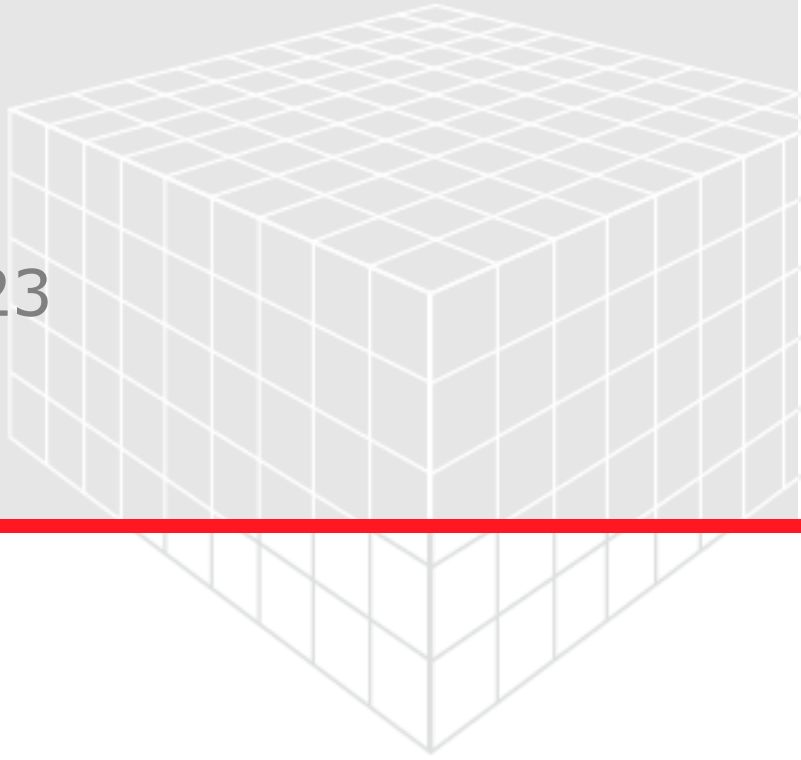
PoroDict



User Guide

GeoDict release 2023

Published: February 14, 2023

GeoDict

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

Citation:
Anne Blumer, Sebastian Rief, Barbara Planas. GeoDict 2023 User Guide. PoroDict handbook. Math2Market GmbH, Germany, doi.org/10.30423/userguide.geodict

The handbooks in the User Guide series of Math2Market GmbH can be obtained from:

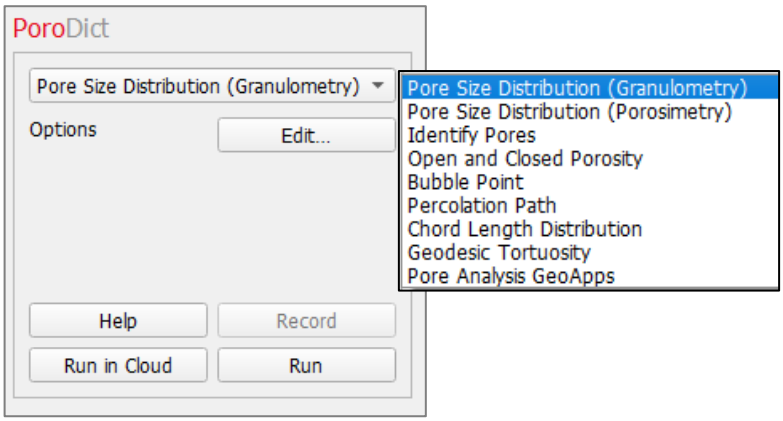
Math2Market GmbH
Richard-Wagner-Strasse 1
67655 Kaiserslautern
Germany

Phone: +49 631 205 605 0
Fax: +49 631 205 605 99
Email: info@math2market.de
Web: www.math2market.de

CALCULATING PORE STRUCTURE CHARACTERISTICS

PoroDict estimates the pore structure characteristics of three-dimensional models of porous media obtained from a µCT or FIB/SEM image or from a 3D model generated with GeoDict.

PoroDict starts by selecting **Analyze** → **PoroDict** in the menu bar. The available commands can be selected from the pull-down menu in the **PoroDict** section.



More commands were available in previous PoroDict versions. These commands (Estimate Surface Area, Estimate Three-Phase Contact Line, Minkowski Parameters, Euclidean Distance Transform) can now be found in MatDict. Since GeoDict 2021 PoroDict's functionality includes the following options:

- In the calculation of the **Pore Size Distribution (Granulometry)**, the algorithm used to determine the size of a pore does not distinguish between through pores, closed pores and blind pores and is in this sense purely geometrical. A pore radius is determined by fitting spheres into the pore volume. To be more precise, a point belongs to a pore of radius *r*, if it is inside a sphere of radius *r*, which can be fitted into the pore space.

- **Pore Size Distribution (Porosimetry)** measurements like Mercury Intrusion Porosimetry (MIP) or Liquid Extrusion Porosimetry (LEP) measure the pore sizes of a media by pressing a non-wetting liquid or gas into the medium and registering applied pressure and absorbed volume. The pressure applied is related to the radius of the pores accessible to the non-wetting liquid, which gives a size distribution of the pores. Due to this method, and in contrast to the approach above, closed pores do not contribute to the pore volume at all. The other pores only contribute to the pore volume fraction if connected to the non-wetting phase reservoir (e.g. the mercury reservoir).

- To **Identify Pores** the Watershed algorithm is used, which is especially useful to optimize mechanical and transport properties of foams and other structures with joined pores. The method introduces a segmentation of the pores, based on a distance transform, which identifies the number of pores, as well as the pore volume. This analysis is also very important to study the complex interconnected pore space in µCT scans of rocks.

- Determination of **Open and Closed Porosity**. In the study of mechanical properties and structural integrity of porous materials, it is important to establish the pore morphology of the porous material. Morphological factors to be determined are the amount and percentage of open and closed pores, and the

total pore volume percentage. Open pores are extensive networks of interconnected pores, leading from the surface to the core in any of the Cartesian directions. In contrast, isolated pores which do not open to the surface in any direction are referred to as closed pores.

- **Bubble point** pressure is defined as the pressure at which the first bubble of gas appears while increasing pressure on a sample filled with a fluid. The bubble point test is done to determine the minimum pressure required to force the fluid out of the largest pore. The bubble point pressure, calculated by PoroDict, must be sufficient to overcome the surface tension of the fluid and it is a direct measure of the effective pore diameter.

- For the calculation of **Percolation Paths**, the method determines the maximal diameters of spherical particles that can move through the medium. In addition, the shortest paths of these particles are calculated and displayed. Furthermore, the shortest path through the medium of a given sphere size can be computed.

- A **Chord Length Distribution** (CLD) is the distribution of the length of a typical chord of a structure. By being essentially unique for any given geometry class, it is a highly precise and sensitive measure to compare the geometries of porous media. The calculation of CLD is particularly useful in 2D tomographic cross-sections, for which the pore size distribution cannot be determined by Granulometry or by Porosimetry.

- The **Geodesic Tortuosity** command computes the tortuosity of paths crossing the material, either through pore space or through solid materials. For every voxel on the outflow plane, the algorithm finds the shortest path through the selected material.

- The **Pore Analysis GeoApps** section contains additional Python macros deployed with GeoDict which are either scripting examples or add-ins for specific applications.

Theoretical Basis: Computation of Pore Sizes by Granulometry or Porosimetry

The computation of a pore size distribution requires a definition of what is meant by the term "pore size". While the definition of diameter for a spherical pore is clear, it is not obvious what is the diameter of a pore for arbitrary 3D geometries.

Granulometry

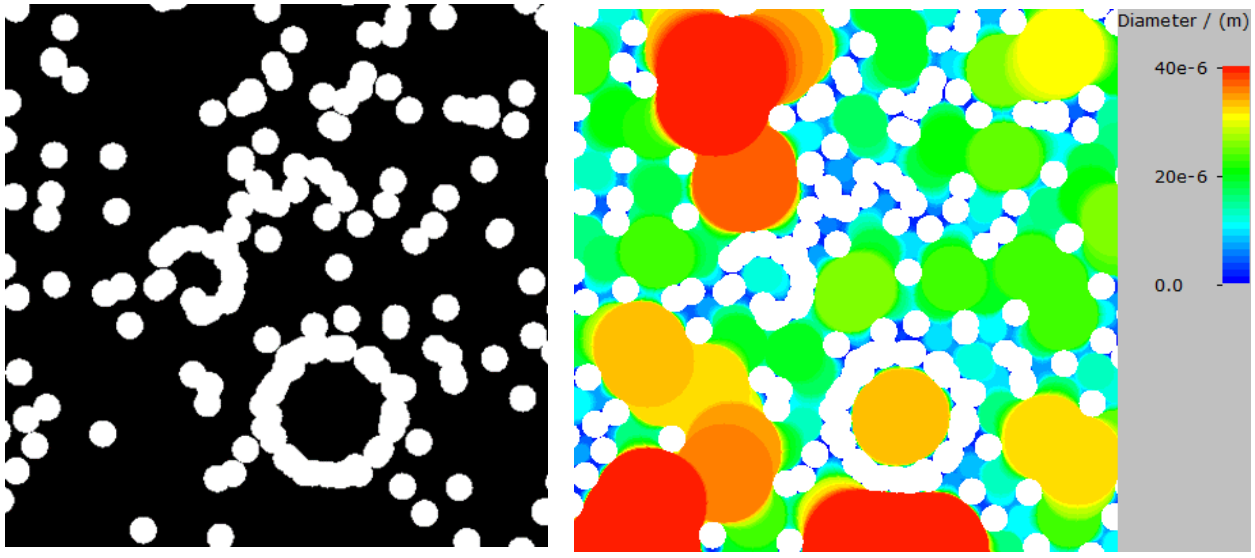
PoroDict uses the following assertion when defining a pore diameter using granulometry:

A voxel is part of a pore with a diameter equal or larger than D, if it is included in a sphere of diameter D, which is completely included in the pore space.

So, if a sphere of diameter 18 µm can be found that contains a certain voxel, but no sphere of diameter 20 µm can be found that contains the voxel, this voxel is assigned a pore diameter of 18 µm.

This means for a pore, that each voxel of this pore is linked to the diameter of the largest sphere that fits inside the pore and contains this voxel. Consequently, the pore diameter is set as the diameter of the largest sphere that fits inside the pore.

The following images illustrate (in 2D) how pore diameters are computed *by granulometry* in PoroDict.



The left image shows a structure with the solid material shown in white and the pore space in black. The image on the right shows the pore volume with diameters colored gradually. The red pore volume describes a pore volume with diameters around 40 µm and larger, green shows areas with diameters around 20 µm and very small diameters are colored in blue.

As shown in this illustration, the pores found by granulometry can be isolated inside the structure, and no connectivity or accessibility to the faces of the structure is required. This kind of pores can only be found by applying geometric algorithms to 3D image data as it can be done with GeoDict with this granulometry approach. With the porosimetry approach below, unconnected pores or large inner pores cannot be detected, since only the pore throats are measured.

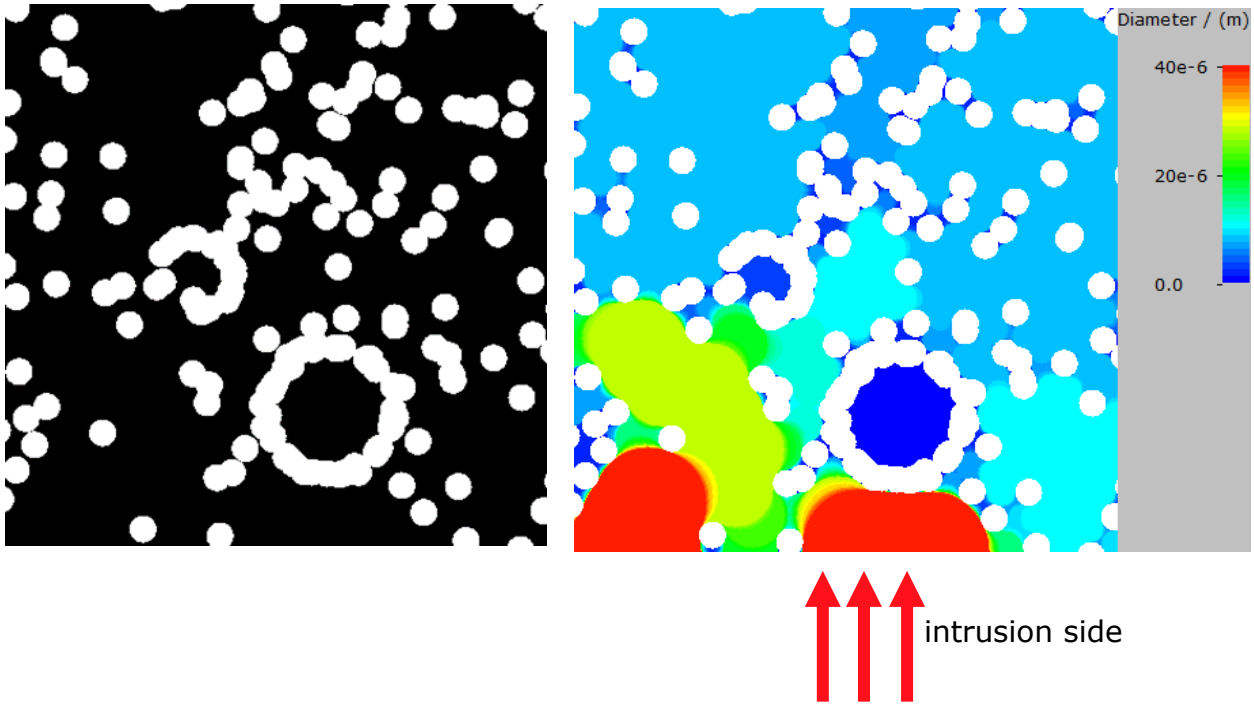
POROSIMETRY

In contrast to the granulometry method, porosimetry is an existing physical method to determine the size of the pore space. When measured by *porosimetry* in laboratory tests (e.g. mercury intrusion porosimetry or liquid extrusion porosimetry), a fluid is pressed through the pores into the structure. The applied pressure is related to the size of the pore throats. The smaller the pore throats, the more pressure is needed to flood the pore volume behind until smaller passages are reached. Thus, the isolated pores are not measured as large pores, because they are hidden behind small pore throats and, therefore, they are only measured as having the diameter of the smallest pore throat. Furthermore, closed pores are not measured as they have no connection to the intrusion side of the fluid.

Consequently, the computed pore size distribution *by porosimetry* takes the connectivity of the pores into account. In this case, the definition of what is a pore diameter changes slightly in PoroDict because in fact pore throat diameters are measured:

A voxel is part of a pore with a diameter equal or larger than D, if it is included in a sphere of diameter D, which is completely included in the pore space ***and can be moved in through the pores from a face of the structure***.

The following images illustrate (in 2D) how pore diameters are computed *by porosimetry* in PoroDict.

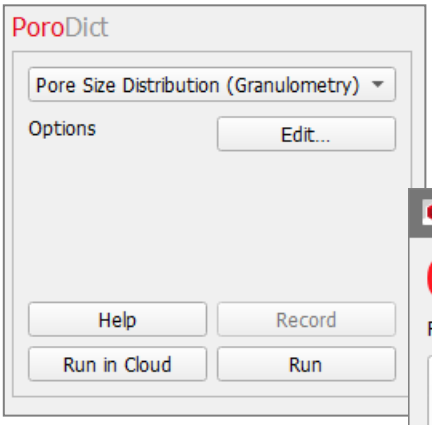


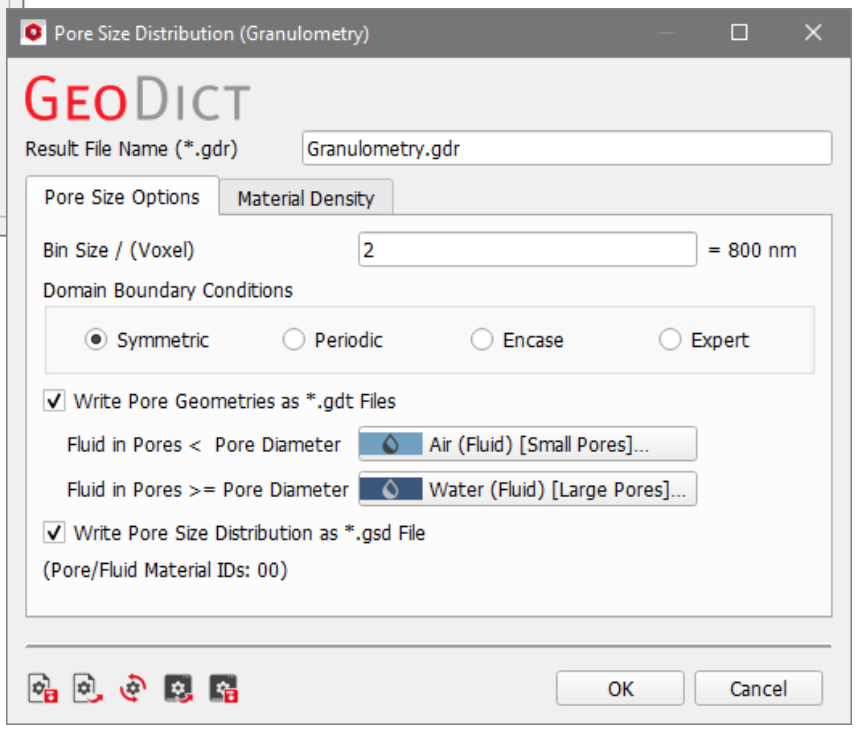
The left image shows a structure with the solid material shown in white and the pore space in black. The image on the right shows the pore volume with diameters colored gradually. The red pore volume describes a pore volume with diameters around 40 µm and larger, green shows areas with diameters around 20 µm and very small diameters are colored in blue.

As shown in this illustration, the pores found by porosimetry must be connected to the fluid intrusion sides of the image (in this example Z-, i.e. the bottom of the image).

Pore Size Distribution (Granulometry)

After selecting **Pore Size Distribution (Granulometry)**, the needed parameters can be entered by clicking the **Options' Edit...** button. The Pore Size Distribution dialog includes the **Pore Size Options** and the **Material Density** tabs.





At the top of the dialog box, enter the **Result File Name** for result files to be saved in the chosen project folder (**File → Choose Project Folder**, in the menu bar).

Pore Size Options

The voxels of the pore space are classified by their diameter into bins, that have equal **Bin Size**, which can be entered in the box. The bin size units are voxels and their equivalent in metric length units is shown. During the granulometry algorithm spheres with decreasing diameter are tried to be placed inside the pore space. Beginning with the largest possible diameter that is divisible by the **Bin Size** the diameter is reduced by the bin size in each step. Every voxel is then assigned the largest possible diameter. Thus, each bin contains pores with a diameter in the range comprised between [(*i* – 1) * Bin size] and [*i* * Bin size], where *i* is the bin number.

For example, when analyzing a porous structure with a voxel size of 1 µm, the user can set the **Bin Size** to 2 or to 4 (voxels) which would come to classify the pores by their diameter in ranges of 2 µm or 4 µm, and would result in the following bins:

Bin number (*i*)	**Pore diameter between [(*i* – 1) * Bin size] - [*i* * Bin size]**	
	Bin Size 2 µm	**Bin Size 4 µm**
1	0 µm - 2 µm	0 µm - 4 µm
2	2 µm - 4 µm	4 µm - 8 µm
3	4 µm - 6 µm	8 µm - 12 µm
..	...	

When choosing the **Bin Size**, be aware that the underlying algorithm to compute the Euclidean distance operates directly on the voxel grid. Thus, the smallest possible distance between to grid points is 1 Voxel, which corresponds to a pore radius of 1 Voxel. This means the smallest pore diameter that the algorithm will find is 2 Voxels.

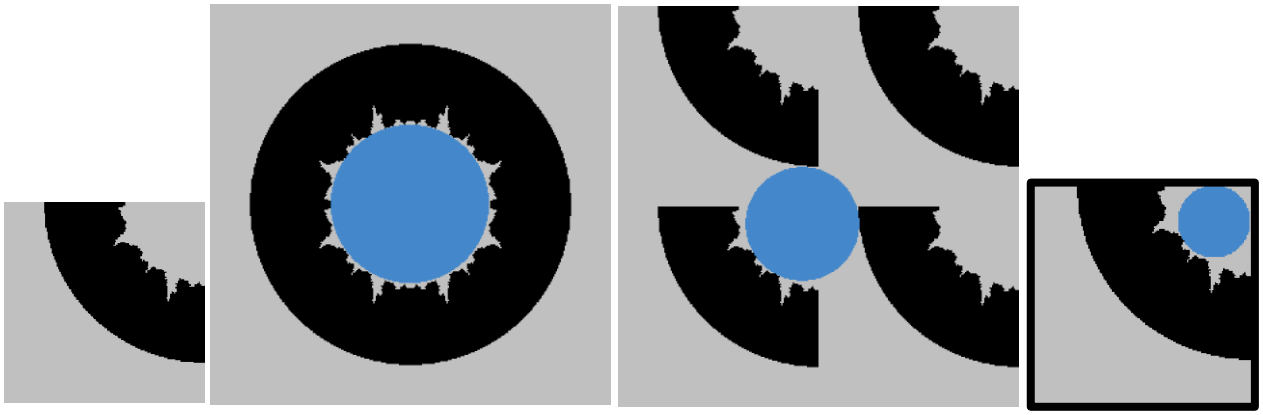
In general, the error made when computing the pore size distribution is of the same order of magnitude as the discretization error of the structure, i.e. 1 Voxel.

