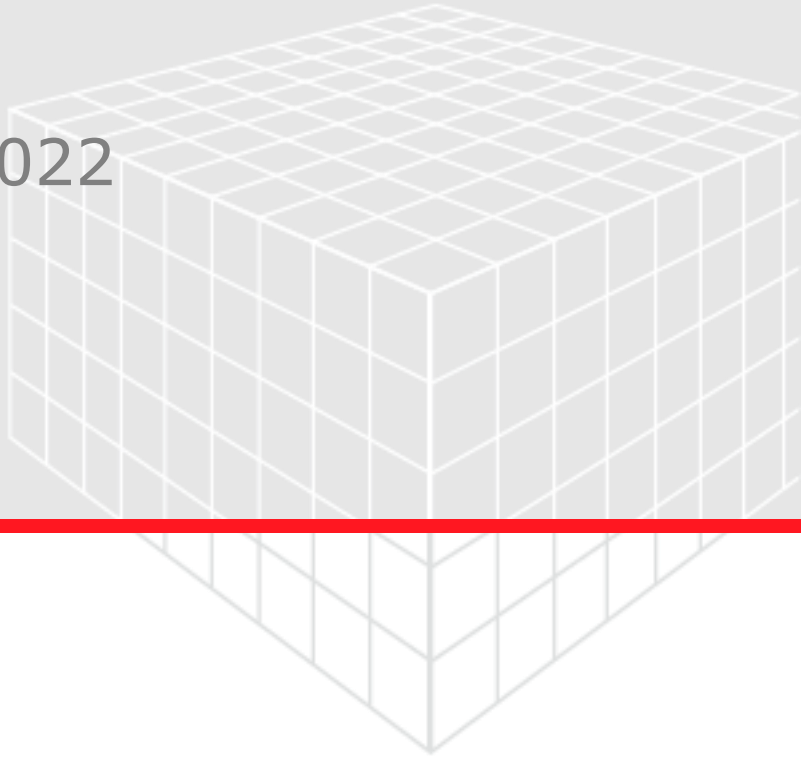
AddiDict

User Guide

GeoDict release 2022

Published: August 27, 2021



GeoDict

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

CALCULATING PARTICLE TRAJECTORIES AND TIME-DEPENDENT SPATIAL PARTICLE DISTRIBUTION

AddiDict is GeoDict's module for the simulation of mass transport by fluid streams. The name of the module stems from the idea to simulate mass transport by advective and diffusive particle movements.

A mass transport simulation develops in the following way:

1. Modeling of a 3D microstructure from 3D image-data (µCT, FIB-SEM, etc.), imported and segmented (with ImportGeo-Vol), or generation of a 3D microstructure model with a GeoDict generator module.
2. Definition of particle characteristics (size, density, etc.) and specification of particle insertion.
3. Definition of fluid characteristics (density, viscosity, etc.).
4. Computation of flow fields, particle motion and trajectories.

Optionally, electrostatic fields may be computed to study the effect of electrostatic forces on the particle motion, and collision points of particles may be recorded to investigate particle-structure interactions.

AddiDict does not incorporate chemical processes while computing the particle trajectories so far. However, since GeoDict 2021, chemical reactions of first order can be considered in the post-processing.

Besides diffusion, mass transport is controlled by the flow field. Mass transport, i.e. transport of solutes or particles, is simulated by tracking particle pathways through the flow enabling geometry.

Based on this data, time-dependent spatial particle distributions can be computed which represent either particle or solute concentrations.

In porous media, a **Breakthrough Curve** describes the evolution of the concentration of a substance within the media. Breakthrough curves are therefore a graphical representation of the transport properties. Within AddiDict, the breakthrough curve is determined by counting the number of particles that leave the computational domain in each time step. Particles can leave the structure on all boundaries defined as **Open** in the simulation, see page 18.

Since GeoDict 2020, the residence time of each particle in each pore or porous material is recorded additionally during simulation and can be visualized in the GeoDict Result Viewer of the result file (*.gdr).

From GeoDict 2021 on, an adsorption time of the particles can be defined for each material available in the simulated structure during post-processing of the results. This simulates a short time adsorption of a particle after entering a porous material or hitting a solid material.

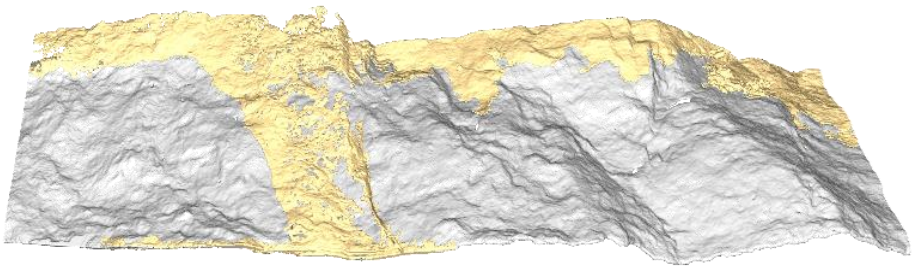
MASS TRANSPORT SIMULATIONS WITH ADDIDICT

A complete AddiDict mass transport simulation consists of the following steps:

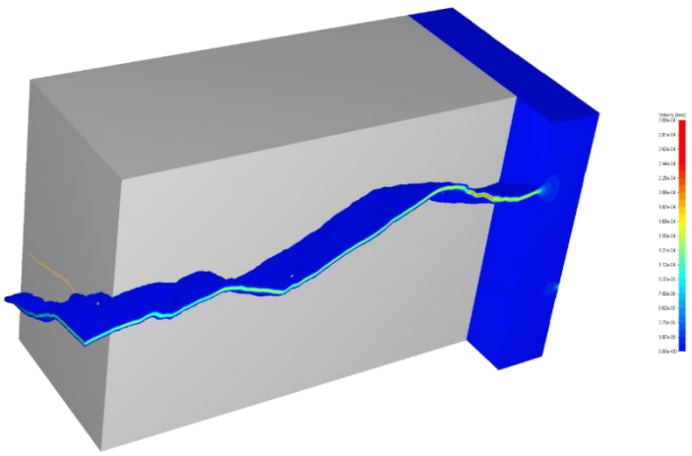
1. Import or generation of the initial 3D model of void space and porous medium,
2. Setting of simulated time and boundary conditions of the experiment,
3. Definition of parameters for the porous medium,
4. Specification of initial particle parameters, particle interaction model and size distribution,
5. Setting of options for the chosen flow solver,
6. Setting of the output of the particle tracking,
7. Running the simulation, and
8. Analysis and visualization of results.

All structures through which a fluid can flow in the transport direction can be used as input for AddiDict. The structure can consist of only solid materials and pores, or of one or several porous materials instead or additionally to the solid material.

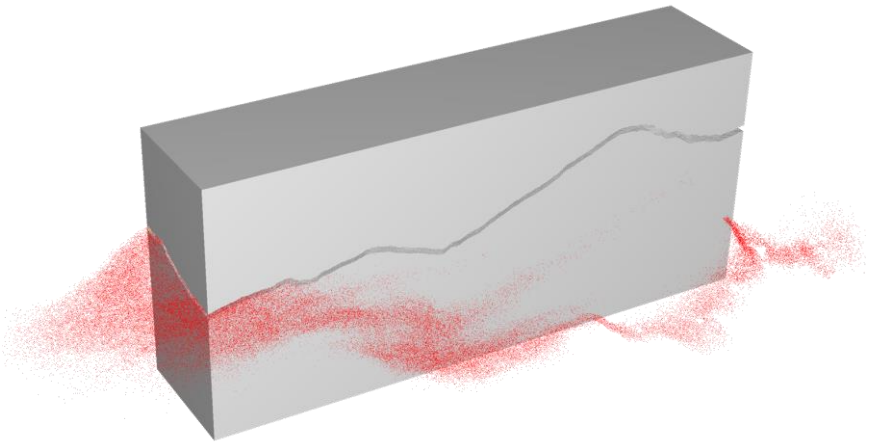
One of the GeoDict case studies (Nanoparticle migration in a natural granite fracture) is the experimental and numerical examination of the transport of particles in a fractured rock. We show here three figures from the case study, the 3D fracture geometry, the water velocity computed in the fracture and a visualization of the particles from the transport simulation.



3D fracture geometry after segmentation of the tomogram data, porous material (gold), solid / mineral matrix (void), pores (grey)



Velocity of water in the fracture for a flow rate of 66.8 µL/min, solid (grey), porous material (gold)

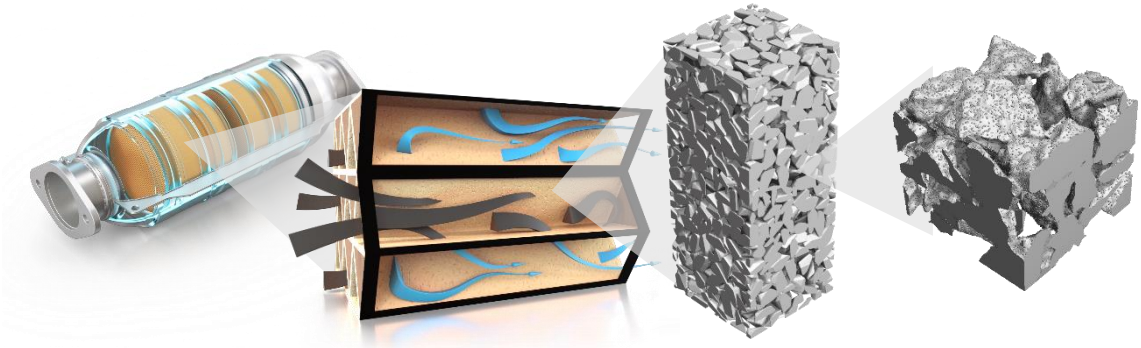


Visualization of the particles (red) in the fracture for a fixed time, solid (grey)

AddiDict for the simulation of Catalytic Converters

Modelling exhaust treatment bears many challenges on different scales. To predict the behavior of a catalytic converter, the following effects have to be taken into account:

- Flow through the support structure channels
- Flow and diffusion through the support structure walls (ceramic)
- Diffusion movement inside the wash coat layer
- Inner-grain (Knudsen-)diffusion to the catalytic reaction sites



Together with the new features introduced first in GeoDict 2021, GeoDict provides the possibility to simulate on all these scales.

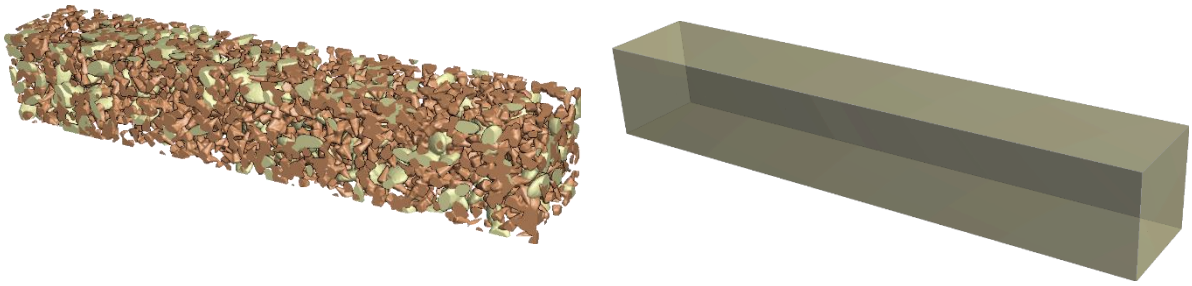
In AddiDict, the features aiming especially on the simulation of catalytic processes and exhaust treatment are:

- Providing residence times in all pore and porous materials
- Computing first order reactions
- Simulate slip flow with improved molecule tracking near surfaces
- Model reflection probability for porous media
- Simulate effective molecule diffusivity

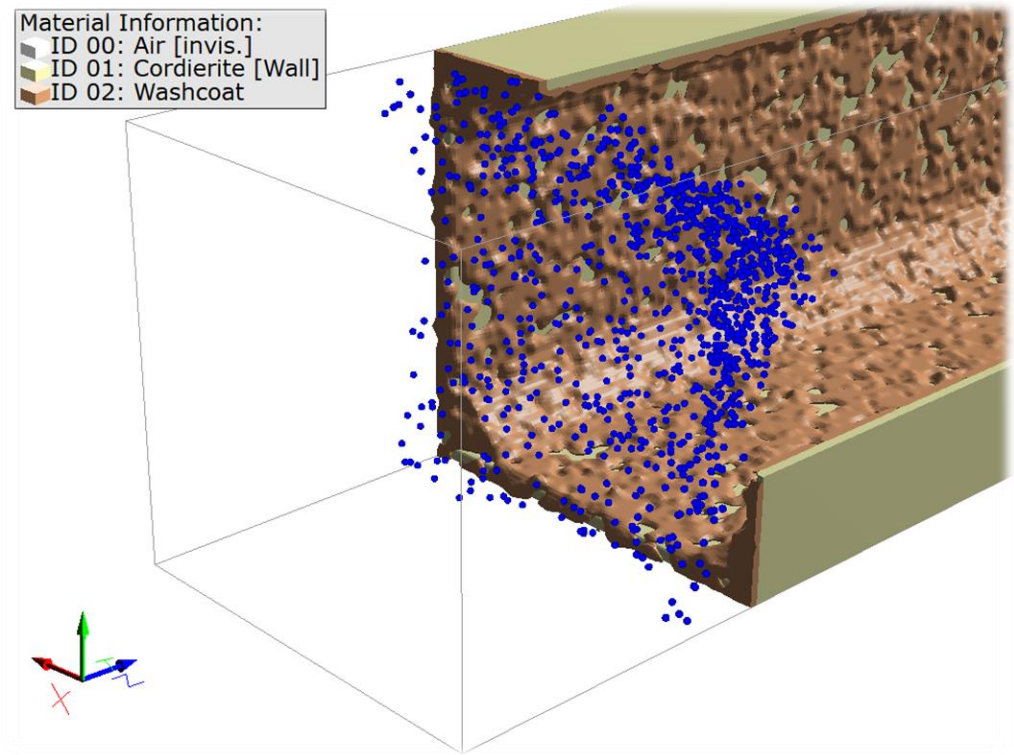
- Simulate the influence of short-time adsorption on surfaces
- Provide the possibility of choosing a maximal displacement as particle end position

To simplify modelling and simulation of catalytic converters, use these features to:

- **Simulate the effective diffusivity of a porous microstructure:** Use the result to simplify the structure by replacing the microstructure with porous voxels and reduce the runtime significantly. See effective diffusivity on page 48 for details. This allows to simulate the behavior on a larger scale but with the correct diffusivity of the microstructure.

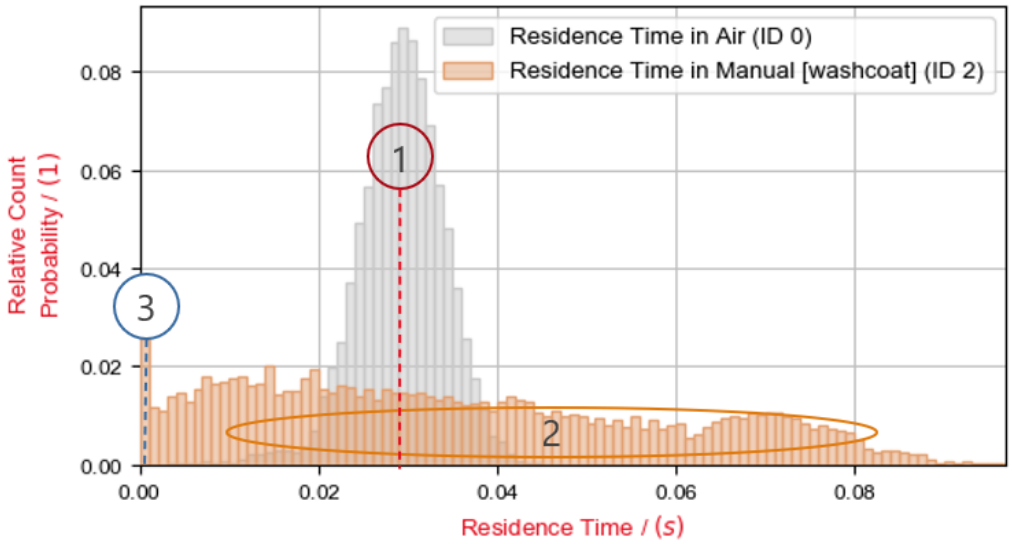


- **Model the wash coat layer of a channel as porous material:** A reflection probability for this material that defines the probability that molecules enter the wash coat layer can be defined, see page 30.



AddiDict tracks the molecules on their way through the channel. Evaluate the residence time of the molecule trajectories in each material, to investigate how long the molecules stay in the reaction zone (the wash coat layer), see page 50.

