. For the resolved pores, the saturation points from this run are taken for the relative permeability calculation, where the entered saturation points are approximated as in the Relative Permeability 91 command.

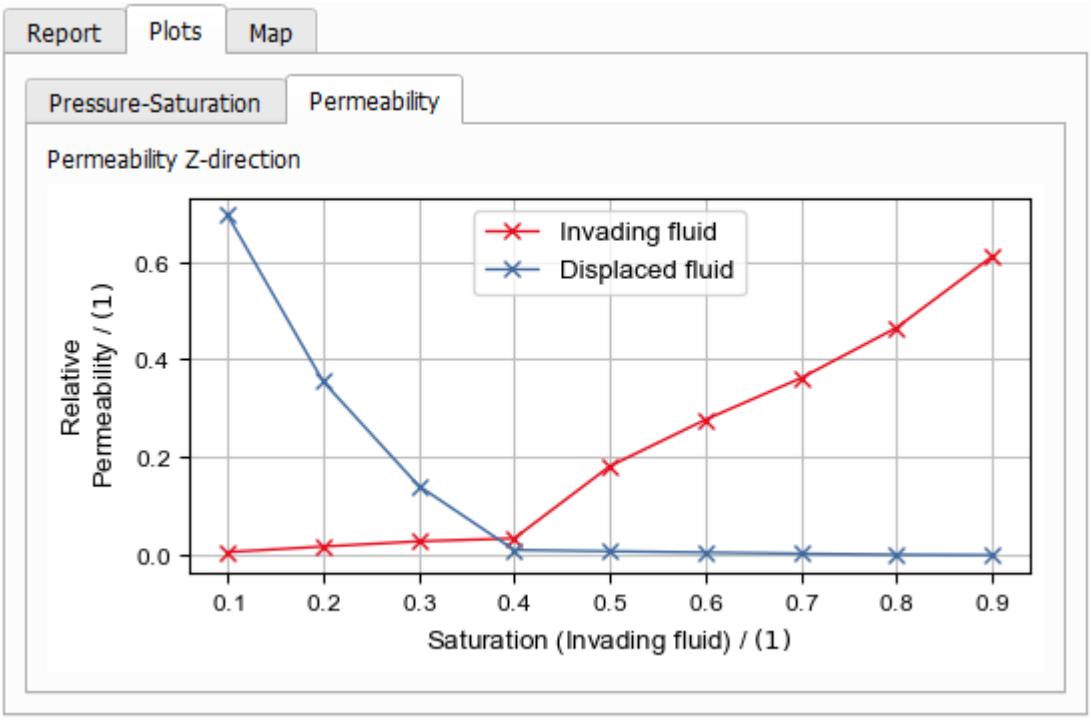
For the unresolved porous materials, the input result files are used for the capillary pressure curve and the relative permeability values.

Results

In the result file, the **Pressure-Saturation** plot shows the capillary pressure curve with the parts for the resolved and unresolved parts similar as in the Upscaling MICP GeoApp 163.



The **Permeability** plot is the same as for the Relative Permeability Plot 94.



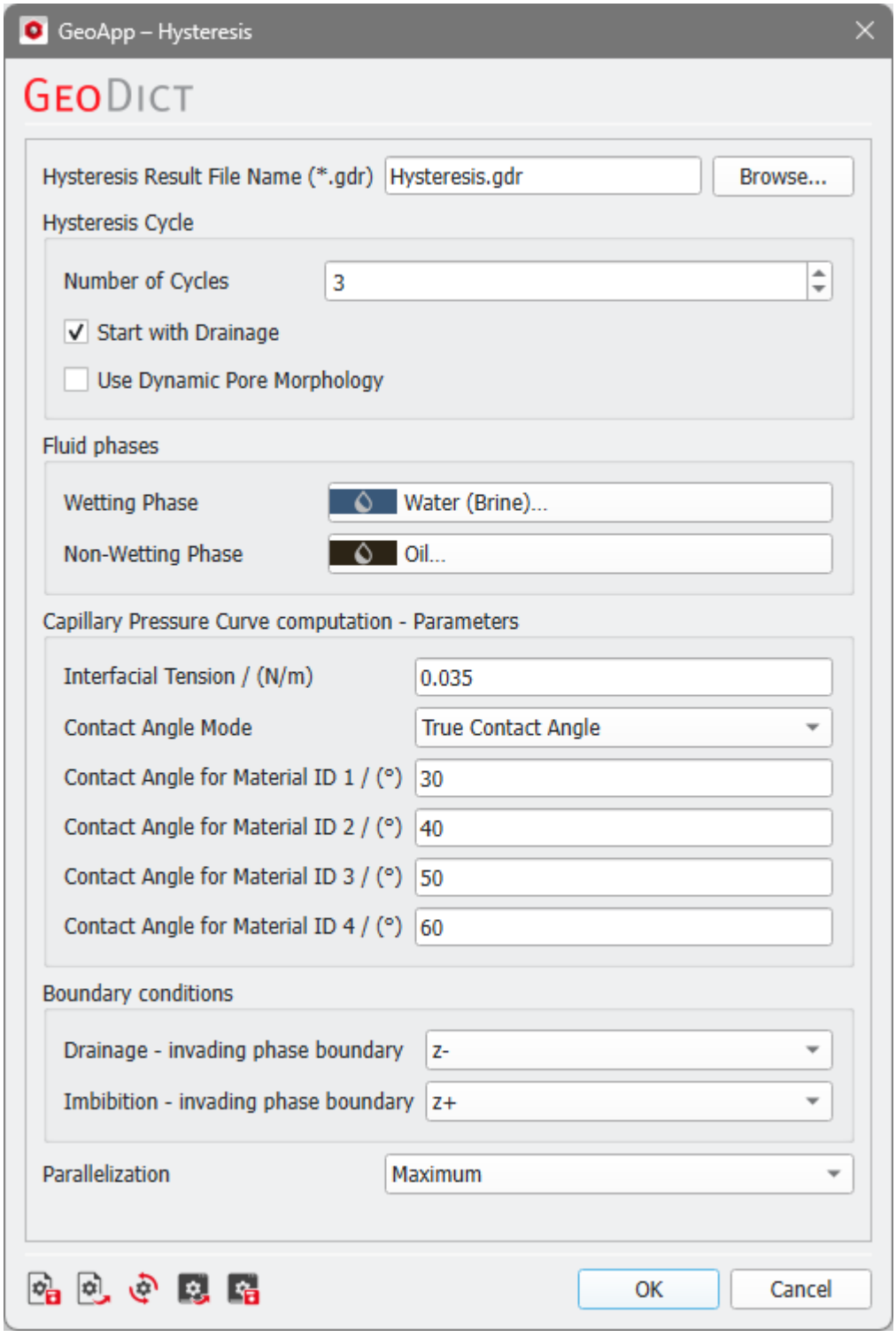
1.8.3 Hysteresis

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 in Capillary Pressure with Hysteresis Effect 44 until the chosen **Number of Cycles** is reached.