The **Domain Boundary Conditions** can be chosen to be **Symmetric**, **Periodic, Encase**, or any combinations of those boundary conditions in all three directions with the choice of **Expert**.

Choosing the appropriate boundary condition depends on the structure's design.

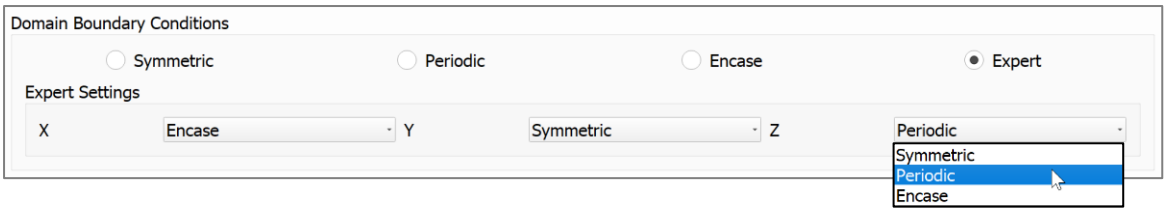
For example, imagine a structure with a cross-section as shown in (a). For the three boundary condition options shown in (b), (c) and (d) the resulting pore size is visualized in blue.

- If the geometry has mirror symmetry (b), **Symmetric** boundary conditions are taken, which would be a good approximation e.g. for a cut-out from a CT image.
- If instead the expected pattern of the geometry is repeated in all directions (c), the pore sizes are computed with **Periodic** boundary conditions. That has the effect that the objects and pores of the structure that end on one side of the structure reappear on the opposite side.
- If the structure is encased in a closed wall (d), the **Encase** boundary conditions are used.

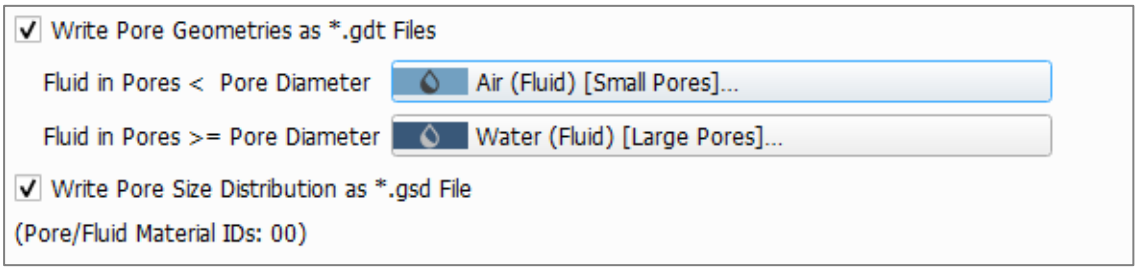


(a) (b) (c) (d)

When different boundary conditions need to be specified, the choice of **Expert** should be used. When **Expert** is checked, the three above mentioned boundary conditions can be selected for each direction separately. For example, the boundary conditions could be chosen to be **Encase** in X-direction, **Symmetric** in the Y-direction and **Periodic** in Z-direction.



When **Write Pore Geometries as *.gdt Files** is checked, files in *.gdt format are saved in the automatically created results folder (e.g. `.../Granulometry/...`) inside the project folder (see page 10). The number of these *.gdt files reflects the number of pore size steps and depends on the entered **Bin Size**. A large bin size results in fewer size steps, and thus, fewer *.gdt files are saved for the visualization. For each bin a separate *.gdt file is written, where every voxel of the pore space is assigned to one of the specified materials.

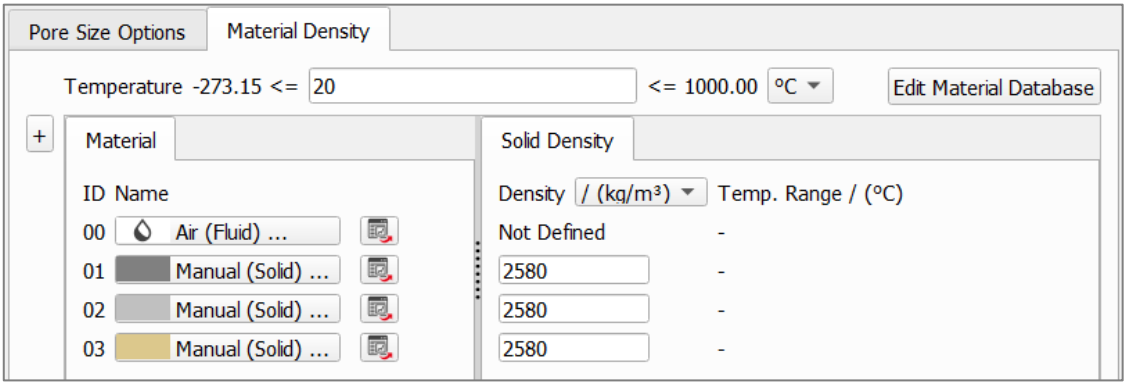


If a voxel belongs to a lower bin number, its corresponding pore diameter is smaller. In this case the voxel is assigned to the first material. Consequently, all voxels from a bin with the same or higher number are assigned to the second material. This results in two different Material IDs for the voxels in the pore space. The materials written into these *.gdt files can be specified after checking **Write Pore Geometries as *.gdt Files**. For example, predefined materials of the **Material Database**, such as Air or Water can be chosen by clicking on the buttons. The current Material IDs for the fluids in the pores are shown at the bottom.

Additionally, when **Write Pore Size Distribution as *.gsd File** is checked, a file with the default name PoreSizeDistribution.gsd, in *.gsd format, is saved in the results folder inside the project folder. The file contains the pore size (diameter of sphere) of each voxel written into a volume field that is used in visualization.

Material Density

Under the **Material Density** tab, the temperature can be edited and the density of every material present in the structure (in kg/m³ or in g/cm³) must be specified unless they are automatically entered (for constituent materials from the GeoDict Material Database).



Results

At the end of the PSD Granulometry calculations, the results are immediately shown in the opening Result Viewer and the result file is saved with the name entered in **Result File Name** (or the default **Granulometry.gdr**) in the chosen project folder (**File → Choose Project Folder**).

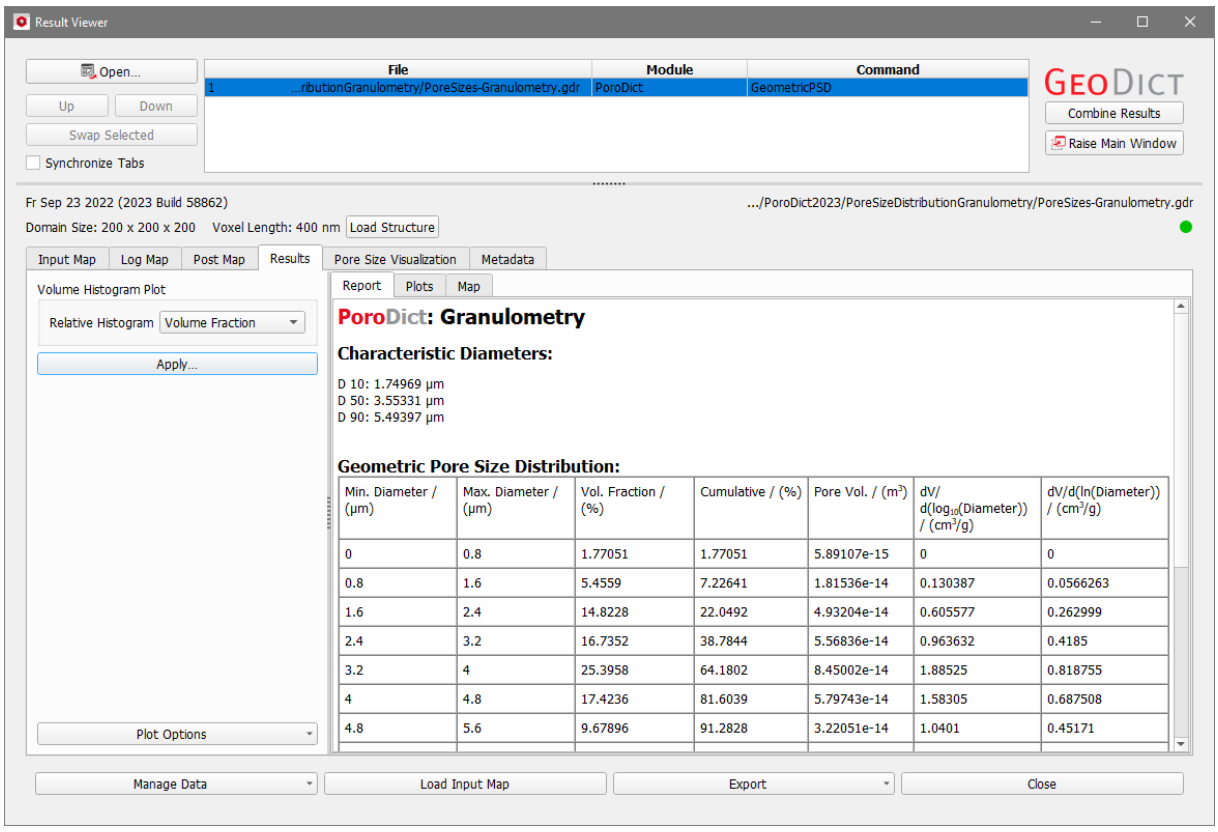
The *.gdr file can also be directly opened, analyzed, and plotted in Microsoft Excel™ by clicking **Export → Excel (generic)** at the bottom of the Result Viewer.

The *.gdr file can also be directly opened, analyzed, and plotted in MATLAB® using GeoLab, after clicking **Export → Matlab** at the bottom of the result file window.

Under the **Results - Report** subtab, on the right-hand side, the **Characteristic Diameters** are shown. For example, here, the D10 value means that 10% of all pores have a diameter smaller than 1.75 µm. The D50 value means that 50% of all pores have a diameter smaller than 3.55 µm. The D90 value means that 90% of all pores have a diameter smaller than 5.49 µm.

The discretization error is less than 1 voxel, which means for the presented example, that the D10 is 1.75 µm ± 0.4 µm.

Underneath, a detailed table lists Maximum and Minimum Diameters, Volume Fraction, Cumulative Volume Fraction, Pore Volume, and the Differential Pore Volume Distribution for every bin. Also, at the bottom of the **Report tab**, the total porosity of the structure is shown.



Under the **Results – Plots** subtab, different relative and cumulative histograms can be plotted. The default relative histogram shows the Volume Fraction [%], but the histogram of interest, can be chosen on the left-hand side. The available options are Volume, Volume Fraction, or the differential pore volume distribution dV/d(log(Diameter)), where the common logarithm ($\log_{10}$) or the natural logarithm (ln) can be chosen.

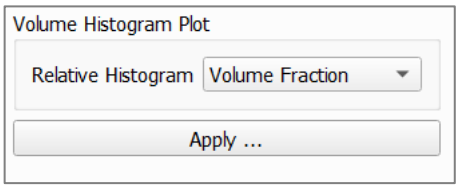
The differential pore volume distribution dV/d(log(Diameter)) is then computed as

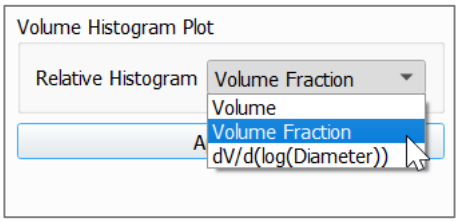
$$\frac{V_{cum}(d_{i+1}) - V_{cum}(d_i)}{(\log(d_{i+1}) - \log(d_i)) \cdot m}$$

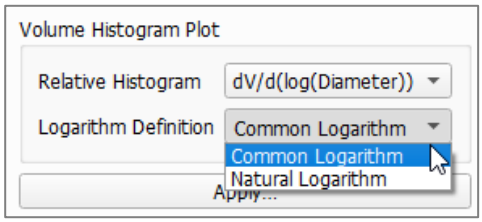
with d_i the pore diameter of the *i*-th bin, V_{cum} the cumulative volume fractions, and m the mass of the structure. The latter is computed using the densities of the solid

constituent materials of the sample. This normalization ensures that the value of dV/d(log(Diameter)) is independent of the domain size.

In the **Volume Histogram Plot** panel on the left-hand side, several histogram types can be selected. After clicking the **Apply ...** button the plots on the right hand-side change accordingly.

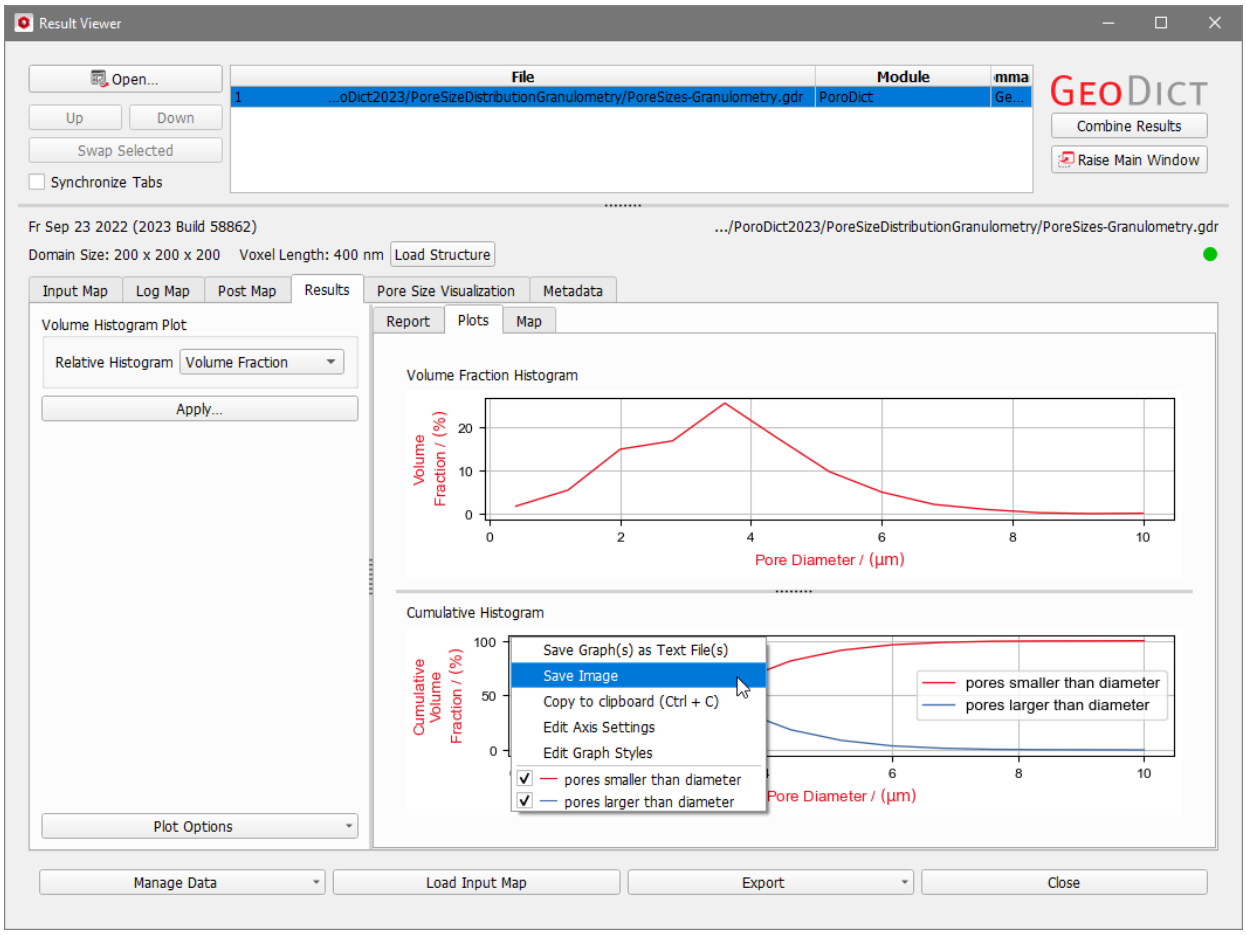




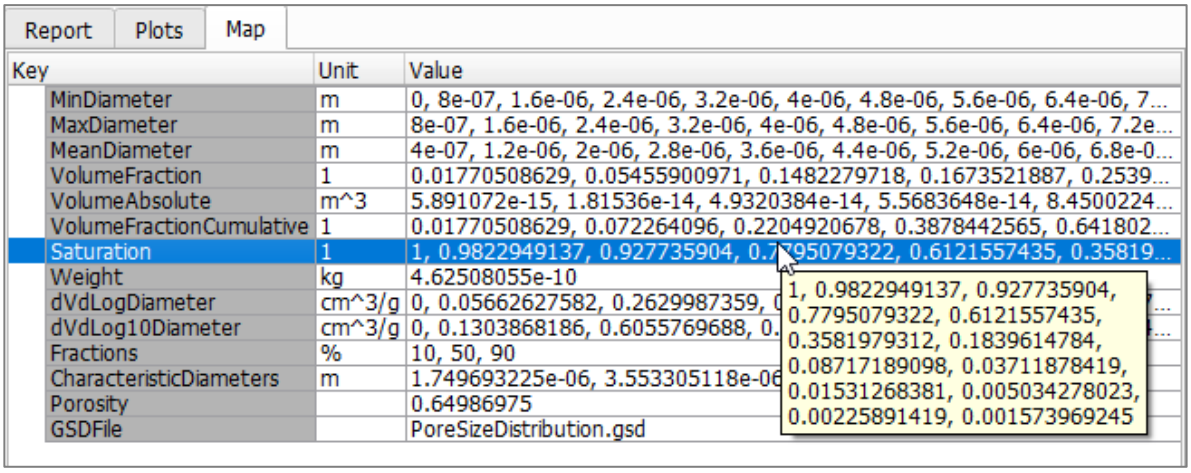


In the **Cumulative Histogram** plot, the red curve shows the volume fraction of pores smaller than a given diameter plotted on the x-axis and the blue curve shows the pores larger than or equal to a given diameter. Both curves sum up to 100% for any given pore diameter.

As usual, the plots can be edited and saved as images or as text files by right-clicking on the graph area.

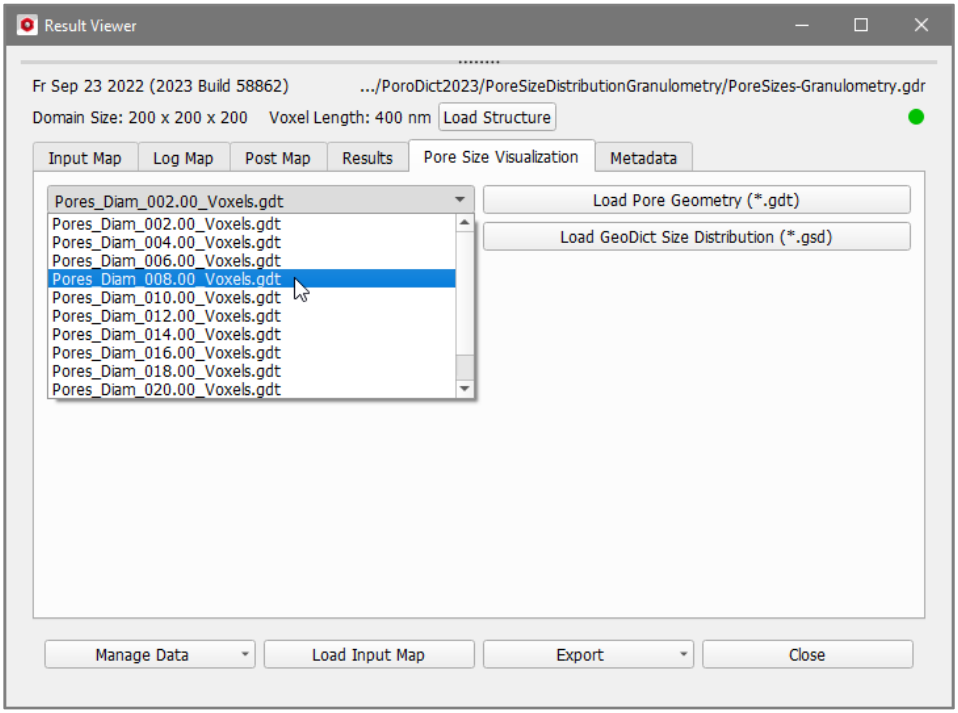


The **Results - Map** subtab gives access to the values of the computed parameters.