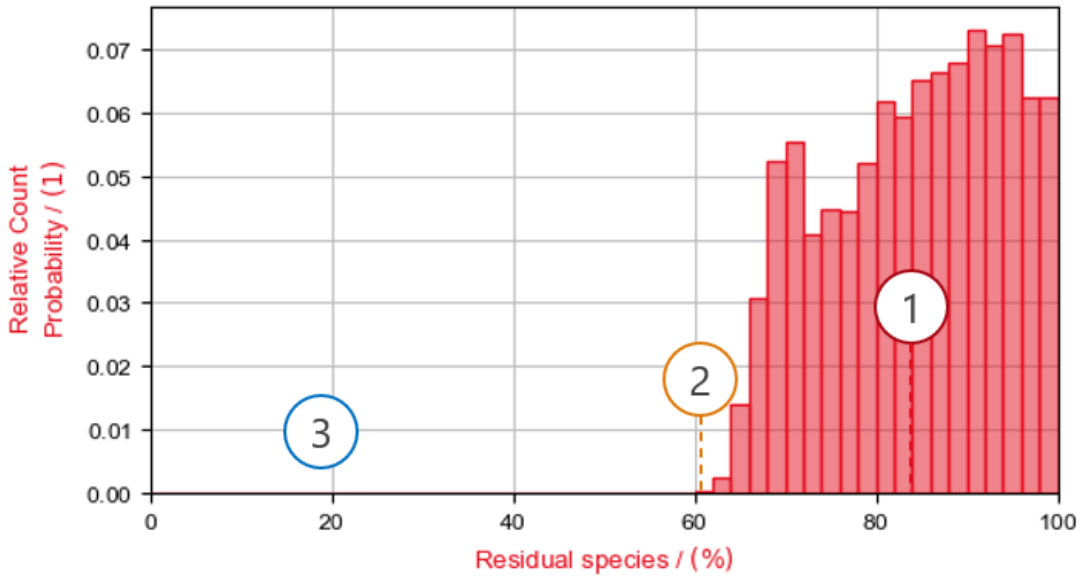
In the example shown here, the following behavior of the molecules can be observed from the residence times:



1. All molecules spent between 0.02 s and 0.04 s in air in the channel.
2. The time spent in the wash coat layer is very different for individual molecules.
3. Some molecules have not spent any time in the wash coat at all.

Finally, the residence times can be used to compute chemical reactions of first order in the AddiDict post-processing by defining reaction rate constants, see page 51.

In the example here, the following behavior can be observed:



1. In average, more than 80% of the molecules did not react at all but left the catalytic converter at the end of the channel.
2. The best reaction was down to only 60% of the initial species amount.
3. There is much room for improvement in the example here.

These results can be used to increase the reaction rate, by varying the channel geometry, the temperature (to change the diffusivity) or the reaction rate of the wash coat layer.

- **Simulate the particle motion in a long, but thin, channel** by simulation of a shorter channel with periodic boundary conditions and a maximum displacement as particle end position, see page 27.

THEORETICAL BASIS OF MASS TRANSPORT SIMULATION

The simulation of mass transport by AddiDict is done in three main steps:

1. The underlying flow through the medium is computed using an appropriate flow solver (Explicit Jump (EJ), SIMPLE Fast Fourier Transform (SimpleFFT) or LIR solver). If the flow is laminar, Stokes or Stokes-Brinkman equations for slow fluid flow can be applied.

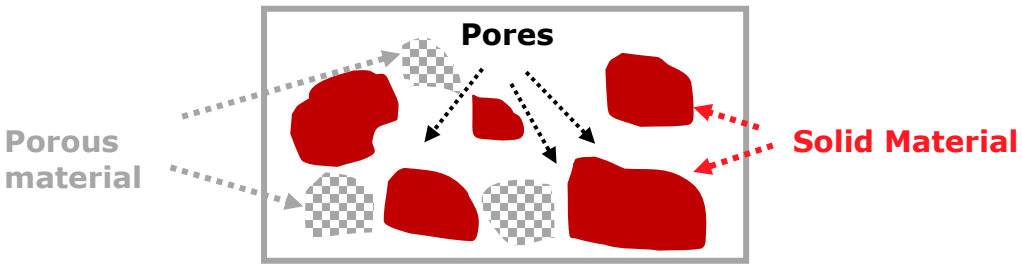
   Since GeoDict 2020, it is also possible to solve Navier-Stokes equations or Navier-Stokes-Brinkman equations to simulate non-laminar flow.

2. A predefined number of particles are tracked in the calculated flow field. Tracking of particles is based on solving an ordinary differential equation and includes electrostatic effects and diffusion. The latter becomes more and more relevant with smaller particle size. Particles are treated as objects moving independently from each other and using a distribution for the particle sizes is possible.

3. The particles have to be inserted into the space enabling fluid flow. The particles can start in pores and in porous material of the structure. The manner of particle injection is crucial for the resulting transport simulation and so a variety of options are implemented. These include different 2d and 3d geometries for particle starting positions, definition of initial particle velocity and injection can also follow a temporal distribution function (Uniform, Gaussian or stepwise defined probability distribution).

FLOW SOLVER PDES (PARTIAL DIFFERENTIAL EQUATIONS)

Besides pores and solid material, the input structures used for AddiDict can contain porous domains i.e. parts of the structure that are not fully resolved in the used discretization. Porous domains are characterized by their flow resistivity. (Navier-) Stokes-Brinkman equations describe the flow in the porous domain. In the pores, the flow is described by the (Navier-) Stokes equations (resistivity (K^{-1}) is zero).



The flow field is computed by solving the (Navier-)Stokes or (Navier-)Stokes-Brinkman equations numerically.

To use the (Navier-)Stokes-Brinkman equations in AddiDict, additional information about the permeability of the porous media has to be provided. Therefore, a permeability has to be assigned to each material.

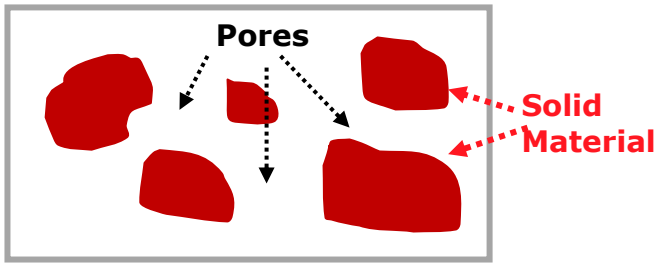
Navier-Stokes Equations

If the geometry of the pores is resolved by the computational grid, all voxels are either pore space or solid material. The fluid flow in the pores is described by the stationary Navier-Stokes equations:

$$-\mu\,\Delta\vec{u} + \rho(\vec{u}\cdot\nabla)\vec{u} + \nabla p = \vec{f} \qquad (1)$$

$$\nabla\cdot\vec{u} = 0 \qquad (2)$$

Here, ρ is the fluid density, μ is the dynamic viscosity, $\vec{u}$ is the velocity vector, p is the pressure and $\vec{f}$ is the force.



Stokes Equations

In the case of slow and laminar flow, the Navier-Stokes equations can be simplified to the Stokes equations, which read as follows:

$$-\mu\,\Delta\vec{u} + \nabla p = \vec{f} \qquad (3)$$

$$\nabla\cdot\vec{u} = 0 \qquad (4)$$

Here, μ is the dynamic viscosity, $\vec{u}$ is the velocity vector, p is the pressure and $\vec{f}$ is the force.

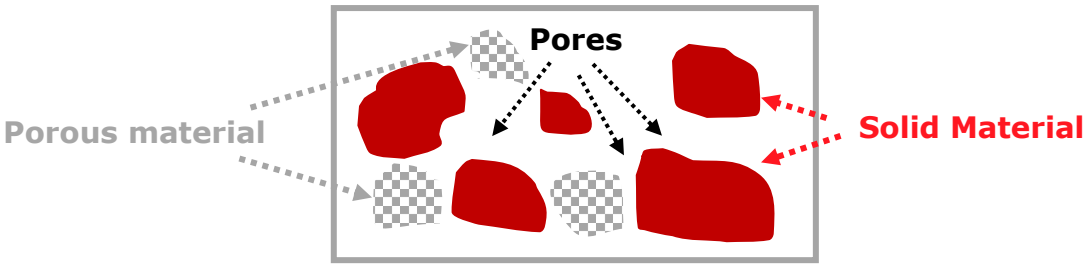
Navier-Stokes-Brinkman Equations

If the geometry of the pores is not fully resolved by the computational grid, a voxel may describe pore space, solid material, or porous material. The Brinkman term allows to describe flow in an unresolved porous medium. The Navier-Stokes-Brinkman equations are given as follows:

$$-\mu\,\Delta\vec{u} + \rho(\vec{u}\cdot\nabla)\vec{u} + \sigma\vec{u} + \nabla p = \vec{f} \qquad (5)$$

$$\nabla\cdot\vec{u} = 0 \qquad (6)$$

Here, $\vec{u}$ is the velocity vector, p is the pressure, $\vec{f}$ is the force, and μ is the effective viscosity. The local viscous flow resistivity σ of a voxel is related to the local permeability by $\sigma = \mu/\kappa$, where κ is the permeability of the voxel. In the pore space, the flow resistivity is zero and the Brinkman term disappears.



STOKES-BRINKMAN EQUATIONS

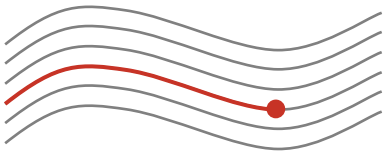
Again, under the assumption of a slow and laminar flow, the equations can be simplified and given as:

$$-\mu\,\Delta\vec{u} + \sigma\vec{u} + \nabla p = \vec{f} \qquad (7)$$

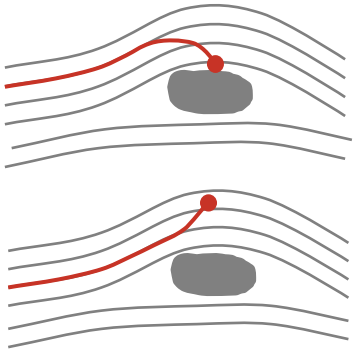
$$\nabla \cdot \vec{u} = 0 \qquad (8)$$

PARTICLE TRACKING

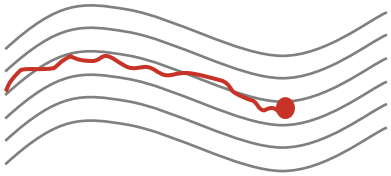
AddiDict simulates mass transport and tracks how particles move through a structure and interact with the solids. The movement of particles in the fluid is influenced by the following factors:



Drag forces are the dominant forces in most cases, and particle trajectories are close to streamlines of the underlying flow field.



Electric attraction. The particles and the surface of the solid parts can be electrically loaded, thus leading to attraction or bouncing effects.



Diffusive (or Brownian) motion. Certain irregularities in the particle surface and collisions among particles lead to small random direction changes of particles.

AddiDict simulates mass transport by considering these three effects. All three effects can be switched off if it is known a-priori that they have no influence on the mass transport process.

Overall, the particle movement is governed by

Particle Momentum = Stokes Drag + External Forces

or, as formula:

$$m\,\frac{d\vec{v}}{dt} = 6\pi\mu\,\frac{R}{C_C}\left(\vec{u} - \vec{v} + \sqrt{2D}\,\frac{d\vec{W}(t)}{dt}\right) + Q\vec{E} + \vec{F} \qquad (5)$$

In the friction coefficient

$$\gamma = 6\pi\mu\,\frac{R}{C_C} \qquad (6)$$

the particle radius R is optionally corrected by the Cunningham correction factor[1]

$$C_C = 1 + \frac{\lambda}{R}\left(1.17 + 0.525e^{-0.78\frac{R}{\lambda}}\right) \qquad (7)$$

[1] values as defined in C.T. Crowe, Multiphase flow handbook, 1st edition, Taylor and Francis, 2006

to account for the reduced drag of very tiny particles that may easily pass between the molecules of the surrounding fluid. The particle diffusivity D computes Brownian motion through

$$D = \frac{k_B\, T}{\gamma} \qquad (8)$$

The Brownian motion may be switched off by the user, and in that case the diffusivity is set to zero. External forces are the electrostatic force $Q\vec{E}$ and an additional force field $\vec{F}$ which is

$$\vec{F} = 0 \qquad (9)$$

by default. The electrostatic field $\vec{E}$ is set to zero if the user decides to switch off electrostatic effects.

Equations (6), (7), (8) and (9) can be changed by the user through user defined functions, e.g. to include gravity, buoyancy forces in $\vec{F}$ or a Cunningham correction with different parameters as in (12). See the Appendix (page 66) for details. The parameter λ for the Cunningham correction factor in (7) can be directly set in the AddiDict options.

The used variables and their units are:

Symbol	Unit	Meaning
$\vec{v}$	m/s	particle velocity
$\vec{u}$	m/s	fluid velocity
γ	kg/s	friction coefficient
μ	kg/m·s	dynamic viscosity
R	m	particle radius
C_c	1	Cunningham correction factor
m	kg	particle mass
λ	m	mean free path

Symbol	Unit	Meaning
Q	C	particle charge
$\vec{E}$	V/m	electric field
k_B	J/K	Boltzmann constant
dW	$\sqrt{s}$	3D Wiener measure
T	K	temperature
D	m²/s	diffusivity
$\vec{F}$	N	external force

The electrostatic charges are assumed as constant given forces on the surface of the solids. A constant charge density ξ is assigned on all voxel walls that belong to this surface. The electric field $E = -\nabla\Phi$ is determined by solving the Poisson equation for the potential Φ (unit:V)

$$\Delta\Phi = -\frac{\xi}{\epsilon_0}\int_{\partial G}\delta \qquad (10)$$

where ξ is the surface charge density (unit: C/m²) and ϵ_0 = 8.854188E-12 F/m is the permittivity. Here, ∂G denotes the solid surface and δ is the Dirac distribution.

Here, ξ is periodic in the tangential directions and should satisfy zero Dirichlet boundary conditions at $-\infty$ and $+\infty$ in flow direction. Numerically, infinity is replaced by $-Z_0$ and $nz + Z_0$ in z-direction.

By construction, these boundaries lay away from the solid material and there is no conflict between singular forces on solid surfaces and these Dirichlet conditions. Due to the periodic boundary conditions, the potential feels a non-integrable amount of charges and tends to infinity in the solid material as the Dirichlet boundary is moved away from the solid. Thus, the potential ξ depends on the position where the Dirichlet condition is located. However, only the electrical field E is needed to determine the movement of the particles in (5) and this remains almost unchanged from the location of the Dirichlet boundary as soon as this boundary is sufficiently far away from the solid material.

Cunningham Correction and Molecular Mean Free Path

In fluid dynamics, the momentum equations for Newtonian fluids are the Navier–Stokes equations and the Stokes equations in the case of low Reynold's numbers. These equations rely on the continuum assumption for the fluid, i.e. the fluids are sufficiently dense to be a continuum, do not contain ionized species, and have flow velocities that are small in relation to the speed of light. For the movement of very small particles through a fluid this assumption is not valid anymore. In consequence, the no-slip condition at the particle – fluid interface does not hold anymore and, so, the drag force acting on a particle moving through a fluid has to be corrected for this effect.

The Cunningham correction factor allows predicting the drag force on a particle moving within a fluid with properties between the continuum regime and free molecular flow. The fluid properties are defined by the dimensionless Knudsen number (Kn), representing the ratio of the molecular mean free path length (λ [m]) to a representative physical length scale (L [m]):

$$K_n = \frac{\lambda}{L} \qquad (11)$$

A typical choice for the representative physical length scale is the pore size of a structure. Different regimes for micro/nano flow fields are distinguished based on the following critical Knudsen numbers:

(a) $0 < Kn < 10^{-2}$ for continuum flow regime

(b) $10^{-2} < Kn < 10^{-1}$ for slip flow regime

(c) $10^{-1} < Kn < 10$ for transition

(d) $10 < Kn$ for free molecular flow regime.

Mean free path lengths in liquid water are reported to be in the order of $3.0\ 10^{-10}$ m (temperature of 20°C and pressure of 1bar) and so Knudsen numbers of above 10^{-2} are reached for pores with radii smaller than $3.0\ 10^{-8}$m. For air at ambient conditions, the mean free path length is reported with 68 nm and so Knudsen numbers of above 10^{-2} are reached for pores with radii smaller than $6.8\ 10^{-6}$m. Hence the Cunningham correction will only be relevant for gas flows. The Cunningham correction factor (C_C) is defined as follows:

$$C_C = 1 + \frac{\lambda}{R} \cdot (A_1 + A_2 \cdot e^{\frac{-A_3 R}{\lambda}}) \quad (12)$$

where λ is the molecular mean free path length [m], R is the particle radius [m] and A_n are experimentally determined coefficients.

Molecular Limit

AddiDict can not only model the movement of finite sized particles, but it can also be used to model the movement of molecules. For molecules, the particle radius R is unknown, and equation (5) cannot be used directly to compute the movement of molecular particles. However, when considering the limit for $R \to 0$ in (5), one observes that the particle mass m is of order R^3, and therefore the left-hand side disappears.

Thus, in case that no electrostatic or external forces are present, the equation simplifies to

$$\vec{u} - \vec{v} + \sqrt{2D}\frac{d\vec{W}(t)}{dt} = 0 \quad (13)$$

such that the particle velocity equals the flow velocity plus a random movement. In that case, only the diffusivity D of the molecule is needed as input.

Collision Models

When a particle touches a solid in a structure, it can be deposited or continue moving. For this, AddiDict offers four different collision models:

Hamaker model

In the **Hamaker** model, the velocity of the particle is compared to the adhesive forces. The particle is caught by the solid if the velocity of the particle, when touching the structure, is sufficiently small. The condition on the velocity is

$$v^2 < \frac{H}{4\pi\rho a_0 R^2} \qquad (14)$$

where H is the **adhesion** (Hamaker constant), ρ is the particle density, a_0 is the adhesion distance (AddiDict uses a value $4 \cdot 10^{-10}$m), and R is the particle radius.

Adhesion (Hamaker constant) and **Restitution**, another parameter, are to be fitted in AddiDict. The restitution parameter determines the amount of energy not absorbed by the collision. The restitution value ranges from 0 to 1. If the restitution parameter is set to 1, no energy is lost, and the particle is reflected with the same speed it had before the collision.

For restitution values smaller than one, energy is absorbed by the collision and the particle slows down. For example, a 0.7 restitution value means that a particle loses part of its velocity in the collision and gets 30% slower.