Modules needed to run this GeoApp:

SatuDict

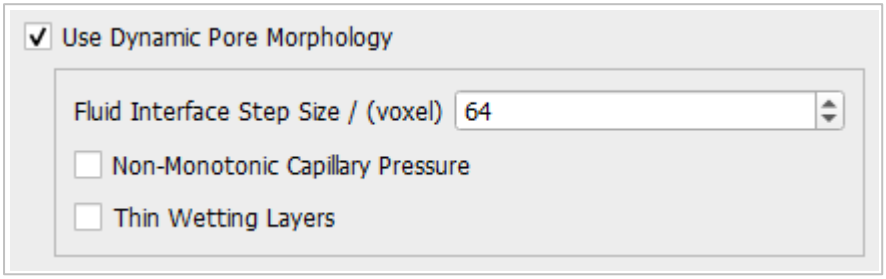
After clicking **Edit...**, enter the **Hysteresis Result File Name** and the necessary parameters.



Hysteresis cycle

Enter the desired **Number of Cycles**, which means the number of SatuDict computations. The minimum value is 2, so that at least one drainage and one imbibition simulation will be performed. Check the box **Start with Drainage?** to first compute a drainage simulation, otherwise an imbibition will be simulated at the beginning. In the example shown above, 3 SatuDict simulations are done: first a drainage, followed by an imbibition, and finally a secondary drainage.

You can decide to **Use Dynamic Pore Morphology** 24, which has the same options as in the Capillary Pressure Curve command. Additionally, you can set the **Fluid Interface Step Size** 28 as in the Solver Parameters tab of Capillary Pressure Curve.



Fluid phases

With **Wetting Phase** and **Non-Wetting Phase** select the fluids involved.

Important! If you start the computations with a **Drainage** simulation, the **Wetting Phase** must be present in the loaded structure. Similarly, if you decide to start with an **Imbibition** simulation, the **Non-Wetting Phase** has to be present at the beginning. The reason is, that in the simulations the corresponding fluid will be displaced.

Capillary Pressure Curve computation - Parameters

Set the **Interfacial Tension**, the **Contact Angle Mode**, and the **Contact Angle** with respect to the **Wetting Phase** for up to four solid material phases. The parameters are similar to those from Capillary Pressure Curve 18, except that the contact angle mode Constant Contact Angle is not available here.

Boundary conditions

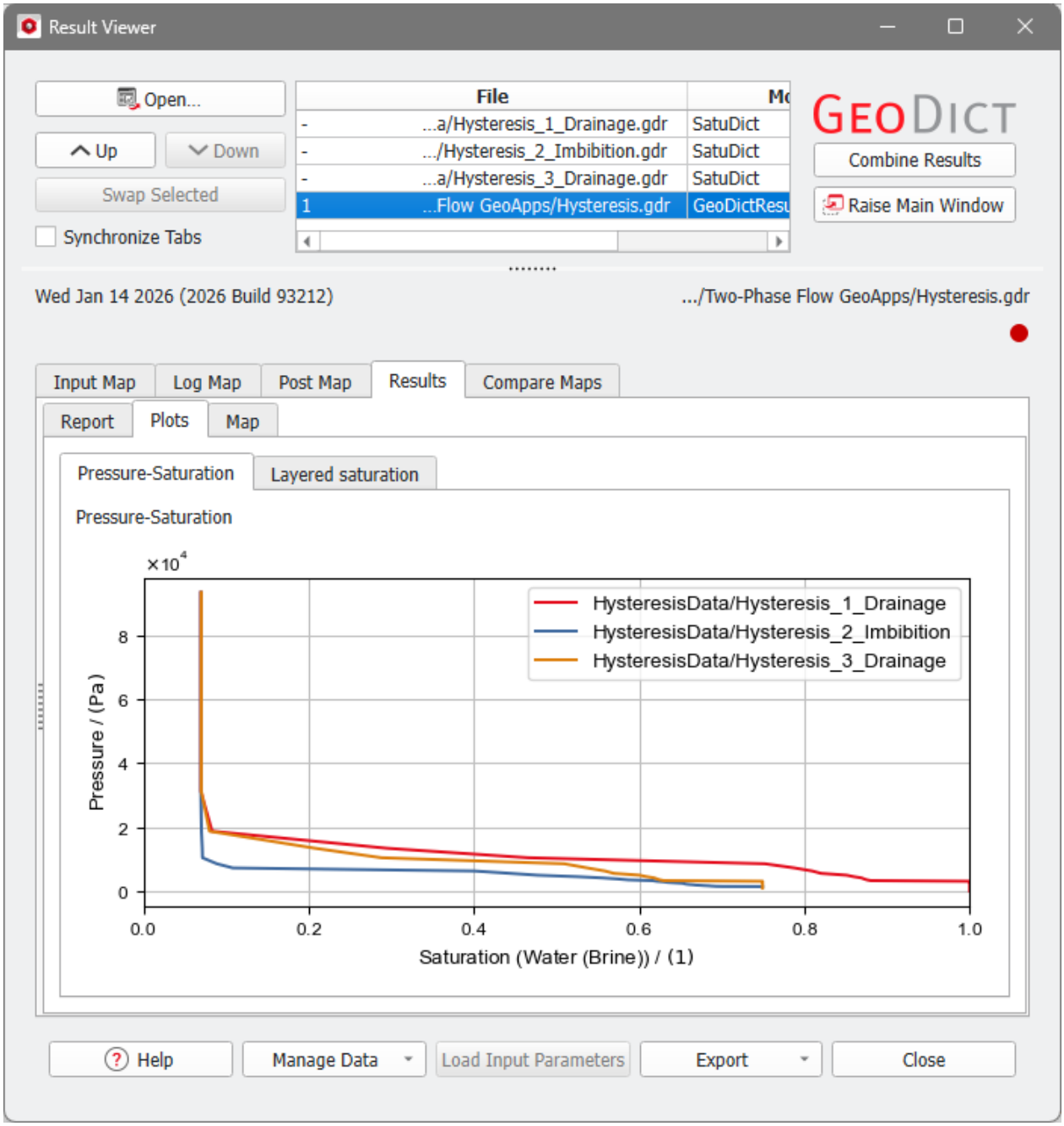
Select the **invading phase boundary** for both Drainage and Imbibition. The other five domain boundary sides are set to **Displaced Fluid Outlet** (see also Boundary Conditions) 25.