Pore Size Visualization

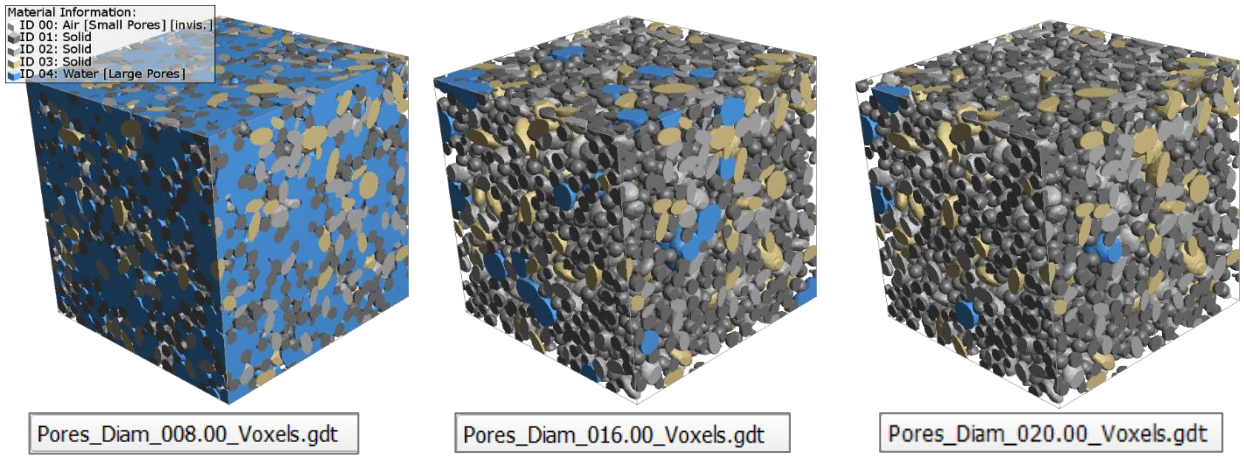
The distribution of pores is observed in the Volume Fraction/Pore Diameter plot but can also be visualized through the **Pore Size Visualization** tab. To load the pore size distribution as specified on page 7 into the visualization area, select the *.gdt file corresponding to a particular pore diameter in the drop down menu. Then, click **Load Pore Geometry (*.gdt)**.



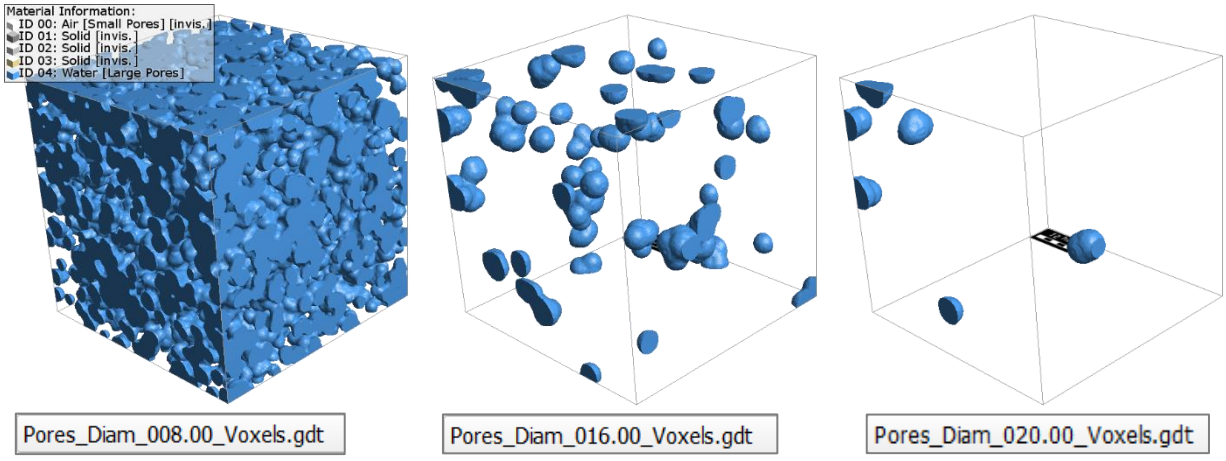
Take for example a Bin Size of 2 voxels. Then the **Pores_Diam_008.00_Voxels.gdt** file shows the pore space separated into two material IDs. Pore voxels which belong to pores with a diameter of 8 voxels (or more) get another Material ID as the pore voxels of smaller pores.

The **Pores_Diam_016.00_Voxels.gdt** file shows the more limited pore space in which spheres with a (large) diameter of at least 16 voxels would fit.

The **Pores_Diam_020.00_Voxels.gdt** file shows that in this structure, the pore space in which spheres with diameter over 20 voxels can fit is very small.

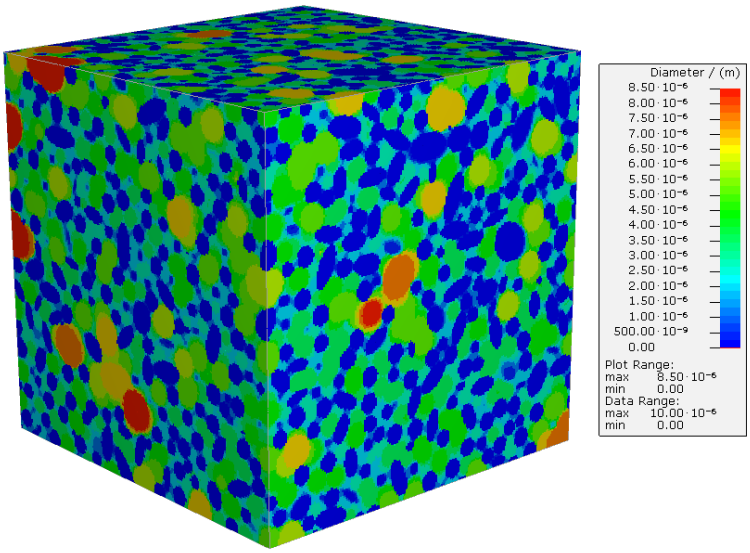


Check or un-check **visible** in **Settings** → **Color & Visibility Settings**, to turn off the materials in the structure (Material ID 01, Material ID 02, and Material ID 03) and see only the pore space filled with water (Material ID 04).

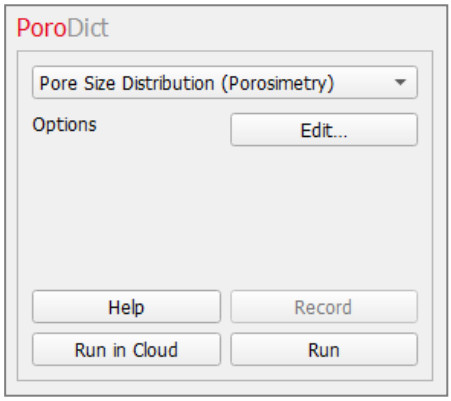


By clicking on **Load GeoDict Size Distribution (*.gsd)** a volume field is loaded which for each voxels is assigned the largest diameter of a sphere, that contains this voxel and fits inside the pore space.

Comparing the volume field with the pores, that have a diameter of 20 voxels or more, one can see that these pores have a red color in the volume field plot.

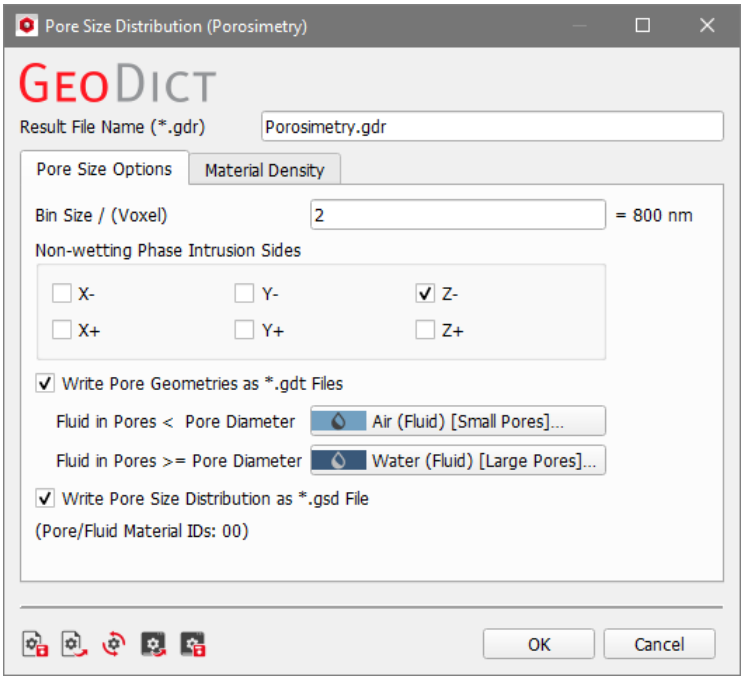


Pore Size Distribution (Porosimetry)



Here, instead of boundary conditions, the direction (or multiple directions) from which the application of the intrusion occurs during the simulation can be chosen.

For **Pore Size Distribution (Porosimetry)**, the parameters can be entered by clicking the **Options' Edit...** button. These parameters are similar to those for Pore Size Distribution (Granulometry), explained above in pages 5ff.



Results

The **Result Viewer** of the porosimetry result file is immediately shown at the end of the calculations. It contains the same information and options as the **Pore Size Distribution (Granulometry)** result file seen above (page 7ff.).

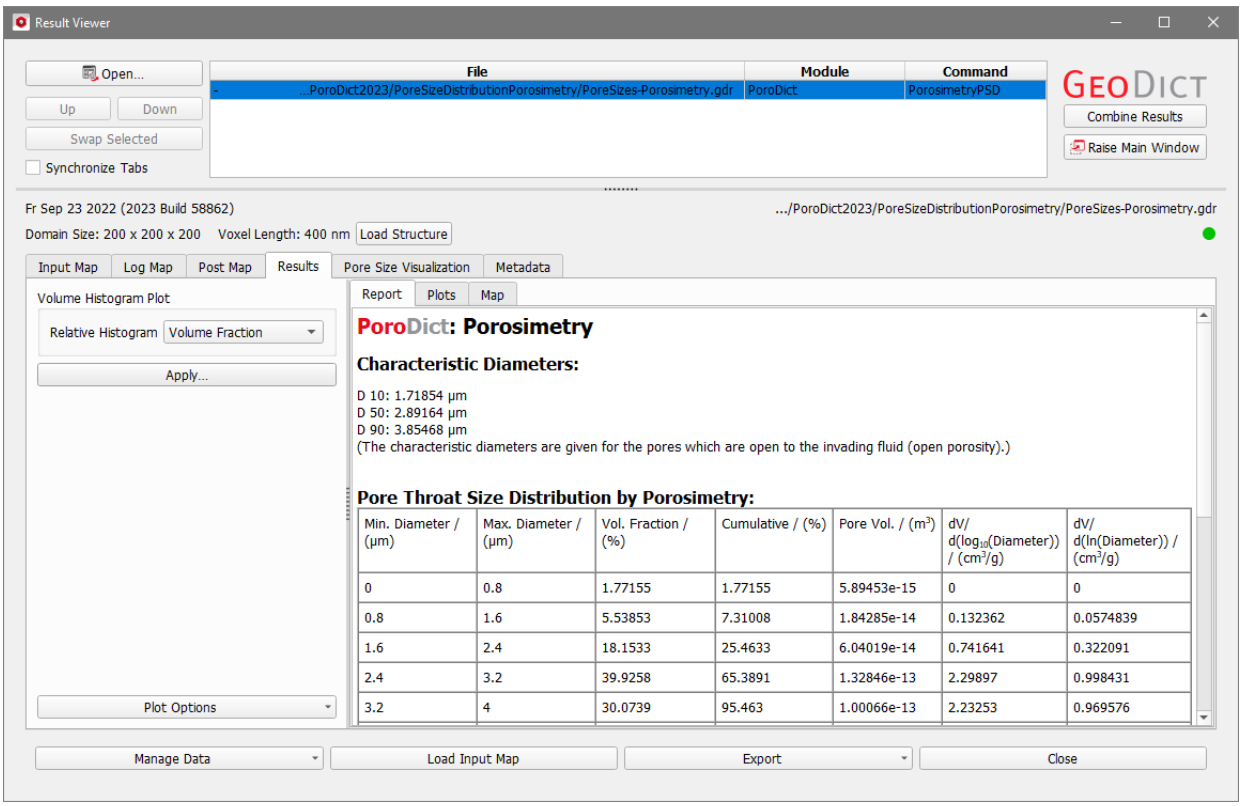
In the **Results** - **Report** subtab, the **Characteristic Diameters** are shown. Here, the D10 value means that 10% of all pores have a diameter smaller than 1.72 µm. The D50 value means that 50% of all pores have a diameter smaller than 2.89 µm. The D90 value means that 90% of all pores have a diameter smaller than 3.85 µm.

Underneath, a detailed table lists Maximum and Minimum Diameters, Volume Fraction, Cumulative Volume Fraction, Pore Volume, and Differential Pore Volume Distribution for every bin. Moreover, the total porosity, the open porosity and the closed porosity are shown.

Fewer large pores are found by porosimetry than by granulometry.

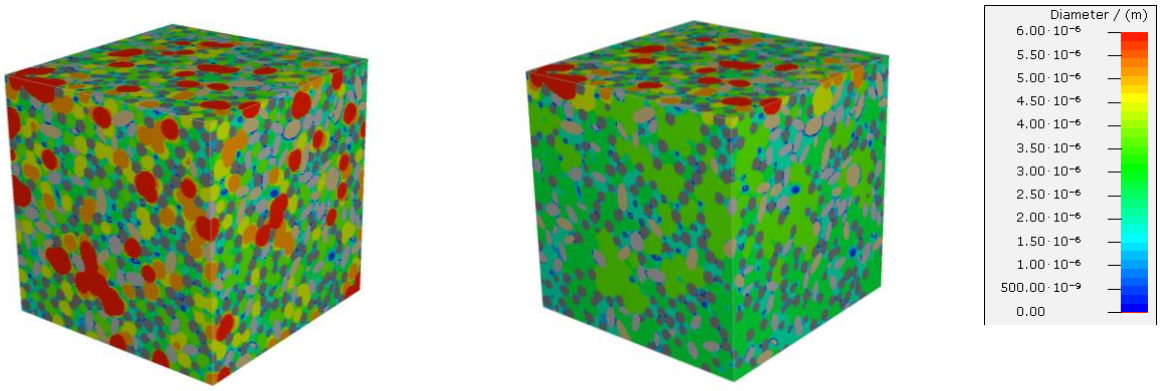
The reason for this is that a big pore in the interior of the volume must be reached from the intrusion sides, usually, through a small diameter pore-throat. The big pore is counted as pore volume of a certain diameter only if a sphere with this diameter can be pushed from the intrusion side through the pore-throat to reach the big pore.

In other words, porosimetry provides a measure of the pore-throat distribution.



Data Visualization

As explained above, the visualization of the pore space is done under the **Pore Size Visualization** tab. The user can select the saved *.gdt file corresponding to a particular pore diameter and click **Load Pore Geometry (*.gdt)**. Furthermore, the pore size distribution can be loaded by clicking on **Load GeoDict Size Distribution (*.gsd)**. Compare the pore size distribution for the same structure computed using granulometry (left) and porosimetry (right). For the porosimetry, the larger pores are all assembled on the intrusion side of the fluid, whereas for the granulometry they are spread all over the structure.



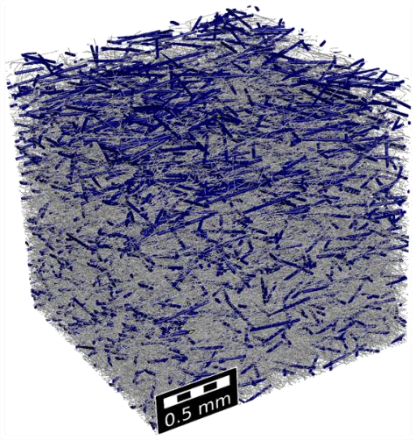
Speed-up through parallelization

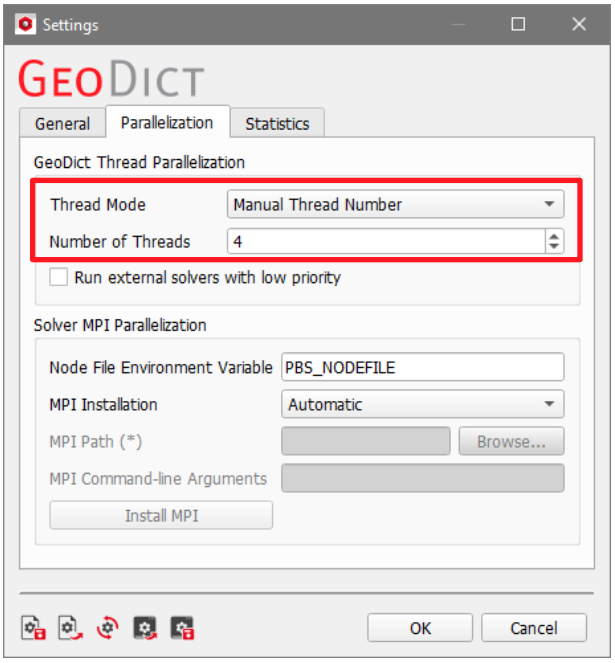
The pore size distribution analyses **Granulometry** and **Porosimetry** can be parallelized with several processes to speed-up the simulation runtime.

By default, the computation is parallelized with the maximal number of available threads on the computer.

To set a manual number of threads, select **Settings** → **Settings** from the menu bar. In the **Settings** dialog move to the **Parallelization** tab and for **Thread Mode** choose **Manual Thread Number** from the pull-down menu. Then enter the desired number of processes for **Number of Threads**.

Click **OK** to close the dialog and run a pore size distribution analysis.

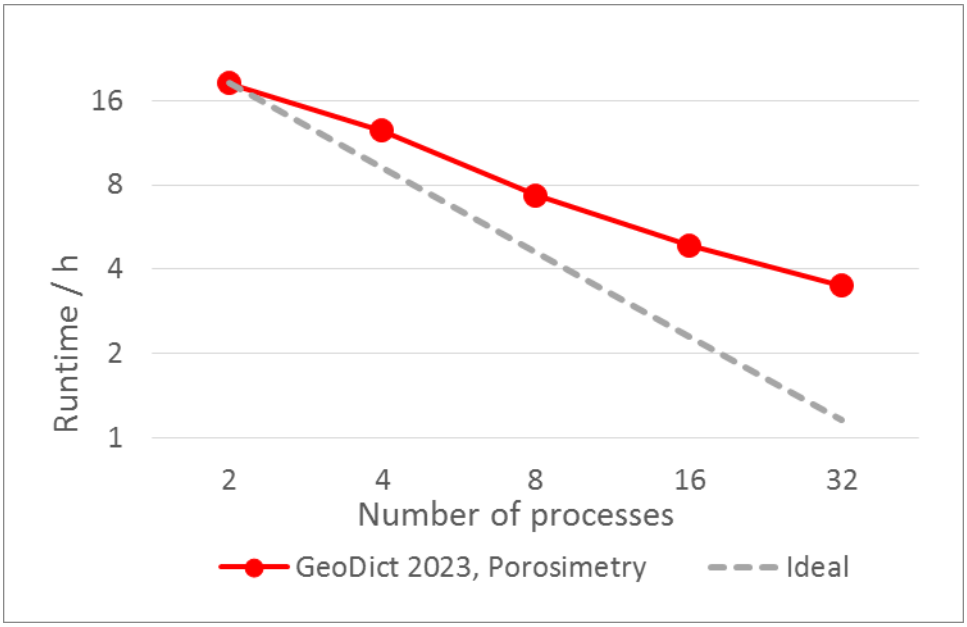




An example of a parallelization benchmark for PoroDict Porosimetry is shown here. The computation was run on a server with 2xIntel E5-2697A v4 processors with 16 cores each, running with a maximum of 3.60GHz.

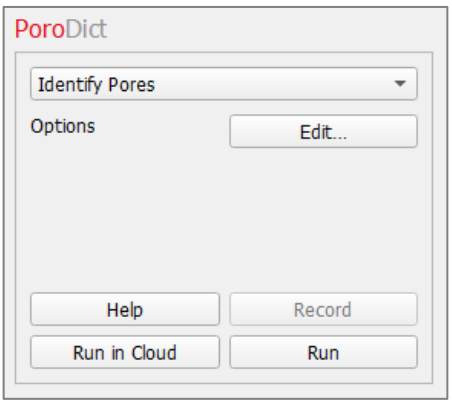
The input structure is a filter structure with linearly increasing density of size 2048x2048x2032 voxels. A **Pore Size Distribution (Porosimetry)** analysis was run on this structure.

The following figure shows the runtime for a different number of processes for the whole simulation. The ideal speedup, i.e. getting half the runtime for twice the number of processes, is also shown as a gray dashed line.



IDENTIFY PORES

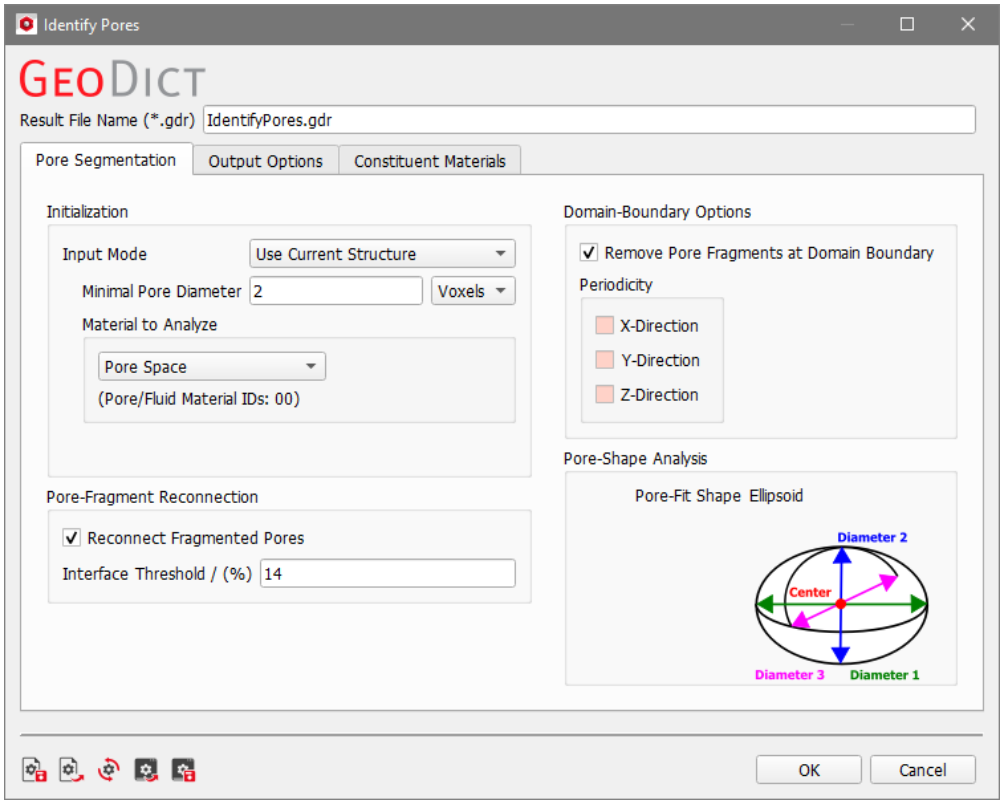
After selecting **Identify Pores** from the pull-down menu, the parameters for the calculation can be modified through the **Edit...** button.