Since the Hamaker model needs the particle diameter as an input, it is only available for finite particle size and not in the molecular limit d=0.

Caught on first touch

Caught on first touch is the simplest of the adhesion models in AddiDict. The particle sticks to the solid as soon as it touches the solid surface.

Sieving

In the **Sieving** model, the particles never stick to the solid, but a particle is caught by the solid if it does not move anymore and simply lies on the solid at two different points. The restitution parameter is used in the same way as in the Hamaker model.

Adsorption

The **Adsorption** model is available for molecules only. The adsorption rate defines the probability that a molecule is trapped if it hits a solid or a porous material.

Post-Processing

Chemical Reactions of first Order

Based on the simulated trajectories of particles, residence times in each pore and porous material can be determined in the AddiDict post-processing. From these residence times, chemical reactions of first order can be computed as a next step.

Chemical reactions of first order are simple chemical reactions that describe a reduction of a reactant A (here a kind of molecules), while the catalyst is not consumed. The change in amount of [A] is determined by the rate constant *k*:

$$-\frac{d[A]}{dt} = k \cdot [A],$$

i.e., the amount of [A] is reduced exponentially, with a half-life time of

$$t_{1/2} = \frac{\ln(2)}{k}.$$

The remaining amount of [A] can therefore simply be computed from the residence times and the rate constant *k*:

$$[A]_t = [A]_0 \, e^{-kt}$$

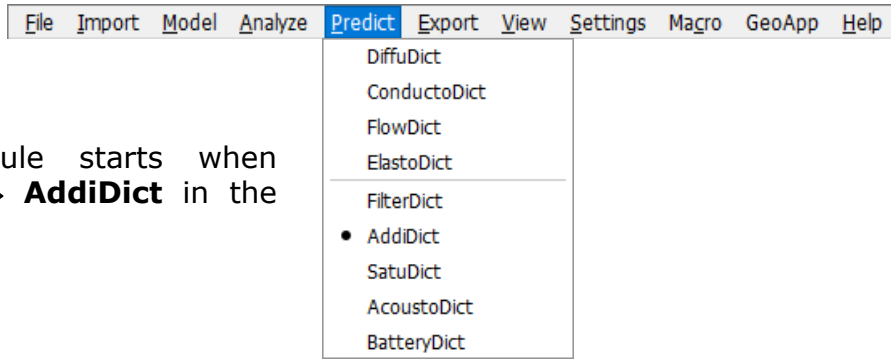
Short-Time Adsorption

Short-time adsorption is the effect, that particles/molecules can stick to some material for a short time interval, before continuing to move due to diffusion and/or advection.

In AddiDict, this effect is so far not taken into account during the simulation of particle trajectories. However, in the post-processing, adsorption times can be defined for each solid and porous material. Each time a particle hits such a material, it is adsorbed there for the defined adsorption time. The travelled displacement of all particles is adapted according to the defined adsorption times and the number of hits with each material.

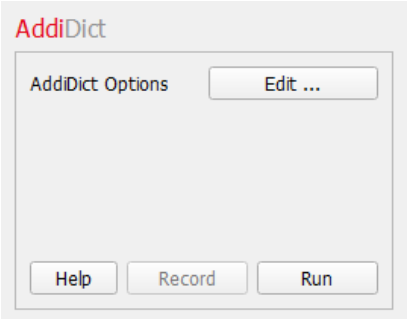
AddiDict Section

A mass transport simulation with AddiDict can be carried out on porous 3D media, modeled from 3D image data (µCT, FIB-SEM, etc.), imported and segmented using ImportGeo-Vol or generated with one of GeoDict's structure generation modules.

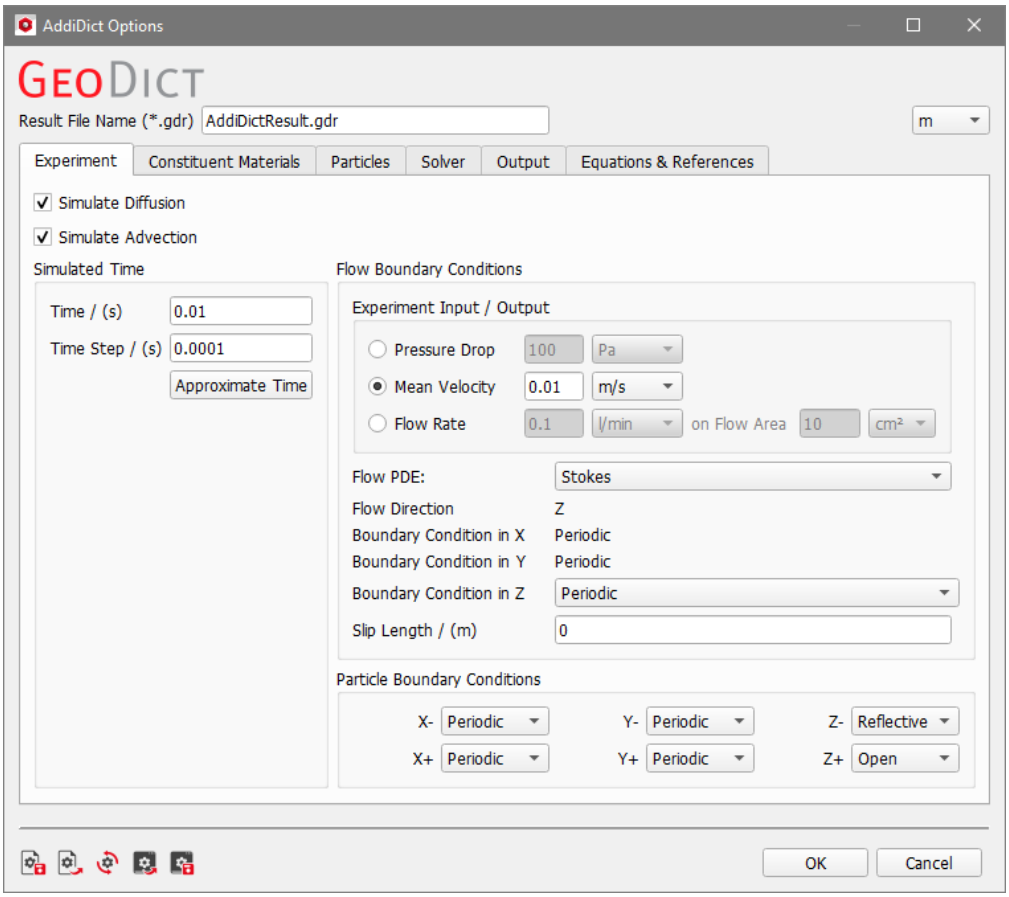


The AddiDict module starts when selecting **Predict** → **AddiDict** in the Menu bar.

The **AddiDict Options** for the simulation can be modified in the AddiDict section, at the left side of the GUI after clicking the **Edit...** button. After editing all necessary options of AddiDict, start the simulation by clicking **Run** in the AddiDict section.



At the top of the **AddiDict Options** dialog box, the result file name can be entered. The parameters needed for the calculations are organized into tabs: **Experiment**, **Constituent Materials**, **Particles**, **Solver**, and **Output**.



The tab **Equations & References** shows the equations solved for fluid flow and particle tracking, together with the input parameters.

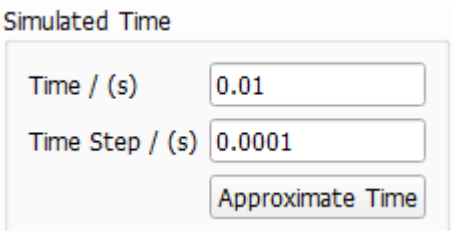
EXPERIMENT

Select whether **Diffusion** and/or **Advection** should be simulated, by checking the boxes in the upper left part of the **Experiment** tab.

Checking **Simulate Diffusion** activates the simulation of random effects in particle movement. If the button is unchecked, the diffusivity is set to $D = 0$ in equation (5).

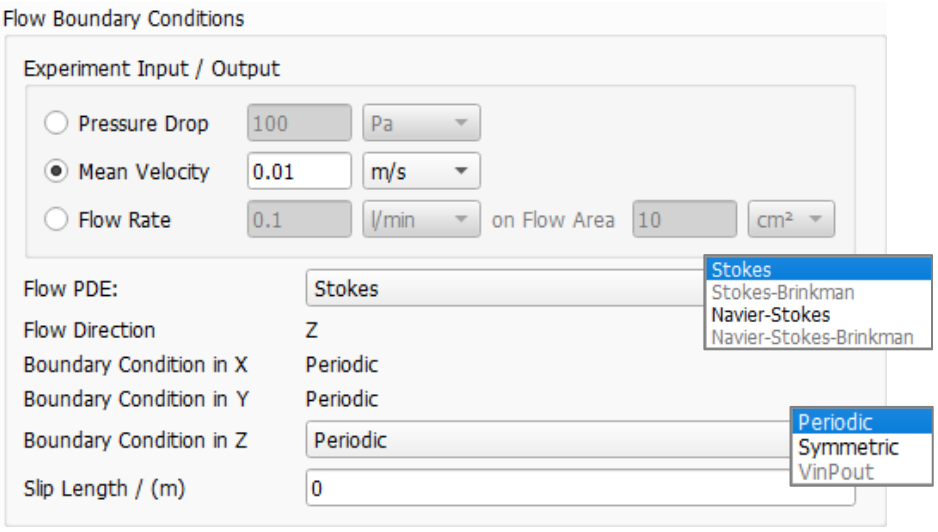
Checking **Simulate Advection** activates the computation of drag forces from the fluid. If it is unchecked, the velocity of the fluid is zero and therefore the particles move by diffusion only.

In the **Simulated Time** panel, the simulated final **Time** can be given. At each **Time Step**, the particle positions are evaluated for the spatial distribution, the breakthrough curve and the residence times.



By clicking the **Approximate Time** button, the simulated time is automatically set such that, for the given average fluid **Velocity** (defined in the **Flow Boundary Conditions** panel), most particle trajectories will pass through the whole geometry and a full pass-through curve is computed. This works only if the flow is the dominant process and not the diffusion. The **Time Step** value is automatically set to be 1% of the **Time**.

In the **Flow Boundary Conditions** panel, the **Pressure Drop**, the average flow **Velocity** or the **Flow Rate** can be entered. In AddiDict, the flow is always computed in z-direction. If another direction is wanted, the 3D model can be rotated with ProcessGeo prior to using AddiDict. Note that this part of the dialog is accessible only if **Simulate Advection** is checked.



From the **Flow PDE** menu, the user specifies the equations to be solved to compute the fluid flow field required to simulate the particle movements and trajectories. **(Navier-)Stokes** equations describe fluid flow in structures containing only solid materials and pores. **(Navier-)Stokes-Brinkman** equations (see pages 7ff.) describe the flow through structures containing porous materials, solids, and pores.

The used flow boundary conditions in X and Y direction are reported and the boundary condition in Z direction can be defined.

The boundary conditions in X and Y direction are set automatically to fit to the chosen boundary conditions for the particle movement: **Reflective** particle behavior fits to **Symmetric** flow boundary conditions and **Periodic** particle movement requires **Periodic** flow boundary conditions.

The boundary condition in Z direction, that can be selected, depends on the Flow PDE chosen above. For Stokes and Stokes-Brinkman equations, the boundary condition can be selected to be **periodic** or **symmetric**, for Navier-Stokes and Navier-Stokes-Brinkman equations, **VinPout** is set as boundary condition.

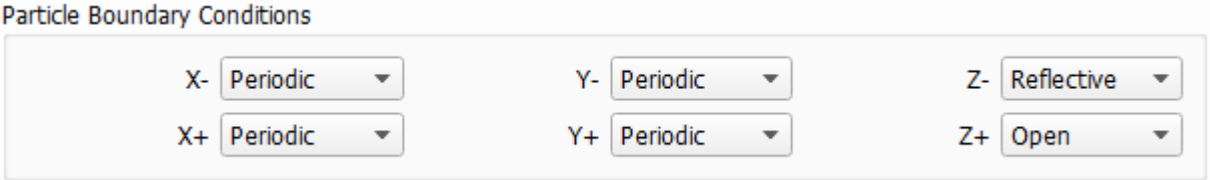
Additionally, the slip length can be defined in the **Flow Boundary Conditions** panel.

The **Slip Length** allows including sliding effects in the 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 **Slip Length** of zero corresponds to a flow velocity of zero along the structure.

A non-zero **Slip Length** simulates the sliding of the fluid along the structure's solid parts, increasing the fluid mean flux and thus, the permeability. 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 GeoDict 2020 the consideration of slip length was improved in the flow computation. Results with the same slip length can therefore deviate from previous versions of GeoDict. More details can be found in the FlowDict handbook of the GeoDict User Guide.

In the **Particle Boundary Conditions** panel, the user can choose what happens when a particle arrives at the domain boundary. This can be done individually for each of the six domain sides. In the **Periodic** case, a particle that leaves through one side



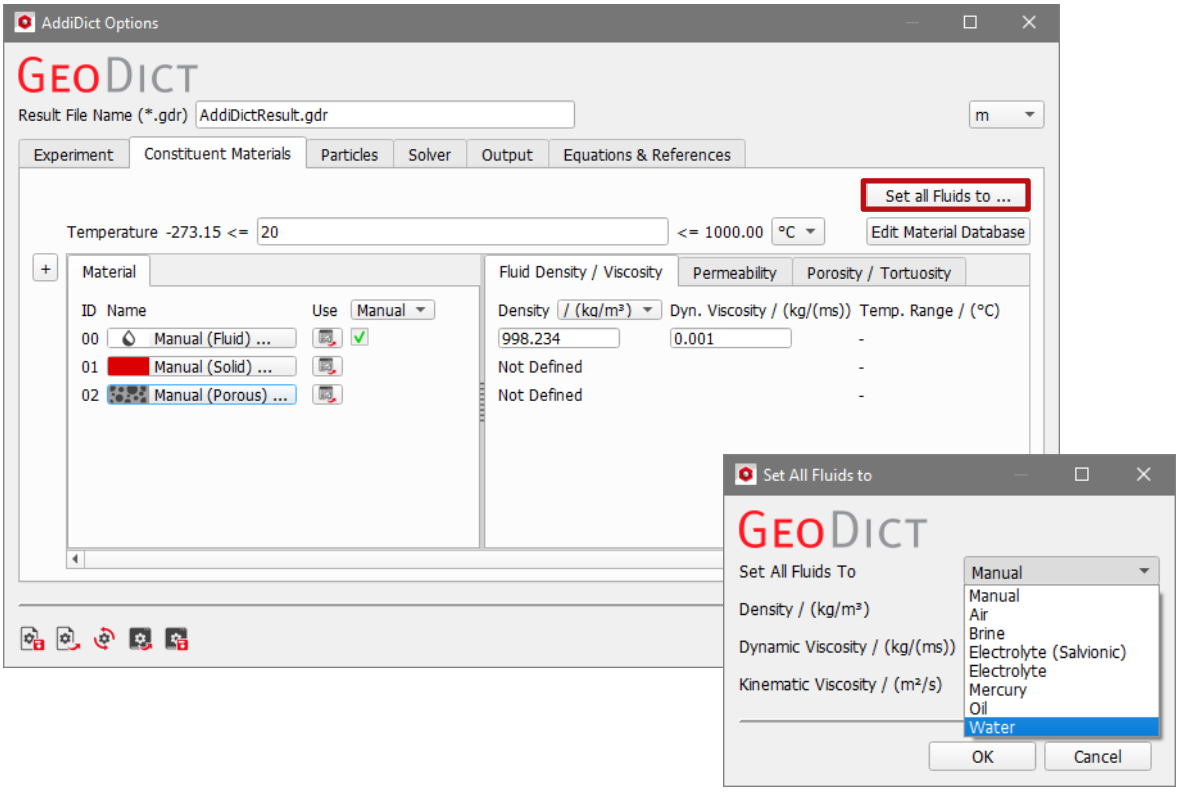
of the domain, enters on the opposite side of the domain. In the **Reflective** case, a particle is reflected at the boundary. In the **Open** case, the particle leaves the domain and is no longer tracked. Those particles are reported in the breakthrough curve.

CONSTITUENT MATERIALS

The **Temperature** at which the mass transport process occurs is selectable in Kelvin [K], Celsius [°C], and Fahrenheit [F], and has a default value of 293.15 K, 20.0 °C, or 68 F, respectively.

For computations of the flow solvers, the materials in the structure and the fluids flowing through it need to be defined under the **Constituent Materials** tab, so that their physical properties are taken into account.