Parallelization

Choose to compute with **Maximum** parallelization or set a **Manual** number of threads.

Results

After the **Hysteresis** computation 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.



1.8.4 Hysteresis for Oil-Water Setups

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

Modules needed to run this GeoApp:

SatuDict

Click **Edit** to open the **Hysteresis for Oil-Water Setups Parameters** dialog.

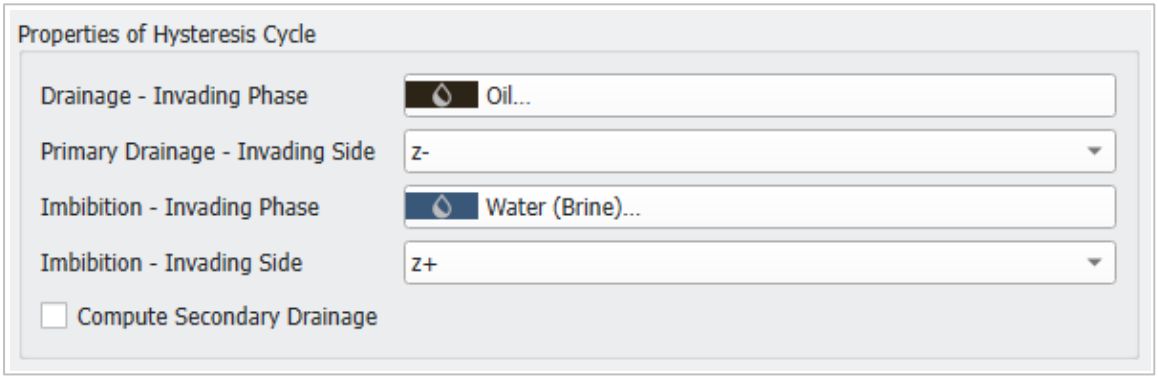
Select a **Result File Name** fitting to the current project.

The parameters are organized into three groups:

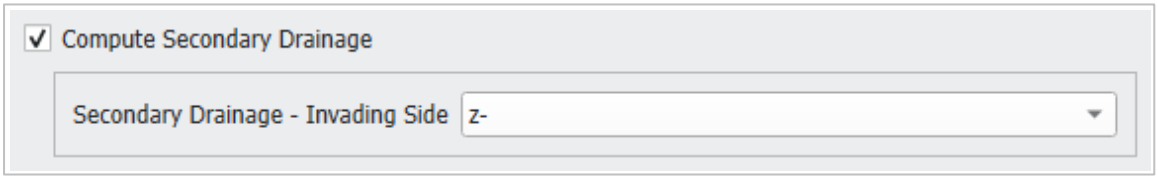
Properties of Hysteresis Cycle

Define the **Properties of Hysteresis Cycle**.

Select a material for the **Drainage – Invading Phase** and set the **Primary Drainage – Invading Side**. Choose an **Imbibition - Invading Phase** and set the **Imbibition – Invading Side**.



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

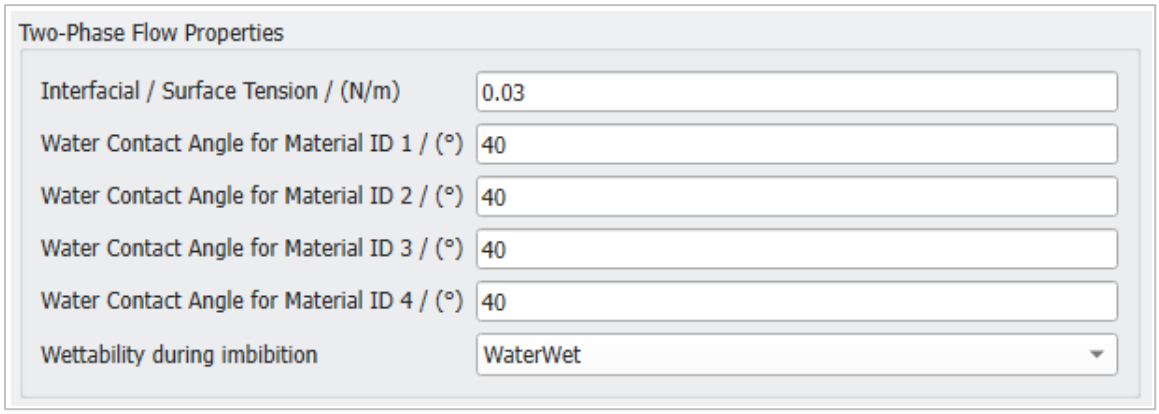


Two-Phase Flow Properties

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

Define the **Interfacial / Surface Tension** in N/m between the two material phases, e.g., water and oil. At the beginning the structure is filled with water and all solids are water-wet. For up to four solid materials the **Water Contact Angle** can be set. During

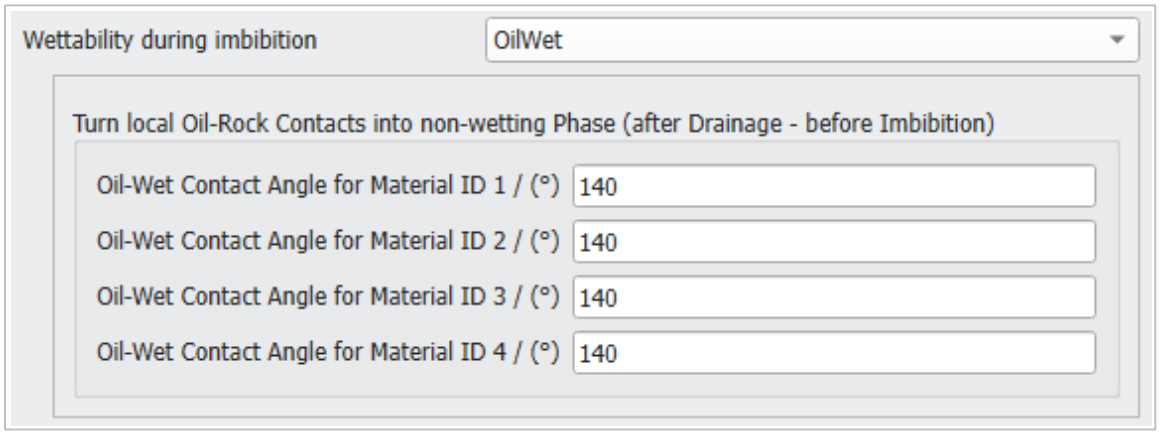
the primary drainage simulation oil enters the structure. The contact angle of the solids to the oil is $180° - \theta_w$, where θ_w is the Water Contact Angle.