In the **Identify Pores** dialog box, enter the **Result File Name (*.gdr)** under which the results are saved in the chosen project folder.

PORE SEGMENTATION

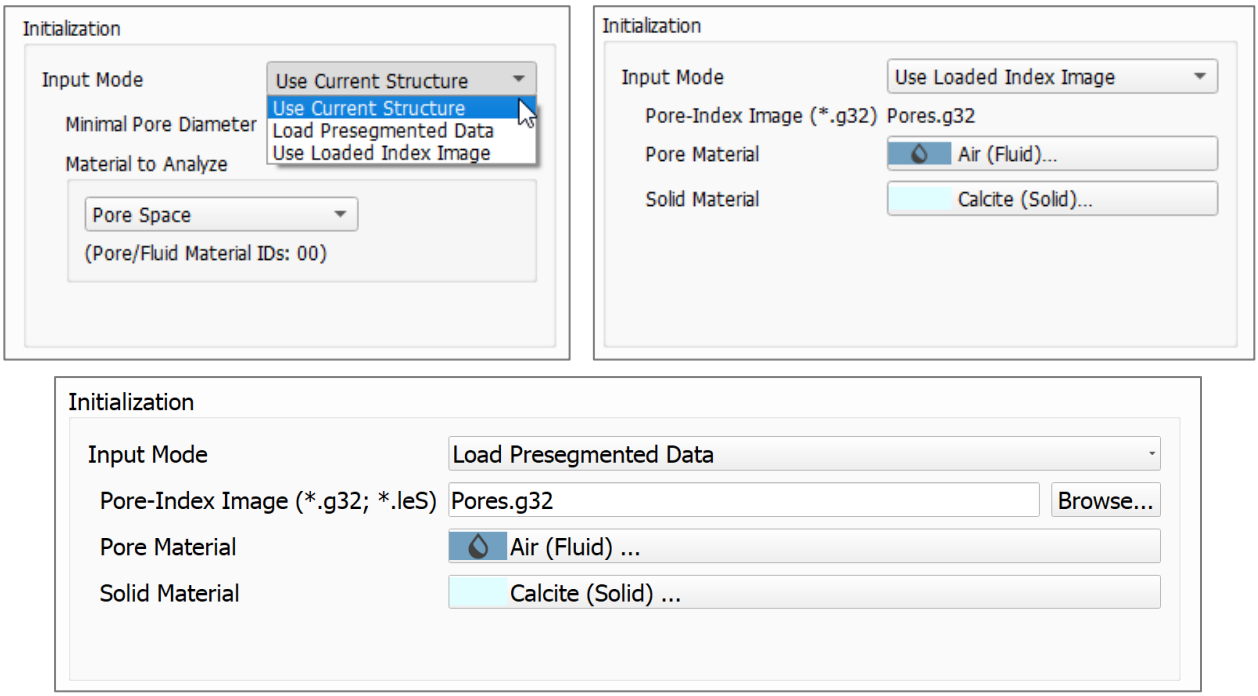
The parameters in the **Pore Segmentation** tab are separated in four panels: **Initialization**, **Pore-Fragment Reconnection**, **Domain-Boundary Options**, and **Pore-Shape Analysis**.



INITIALIZATION

The parameters in the **Initialization** panel define the basis for the analysis. The structure to be evaluated is chosen through the **Input Mode** and the material to be analyzed is selected through **Material to Analyze**.

For the **Input Mode**, three options are available: use the structure currently in memory (**Use Current Structure**), import already segmented data from an index-image file, *.g32 or *.leS (**Load Presegmented Data**), or use the currently loaded *.g32 file (**Use Loaded Index Image**).



The initialization (the watershed algorithm) might be time consuming for large structures. Thus, the options **Load Presegmented Data** or **Use Loaded Index Image** are useful when performing parameter studies with PoroDict – Identify Pores, where the initialization is kept unchanged while other parameters are varied.

For **Load Presegmented Data**, the difference between the *.g32 and *.leS formats is that *.g32 is a binary format, which produces comparatively smaller files but is not human readable, and *.leS is an ASCII-format which is human readable, but produces larger files. Furthermore, loading a *.g32 file into GeoDict is much faster than loading a *.leS file. Therefore, we recommend to use the *.g32 option.

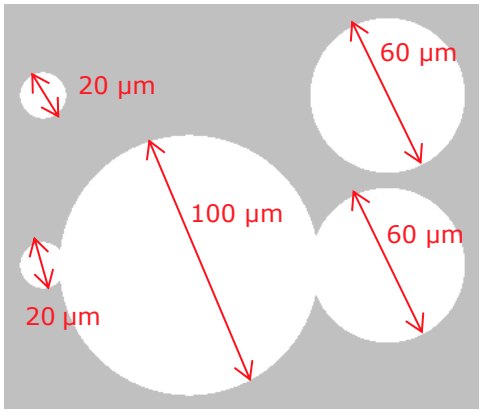
Alternatively, **Use Loaded Index Image** can be used if the presegmented data is already loaded into GeoDict. In that case, it can be used directly and it is not necessary to load it again.

In the **Use Current Structure** mode, the **Minimal Pore Diameter** defines the minimal size an individual pore must have for the analysis. The unit of **Minimal Pore Diameter** can be selected as **Voxels** or **m**.

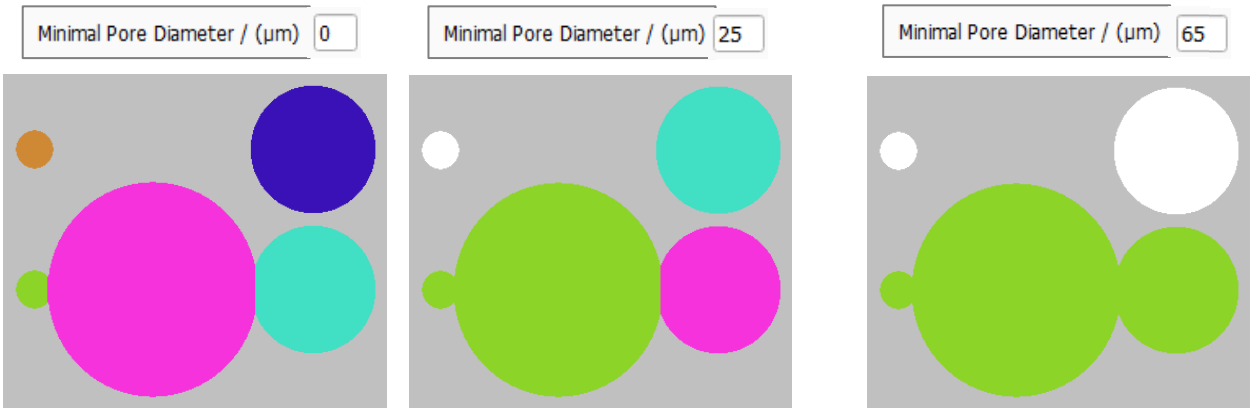
This parameter determines which pores to keep and which pores to neglect or merge with others. If smaller pores exist which are connected to larger pores, the pores are merged. Single pores with a diameter smaller than **Minimal Pore Diameter** are neglected.

In the next figure, the effect of the choice for **Minimal Pore Diameter** in the initialization step (of the watershed algorithm) is illustrated using the visualization of *.g32 files.

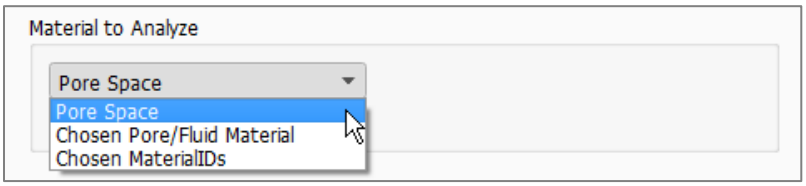
The original structure, shown on the right, contains spherical pores with diameters 100 µm, 60 µm, and 20 µm, and some pores touch so they share an interface.

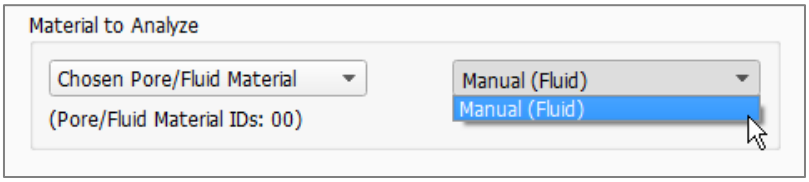


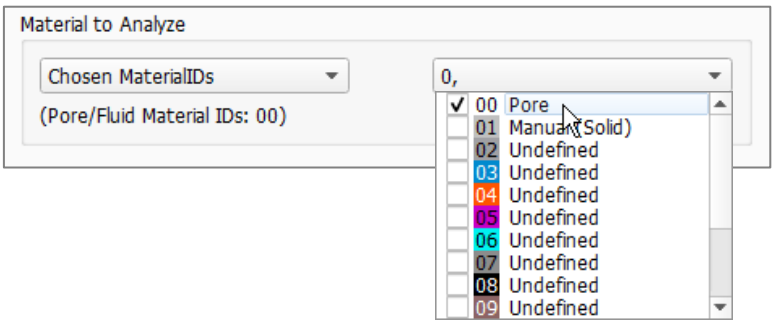
With **Minimal Pore Diameter** set to zero, all five pores are identified as single pores. When setting the **Minimal Pore Diameter** to 25 µm, the single 20 µm pore is neglected (shown in white), while the 20 µm pore connected to the larger pore is merged and so only three pores are identified. Analogously, for a choice of 65 µm, only one single merged pore is detected while the smaller pores are neglected.



Under **Material to Analyze**, the user defines the part of the structure to be considered. Either the complete structure can be analyzed (**Pore Space**), an individual material in the pore space can be selected (**Chosen Pore/Fluid Material**) or a choice of material IDs in the pore space can be made (**Chosen Material IDs**).

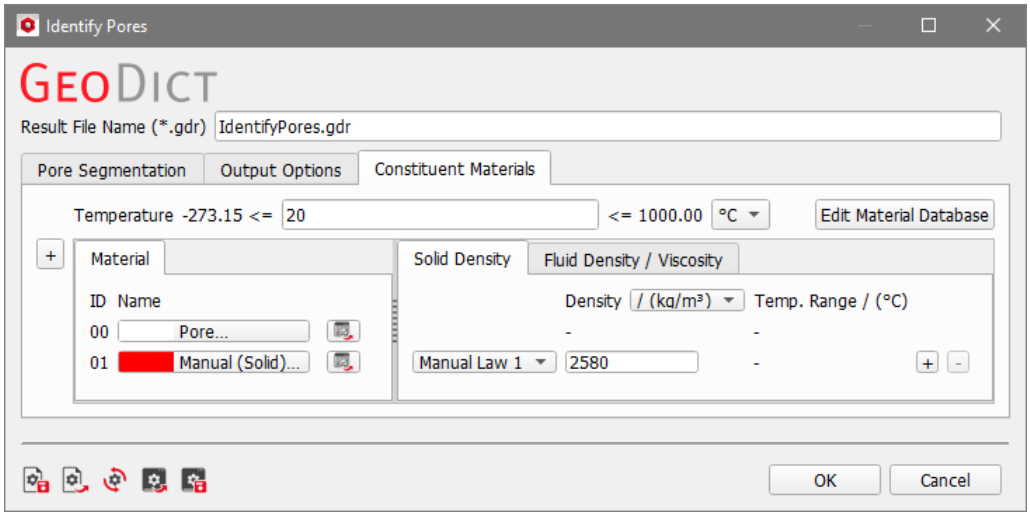






With **Chosen Material IDs**, one or multiple IDs can be chosen, which are then combined and analyzed as one single material. For example, when the pore space is occupied by brine and oil during the simulation of drainage or imbibition, choosing the material to analyze allows computing the amount of the pore space occupied by each of the two fluids.

When choosing an index image as input the user can define the Material of the pores and the surrounding solid material by clicking on the corresponding buttons. If the loaded structure is used the materials can be selected in the **Constituent Materials** tab. The material info is used in the Results Viewer to compute the grain mass and the moment of inertia.

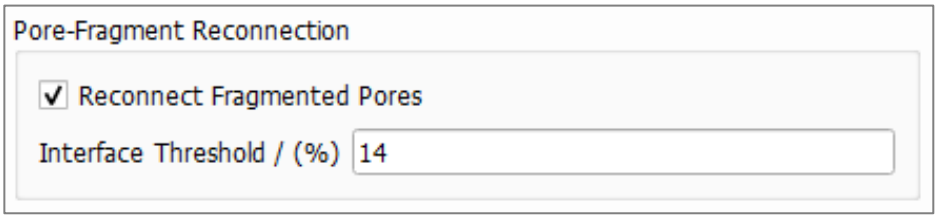


Pore-Fragment Reconnection

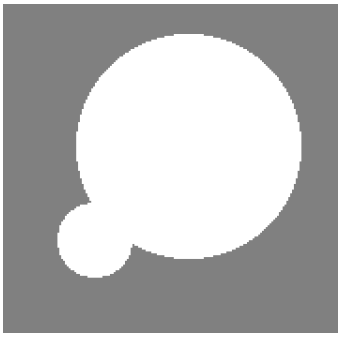
In some cases (e.g. for complex pore shapes), the watershed algorithm in step 1 tends to over-segment the pore space. This means, that sometimes pores are identified as multiple pores (**Fragmented Pores**) when, in fact, they may be a single pore with a complex shape.

By checking **Reconnect Fragmented Pores**, it is possible to handle this over-segmentation by merging pores depending on the size of their shared interface. After checking **Reconnect Fragmented Pores**, the merging of connected pores can be controlled using the values entered for **Interface Threshold**.

The interface of two pores that touch is compared to the total surface of the smaller pore. If the ratio of interface to total surface is larger than the value chosen for **Interface Threshold** (in %), the two pores are merged and only one pore is reported as identified.

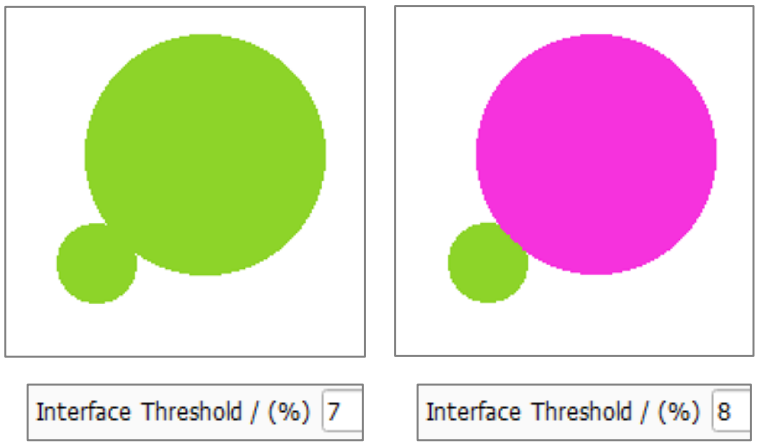


For example, if the **Interface Threshold** is set to the default **14**, the shared interface of two pores must be larger than 14% of the total surface of the smaller pore for the two pores to be merged. The next images show two examples in which a big pore and a small pore touch with different interface surface between them.



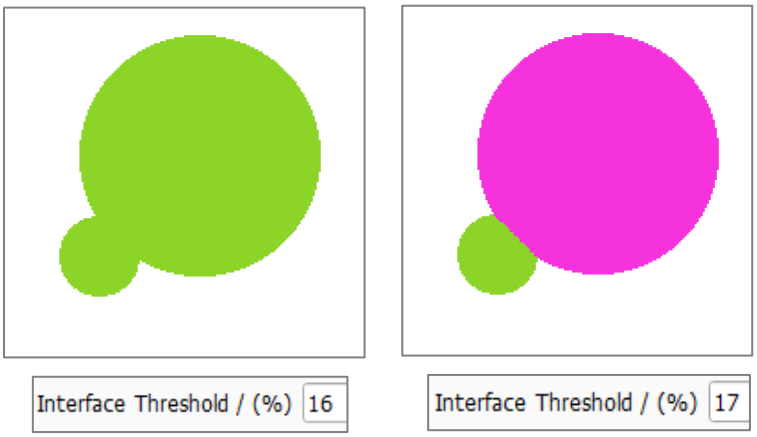
Depending on the surface of the interface, the value of **Interface Threshold** at which the two pores stop being reconnected and are detected as two (instead of only one) is very different.

When the two pores share a small interface, a low value of **Interface Threshold** (8) is enough to separate the two pores.



When the two pores share a large interface, a higher value of **Interface Threshold** (17) is needed to separate the two pores.

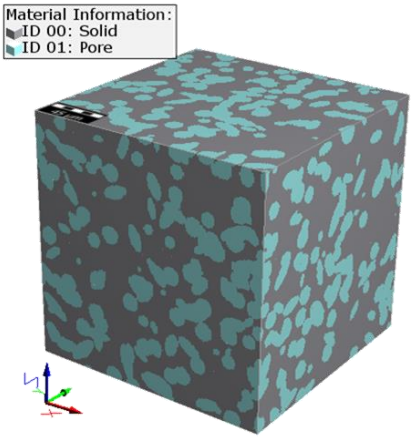
The default value of **Interface Threshold** (14) would be appropriate to separate the two pores sharing a small interface, but not the pores sharing a large interface.

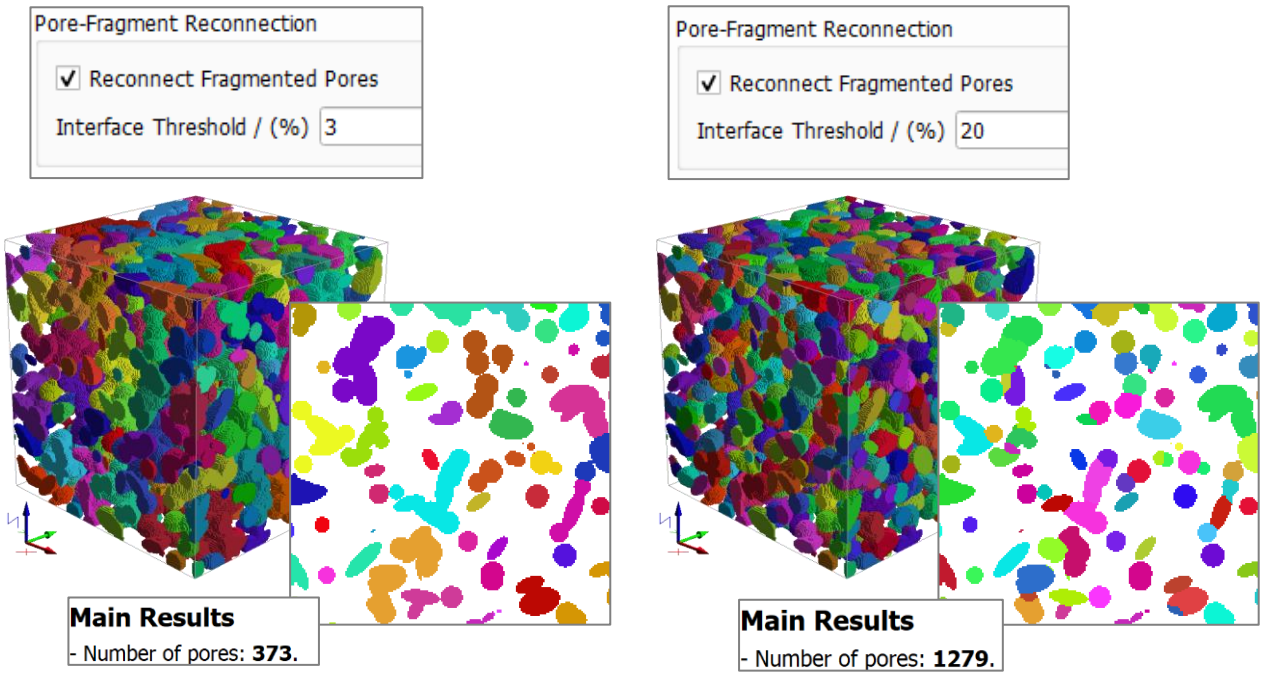


The value for the **Interface Threshold** must be chosen carefully depending on the size of pores in the structure. With a low threshold, more pores are merged (and less pores are identified).