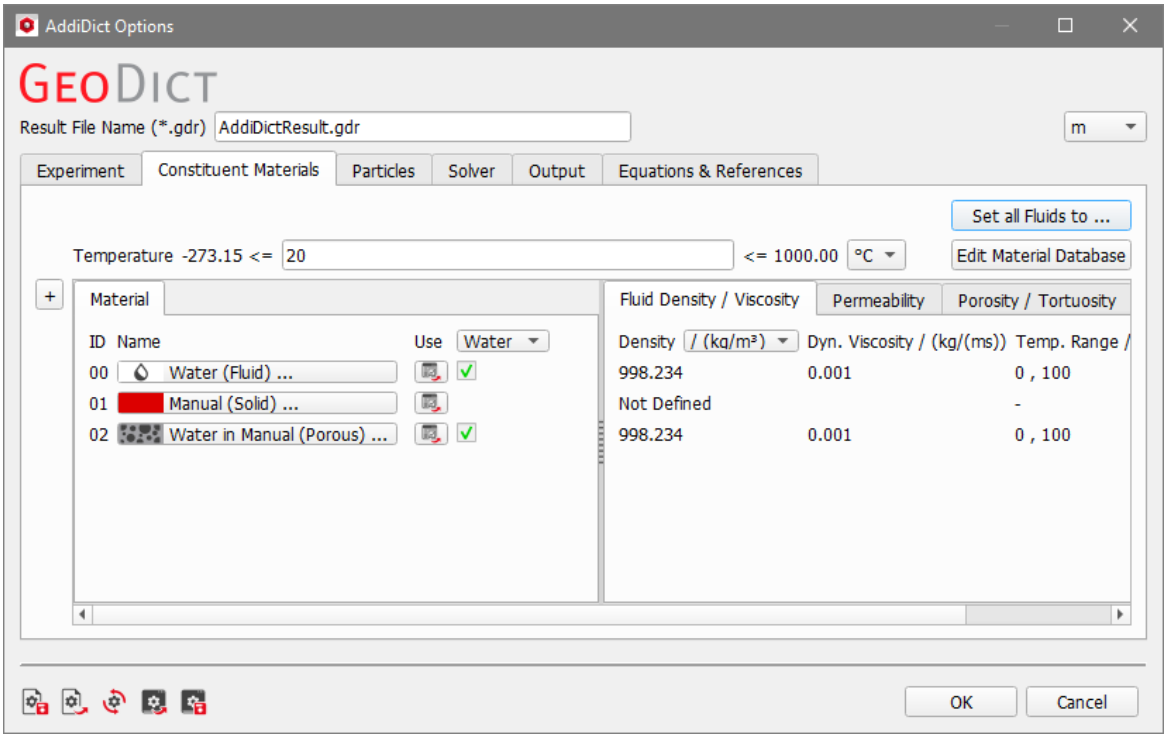
The fluid flowing through all pore and porous materials can be set by clicking **Set all Fluids to ...**. and selecting it from the pull-down menu.



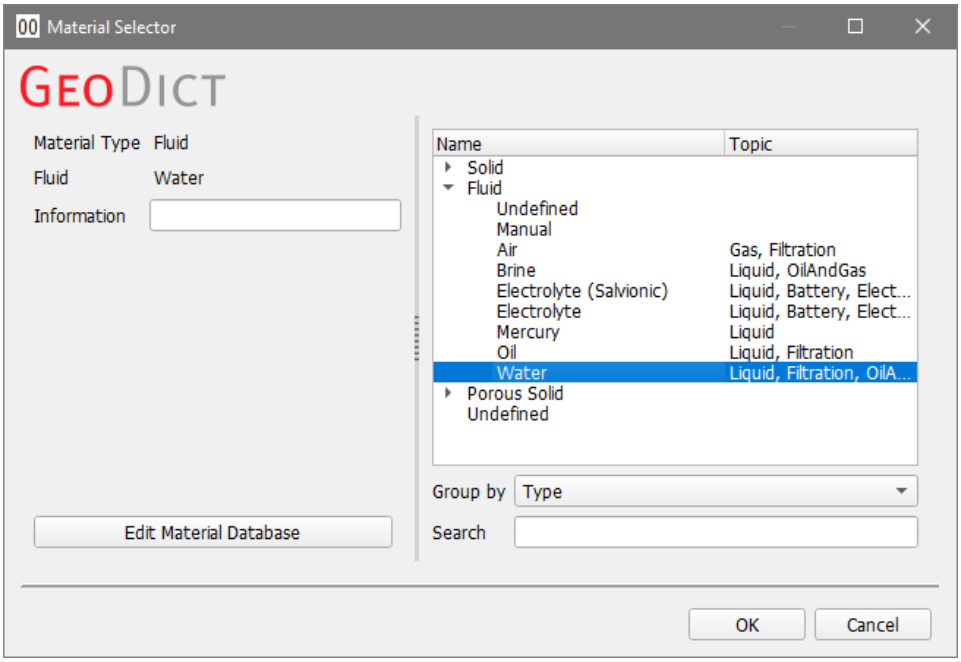
If one of the seven predefined fluids (Air, Brine, Electrolyte (Salvionic), Electrolyte, Mercury, Oil, or Water) is used, the values for **Density**, **Dynamic Viscosity** and **Kinematic Viscosity** are taken from the GeoDict Material Database and are dependent on the given **Temperature** value. If **Manual** is chosen, these values can be entered manually.

Any values entered manually, e.g. those for a special type of oil, can also be added to the material database through the **Edit Material Database** button. More information on editing, expanding, and using the GeoDict Material Database is available.

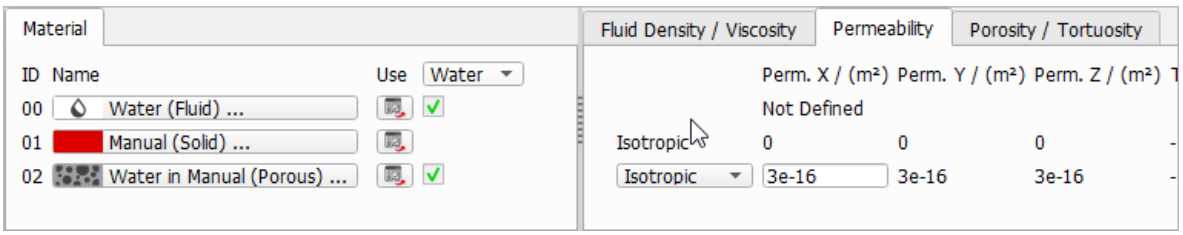
As soon as the user sets the fluid in the pull-down menu, this choice appears under the **Material** subtab. Now this fluid is shown to occupy the previously unassigned pore space with the ID 00 and in the porous material with the ID02. The density and the dynamic viscosity of this fluid, at the selected temperature range, is shown under the **Fluid Density/Viscosity** subtab.

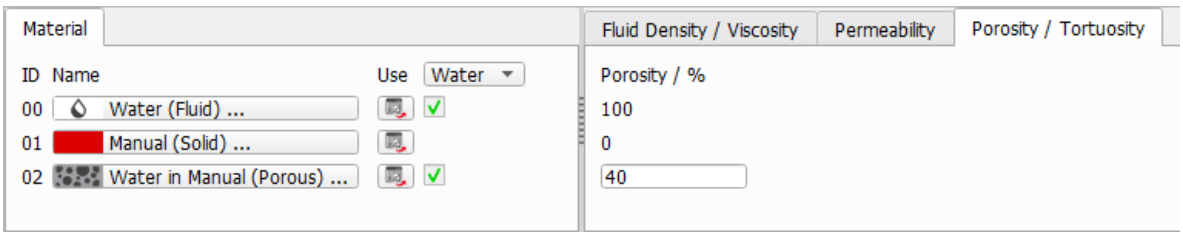


The materials assigned to the material IDs, which fall into one of the material categories (pore, porous or solid), can be selected through the **Material Selector** dialog box, by clicking on the material's buttons. Fluid flow can happen in pores and in porous materials, but not in solid materials.



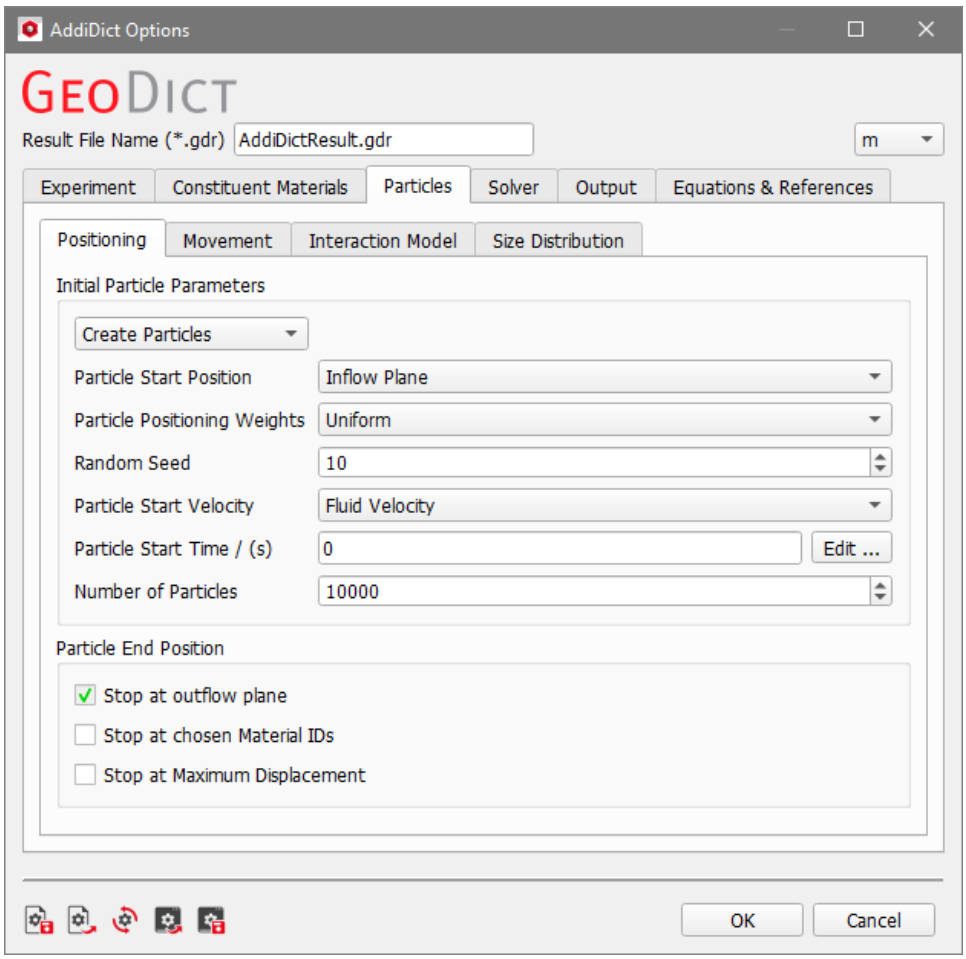
For porous materials, also the information about the permeability needs to be defined on the **Permeability** subtab. If the **Pass Through Model Reflection Probability** will be chosen later on for a porous material and the reflection probability is not selected manually, also the porosity of a porous material needs to be defined on the **Porosity** subtab (see page 30 for details about the reflection probability).


Material
ID Name
Use
Water
00 Water (Fluid) ...
01 Manual (Solid) ...
02 Water in Manual (Porous) ...
Fluid Density / Viscosity
Permeability
Porosity / Tortuosity
Perm. X / (m²)
Perm. Y / (m²)
Perm. Z / (m²)
Not Defined
Isotropic
0
0
0
Isotropic
3e-16
3e-16
3e-16


Material
ID Name
Use
Water
00 Water (Fluid) ...
01 Manual (Solid) ...
02 Water in Manual (Porous) ...
Fluid Density / Viscosity
Permeability
Porosity / Tortuosity
Porosity / %
100
0
40

PARTICLES

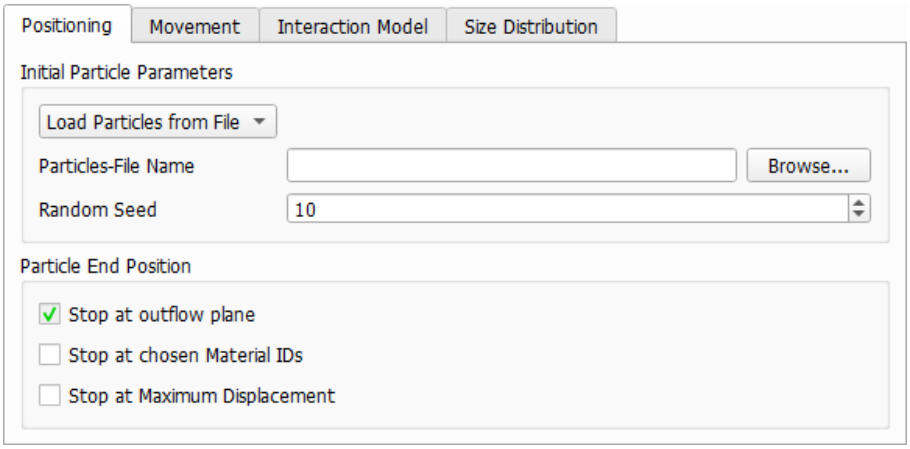
The initial particle parameters and parameters defining the particle movement are defined under the subtabs of the **Particles** tab.



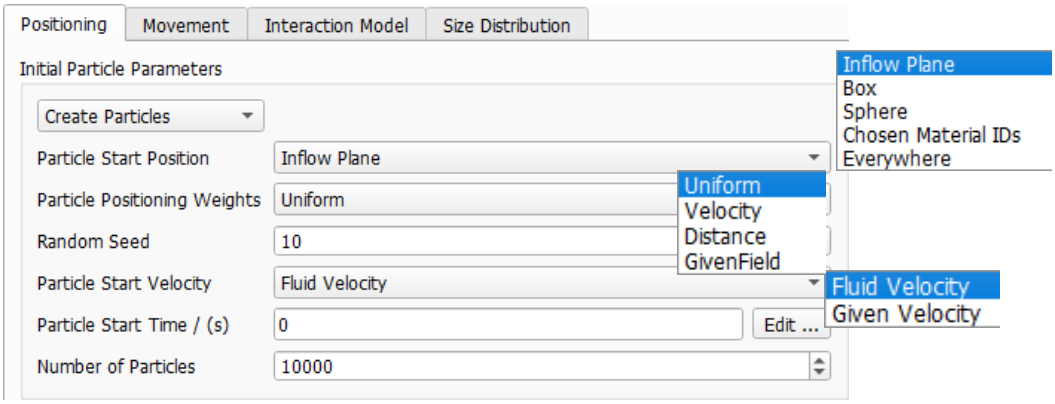
POSITIONING

On the **Positioning** subtab, initial particle parameters and end position of the particles are defined.

For the **Initial Particle Parameters**, the user can choose to **Create Particles** according to the options set afterwards or to **Load Particles from File**. For the second option, the user browses, selects, and opens an existing .gpp (GeoDict particle parameters) file. This file may origin from a previous AddiDict simulation or may be generated using GeoLab, GeoDict's Matlab library.

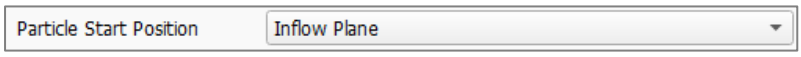


When the user selects **Create Particles**, the parameters for the particles can be set.

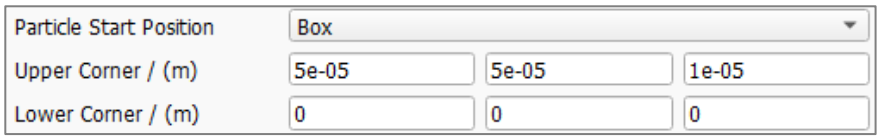


The position of the particles at the beginning of the injection, are chosen from the **Particle Start Position** pull-down menu:

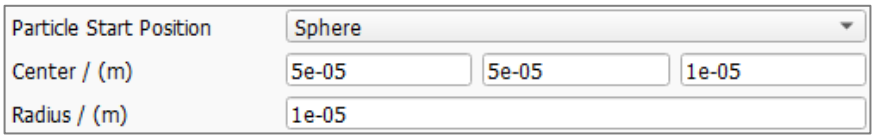
- **Inflow Plane** assigns all particles to start from a single inflow plane.



- With **Box** all particles are positioned in a rectangle whose size can be defined by setting valid ranges for each spatial direction.

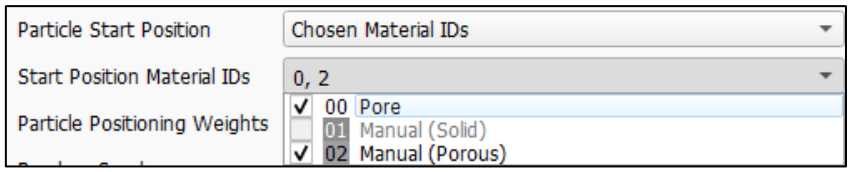


- With **Sphere** a spherical injection volume for the particles is defined by entering center and radius of the sphere.



The unit used to define the lower and upper corner of the box for each coordinate direction, or the center and radius of the sphere, can be defined at the right top of the AddiDict Options dialog box.

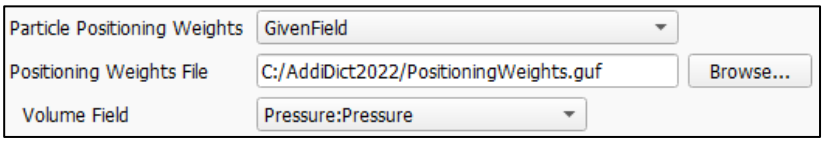
- With **Chosen Material IDs**, the material(s) where the particles start can be selected. Each pore and porous material is possible as particle start position.



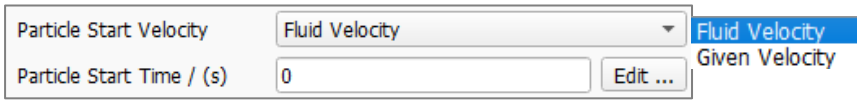
- With **Everywhere** selected, the particles can start in each pore and porous material available in the structure in memory.

The **Particle Positioning Weights** allow to define the distribution of the particle start positions to the possible positions, defined under **Particle Start Position**.