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

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

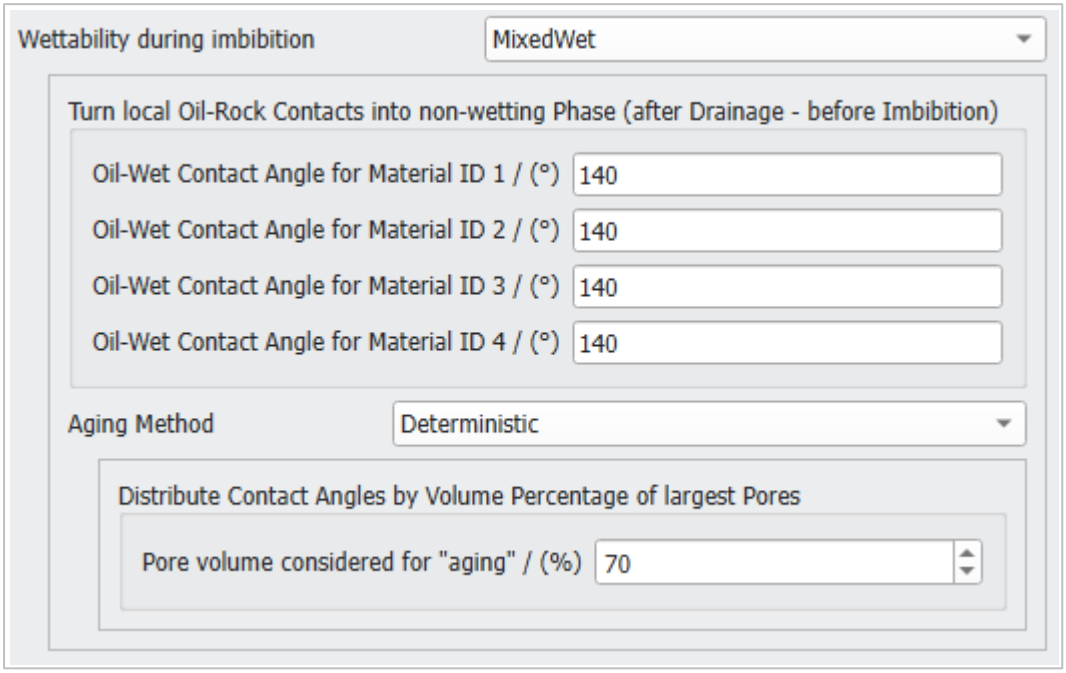
In the case of a changing wettability, the new contact angles for the oil-rock contacts must be defined. Again, for up to four solid material IDs the **Oil-Wet Contact Angles** can be defined.



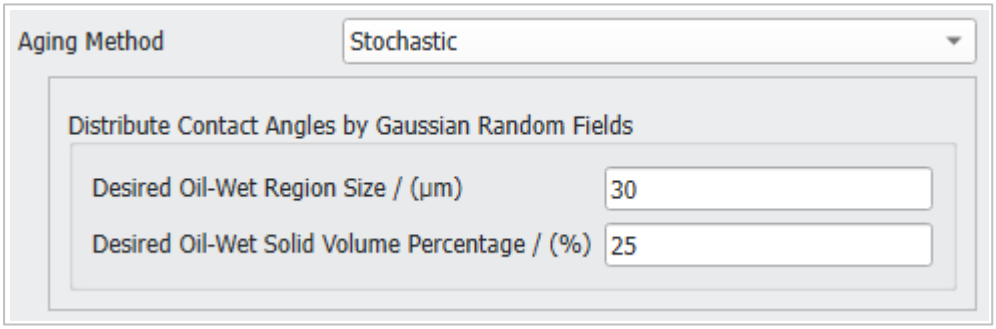
For a **MixedWet** set-up additionally the distribution of the oil-wet solids must be specified. First, select an **Aging Method** and then set the corresponding parameters. The aging method introduces which surfaces change their wettability after the primary drainage and before the imbibition.

For a **Deterministic** aging method, the wettability is changed at surfaces in large pores and in contact with the invading oil. The **Pore volume considered for "aging"** defines

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



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

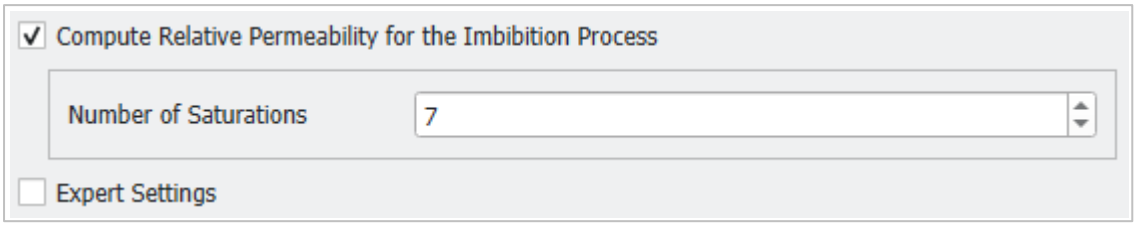


Find out more about the aging methods in the Simulate Aging GeoApp chapter.

Others

To compute the relative permeability during the imbibition check **Compute Relative Permeability for the Imbibition Process**. Define the **Number of Saturations** for

which to compute the relative permeability. The default number of 7 means that for seven different saturations of the structure the permeability is computed. Increase the number to obtain more data points on the relative permeability curve.



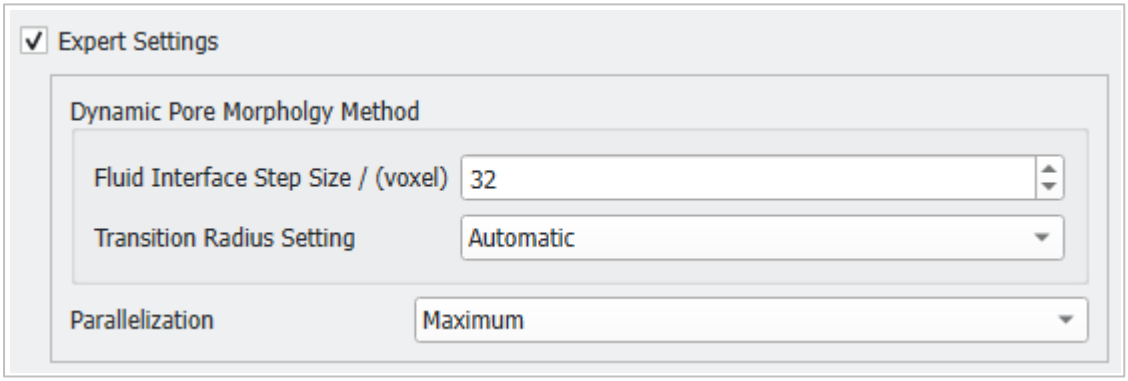
Finally, determine the **Expert Settings**. Here, define the **Dynamic Pore Morphology Method** parameters and the **Parallelization**.