In the figures below (using the visualization of *.g32 files), observe the effect of different choices for the **Interface Threshold**. For this example, the **Minimal Pore Diameter** is always 2 µm and **Remove Pore Fragments at Domain Boundary** has been unchecked.

With a very low value of 3%, several large and complex pores are identified in the structure that may not correspond to single pores. With a value of 20%, the pore space may be over-segmented with many small pores being detected.

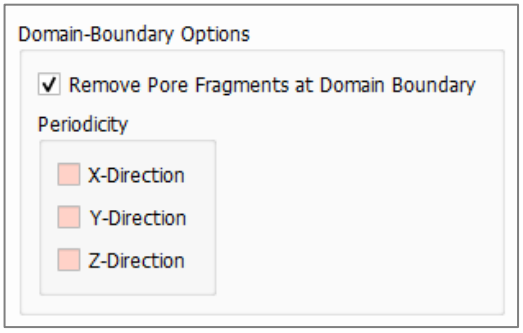




To help the user finding the correct **Interface Threshold** for the structure, the **Reconnection Indicators** histogram under the **Results** → **Plots** subtab in the Result Viewer can be used.

Domain-Boundary Options

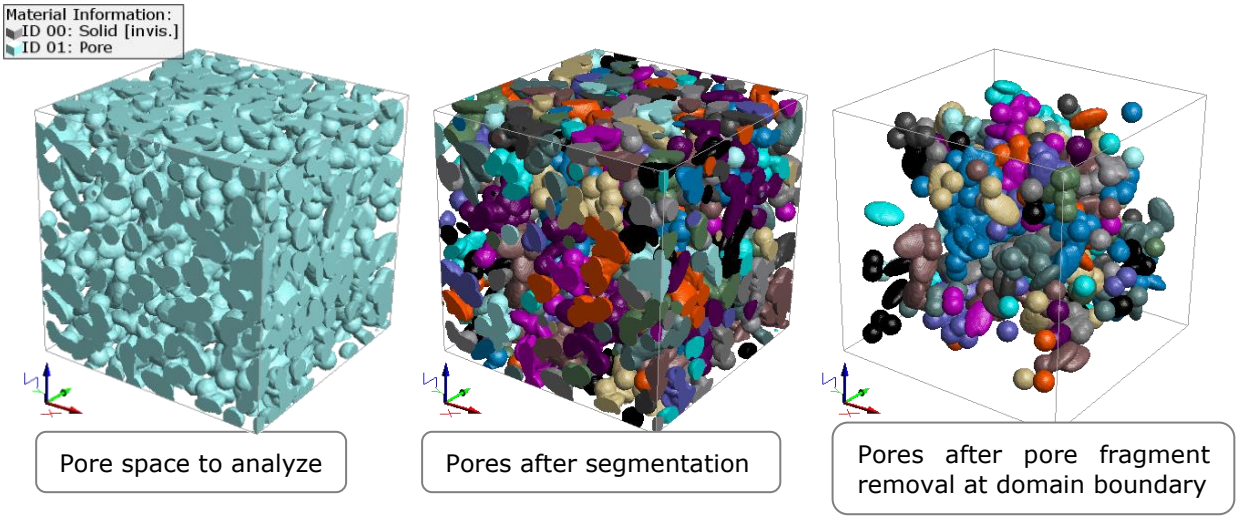
In the **Domain-Boundary Options** panel, the handling of boundary pores is defined. When **Remove Pore Fragments at Domain Boundary** is checked, all pores touching the domain boundary, after the initialization and the pore-fragment reconnection are done, are removed. This might improve the results, since boundary pores which do not lay completely in the domain might lead to wrong estimates for the pore shapes.



When **Remove Pore Fragments at Domain Boundary** is unchecked, the **Periodicity** options become available. By checking the X-, Y- or Z-Direction checkboxes, the pore space is treated as periodic in the chosen direction(s) before the pore segmentation.

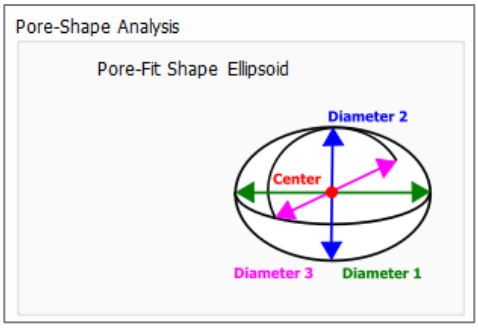
This option should only be chosen for real periodic structures, otherwise it might lead to strange results (with pores which are treated as connected but are distant from each other in reality).

Otherwise, when **Periodicity** is not chosen in a direction, the structure is assumed to end at the domain boundary.



PORE-SHAPE ANALYSIS

After the pore identification step (defined by the parameters under **Initialization**, **Pore-Fragment Reconnection** and **Domain-Boundary Options**), the shape of the pores is analyzed.



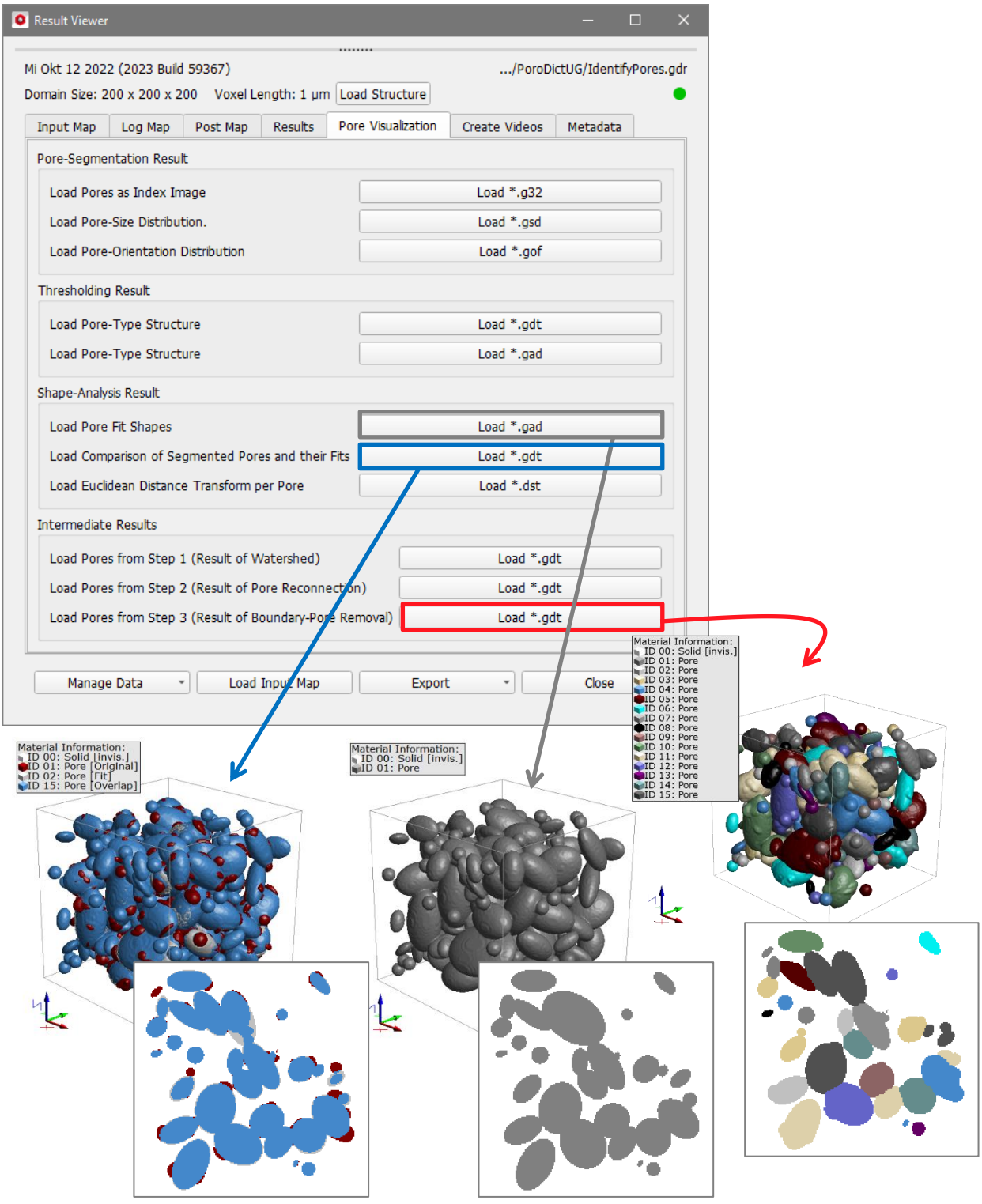
This analysis is done by fitting ellipsoids into the identified pores.

The figure below shows the results of **Pore-Shape Analysis** on a porous structure. These visualizations are loaded from the Results Viewer of the *.gdr result file (under the Pore Visualization tab).

On the right, the structure is shown after pores are identified, and the pore fragments are removed at the domain boundary.

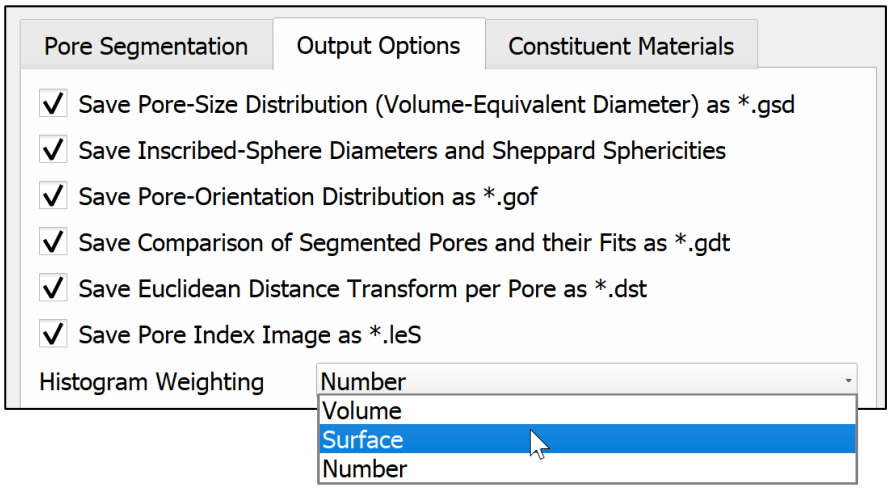
The middle image shows the shapes of ellipsoids fitted to the pores.

The left image shows a comparison between the identified pores (red) and the ellipsoid shapes fitted to them (grey). The matching voxels are shown in blue. This visualization provides a validation of the fitting to the ellipsoid shapes. A fitting is very good when a high percentage of blue is observed, meaning that the fitted ellipsoids overlay the pores with great accuracy.


Result Viewer
Mi Okt 12 2022 (2023 Build 59367)
.../PoroDictUG/IdentifyPores.gdr
Domain Size: 200 x 200 x 200
Voxel Length: 1 µm
Load Structure
Input Map
Log Map
Post Map
Results
Pore Visualization
Create Videos
Metadata
Pore-Segmentation Result
Load Pores as Index Image
Load *.g32
Load Pore-Size Distribution.
Load *.gsd
Load Pore-Orientation Distribution
Load *.gof
Thresholding Result
Load Pore-Type Structure
Load *.gdt
Load Pore-Type Structure
Load *.gad
Shape-Analysis Result
Load Pore Fit Shapes
Load *.gad
Load Comparison of Segmented Pores and their Fits
Load *.gdt
Load Euclidean Distance Transform per Pore
Load *.dst
Intermediate Results
Load Pores from Step 1 (Result of Watershed)
Load *.gdt
Load Pores from Step 2 (Result of Pore Reconnection)
Load *.gdt
Load Pores from Step 3 (Result of Boundary-Pore Removal)
Load *.gdt
Manage Data
Load Input Map
Export
Close
Material Information:
ID 00: Solid [invis.]
ID 01: Pore [Original]
ID 02: Pore [Fit]
ID 15: Pore [Overlap]
Material Information:
ID 00: Solid [invis.]
ID 01: Pore
Material Information:
ID 00: Solid [invis.]
ID 01: Pore
ID 02: Pore
ID 03: Pore
ID 04: Pore
ID 05: Pore
ID 06: Pore
ID 07: Pore
ID 08: Pore
ID 09: Pore
ID 10: Pore
ID 11: Pore
ID 12: Pore
ID 13: Pore
ID 14: Pore
ID 15: Pore

Output Options

Under the **Output Options** tab, additional results to be computed and saved can be chosen. They are displayed later for visualization in the Result Viewer under the **Pore Visualization** tab. Some of these options need an additional computing effort and are unchecked by default.



- Check **Save Pore-Size Distribution (Volume-Equivalent Diameter) as *.gsd** to save the computed pore size distribution as a volume field. This information can be used e.g. for visualization of the volume field of the Volume-Equivalent Diameter (see page 32) or for further analysis with Python.
- When **Save Inscribed-Sphere Diameters and Sheppard Sphericities** is checked, the diameter of the inscribed sphere for every pore is calculated as volume field and saved. The results of this volume field are saved in a *.gsd file and can be loaded with it. The Sheppard sphericities and the inscribed sphere diameters can be found in the Result Viewer (Results – Plots – Sphericities tab and Diameters tab, see page 25). Both options need additional computing effort and are unchecked by default.
- Check **Save Pore-Orientation Distribution as *.gof** to use the orientation information in simulations or for later analysis.
- The checked-by-default **Save Comparison of Segmented Pores and their Fits as *.gdt** is useful to evaluate the quality of the fitted GAD-objects (Ellipsoids). A good accordance of the pore fit shapes and the identified pores is important as a basis for generating good digital twins.
- After checking **Save Euclidean Distance Transform per Pore as *.dst**, the EDT for every pore is calculated individually and the result is saved in one single file (*.dst format). This option needs additional computing effort and is unchecked by default.
- The resulting pore index image is saved by default in the binary *.g32 format. With the last option, **Save Pore Index Image as *.leS**, it can be additionally saved as an ASCII file. This format takes more space and needs longer to write and load into GeoDict, but it is human-readable and can easily be imported into other software.

Choosing **Histogram Weighting** as **Volume**, **Surface** or **Number** changes the values on the Y-axis of the resulting histogram plots. Then, either the pore volume probability, the pore surface area probability, or the pore count probability is shown. The histogram weighting can be changed in the result viewer after the simulation has been run.

PORE IDENTIFICATION RESULTS

The pore identification results are saved in a GeoDict result file (*.gdr) with the given Result File Name and after the run has finished the **Result Viewer** opens automatically.

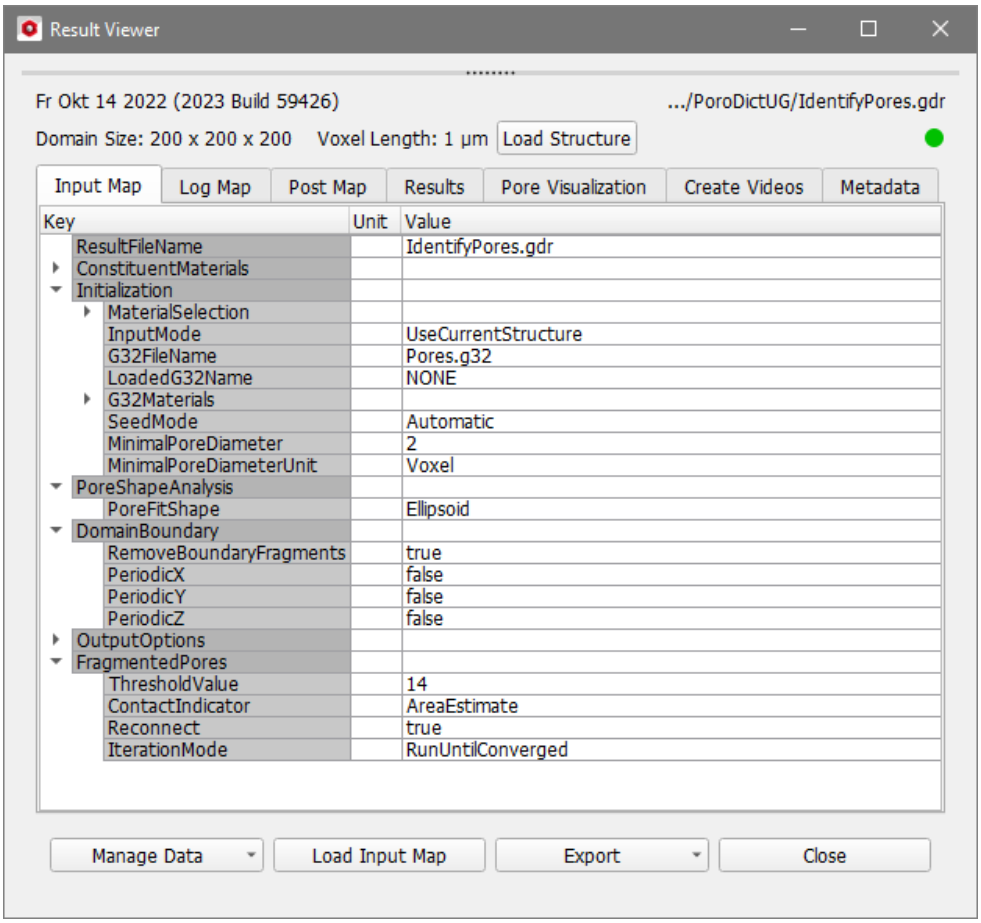
By clicking **Load Structure**, the analyzed structure can be imported into the Visualization area of the GeoDict GUI . Observe the dot at the right side of the **Load Structure** button: a green dot means that the currently loaded structure corresponds to the results shown in the Result Viewer. A red dot means that the structure does not correspond to the results.

The Result Viewer contains several tabs. **Input Map**, **Log Map**, and **Post Map** contain the parameters concerning the pore identification process. The **Log Map** contains information about the identification process, as e.g. the runtime and the used computer. The **Post Map** contains all information about the post-processing in the result viewer, as e.g. the chosen plots and their parameters. Only the **Input Map** is shown below in detail, the other two are structured analogously. The **Result** tab shows the report of the run as well as several plots, which are described in the Results section. In the **Pore Visualization** tab additional result files can be loaded depending on the choice made in the Output Options. A video of single pores and their fit object can be generated in the **Create Videos** tab. The **Metadata** tab contains some meta information about the result file.

At the bottom of the Results Viewer, several options for the results are available. Under **Manage Data** by choosing **Clean Up/Pack** either old results files can be deleted (Clean Up) or the results can be packed to a *.zip file. Clicking **Rename** allows to change the name of the *.gdr file. With **Load Input Map**, the parameters of the input map are loaded in the GUI and can be used to analyze different structures. With the **Export** button, selecting **Excel (generic)** or **Matlab**, the content of the *.gdr result file can be loaded into Microsoft Excel® or MATLAB®. These options only work when the chosen software is installed on the computer. Alternatively, the information in the result file in *.html format can be saved by clicking **Store As HTML**. **Save Plots** allows to save all plots of the Results Plots subtab at once. Also, the user can save the **Input Map as Python** file to re-execute the run as macro with the same settings.

INPUT MAP

The **Input Map** contains a table with all chosen input parameters for **Identify Pores** written down as key-value pairs. For example, it is shown that **Reconnect Fragmented Pores** was enabled, and that the **Interface Threshold** was 14%.



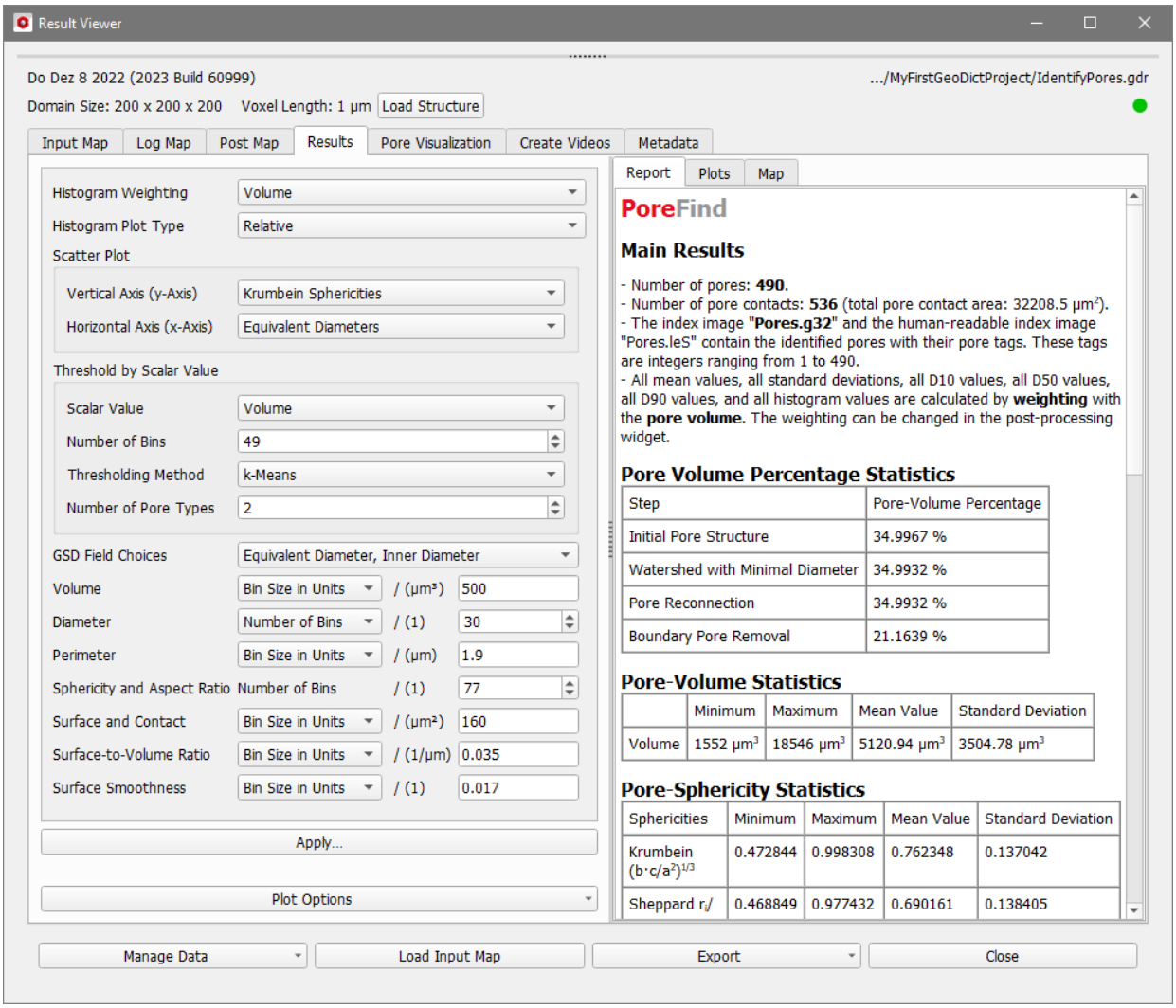
RESULTS

The **Results** tab is the central point for the analysis of the identified pores. It is grouped in three subtabs: **Report**, **Plots** and **Map**. The **Report** tab shows statistics about the identified pores and the **Plots** tab contains plot options for the analysis of the results. The **Map** tab contains all resulting data from the **Identify Pores** run. This data is the basis for the tables in the **Report** tab and for the plots in the **Plots** tab.