- With **Uniform**, all possible start positions have the same probability that particles start there.
- For **Velocity**, the probability of particles starting at a possible position, depends on the fluid velocity. The higher the velocity, the higher the probability that a particle will start at a specific position. This will lead to uniform particle concentration in the flow.
- With **Distance**, the probability depends on the distance from solid voxels. Choosing this option leads to more particles in the core flow and less particles near surfaces of solid voxels.
- Choose **GivenField**, to define the starting probability dependent on a predefined field. This field is defined as a GeoDict volume file (.guf, .vol, etc.). If this file is loaded, the Volume Field that should be used for the particle positioning can be selected.



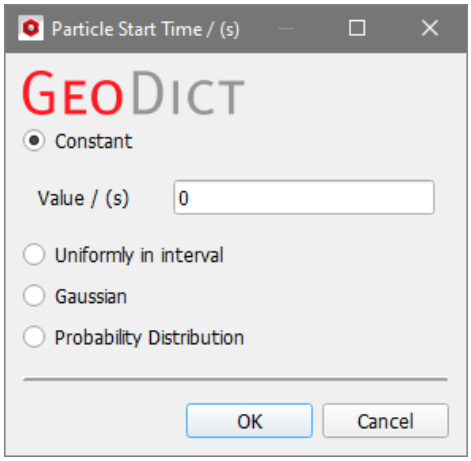
The **Particle Start Velocity** determines the initial particle velocities at the starting positions. If **Fluid Velocity** is chosen, every particle starts with the local velocity of the fluid flow. If **Given Velocity** is chosen, every particle starts with the entered velocity. The given velocity can be applied in all three directions or only in z-direction.

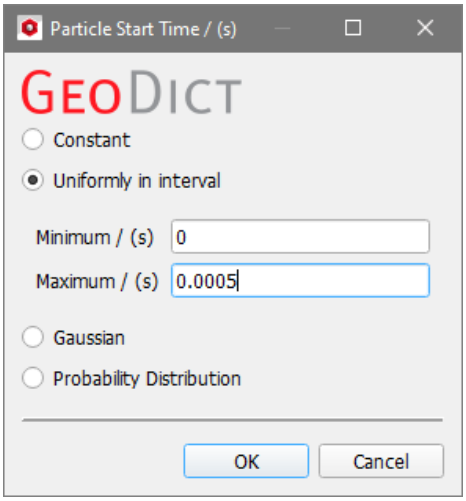


The **Particle Start Time** defines when the particles are released to the flow. Through the **Edit...** button, the particle start time can be set to be constant, or to follow a distribution: Uniformly in interval, Gaussian, or an arbitrary Probability Distribution.

A **Constant** particle start time releases all particles at the same time, defined under **Value**.

Particles can be released **Uniformly in Interval** by specifying the beginning and ending of the time interval.

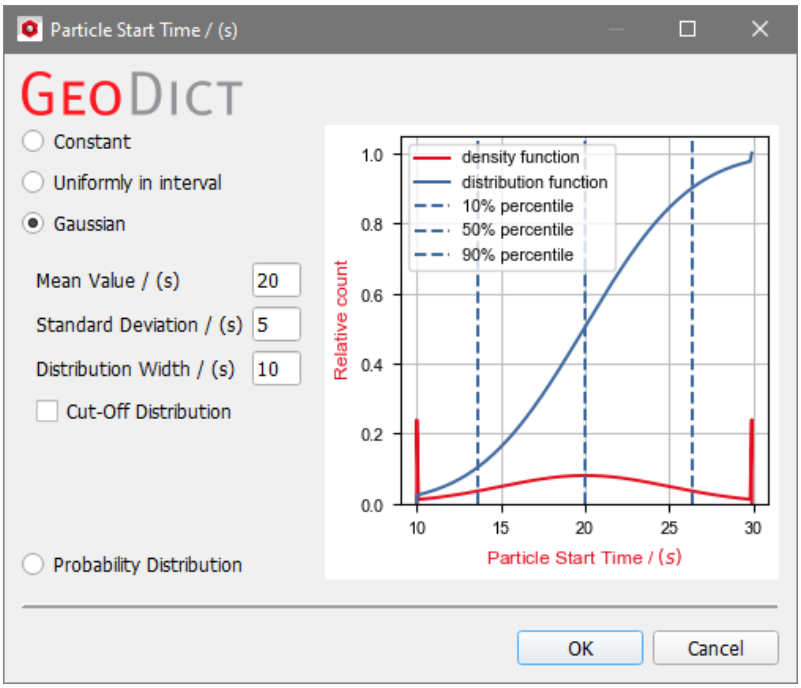




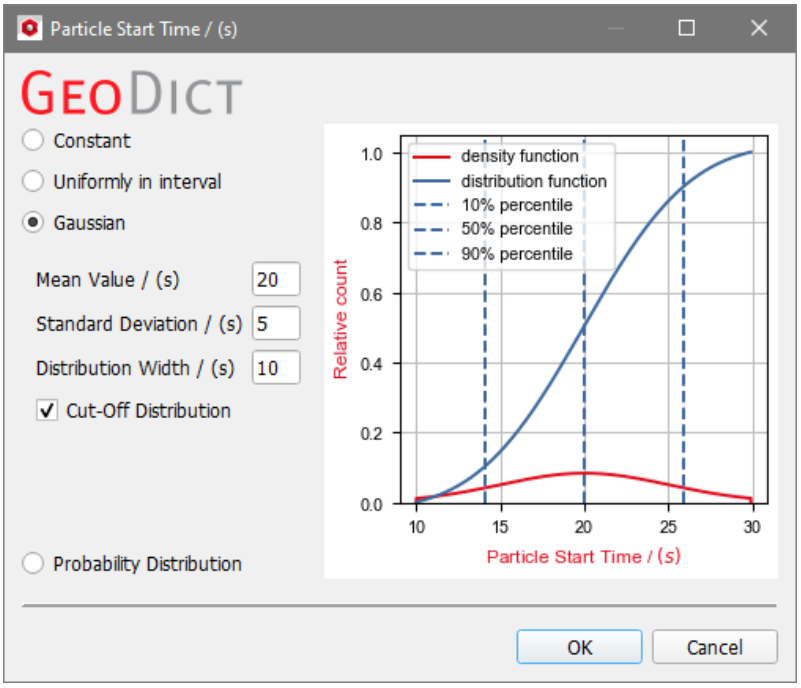
For particles to be released following a **Gaussian** distribution, the **Mean Value**, the **Standard Deviation**, and the **Distribution Width** of the distribution need to be defined. The particle release times are centered on the **Mean Value** and they vary according to the **Standard Deviation**.

The value in **Distribution Width** corresponds to the range on both sides of the mean value limiting the particle release time value that is accepted. A **Distribution Width** of 10 means that release time values may deviate only from -10 s to +10 s from the given **Mean Value**.

The parameters must be set so that no negative values are possible. For example, a release time mean value of 20 s and a distribution width of 25 s would lead to an error message appearing, as the time could reach a value less than zero.

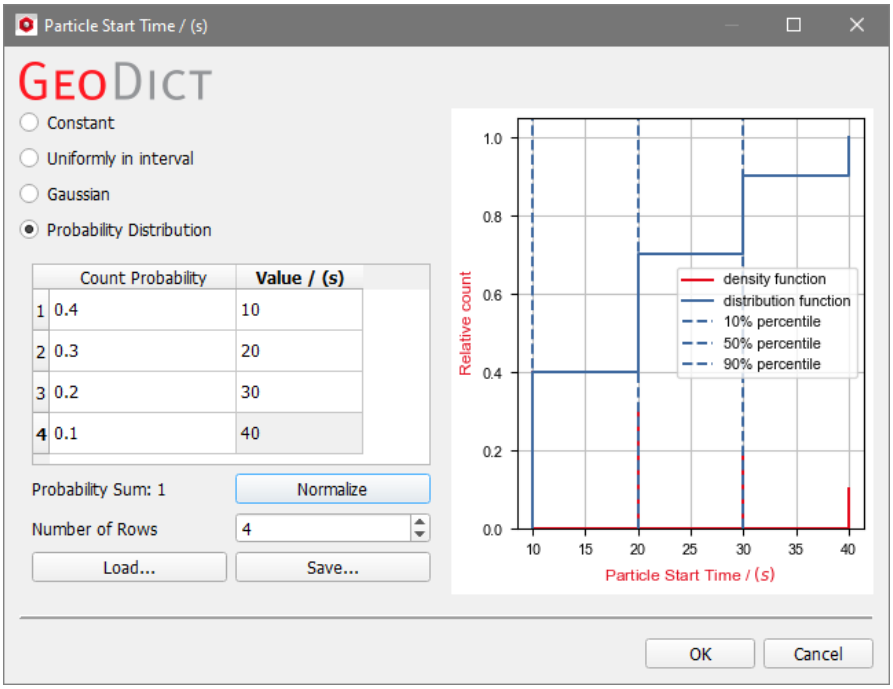


Checking **Cut-Off Distribution** restricts the start times selected by the random number generator to the interval defined by the distribution bound. Otherwise, random numbers outside of this interval are set to the distribution bounds.



With **Probability Distribution**, a discrete distribution for the particle release time can be defined.

The table describes the probability (**Count Probability**) of a release time taking a certain **Value**.



The sum of all Count Probabilities defined in the table needs to sum up to one. Especially for large tables, the **Normalize** button for this **Probability Sum** can be helpful, that scales the count probabilities to sum up to one.

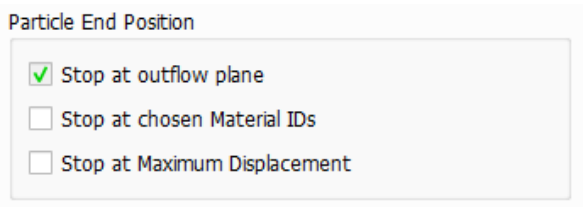
The **Number of Rows** can be increased or decreased to enter the desired number of release time **Values** and their **Count Probability**, between 0 and 1.

The buttons **Load** and **Save** allow loading a previous defined probability distribution and saving the current one for later use.

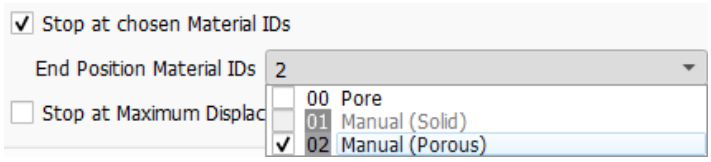
Particles to be transported are placed randomly in the Particle Start Position volume and may move randomly due to Brownian motion. The **Random Seed** sets the seed of the underlying random number generator. The same random seed produces identical results, whereas results with different random seeds are similar but not identical.

The **Number of Particles** determines the number of particles inserted into the geometry over the entire simulation period.

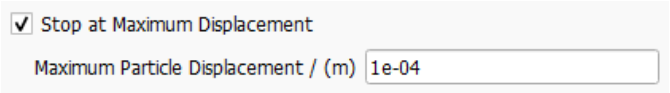
For the **Particle End Position**, three options are possible.



- Particles always leave the simulation when they leave the computational domain at a defined outflow plane.
- Optionally, particles can also leave the simulation when they hit a voxel with one of the defined material IDs, i.e., they are not considered anymore in the computation.



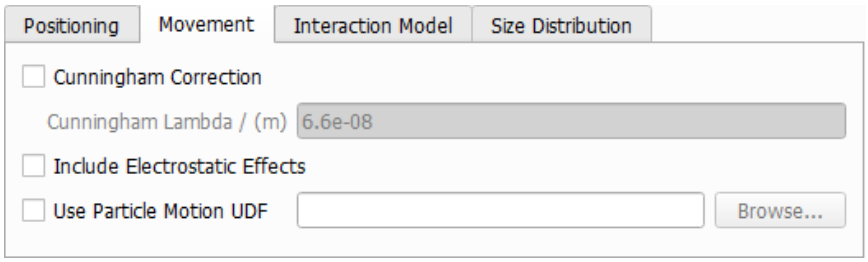
- Additionally, they can stop moving and leave the simulation if the particle displacement is larger than a predefined maximum value.



  This option can be used e.g., to simulate a long channel (like in a catalytic converter) that is much longer in flow direction compared to the other two directions. By defining a maximum displacement, the simulation can be run on a much shorter channel in flow direction but with periodic boundary conditions.

MOVEMENT

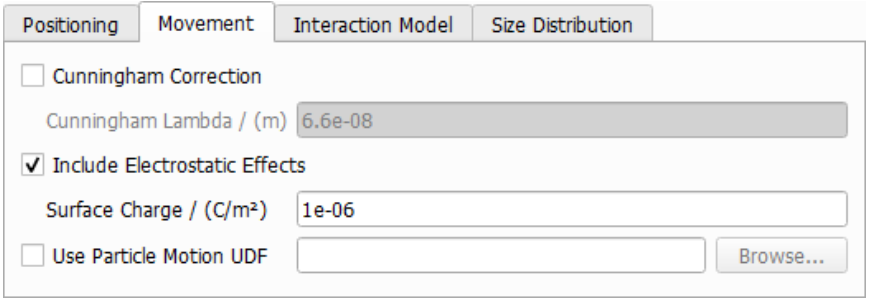
In the **Movement** subtab of the **Particles** tab, the particle movement is controlled by changing the terms of the governing equation (5) on page 10.



Checking **Cunningham Correction** activates the corresponding correction method and adjusts the drag force using equation (7) of page 10. If this button is unchecked, the Cunningham correction factor is set to $C_c = 1$. If the button is checked, the value of the mean free path λ can be entered.

If **Include Electrostatic Effects** is checked, electrostatic effects between solids and particles in the fluid are considered. That is, the electrostatic forces are set to $Q\vec{E} = 0$ if the button is unchecked.

The **Surface Charge** (C/m²) corresponds to ξ in equation (10) of page 11. To model electrostatic effects, it is also necessary to enter a value for the particle charge under the **Particles – Interaction Model** subtab as described below on page 32. Pay attention that to simulate attraction of particles and surfaces, a positive value for the surface charge and for the particle charge needs to be set.

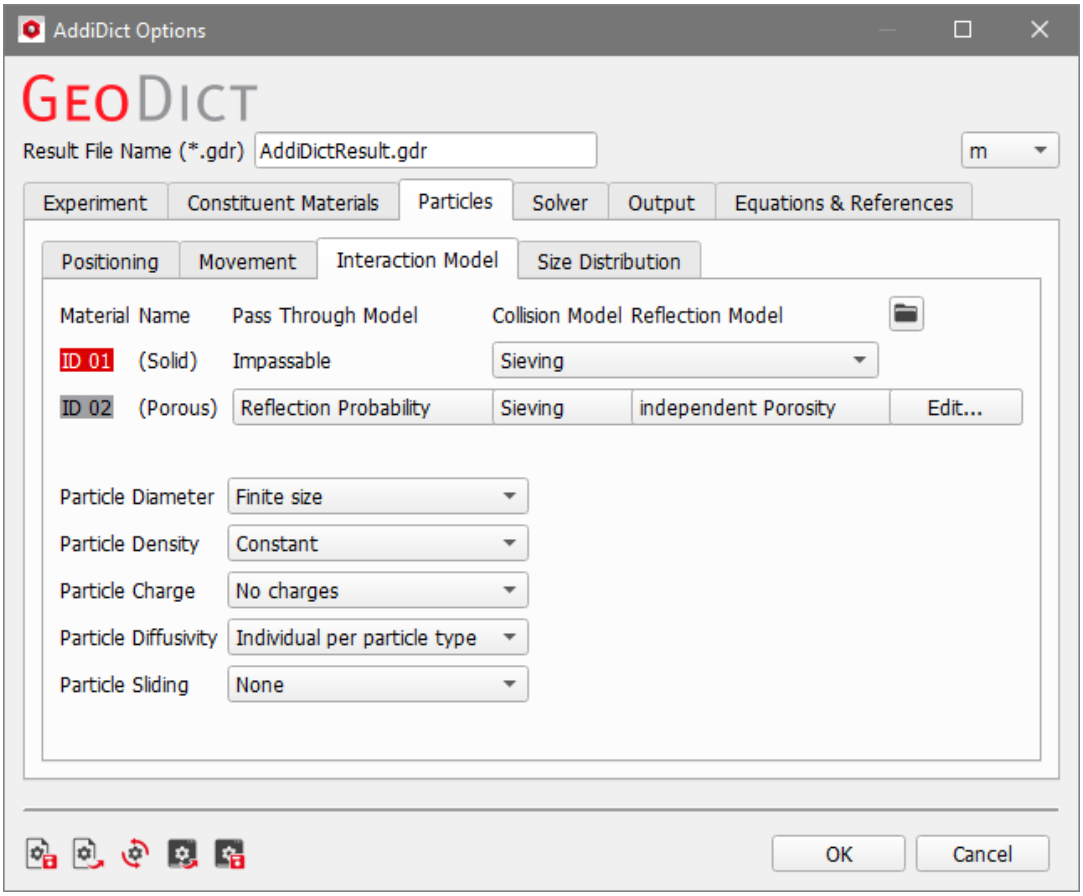


With the **Use Particle Motion UDF** option, the user can replace formulas (6)-(9) of page 10 by own formulas. When **Use Particle Motion UDF** is checked, the formulas in the (modified) UDF file are used for all four formulas in the AddiDict simulation instead of the built-in equations.