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

The imbibition starts with the spontaneous imbibition part. At some point, defined by the **Transition Radius**, the imbibition changes from spontaneous to forced:

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

For the **Parallelization** of the execution either use the **Maximum** number of cores or enter a **Manual** value.



Click **OK** to save the settings. Click **Run** to perform the hysteresis simulation.

Results

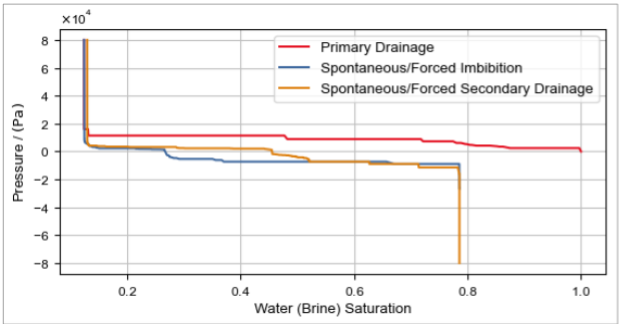
When the simulation is finished, the result file automatically opens in the **Result Viewer**.

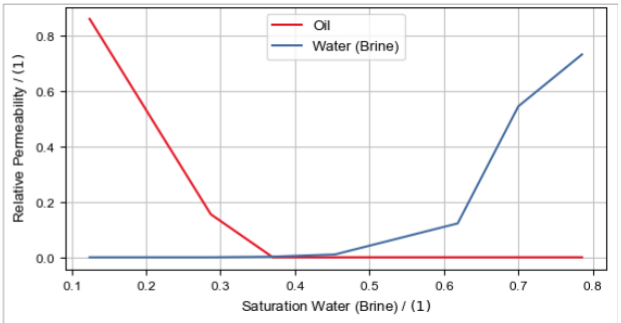
The **Results - Plots** tab contains plots for **Hysteresis**, **Relative Permeability**, and **Relative**

Permeability at irreducible Water (Brine) Saturation.

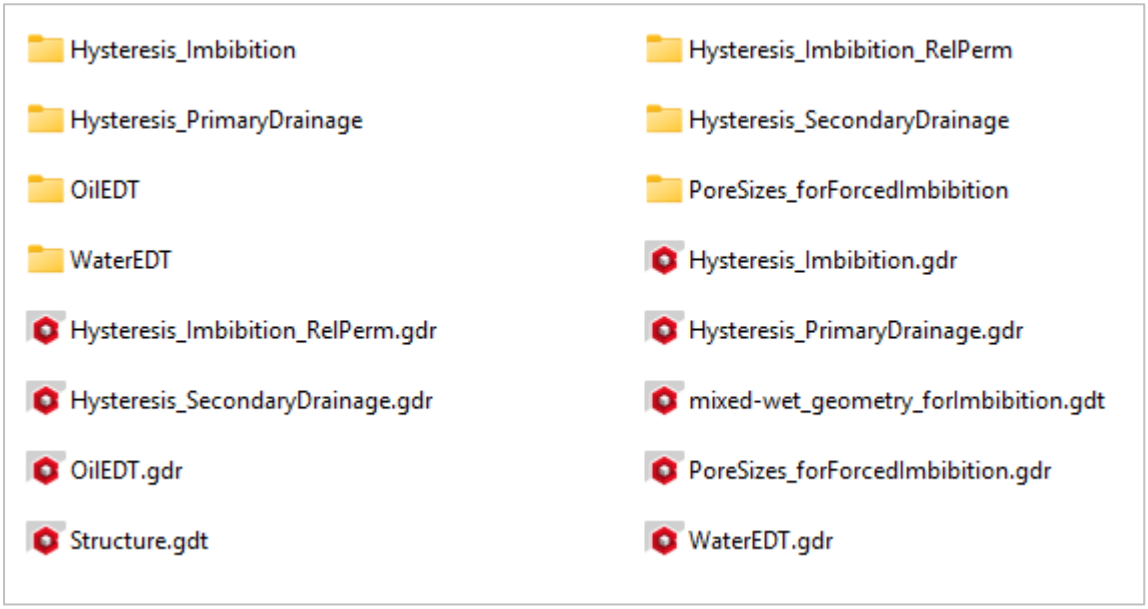
To obtain the **Relative Permeability** values, the permeabilities of the different saturation steps are divided by the absolute permeability.

For the **Relative Permeability at irreducible Water (Brine) Saturation** the effective permeability of the state with irreducible water saturation (at the end of the primary drainage) is used for normalization.





Several result files and result folders are generated and can be found in the project folder. The prefix is based on the chosen **Result File Name** (default is Hysteresis).



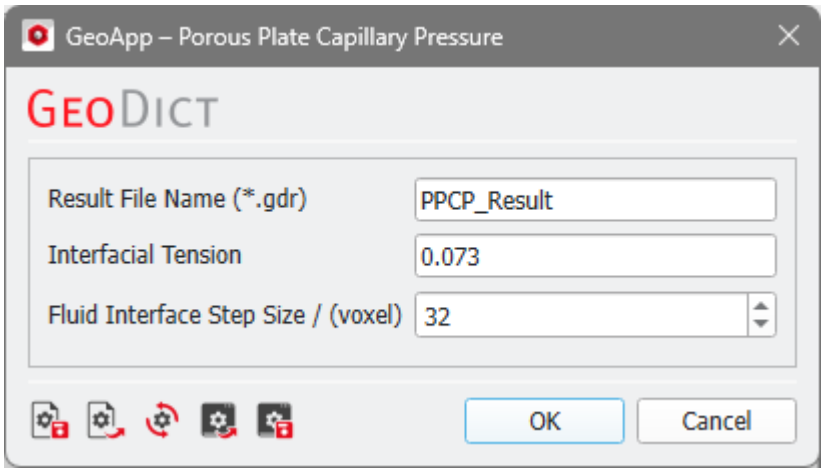
1.8.5 Porous Plate Capillary Pressure

The **Porous Plate Capillary Pressure** GeoApp fills the pore space of the current structure with water. Then, air invades the structure from all but one side. The face in Z- direction is connected to a porous plate. The **Porous Plate Capillary Pressure** app is similar to the MICP 49 command, but here air displaces water.