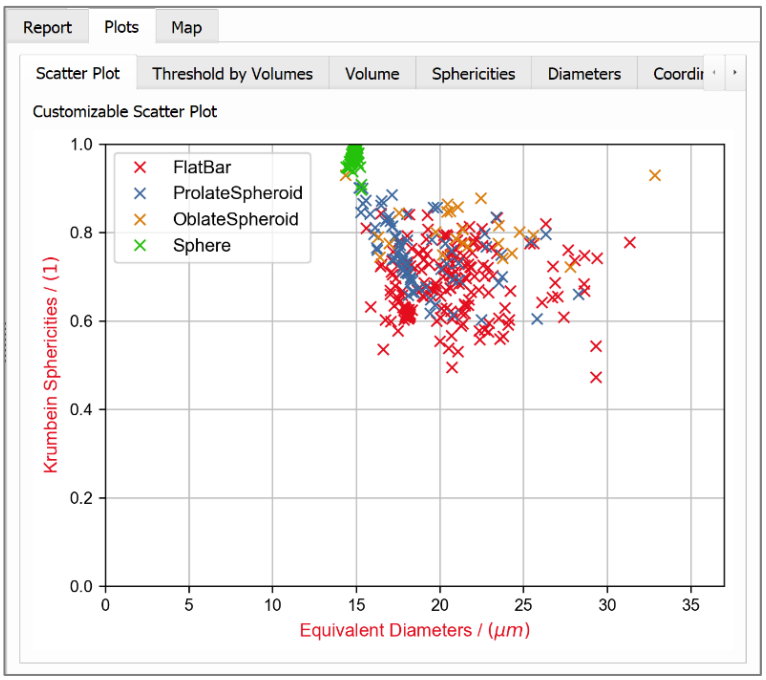
The **Plots** tab offers several plots to show the relationship between pore parameters: **Scatter Plot**, **Threshold by Scalar Value** histogram, **Volume** histogram, **Diameters** histogram, **Perimeter** histogram, **Sphericities** histogram, **Aspect ratio** histogram, **Surfaces and Contacts** histogram, **Coordination Number** histogram, the **Orientation** polar plot and the **Reconnection Indicators** histogram.

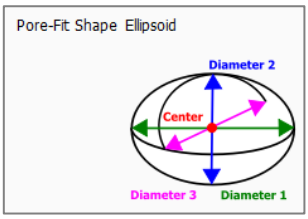
For the **Threshold by...** histogram, the threshold parameter must be selected under **Threshold by Scalar Value** on the left (See page 30 for more explanations). The default is **Threshold by Volume**.

Settings for these plots can be selected in the panel at the left side of the **Plots** tab. After changes, click **Apply...** to use the new values. The changes are also applied to the table under the **Report** subtab.

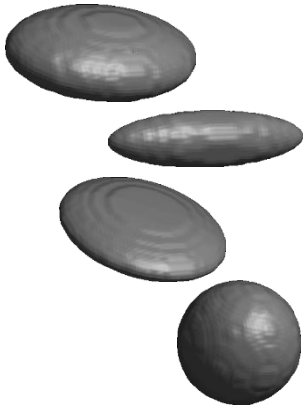


In the example, observe in the **Scatter Plot** that the found spherical pores have an equivalent diameter of 15 µm, while the found ellipsoidal spheres have equivalent diameters between 15 and 32 µm.





The plots Scatter Plot and Orientation distinguish between the four shapes Flat Bar, Prolate Spheroid, Oblate Spheroid and Sphere. These are the four possible shapes for the ellipsoids that are fitted into the pores.

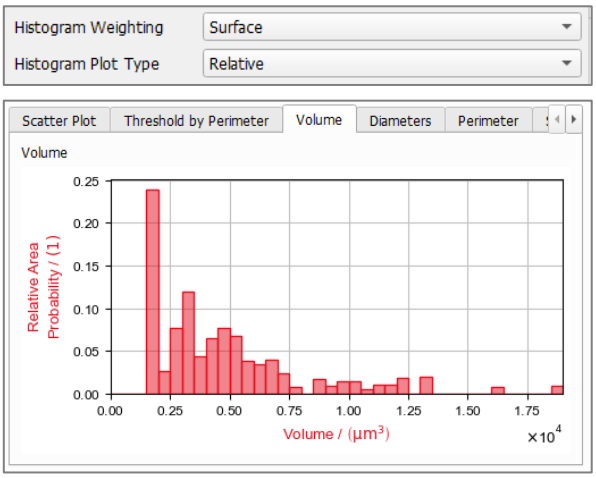


- An ellipsoid is formed as a **Flat Bar**, if all three diameters differ much from each other.
- A **Prolate Spheroid** has one bigger and two similar smaller diameters. Its shape is similar to a cigar.
- The two bigger diameters of an **Oblate Spheroid** are similar. Thus, it can be compared to a disk.
- For a **Sphere** all three diameters are similar.

Plot Options Panel

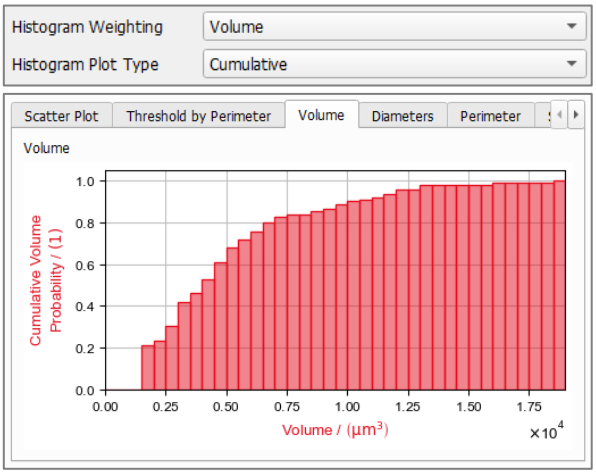
Histogram Weighting and Histogram Plot Type

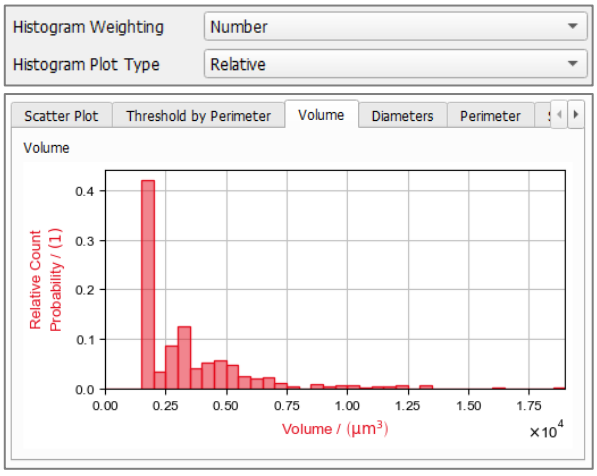
The values on the Y-axes of the histograms in all plots (except **Scatter Plot, Threshold by Scalar Value, Orientation** and **Reconnection Threshold**) can show Count Probability (weighting by **Number**), Area Probability (weighting by **Surface**) or Volume Probability (weighting by **Volume**), as a **Relative** or **Cumulative** plot. This can be set by adjusting the **Histogram Weighting** and **Histogram Plot Type**.



The Area (or Surface) Probability is defined by computing the surface area of each segmented pore (using the same algorithm as in MatDict's Estimate Surface Area command) and then weighting the pores by that value. The computed surface area does also include the surface between different pores, not only the area between pore and solid material.

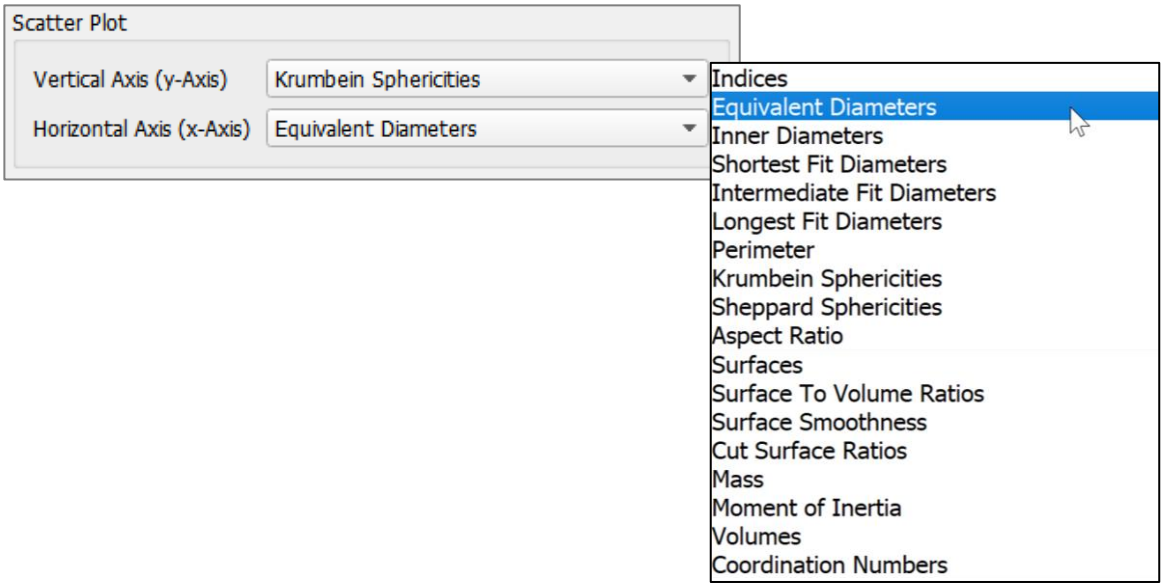
The example on the left-hand side shows, that the smallest pores make up nearly 25% of the total Surface area. Compared to the weighting with numbers, 42% of the pores belong to the smallest pores in the structure.





Scatter Plot

Under **Scatter Plot**, the variables for the X- and Y-axis in the scatter plot can be chosen. More on the variables can be found in the next section.



Threshold by Scalar Value

In **Threshold by Scalar Value**, several options for thresholding the structure depending on the results are available.

The choice of the **Scalar Value** affects the plot that is created under the **Plots** - **Threshold by ...** subtab. Additionally, a structure containing the materials of the thresholded pores will be created, that can be accessed through the **Pore Visualization** tab → **Load Pore-Type Structure** → click **Load *.gdt** or **Load *.gad** button.

The following Scalar Values are available for thresholding:

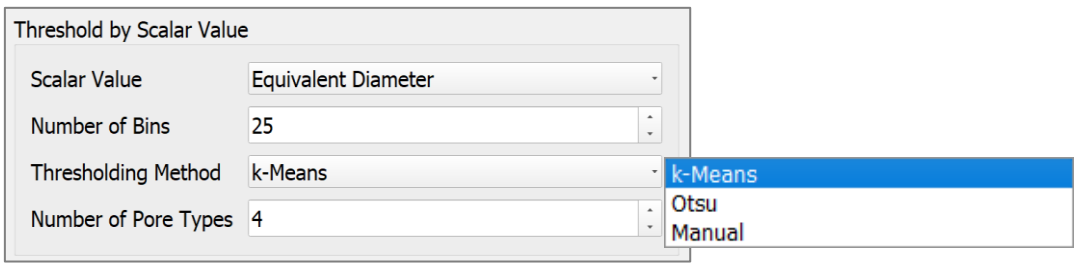
- **Equivalent Diameter**: the diameter of the volume-equivalent sphere.
- **Inner Diameter**: the diameter of the largest sphere that can be inscribed into the pore.
- **Shortest Fit Diameter**: the shortest diameter of the ellipsoid fitted onto the pore.
- **Intermediate Fit Diameter**: the intermediate diameter of the ellipsoid fitted onto the pore.
- **Longest Fit Diameter**: the longest diameter of the ellipsoid fitted onto the pore.
- **Perimeter**: three diameters are needed to define the ellipsoid fitted into the pore. The perimeter is the shortest perimeter around this ellipsoid, which means it is computed as the perimeter of the ellipse formed from the two smallest of those three diameters.
- **Krumbein Sphericity**: measure for the sphericity $P_K = \sqrt[3]{\frac{bc}{a^2}}$ based on the three principal axes (a,b,c) of the ellipsoid fitted into the pore.
- **Sheppard Sphericity**: the diameter of the inscribed sphere divided by the diameter of the volume-equivalent sphere.

- **Aspect Ratio:** the ellipsoid fitted into the pore is defined by three diameters. The aspect ratio is the shortest diameter divided by the largest of those diameters.
- **Surface Area**: surface of the pores estimated by an algorithm based on MatDict's **Estimate Surface Area** command (see [1] and MatDict handbook).
- **Surface-to-Volume Ratio**: estimated surface of the pore divided by the volume of the pore.
- **Surface Smoothness**: the surface of a fitted ellipsoid divided by the estimated surface. Usually the estimated surface is larger than the surface of the fitted ellipsoid. Hence, the surface smoothness is usually below 1. Only if the shape of the pore is very ellipsoidal, then the surface estimation might be a little smaller than the surface of the fitted ellipsoid.
- **Cut-Surface Ratio**: the interface of the pore with the domain boundary over the remaining surface of the pore. The **Cut-Surface Ratio** measures how much of the pore surface is part of the domain boundary. It is a measure for the quality of boundary pores. For example, a **Cut-Surface Ratio** of 1 means that the interface of the pore with the domain boundary is as large as the remaining surface of the pore.

  NOTE that the domain boundaries, that were set to be periodic, do not contribute to the interface of the pore with the domain boundary. Particularly, if all domain boundaries are set to be periodic, the cut-surface ratio will always be zero. Also, if **Remove Pore Fragments at Domain Boundary** was activated (page 20), then the cut surface ratio is zero, too, because there will be no pores left that have an interface with the domain boundaries.
- **Mass:** if a density is assigned to the porous space in the constituent materials tab under the Fluid Density tab, each pore has a mass which can be calculated from its volume.
- **Moment of Inertia:** depends on the mass distribution of the pores and only works if a density is assigned.
- **Volume**: the volume of the pore, simply determined by the number of voxels the pore contains.
- **Coordination Number**: the number of contacts of a pore to other pores.

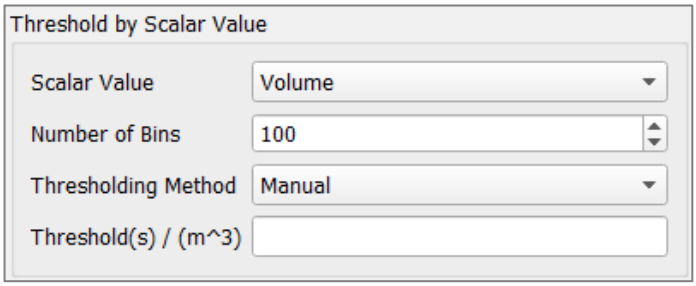
NOTE that the choice of **Inner Diameter** and **Sheppard Sphericity** are only available if the option **Save Inscribed-Sphere Diameter and Sheppard Sphericities** was checked in the **Output Options** of the pore-identification options (page 23).

The **Number of Bins** defines how many bins the histogram **Threshold by ...** has.



The following **Thresholding Methods** are available:

- **k-Means**: uses the k-Means algorithm to find thresholds for the chosen **Number of Pore Types**.
- **Otsu**: uses the Otsu algorithm to find thresholds for the chosen **Number of Pore Types**.
- **Manual**: define your own thresholds by writing a comma-separated list of thresholds into **Threshold(s)**. They will then be applied to the computed pore index image.

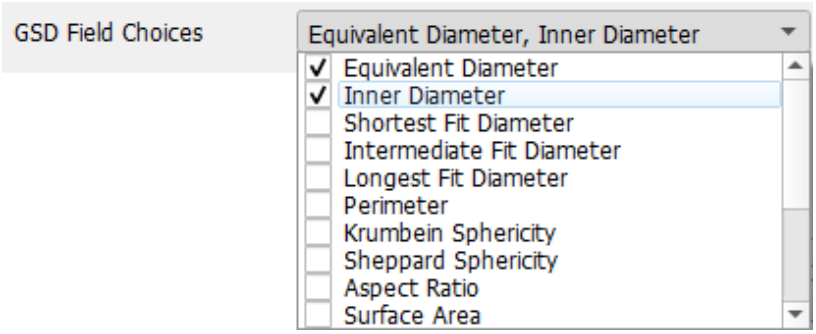


GSD Field Choices

The GeoDict size distributions (GSD) files allow to visualize the various scalar pore properties that are a result of the pore identification.

See the options for the configuration of a GeoDict size distribution (GSD) file in the figure below. For every chosen pore property, a volume field is created containing the 3D distribution of this pore property. These volume fields are saved together in a GSD file (*.gsd). This file can be accessed through the **Pore Visualization** tab → **Load Pore-Size Distribution** → click **Load *.gsd** button.

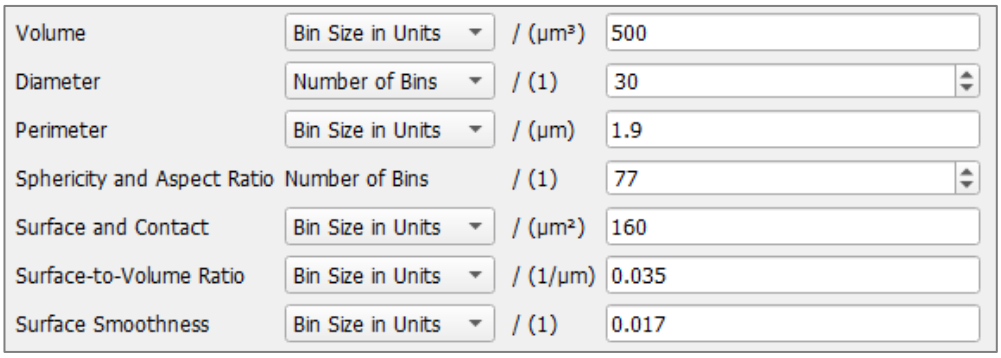
For example, by choosing **Equivalent Diameter** and **Inner Diameter**, the *.gsd file will contain two volume fields: one with the size distribution of the diameters of volume-equivalent spheres, and one with the inner diameter.



The same measures for assembling a customized size distribution are available as for the thresholding (see page 28).

Histogram Bin Sizes

The bin sizes used in the plotted histograms can be customized.



In general, it is possible to choose between:

- **Number of Bins**: choose how many bins the histogram should have.
- **Bin Size in Units**: choose the bin size for the histogram using the value in the appropriate unit (m, µm, nm, etc.).
- **Bin Size in Voxels**: choose the bin size for the histogram using the value measure in voxel lengths.