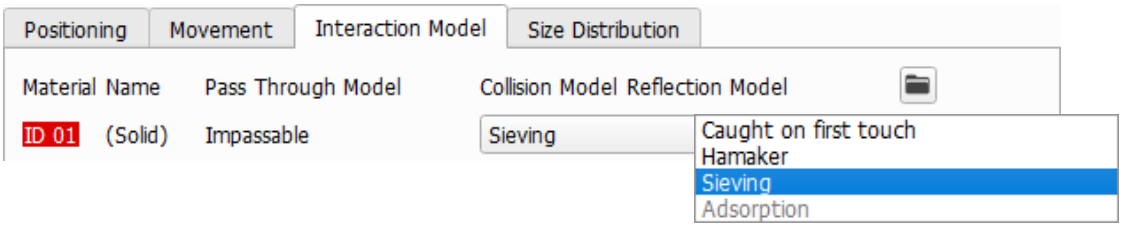
For details on how to modify and compile user defined functions, refer to the Appendix on UDF.

Interaction Model

Under the **Interaction Model** subtab, properties of the particles as well as their interaction with the solid and porous materials, available in the structure, are defined. The choice of parameters under this subtab affects the entries and columns shown in the table under the **Size Distribution** subtab.



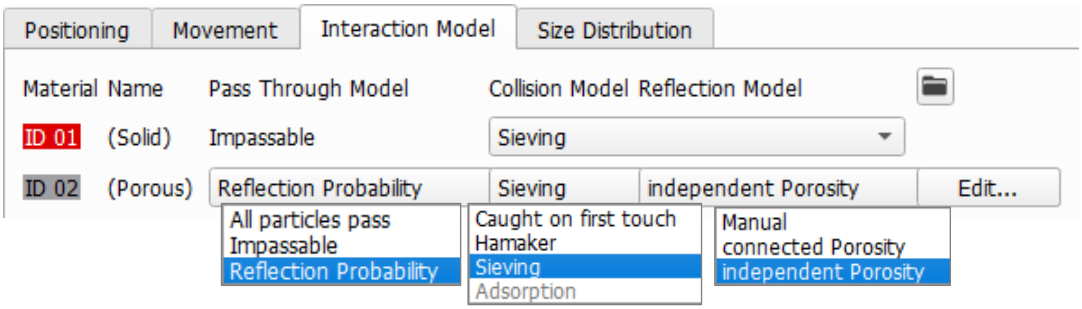
For all materials in the model, a **Pass Through Model** and a **Collision Model** must be set. It depends on the choice of the **Pass Through Model** whether a **Reflection Model** needs to be selected additionally, or not.



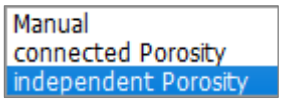
Solid materials are always **Impassable** for particles, and for them, only the collision model among **Caught on first touch**, **Hamaker**, **Sieving** and **Adsorption** must be chosen. Hamaker model can be selected only for particles with finite size diameter, Adsorption only for molecules. Additional columns appear in the table under the **Size Distribution** subtab when Hamaker (columns Restitution and Adhesion), Sieving (column Restitution) or Adsorption (columns Restitution and Adsorption rate) are chosen as Collision Model.

Additional collision models can be defined by the user in user defined functions (UDF) and accessed by adding an UDF Search Folder by clicking the file button on the top right of this tab. This is more often used for filter simulations. Details can therefore

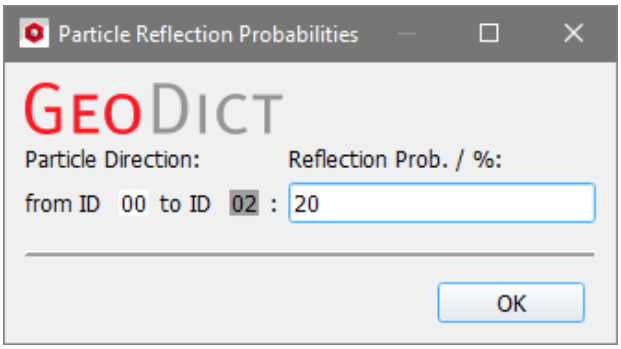
be found in the FilterDict handbook of this GeoDict User Guide, in the appendix 1: **User-Defined Functions**.



For porous materials, one of the three Pass Through Models **All particles pass, Impassable** or **Reflection Probability** must be chosen. If set to **Impassable**, the material is treated as a solid material and particles cannot enter. If set to **All particles pass**, particles can move through the material. In that case, no Collision Model is selected. If the Pass Through Model is set to **Reflection Probability**, part of the particles can enter the porous material, others collide with the material. I.e. the same behavior of the porous material is simulated that one would expect, if the porous material would be fully resolved in the simulation. Part of the particles enter the material (the ones that hit the material at a pore), others collide with the material (the ones that hit the solid part). This option should be chosen only if the particles are smaller than the pore sizes of the porous material, i.e. they can really enter the material. The percentage of the particles that enter the material, depends on the choice of the **Reflection Model**. **Manual**, **connected Porosity** or **independent Porosity** can be selected.



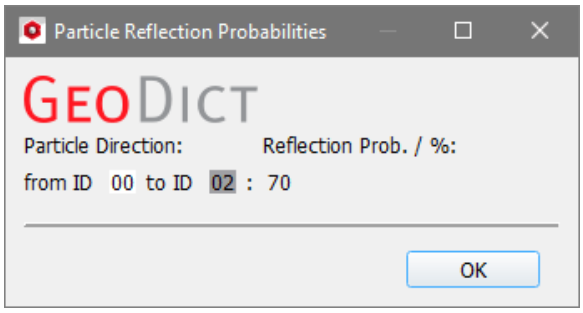
If **Manual** is selected, the user defines the probability of a particle to be reflected at the interface between pore space and porous material by clicking the **Edit...** button. In the example shown, the probability of a particle to be reflected, if it reaches the interface between material with ID 0 and the porous material with ID 2, is 20%. With probability 80%, the particle enters the porous material.



For **connected Porosity,** the reflection probability depends on the porosity of the material the particle is entering (porosity_to) and the material the particle is leaving (porosity_from). The reflection probability is (porosity_from-porosity_to) / porosity_from. If the particle is moving from a region with low porosity to one with higher porosity, it will never be reflected, i.e., the reflection probability is always kept between 0% and 100%. This Reflection Model should be selected for the case of materials with different porosity, with pores that are connected and change only their width at the interface between materials.

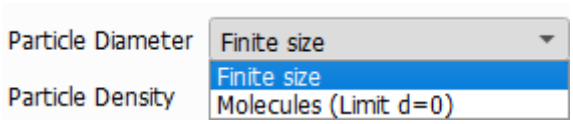
If **independent Porosity** is selected, the reflection probability is 1-porosity_to, i.e., if the porous material has a porosity of 30%, 30% of the particles reaching the interface enter the porous material and 70% are reflected.

In the example shown here, with only an interface between pore and porous material, connected and independent porosity both give the same value. Clicking the **Edit...** button shows the value used.

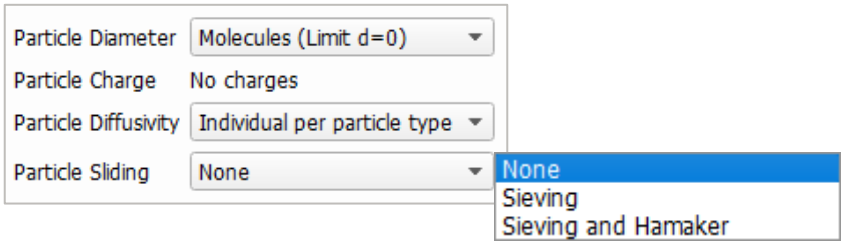


For **connected Porosity** and **independent Porosity**, the porosity value(s) of the porous material(s) need to be set correctly on the tab Constituent Materials (see page 19).

The two choices of **Particle Diameter** are **Finite Size** (default) and **Molecules (Limit d=0)**.

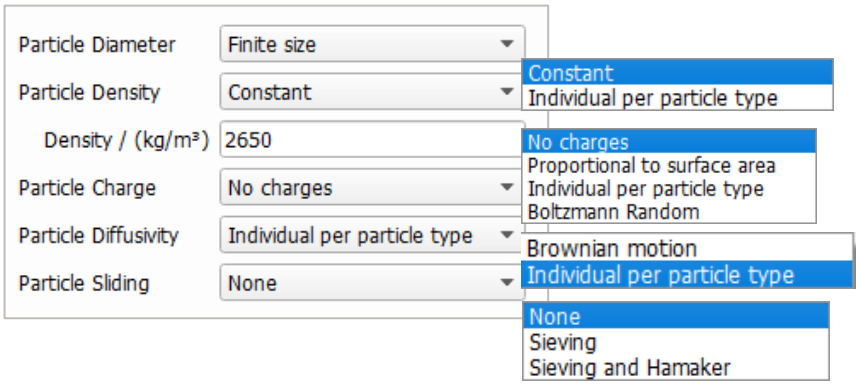


In the case of **Molecules**, the simplified equation (13) on page 13 is solved to model the particle movement. In this case, no density value has to be entered, particle charges are set to zero, and diffusivities have to be defined individually per particle type.

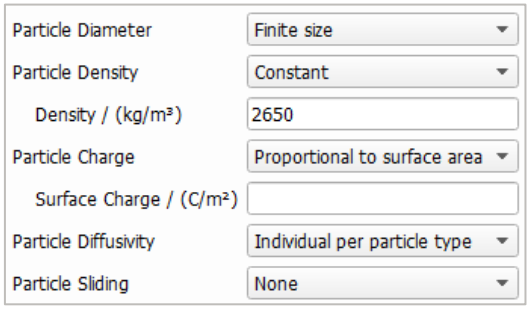


For Particle Sliding **None**, **Sieving** or **Sieving and Hamaker** can be selected. The selection defines for which material the sliding will be considered. For none of the materials, for those with Collision Model Sieving or for those with Collision Models Sieving and Hamaker.

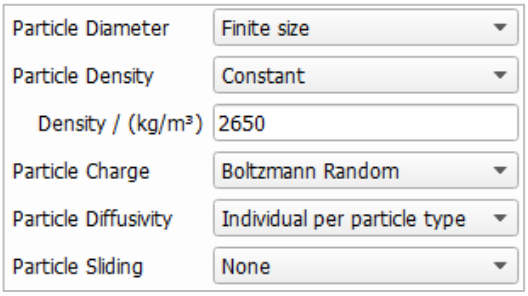
If **Finite Size** is set for the **Particle Diameter**, equation (5) on page 10 is solved to model the particle movement.



For finite sized particles, a **Particle Density** has to be given. If **Constant** is chosen, one density is set for all particle sizes. If **Individual per particle type** densities are chosen, the field to set the **Density** in (kg/m³) disappears and individual density values have to be entered in the particle size distribution table, under the **Size Distribution** tab.



Similarly, a **Particle Charge** may be entered that is **Proportional to surface area**, in which case a general particle **Surface Charge / (C/m²)** can be given, or **Individual per particle type**, in which case the particle charges have to be entered into the particle size distribution table (under the **Size Distribution** subtab). Pay attention that to simulate attraction of particles and surfaces, a positive value for the particle charge needs to be set here, like for the surface charge, see page 27.



If **Boltzmann Random** is chosen for the **Particle Charge**, particle charges are randomly distributed according to a normal (or Gaussian) distribution with mean value $\mu = 0$ and standard deviation $\sigma = \sqrt{2d\varepsilon_0 kT\pi}/e$. Here, d denotes the particle diameter, ε_0 the dielectric constant, k the Boltzmann constant, T the temperature and e the charge of an electron. This can be used e.g. to model the particle charge of dust in air, that follows a Boltzmann distribution.

For **Particle Diffusivity**, the user may choose between **Brownian Motion** and **Individual per particle type**. For Brownian motion, the diffusivity coefficient is determined by equation (8):

$$D = \frac{k_B T}{\gamma}$$

For **Individual per particle type**, the value of D must be entered into the particle size distribution table (under the **Size Distribution** subtab) for each particle type:

Positioning | Movement | Interaction Model | Size Distribution

	Diameter / (m)	Count Percentage	Restitution (in [0,1]) for Sieving	Restitution (in [0,1]) for Sieving	Diffusivity in Pore / (m²/s)	**Diffusivity in Media / (m²/s)**
1	1e-06	10	0.5	0.5	3.2e-07	1.6e-07
2	2e-06	75	0.5	0.5	1.2e-07	6e-08
3	3e-06	10	0.5	0.5	1e-07	5e-08
4	4e-06	5	0.5	0.5	9e-08	4.5e-08

The values entered in the **Diffusivity in Pore** column are used to model the diffusion of the particles in the pores and the values entered in a **Diffusivity in Media** column are used to model the diffusion inside of this porous material.

In the table, one column appears for each porous material which allows particles to pass, i.e., for which the **Pass Through Model** is set to **All particles pass** or to **Reflection Probability**.

SIZE DISTRIBUTION

The **Size Distribution** subtab contains a table with the size distribution of the particles.

For the default settings of **Finite Size** as **Particle Diameter**, **Constant** as **Particle Density**, **Caught on first touch** as **Collision Model** and **Brownian Motion** as **Particle Diffusivity** (chosen under the **Interaction Model** tab, page 29), the first column lists the different particle diameters (m) of the particle size distribution. The second column contains the particle percentages of each particle size in relation to the entire size distribution. The percentage of the entire particle size distribution can be defined in percentage of mass (**Mass %**), volume (**Volume %**) or total number of particles (**Count %**), to be selected on the right of the table.

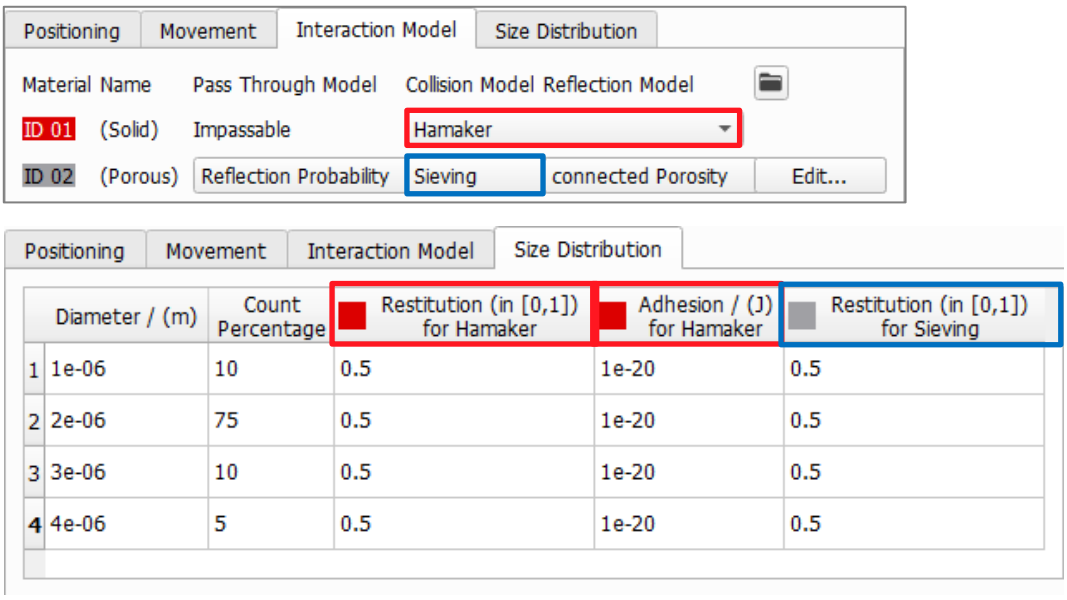
Additional columns appear under the **Size Distribution** tab, depending on the user choices under the **Particle Model** tab.

If the limit d = 0 for **Molecules** is selected as **Particle Diameter**, the column **Diameter** disappears, and the percentages of the particle distribution can be defined only in percentage of the total number of particles (**Count %**).

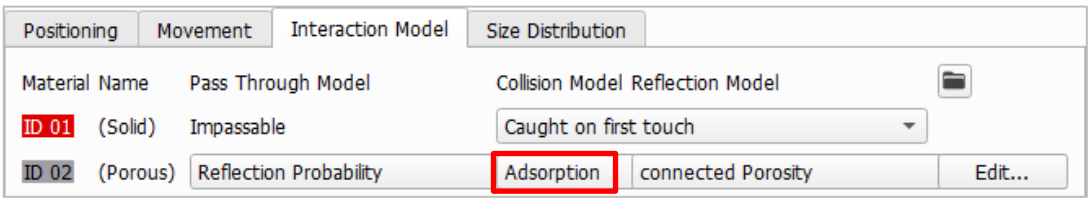
As mentioned above, the choice of an **Individual per particle type** density makes the Particle Density [kg/m³] column appear.

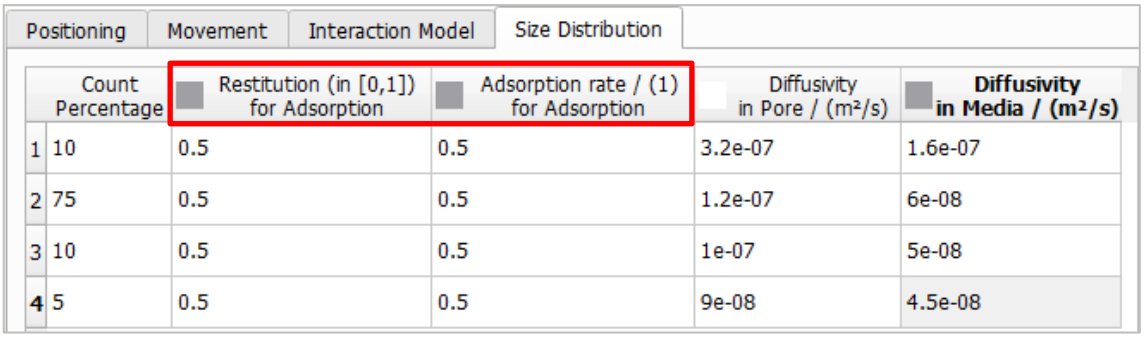
Depending on the choice for the solid and porous material IDs collision models, an individual column for each material ID may appear. After choosing **Caught on first touch**, no additional columns appear.