Modules needed to run this GeoApp:

SatuDict

Click **Edit** to open the **Porous Plate Capillary Pressure Parameters** dialog.



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

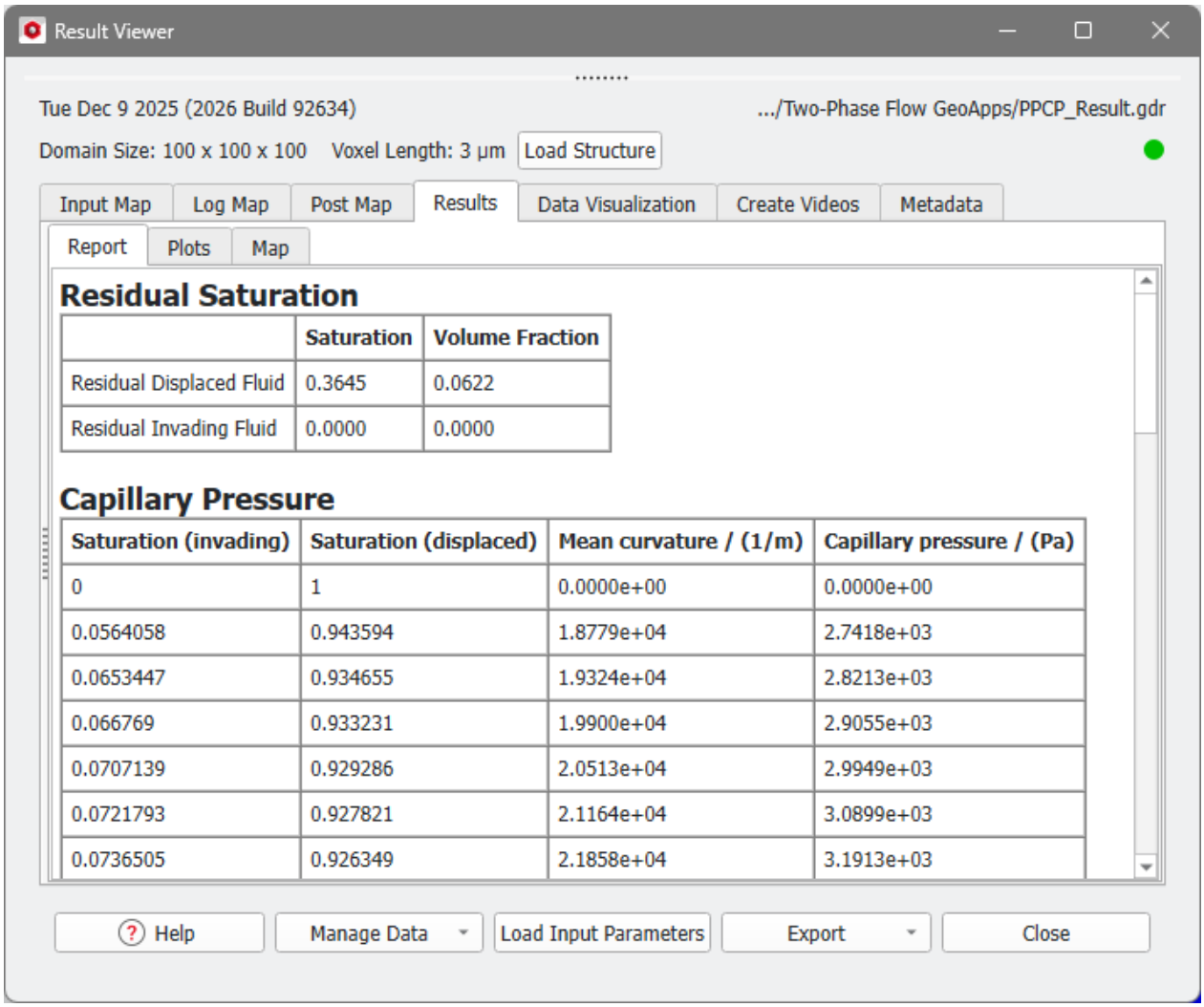
Two parameters can be defined:

- Set the **Interfacial Tension** in N/m between water and air. The given default value refers to the value at 20°C for an air contact angle of 140°. The air contact angle cannot be changed.
- The **Fluid Interface Step Size** determines the range of voxels that can be maximally saturated within one pressure step. Lower values might increase the runtime and the number of saturation steps significantly, but give a more realistic development of the saturation process.

Click **Run** to perform the porous plate capillary pressure simulation. The pore space is filled with water, then air invades the structure from all sides except for Z-.

Results

After the simulation is finished, the result file is opened in the Result Viewer. Refer to the Capillary Pressure Curve Results 31 chapter for more details regarding the results.