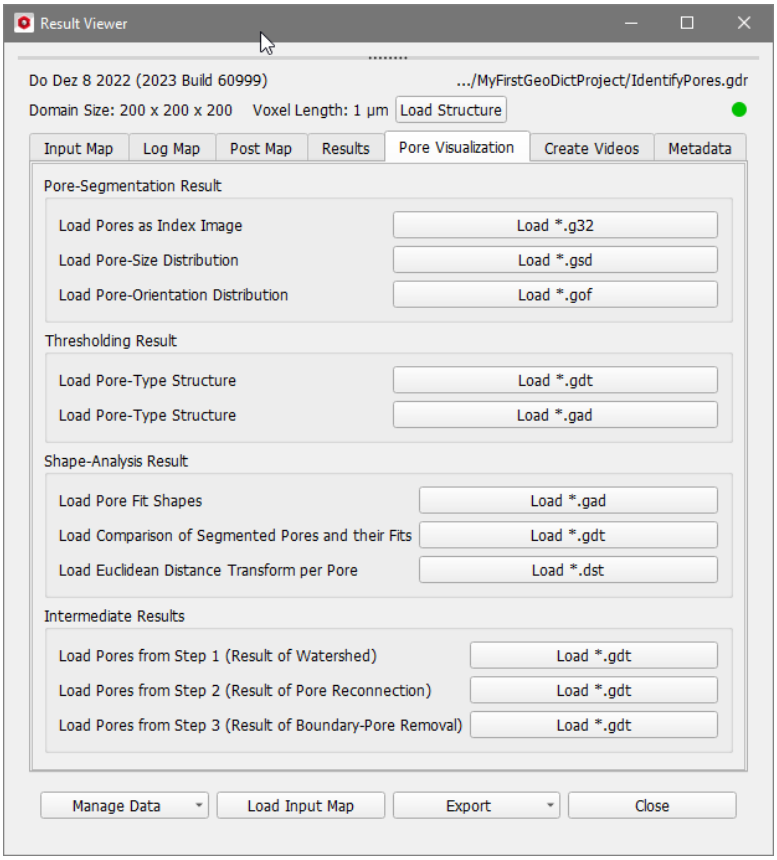
As the different histogram plots show different results, only those choices are available which make sense for the corresponding plot.

- The selection made under **Volume** changes the bin size for the plot under the **Volume** tab.
- The selection made under **Diameters** changes the bin size for all plots under the **Diameters** tab.
- The selection made under **Perimeter** changes the bin size for the plot under the **Perimeter** tab.
- The selection under **Sphericity and Aspect Ratio** cannot be changed, this affects the bin size for the plots under the **Sphericities** tab and the plot under the **Aspect Ratio** tab.
- The selection made under **Surface and Contact** changes the bin size for the **Surfaces** and **Contacts** plots under the **Surfaces And Contacts** tab.
- The selection made under **Surface-to-Volume Ratio** changes the bin size for the **Surface-to-Volume Ratios** plot under the **Surfaces And Contacts** tab.
- The selection made under **Surface Smoothness** changes the bin size for the **Surface Smoothnesses** plot under the **Surfaces And Contacts** tab.

Pore Visualization

The **Pore Visualization** tab is used to import structures and computed volume fields which illustrate the pore identification process and its results.

Under the **Pore Visualization** tab, several options are available for the visualization of the different steps of **Identify Pores** and for the evaluation of the quality of the results. Some options might be unavailable, depending on the previously chosen parameters in the **Identify Pores** dialog (Output Options tab. see page 23). The visualization options are grouped into panels.



Pore-Segmentation Result

In the first panel, several options for the analysis of the identified pore shapes are available. With **Load Pores as Index Image**, all identified pores are assigned to a unique 32-bit color and can be investigated in the Visualization area. The 2D-view of *.g32 files is particularly suited for visual analysis of the correct segmentation.

The **Load Pore-Size Distribution** and the **Load Pore-Orientation Distribution** are greyed out when these two options have not been previously checked under the **Output Options** tab of the **Identify Pores** dialog (see page 23).

Thresholding Result

The structure that contains the thresholded pore materials is loaded by clicking the **Load Pore-Type Structure** button. Here, either **Load *.gdt** or **Load *.gad** can be chosen. The options for the thresholding can be found in the **Results** tab as mentioned above in Thresholding.

Shape-Analysis Result

With **Load Pore Fit Shapes**, the best-fit shapes for the individual pores are imported into GeoDict as *.gad file and can be visualized.

The option to **Load Comparison of Segmented Pores and their Fits** is closely related to **Load Pore Fit Shapes**. The identified pores and their best-fit shapes are both imported into GeoDict and shown as different materials (**Original** and **Fit**). This is a good indicator for evaluating the performance of pore identification with the chosen options (compare the figure on page 21 for reference).

With **Load Euclidean Distance Transform per Pore**, the results of the Euclidean Distance Transform for each pore can be imported if **Save Euclidean Distance Transform per Pore as *.dst** was previously checked under the **Output Options** tab of the **Identify Pores** dialog (see page 23).

Intermediate Results

In the **Intermediate Results** panel, results from the identification steps can be loaded.

With **Load Pores from Step 1 (Result of Watershed)**, the segmented pores after the watershed transform are shown without any post-processing. Depending on the structure and the chosen **Minimal Pore Diameter**, this step might already be good enough to identify the pores. Otherwise, this option is useful to check the initialization options – mainly if the **Minimal Pore Diameter** was chosen correctly for the analyzed pore space.

By clicking **Load Pores from Step 2 (Result of Pore Reconnection)**, the pore space after the Pore-Fragment Reconnection is loaded in GeoDict. This way it can be assessed whether the chosen value for **Interface Threshold** suits the analyzed pore space. This is only available if **Reconnect Fragmented Pores** was checked in the **Pore Segmentation** tab of the **Identify Pores** dialog (see page 18).

Load Pores from Step 3 (Result of Boundary-Pore Removal) imports the identified pores resulting from the removal of pore fragments defined in the **Domain-Boundary Options**. This is only available if **Remove Pore Fragments at Domain Boundary** was checked in the **Pore Segmentation** tab of the **Identify Pores** dialog (see page 20).

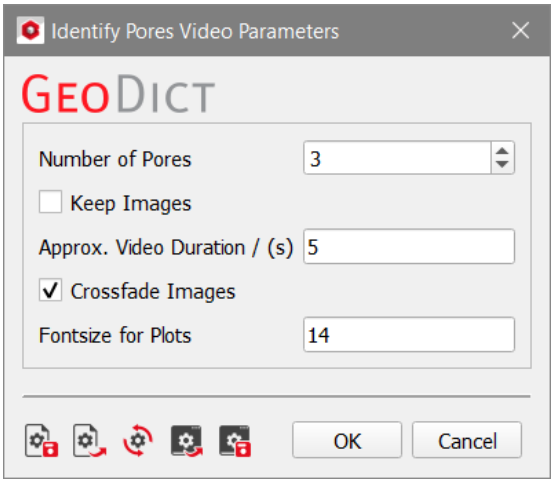
For the visualization of the identified pores, remember that the visibility of all material IDs must be set to visible in **Settings** → **Color & Visibility Settings** → **visible**. The identified pores are assigned 15 random colors, which are unrelated to their size.

The visibility of the non-pore space (ID 00) should be unchecked and thus it will not be rendered.

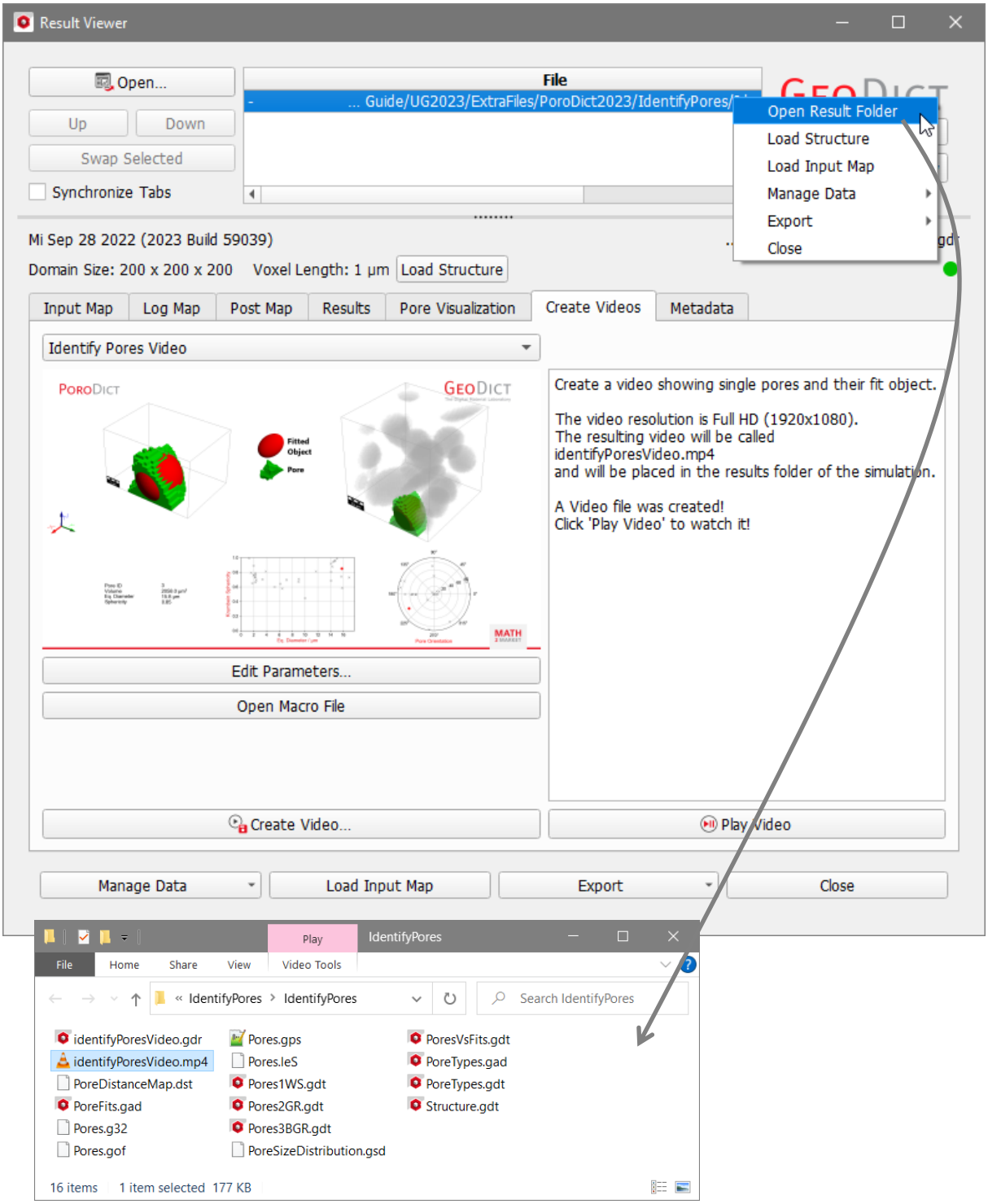
CREATE VIDEOS

With **Create Videos**, it is possible to automatically generate a video showing the largest identified pores compared to their fit shapes.

Click **Edit Parameters...** to choose the number of pores that should appear in the video. Additionally, the video duration and the fontsize for the plot labels can be edited.

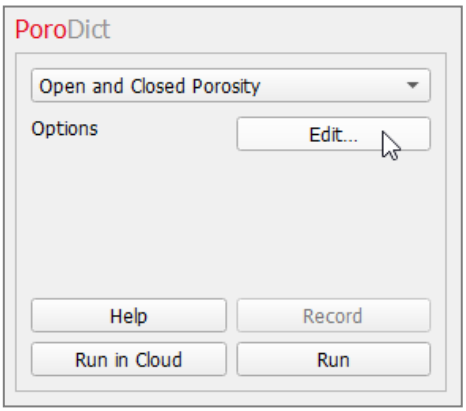


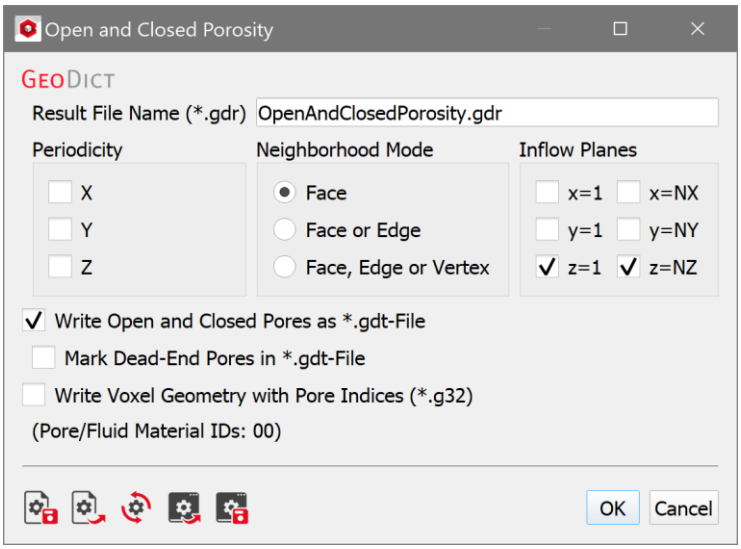
Clicking the **Create Video ...** button starts the creation of the video. When the video is finished, the video file is saved in the results folder belonging to the loaded *.gdr file. The result folder can be opened by right-clicking on the file name or file path in the Result Viewer Header section box and choosing **Open Result Folder**.



Open and Closed Porosity

When selecting **Open and Closed Porosity** from the pull-down menu, the connectivity of the pores to one or more specified directions can be calculated. The settings for this can be modified through the **Options**' **Edit...** button.



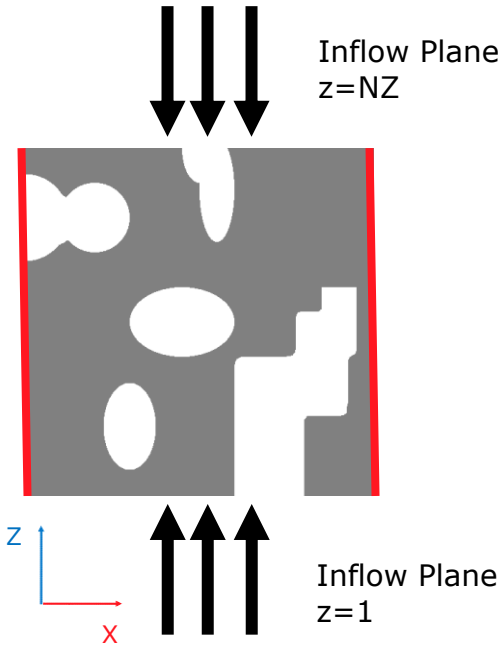


In the **Open and Closed Porosity** dialog box, the name for the file (**Result File Name**) where the results are saved in the chosen project folder can be entered. Then select whether to apply **Periodicity** to the structure in one or more directions.

The **Neighborhood Mode** determines how many voxels from the pore space material in the structure are perceived as belonging to a connected group. Checking **Face** is more restrictive than choosing **Face or Edge**. The most permissive **Neighborhood Mode** condition is **Face, Edge or Vertex**.

The selection of **Inflow Planes** determines to which surface the pores should be open to be considered part of the open pore network.

For example, here with the default z=1 (x-y-plane through z=1) and z=NZ (x-y-plane through z=NZ) checked, pores that do not open to the Z-inflow planes (at the top and at the bottom of the volume) are deemed to be closed.



When **Write Open and Closed Pores as *.gdt-File** and/or **Write Voxel Geometry with Pore Indices (*.g32)** are checked, .gdt and/or .g32 files are saved in the results folder (inside the project folder) with the default names **OpenAndClosedPores.gdt** and **PoreIndex.g32**. The files in *.g32 format are considerably larger than those in *.gdt format and contain all identified pores with the index per pore.

By checking **Mark Dead-End Pores in *.gdt File** the open pores can be subclassified in

- dead-end pores, which have contact with only one of the specified inflow planes
- through pores, which connect multiple specified inflow planes.

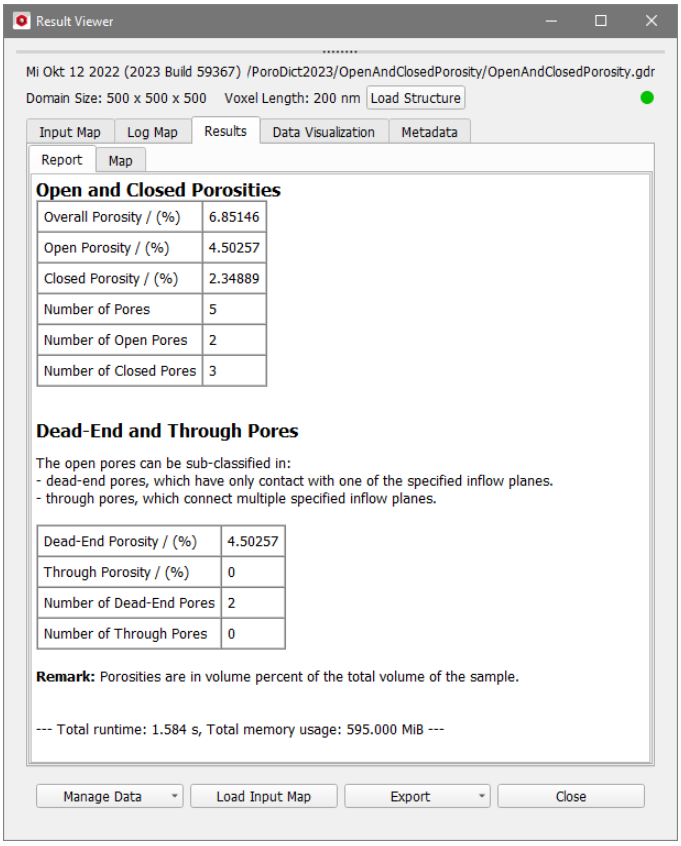
This classification only makes sense if multiple inflow planes are chosen.

Results

The Result Viewer opens at the end of the calculations.

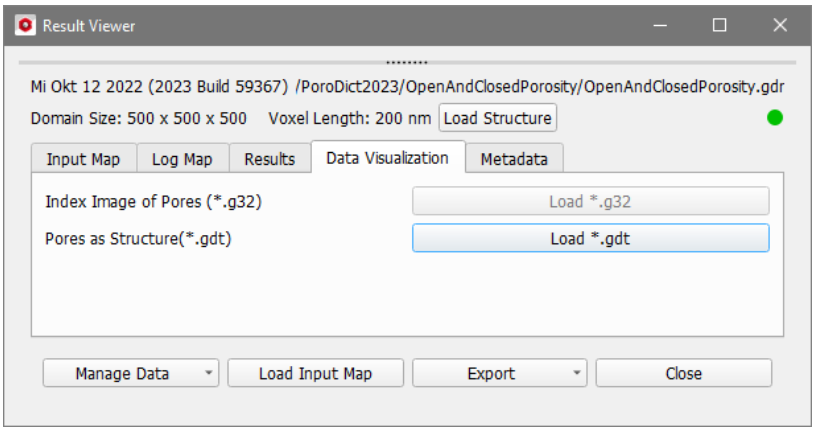
Under the **Results - Report** subtab, a table shows the calculated overall porosity, open porosity, and closed porosity, as well as the total number of pores, the number of open pores, and the number of closed pores.

A second table shows the dead-end porosity and the through porosity, as well as the number of dead-end pores and the number of through pores.



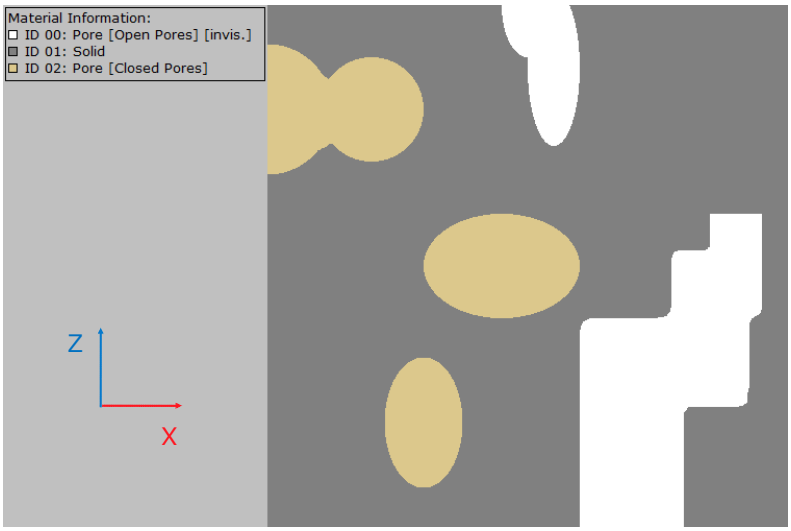
Data Visualization

Under the **Data Visualization** tab, click **Load *.gdt** to observe the open and closed pores network.



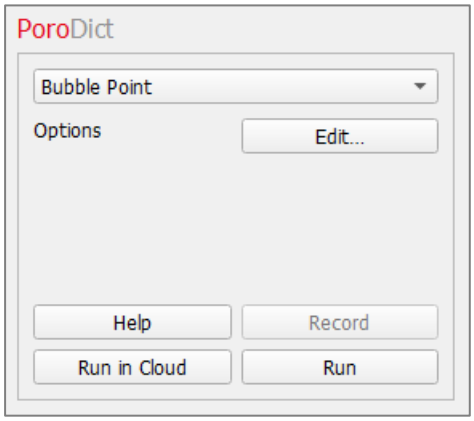
The material ID 00 is assigned to the Open Pores and is invisible per default.