When choosing the **Hamaker** collision model for a material, the columns Restitution and Adhesion appear. In the case of **Sieving**, only the Restitution column appears.



Choosing **Adsorption** as collision model, columns for restitution and adsorption rate appear.





	Count Percentage	Restitution (in [0,1]) for Adsorption	Adsorption rate / (1) for Adsorption	Diffusivity in Pore / (m²/s)	**Diffusivity in Media / (m²/s)**
1	10	0.5	0.5	3.2e-07	1.6e-07
2	75	0.5	0.5	1.2e-07	6e-08
3	10	0.5	0.5	1e-07	5e-08
4	5	0.5	0.5	9e-08	4.5e-08

The values in the **Restitution** column(s) determine the amount of energy not absorbed by a collision with the solid material. The restitution value ranges from 0 to 1. If the restitution value is set to 1, no energy is lost, and the particle is reflected with the same speed it had before the collision. For restitution values smaller than one, energy is absorbed by the collision and the particle slows down. For example, a restitution value of 0.7 means that a particle loses 30% of its velocity in the collision and gets 30% slower.

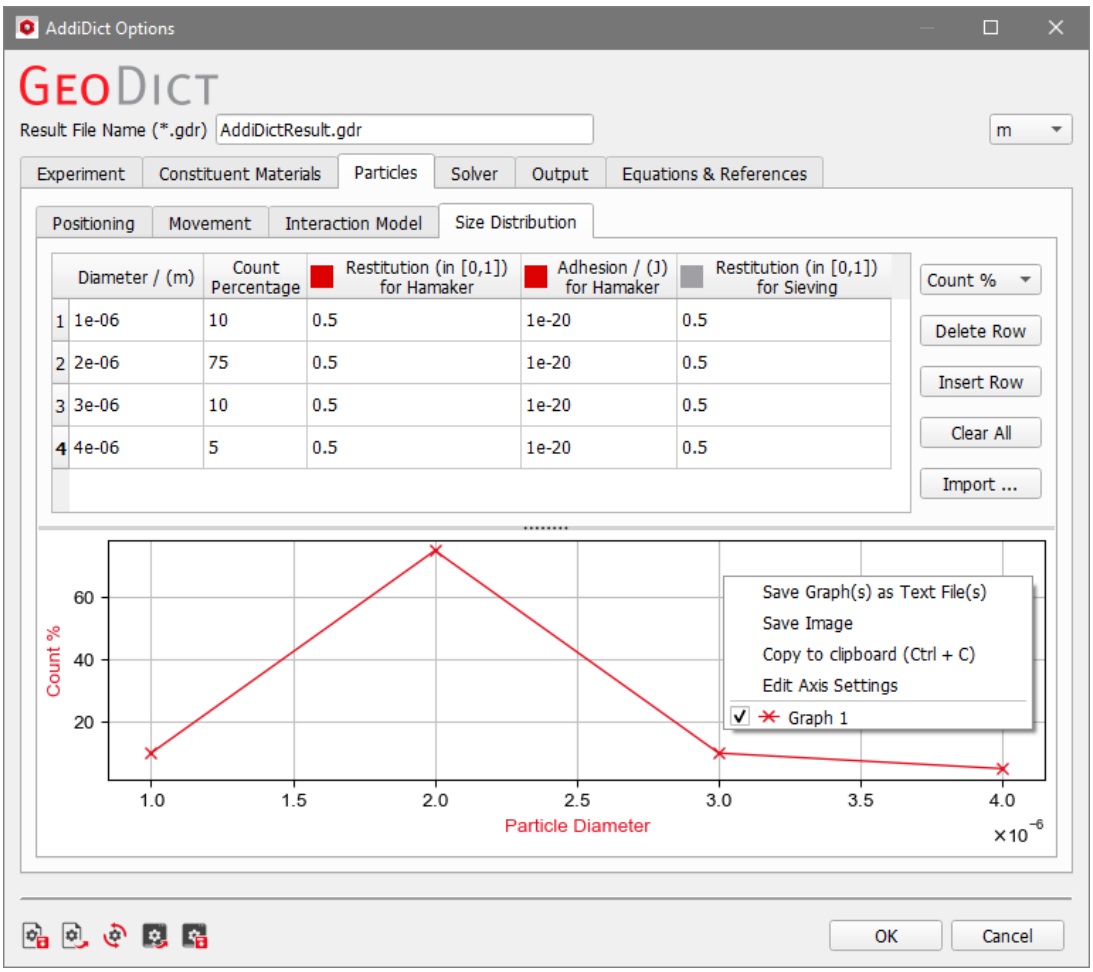
The **Adhesion** column defines the Hamaker constant (Adhesion / (J)) which lies generally in the range of 10^{-19} to 10^{-20} Joule.

The **Adsorption rate** defines the probability that a particle is trapped if it hits a solid or porous material.

Choosing **Molecules** for the **Particle Diameter** or a **Particle Diffusivity Individual per particle type** for the **Particle Diameter Finite size**, adds a column for the diffusivity in the pore space and for each porous material with **Pass Through Model All particles pass** or **Reflection Probability**.

Choosing a **Particle Charge Individual per particle type** adds a column for the Particle Charge.

Below the size distribution table, a graphical presentation of the particle size distribution is displayed, if particles with finite size are selected. The graph is automatically updated after changes in the table.



Clicking **Delete Row**, on the right of the table, deletes the currently selected row.

Clicking **Insert Row** inserts a row below the currently selected one. The inserted row is a copy of the currently selected row and contains the same data.

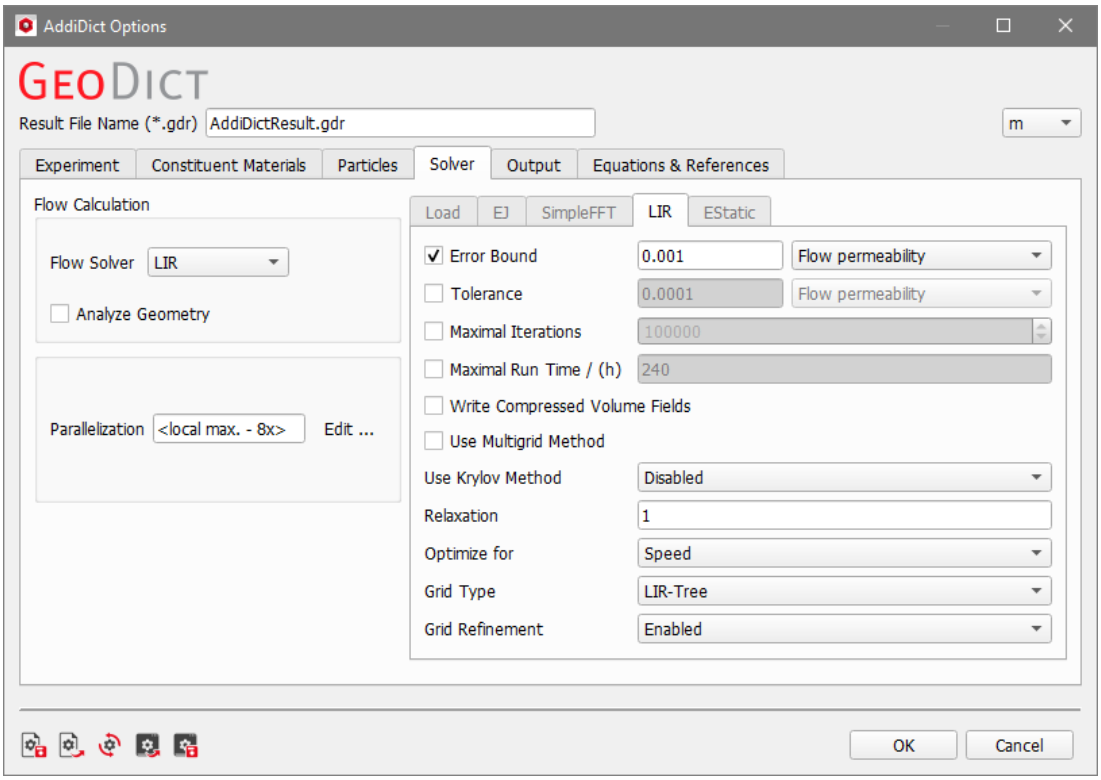
Clicking **Import...** allows to import data from ASCII text files that contain two columns, for diameter (in [m]) and count percentage.

After loading a text file, a chart of the particle size distribution is automatically displayed. The x-axis shows the particle diameter, and the y-axis the Mass, Count, or Volume percentage. Right-click the plot to store the graph again as a .txt file (perhaps after modifications), to save the graph as image, to copy the values to the clipboard or to edit the plot settings. Percentages of the .txt file are always considered as count percentages. Change the displayed values to **Count %** before saving, to reproduce your values during import of a file.

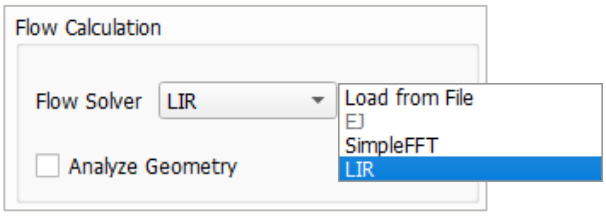
After editing a distribution table and clicking **OK**, a warning message appears if the new percentages do not add up to 100%. The values can be automatically normalized by clicking **Yes**, or manually by clicking **Cancel** and returning to the particle distribution table.

SOLVER

Under the **Solver** tab, the settings for the AddiDict solver can be chosen and its parameters can be defined. The tab is subdivided into three panels.



In the **Flow Calculation** panel on the top left, select the **Flow Solver** to be used for solving the chosen partial differential equations from the pull-down menu (EJ, SimpleFFT, or LIR). EJ can be selected for solving (Navier-)Stokes equations only.



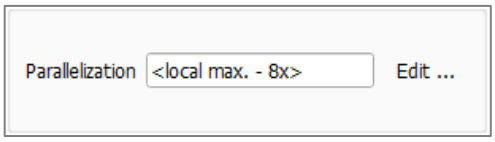
It is also possible to choose **Load from file** to import the flow field (.vap) of a fluid flow simulation previously executed with FlowDict or AddiDict. In this case, computational time is saved by re-using this result, and no additional flow simulation must be executed.

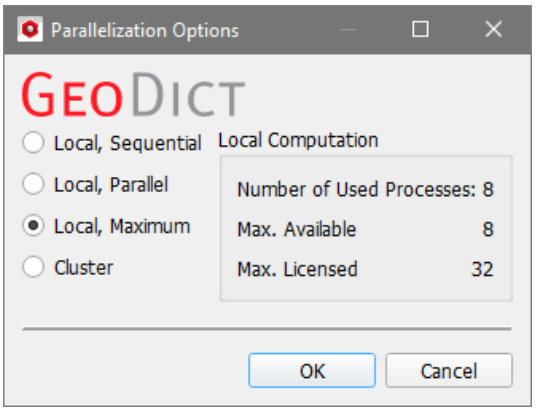
Check the **Analyze Geometry** button to check whether a through path for the flow through the structure exists. For very large structures, this can take some time, thus it can be turned off in this case.

Irrespective of the flow solver, the fluid flow is simulated only in **z-direction**. If mass transport and particle trajectories should be simulated for a different flow direction, the structure has to be rearranged in a way that the direction of interest coincides with the z-direction. This can be achieved by applying **Permute** in ProcessGeo prior to an AddiDict simulation.

In the lower left panel, calculations can be parallelized if the user's license and hardware allow it.

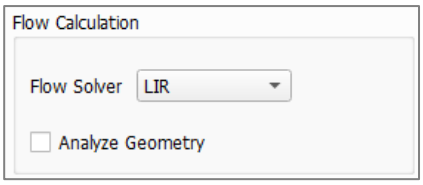
The **Parallelization Options** dialog box opens when clicking the **Edit...** button, to choose between **Local, Sequential**, **Local**, **Parallel, Local, Maximum** or **Cluster**. When **Local, Parallel** is selected, the **Number of Threads** can be entered. If **Local, Maximum** is selected, the maximum number of parallel processes is used. The maximum number depends on the available hardware and on the maximum number of processes licensed.

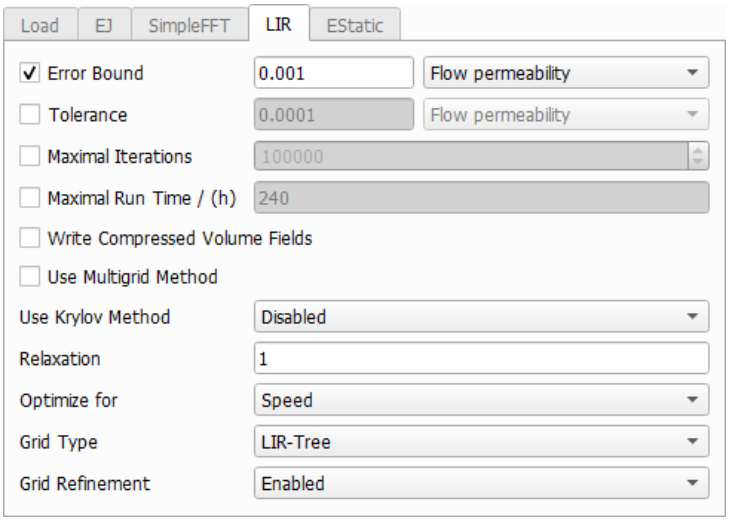




The choice of **Cluster** is for computations on Linux clusters. See the **High Performance Computing** handbook of the GeoDict User Guide for information on how to license GeoDict for these options and how to perform GeoDict computations on a cluster.

In the right panel of the **Solver** tab, the subtab of the solver chosen to solve the equations governing the fluid flow is selectable after choosing a method (Load from File, EJ, SimpleFFT or LIR solver) in the Flow Calculation panel on the left.

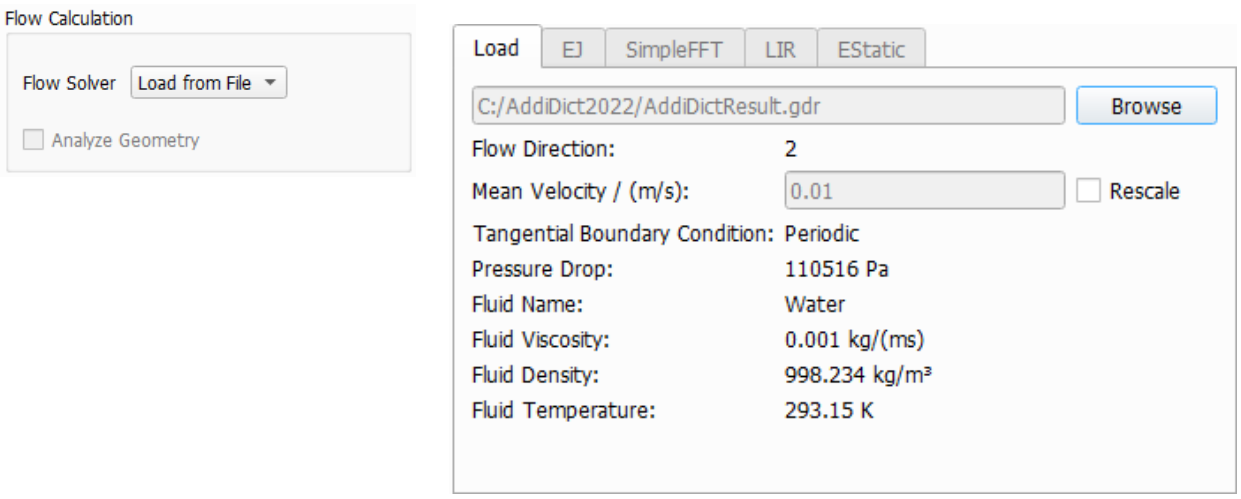




The options for the selected solver are set in the subtab for that solver (here, shown for the LIR solver).

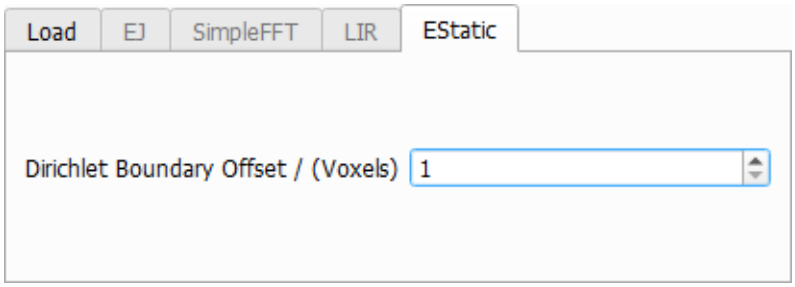
If **Load from File** has been selected from the **Flow Solver** menu in the **Flow Calculation** panel above, choose a GeoDict result file of a previously run computation.

Some information about the computation is shown. The mean velocity of the computation can be rescaled to another one by checking **Rescale** and editing the mean velocity.



The **EStatic** subtab is only selectable when **Include Electrostatic Effects** has been checked previously under the **Particles-Movement** tab.

The **Dirichlet Boundary Offset** has to be specified under the **EStatic** subtab if electrostatic effects are considered in the simulation.