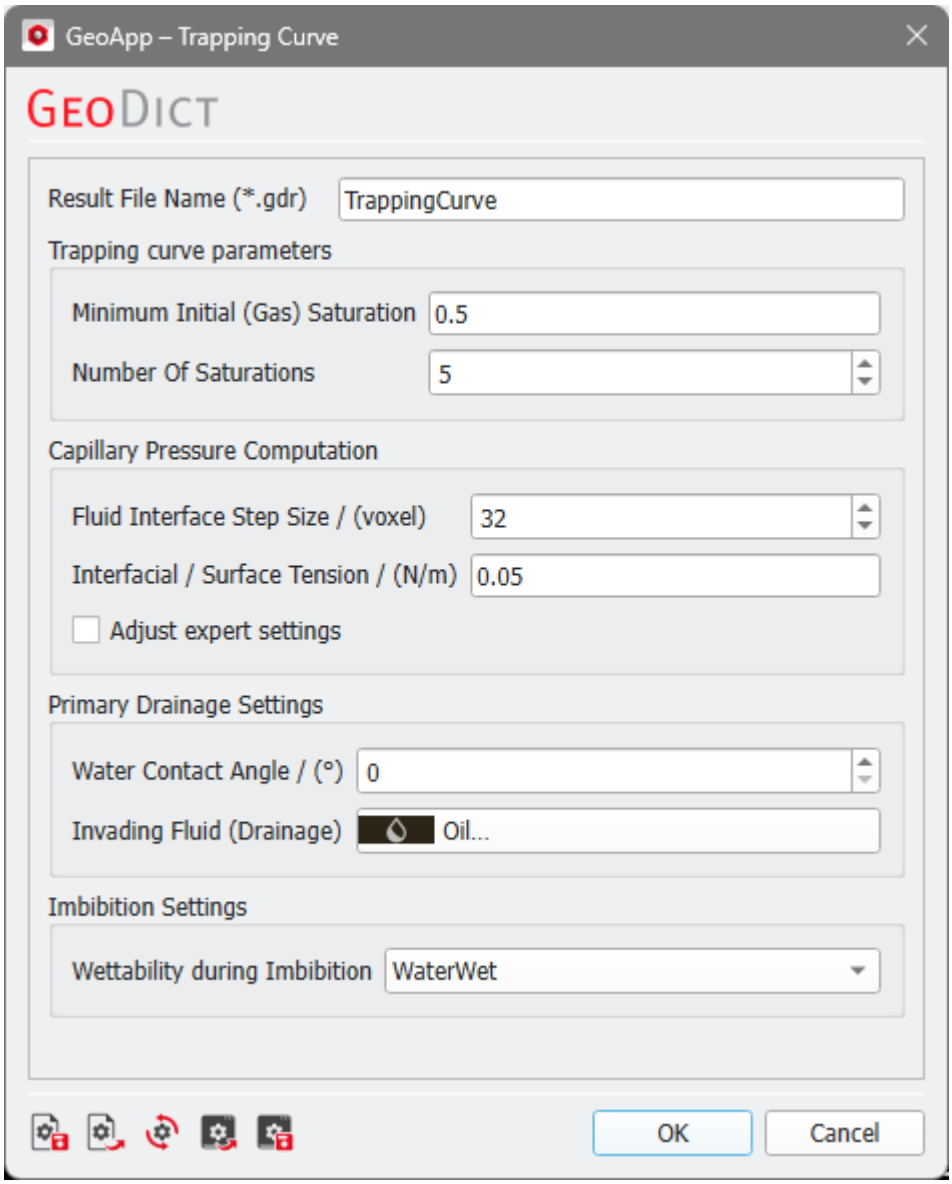
1.8.6 Trapping Curve

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

Modules needed to run this GeoApp:

SatuDict

Click **Edit** to open the **Trapping Curve Parameters** dialog.



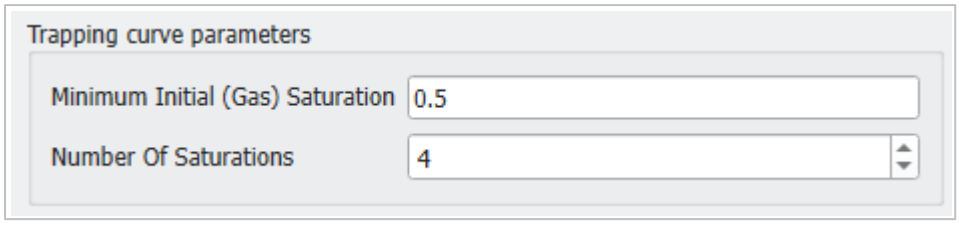
The parameters are organized in four groups:

Trapping curve parameters

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

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

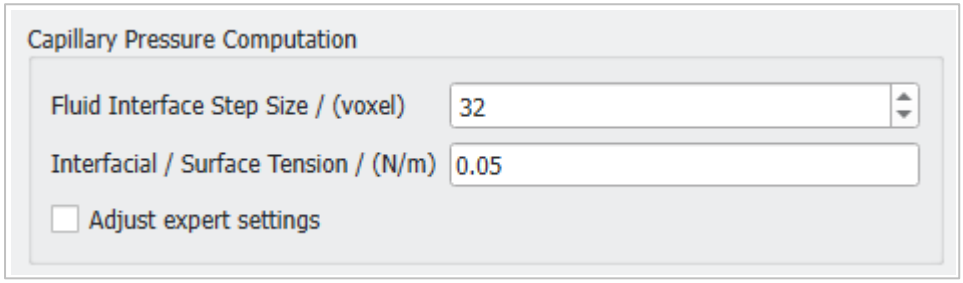
The starting saturations of the invading fluid for the imbibition are distributed between the value entered in Minimum Initial Saturation and 1.



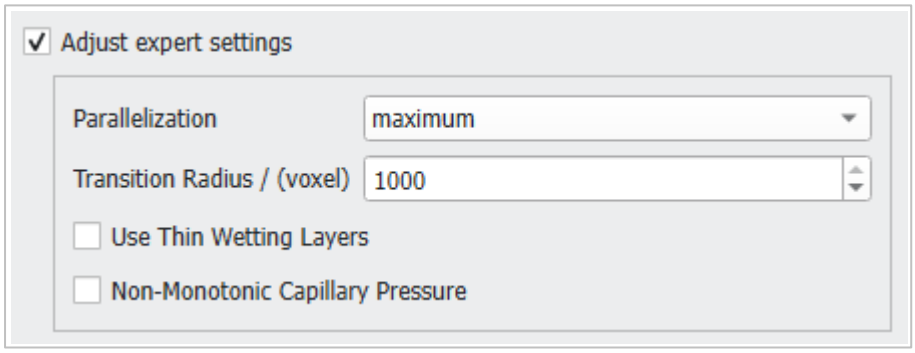
Capillary Pressure Computation

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

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

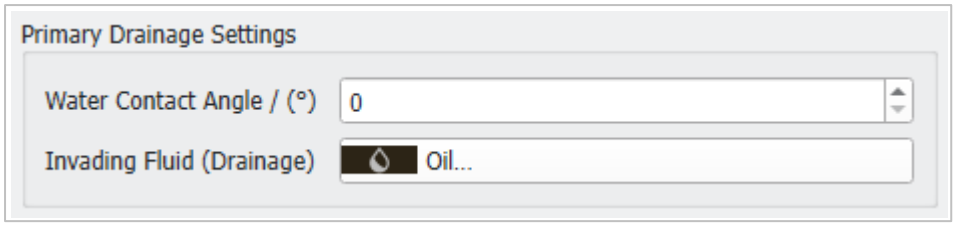


The available **expert settings** include **Parallelization**, **Transition Radius**, and whether **Thin Wetting Layers** and/or **Non-Monotonic Capillary Pressure** should be applied. Refer to the Capillary Pressure Curve 23 chapter for a detailed explanation of these saturation experiment parameters.