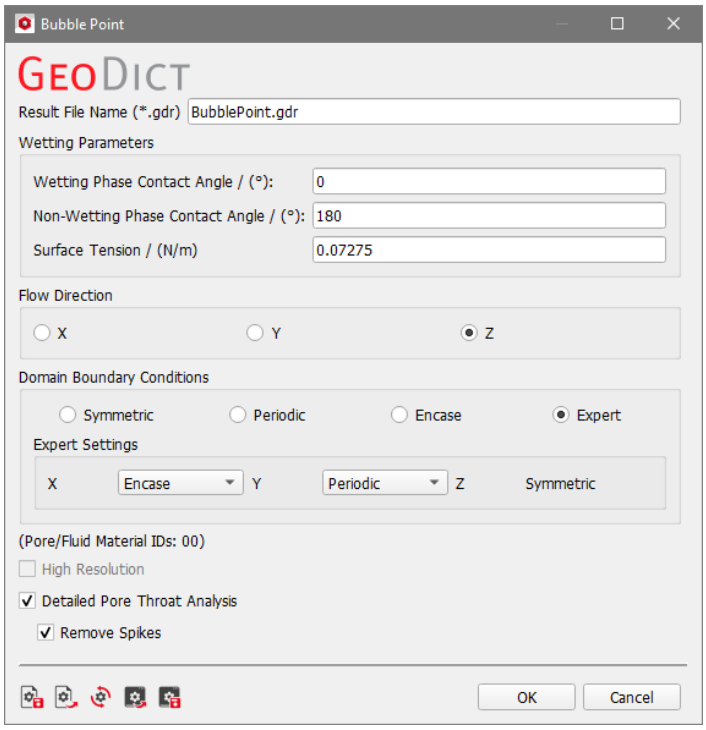
The Closed Pores are assigned the next available ID after the solid material IDs (all Solid). Here it is material ID 02, shown in beige. One of the closed pores is closed to the Z-inflow planes but would be assigned to open pores if x=1 was chosen for Inflow Plane.


Material Information:
ID 00: Pore [Open Pores] [invis.]
ID 01: Solid
ID 02: Pore [Closed Pores]
Z
X

Bubble Point

When selecting **Bubble Point** from the pull-down menu, the **Wetting Parameters, Flow Direction** and **Domain Boundary Conditions** can be modified through the **Edit...** button.

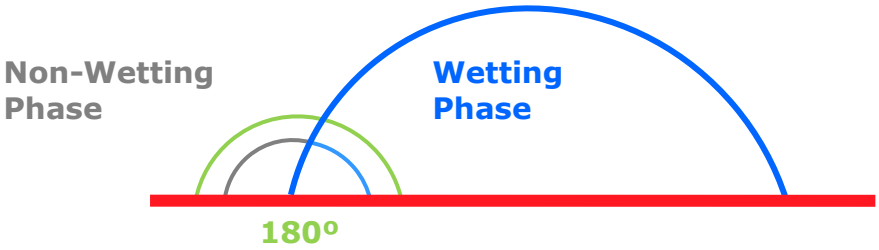




In the **Bubble Point** dialog, enter the **Result File Name**.

Then, choose the **Wetting Phase Contact Angle** and the **Non-Wetting Phase Contact Angle**.

The sum of the contact angles is 180º, (shown in the picture are 25º and 155º) and they are adjusted automatically when changing one of the two values.



Enter the **Surface Tension** of the fluid or use the default value corresponding to the surface tension of water.

The direction of the flow (**X**, **Y**, or **Z**) can also be defined.

The **Domain Boundary Conditions** can be chosen to be **Symmetric**, **Periodic, Encase**, or any combinations of those boundary conditions in all three directions with the choice of **Expert**. A detailed explanation of the different conditions can be found on page 6.

To run the calculations in **High Resolution** might be useful when the pore space is assumed to be especially narrow. The standard algorithm computes pore sizes and distances directly on the voxel grid, i.e. when determining the pore size, only the distances from the center of a pore voxel to the center of a solid voxel are taken into account. High Resolution also takes the voxel surfaces and edges into account, so the computed distances correspond to the distance to the next solid surface or edge.

The disadvantage of the **High Resolution** mode is that the calculation runtime and memory usage may increase by a factor of eight.

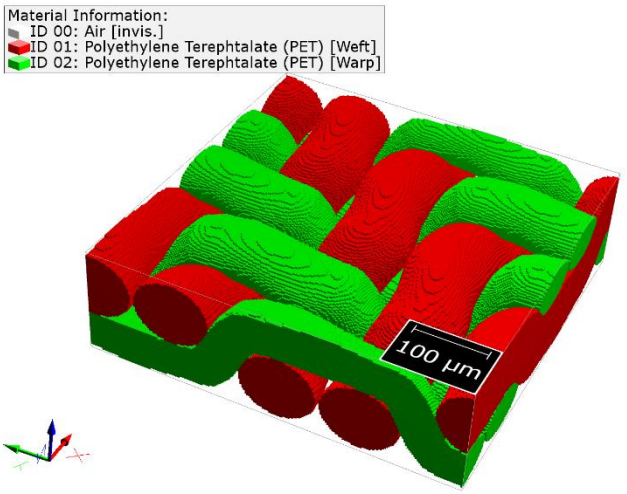
If **Detailed Pore Throat Analysis** is selected, the location and the shape of the smallest pore throat is found and geometrically analyzed. Multiple candidate throat planes along the percolation path will be tested by constructing planar ray-traced planes with varying tilt angles. The plane with the smallest area will be used for further analysis. This includes calculation of the hydraulic diameter, a detailed plot of the pore throat and enables loading the voxelized pore throat into GeoDict.

The circumference of this pore throat may exhibit spike-like extrusions, which have a strong influence on the geometrical analysis run. With the **Remove Spikes** option, those are removed before running the geometrical analysis. We advise to always have a look at the pore throat plot, to identify spikes in the pore circumference.

Either **High Resolution** or **Detailed Pore Throat Analysis** can be chosen, not both at the same time.

Results

The Result Viewer opens at the end of the computations and the results are automatically saved in the project folder.

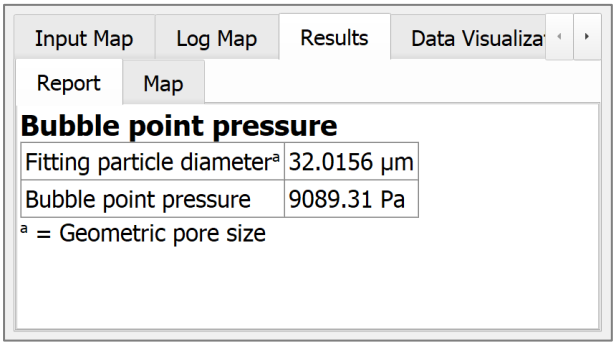


The bubble point pressure p_c is computed from the determined largest through pore radius r using the Young-Laplace equation:

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

where α is the wetting phase contact angle and σ is the surface tension, both entered in the **Bubble Point** dialog.

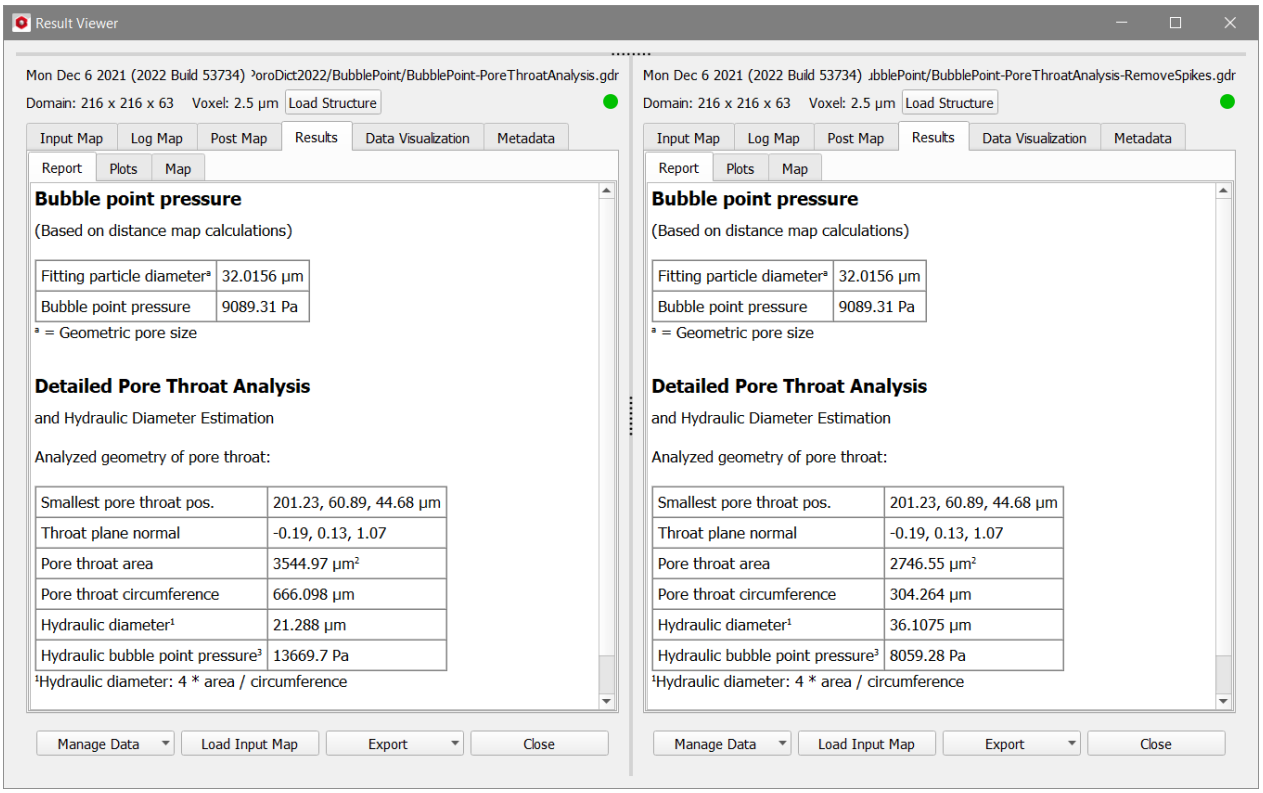
When the **Detailed Pore Throat Analysis** was switched off, the report only states the fitting particle diameter and the corresponding bubble point pressure as computed with the Young-Laplace equation. The fitting particle diameter is the largest through pore diameter as computed with the **Percolation Path** command (see the MatDict handbook of this User Guide for reference).



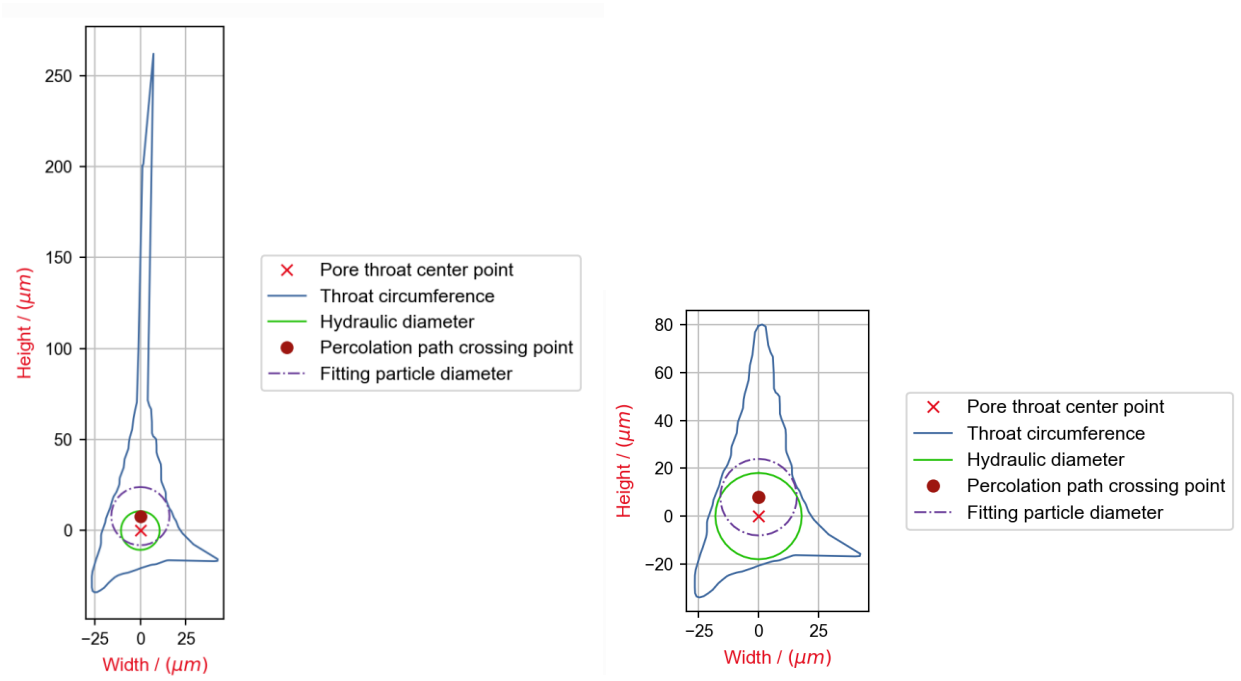
If a **Detailed Pore Throat Analysis** is run, the standard results are also reported, but additionally, the smallest pore throat is found, and its shape is analyzed.

The user can find the pore throat's position, normal direction, area, circumference, diameter and bubble point pressure in the result Viewer of the result file. Based on the area and circumference, the hydraulic diameter is calculated and used to predict a more precise bubble point pressure.

The results may vary depending if **Remove Spikes** was chosen or not, the screenshot below shows the results without this option on the left, and with this option on the right:



The pore throat cross section and the computed diameters are shown as 2D plot under the **Plots** tab:



If the plot looks like the one on the left side, please enable the **Remove Spikes** option, as described above.

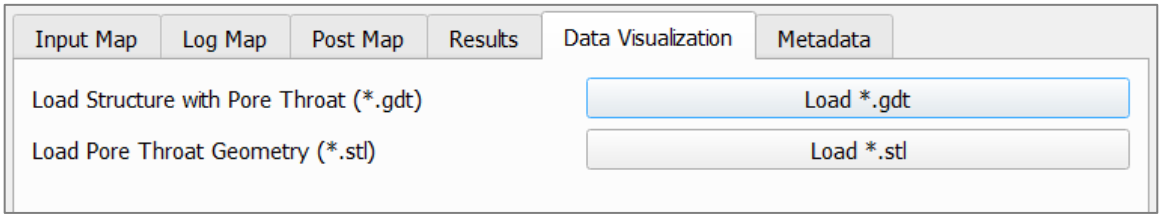
When **Remove Spikes** is used, the spikes seen in the circumference are removed before calculating the fitting diameters (see plot on the right side).

In the **Pore Throat Area Top View** up to six types of plot data can be shown:

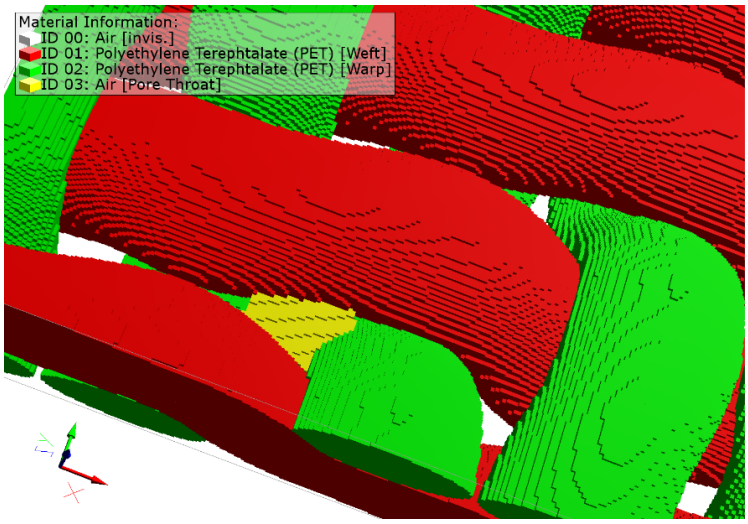
- The **Pore throat center point** is the center of the pore throat calculated as center point of the pore throat fitting diameter circle.
- The **Throat circumference** is the outline of the pore throat.
- The **Pore throat fitting diameter** describes the maximal circle around the pore throat center point. This parameter considers only the two dimensions of the cross section. Thus, it is only used for visualization and not for the bubble point computation. The corresponding plot is disabled by default. It can be enabled by right-clicking in the plot and checking the corresponding box.
- The **Hydraulic diameter** is a result of throat area and calculated bubble point pressure. For detailed information refer to the Wikipedia page. It can be quite different from the **Fitting particle diameter**, especially for pore throats with sharp angles.
- The **Percolation path crossing point** is the point, where the percolation path crosses the pore throat. As the percolation path considers all three dimensions, the percolation path crossing point and the pore throat center point can be different.
- The **Fitting particle diameter** is the diameter of the circular particle fitted into the pore throat when computing the percolation path. The percolation path crossing point is the center point of the circle described by this parameter.
-

Data Visualization

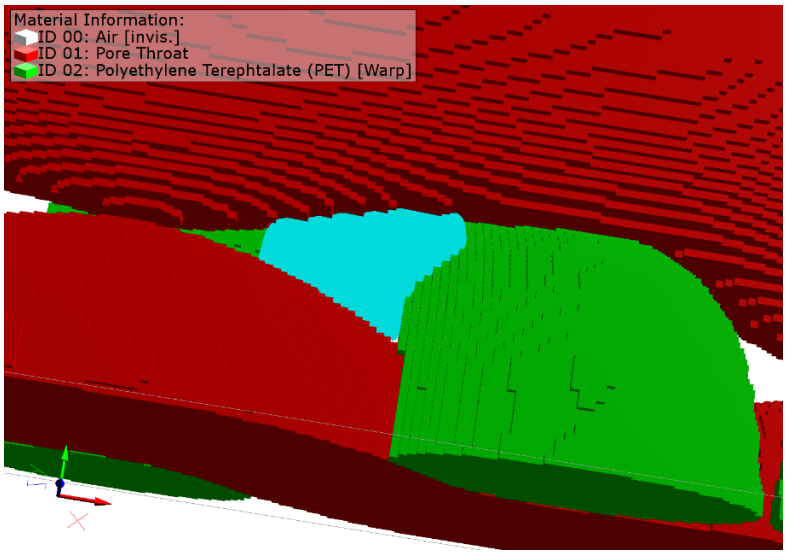
When the **Detailed Pore Throat Analysis** was switched off, no additional visualization options are available under the **Data Visualization** tab. If the option was switched on, two options are available:



Load Structure with Pore Throat (*.gdt) loads a GDT file, where the pore throat voxels are marked with another material ID, in this example ID 03.



Load Pore Throat Geometry (*.stl) shows the same pore throat. In this case the pore throat is loaded as a surface triangulation, and not as marked voxels.



Percolation Path

This command is also available in MatDict, and a description can be found in the MatDict handbook of this User Guide.

Chord Length Distribution

This command is also available in MatDict, and a description can be found in the MatDict handbook of this User Guide.

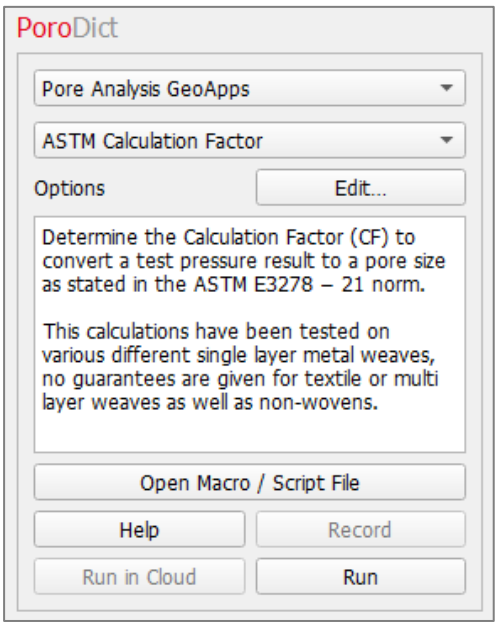
Geodesic Tortuosity

This command is also available in MatDict, and a description can be found in the MatDict handbook of this User Guide.

Pore Analysis GeoApps

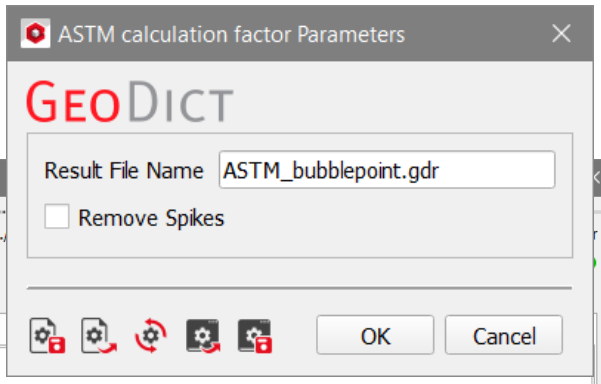
The Pore Analysis GeoApps section contains a GeoApp for the calculation of the ASTM pore size calculation factor according to the ASTM E3278-21 standard.

The computation of the ASTM pore size calculation factor was tested and optimized on several metal wire weaves. In the ASTM test, the wire weaves are put in a containment filled with water, while air is injected from below the weave. The bubble point pressure is reached when the first air bubble pushes through the weave layer.



For the calculation, a precise analysis of the pore throats in the weaves is of major interest. Especially, the shape of the pore throat is a key parameter. Additionally, a correction factor for metal wire weaves is computed.

Further information about GeoDict in the ASTM E3278-21 can be found on the GeoDict website.



REFERENCES

[1] J. Ohser, F. Mücklich; 2000; Statistical Analysis of Microstructures in Materials Science; Wiley and Sons, page 115.

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

Technical documentation:

Anne Blumer

Sebastian Rief

Barbara Planas

MATH 2 MARKET

Math2Market GmbH

Richard-Wagner-Str. 1, 67655 Kaiserslautern, Germany
www.geodict.com