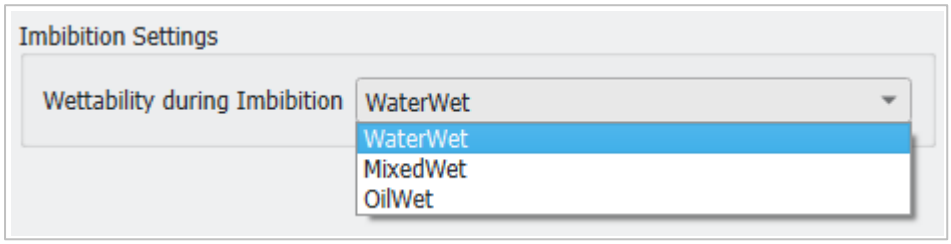
Primary Drainage Settings

By default, the initial pore fluid is water. Enter the **Water Contact Angle** that is used for the primary drainage computation. Select the **Invading Fluid** for the primary drainage from the Material Database.



Imbibition Settings

Set the **Wettability during Imbibition** as explained for the Hysteresis for Oil-Water Setups 174 GeoApp. Note, that here oil-wet means that the solid surfaces covered with the invading fluid (not necessarily oil) change their wettability.

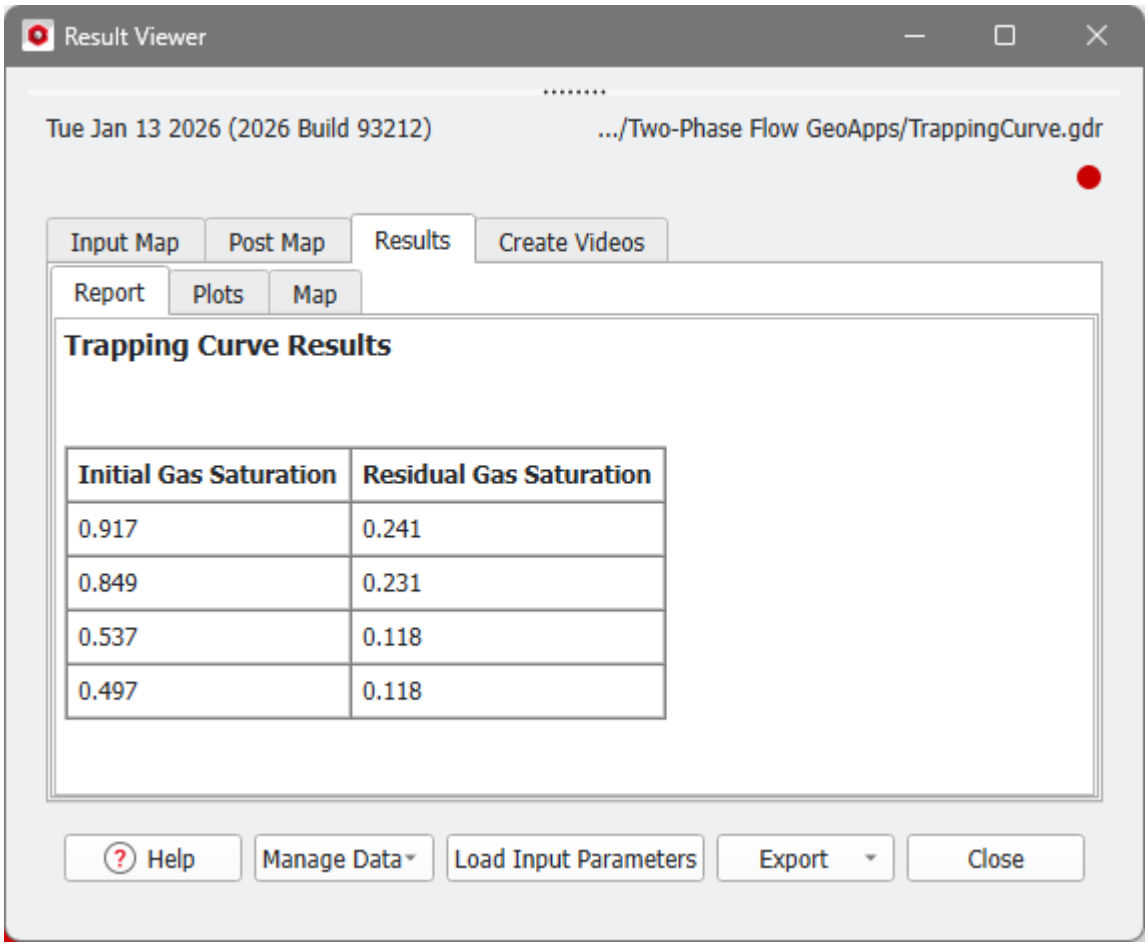


Click **Run** to create the trapping curve.

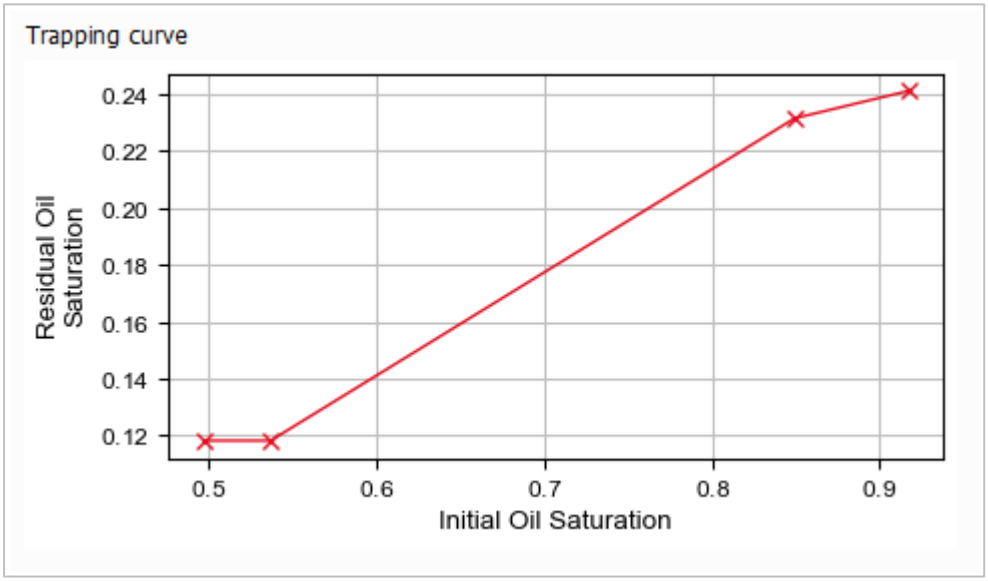
Results

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

The **Results - Report** subtab of the **Result Viewer** shows a table with the saturation of the invading fluid at the beginning of the imbibition (**Initial Gas Saturation**) and after the imbibition (**Residual Gas Saturation**).



These values are also plotted in a **Trapping curve** available in the **Plots** subtab.



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