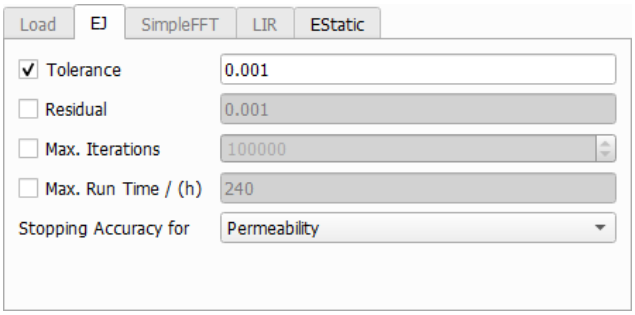
This value defines the distance to the computational domain, at which the Dirichlet boundaries for the electric field are installed in the flow direction of the fluid. Essentially, this value should be infinite, but a practical value must be given to run the calculations, see page 11 for more details.

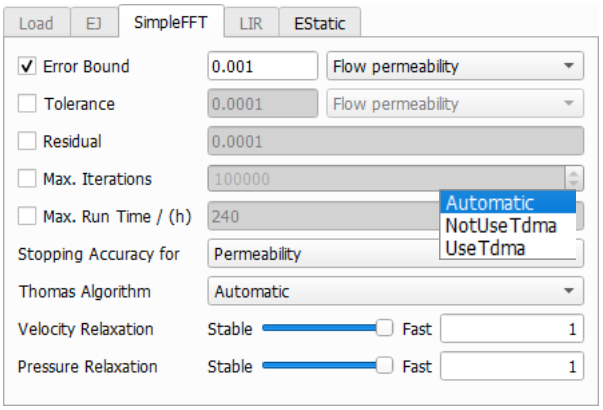
EJ Solver and SimpleFFT Solver

With the **EJ solver** and the **SimpleFFT solver**, the flow field is determined by iteratively solving the partial differential equations describing the flow field. The SimpleFFT solver can be selected in the GUI for solving (Navier-)Stokes or (Navier-) Stokes-Brinkman equations, EJ for solving (Navier-)Stokes equations. The basic idea of an iterative method is to:

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

The iterative process is controlled for the EJ and the SimpleFFT solvers by selecting one or several stopping criteria and setting values for them. Stopping criteria **Tolerance**, **Residual**, **Maximal Iterations**, **Maximal Run Time/(h)** are available for both EJ and SimpleFFT and can be selected by checking the boxes. For SimpleFFT the additional stopping criterion **Error Bound** is available.





For **Thomas Algorithm**, **Automatic**, **NotUseTdma** or **UseTdma** can be selected. The tridiagonal matrix algorithm (Tdma) can help to improve the converge for structures with high porosity and therefore speedup the computation with SimpleFFT. With **UseTdma** / **NotUseTdma** it can be switched on or off. Choosing **Automatic** makes the selection based on the porosity of the structure and on the partial differential equation for the flow solver. For Navier-Stokes, Tdma is switched on for a porosity larger than 45%, for Stokes equations it is always switched off.

Depending on the material parameters, the geometry of the structure and the flow velocity, 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.

The management of this balance is done through the **Velocity Relaxation** and **Pressure Relaxation: Stable ↔ Fast** slide bars for the SimpleFFT solver. 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.

LIR SOLVER

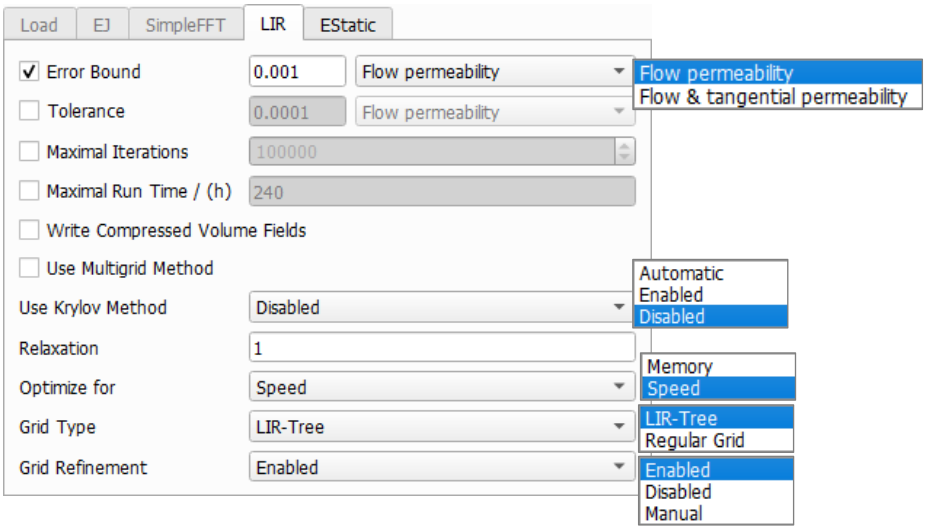
For the LIR solver, the flow field is determined by solving the partial differential equations for the flow field iteratively with an adaptive tree structure. Stopping criteria **Error Bound**, **Tolerance, Maximal Iterations**, and **Maximal Run Time** can be selected.

The LIR solver can be used with a multigrid method to speed up the computation. Check the box **Use Multigrid Method** to use this option.

Additionally, the flow field can be exported in a compressed form, by checking **Write Compressed Volume Fields**.

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

If the Krylov method is used, the relaxation parameter will be chosen automatically by the solver.



The **Relaxation** parameter is very similar to the **Velocity relaxation** and **Pressure relaxation** for the SimpleFFT solver. For the LIR solver, this balance is managed through the **Relaxation: Stable (<1.0) ↔ Default (=1.0) ↔ Fast (>1.0)**.

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.

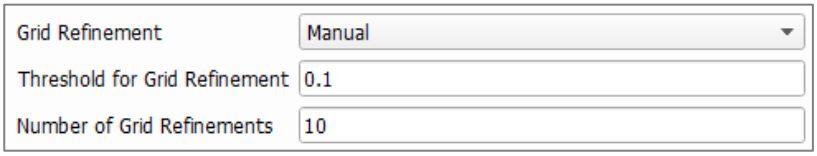
The **Grid Type** decides what kind of tree structure is used for the simulation.

The default option is **LIR-Tree** and should always be used. The solver uses an adaptive tree 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 velocity and pressure field during the computation and improves the adaptive grid in places where more accuracy is needed. The LIR solver splits cells where a high velocity-gradient or high pressure-gradient occurs. The analysis is enabled if the **Grid Refinement** option is set to **Enabled** or **Manual**.

If the **Grid Refinement** is set to **Enabled**, the solver chooses the **Threshold for Grid Refinement** and **Number of Grid Refinements** automatically. If the **Grid Refinement** is set to **Manual,** the user enters these parameters.

The **Number of Grid Refinements** controls how many velocity-based and pressure-based grid refinements are allowed during the simulation.



The value should be between 0 and 10. The number of grid refinements may increase the number of iterations, runtime, and memory requirements.

Cells are split where the current velocity gradient (or pressure gradient) is greater than the **Threshold for Grid Refinement** times the maximal velocity gradient (or pressure gradient). This threshold must be between 0.0 and 1.0. The recommended value range is between 0.05 and 0.1.

STOPPING CRITERIA FOR FLOW SOLVERS

The **Error Bound** stopping criterion uses the results of previous iterations and predicts the final solution based on linear and quadratic extrapolation. The solver stops if the relative difference with respect to the prediction is smaller than the specified error bound. The stopping criterion can recognize 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 with respect to the damped convergence curve. Error Bound is the default stopping criterion for SimpleFFT and LIR.

The **Tolerance** stopping criterion looks for stagnation of the method when the process becomes stationary. This occurs when from iteration to iteration the improvement in the computed value(s) becomes extremely small. If the relative change is smaller than the value entered for **Tolerance**, the iteration is stopped. When there is doubt about the quality of the solution, decrease the **Tolerance** value by a factor of ten for that solver.

For **Error Bound** and **Tolerance** as stopping criterion, it is possible to choose if the stopping criterion should look at the permeability in flow direction only or at the permeability both in flow and in tangential directions. For flow simulations where the permeability in flow direction converges much faster than the permeability in tangential directions, it is recommended to choose **Flow & tangential permeability**.

By checking **Residual** as stopping criterion, 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.

```
SIMPLE-FFT        0  norm of res. 1.27e-02   scaled res. 1.00e+00
SIMPLE-FFT        1  norm of res. 2.26e-02   scaled res. 1.78e+00
SIMPLE-FFT        2  norm of res. 1.88e-02   scaled res. 1.49e+00
SIMPLE-FFT        3  norm of res. 1.58e-02   scaled res. 1.25e+00
SIMPLE-FFT        4  norm of res. 1.32e-02   scaled res. 1.04e+00
SIMPLE-FFT        5  norm of res. 1.17e-02   scaled res. 9.28e-01
SIMPLE-FFT        6  norm of res. 1.13e-02   scaled res. 8.91e-01
SIMPLE-FFT        7  norm of res. 1.11e-02   scaled res. 8.78e-01
SIMPLE-FFT        8  norm of res. 1.07e-02   scaled res. 8.49e-01
SIMPLE-FFT        9  norm of res. 1.01e-02   scaled res. 8.00e-01
SIMPLE-FFT       10  norm of res. 9.45e-03   scaled res. 7.47e-01
```

When the solver stops because the **Maximal Iterations** value or the **Maximal Run Time/(h)** has been reached, no guarantee on the quality of the solution can be given.

For the SimpleFFT and LIR solver we recommend using **Error Bound**, as this stopping criterion approximates "relative deviation from the final solution"!

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.

The **Stopping Accuracy for** can be set to **Permeability** or **Residual** for SimpleFFT and EJ. This defines whether the stopping criterion chosen above applies for the computed permeability or for the residual of the computation.

Which stopping criterion was the relevant one to stop the simulation, if several criteria where selected, can be seen later in the GeoDict result file (.gdr).

OUTPUT

In the **Trajectory File** panel, the user can set how accurately the particle trajectories are stored. These settings influence greatly the size of the created file. The **Trajectory File Accuracy** pull-down menu has four options (Minimal, Intermediate, Precise and User Defined).

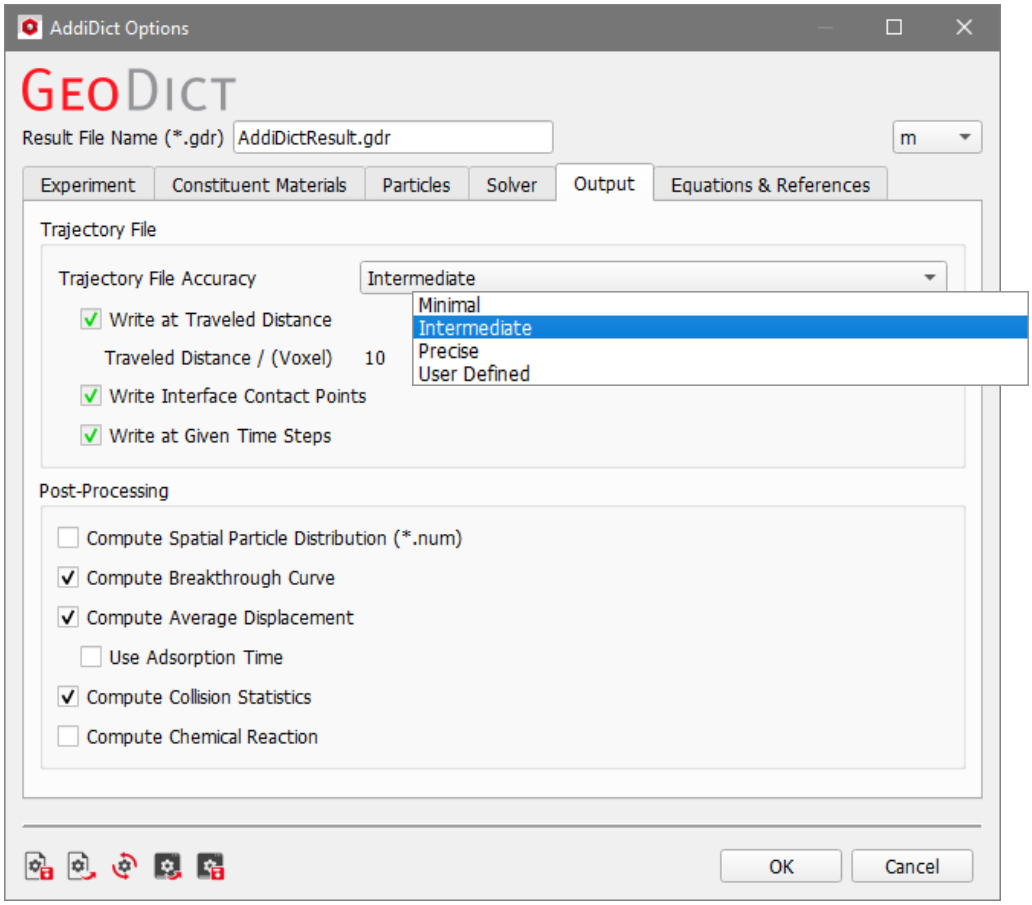
This choice determines the selection of the settings for **Write at Traveled Distance** and **Write Interface Contact Points**.

The **Write at Given Time Steps** option is always checked. This causes that the particle positions at the time steps defined in the **Experiment** tab are always stored.

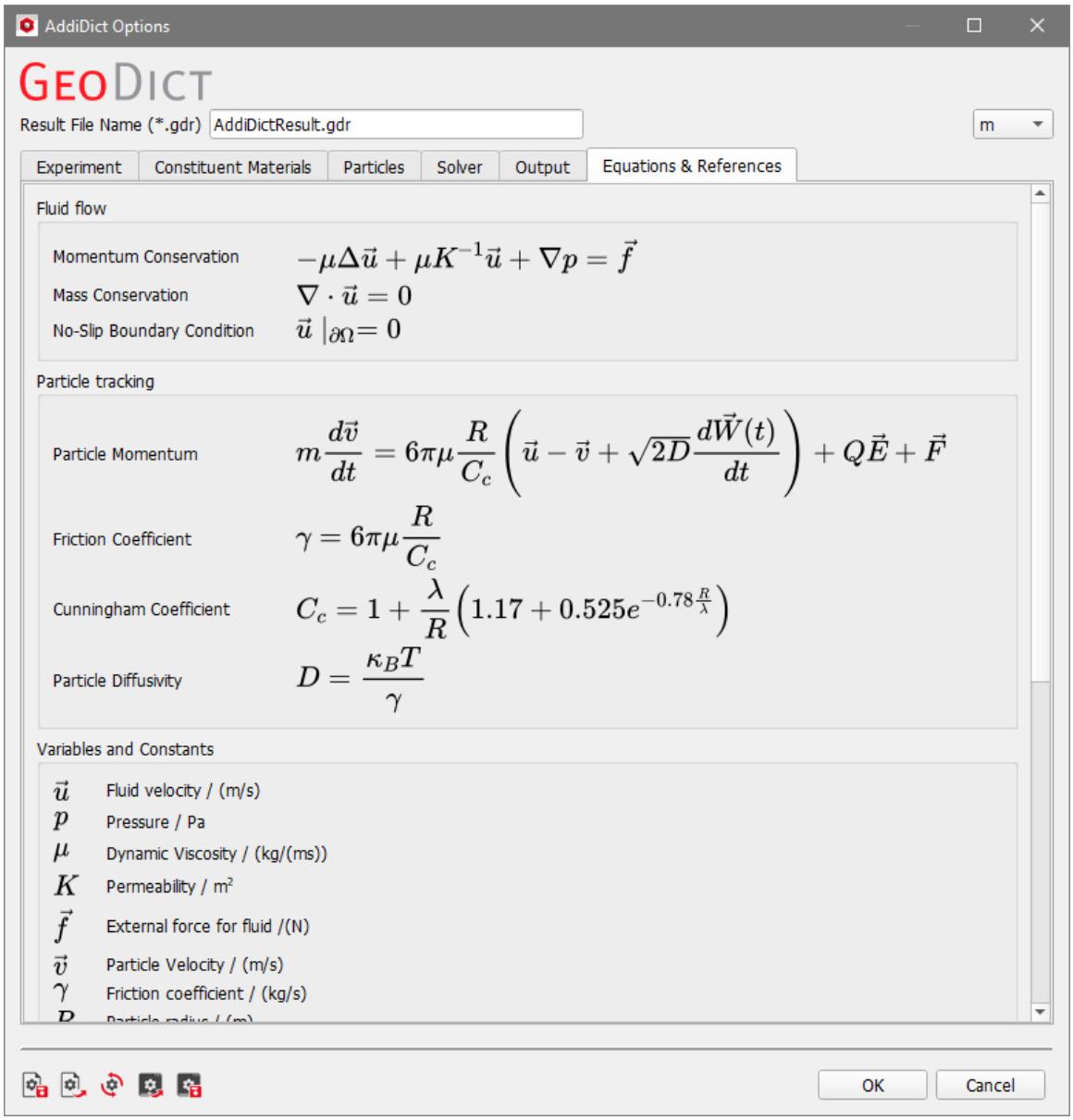
When **Write Interface Contact Points** is checked, all locations at which the particles collide with a solid are added to the file. Only for the option **User Defined**, this box can be checked off.

When **Write at Traveled Distance** is checked, it writes the position of each particle to its trajectory if the particle moved the distance specified in **Traveled Distance / (Voxel)** since its last record. For the option **Precise**, the **Traveled Distance** is set to 1 voxel. For the option **Intermediate**, it is set to 10 voxels. For the option **User Defined**, the **Traveled Distance** can be specified by the user, or the box can be unchecked.

In the **Post-Processing** panel, the user can choose the features to be included in the created report. These choices only determine the content of the initially created report. It is possible to change those settings at any time after the computation, and then a modified report will be created. Read below the information for the **Results - Report** subtab on page 46 for more details.



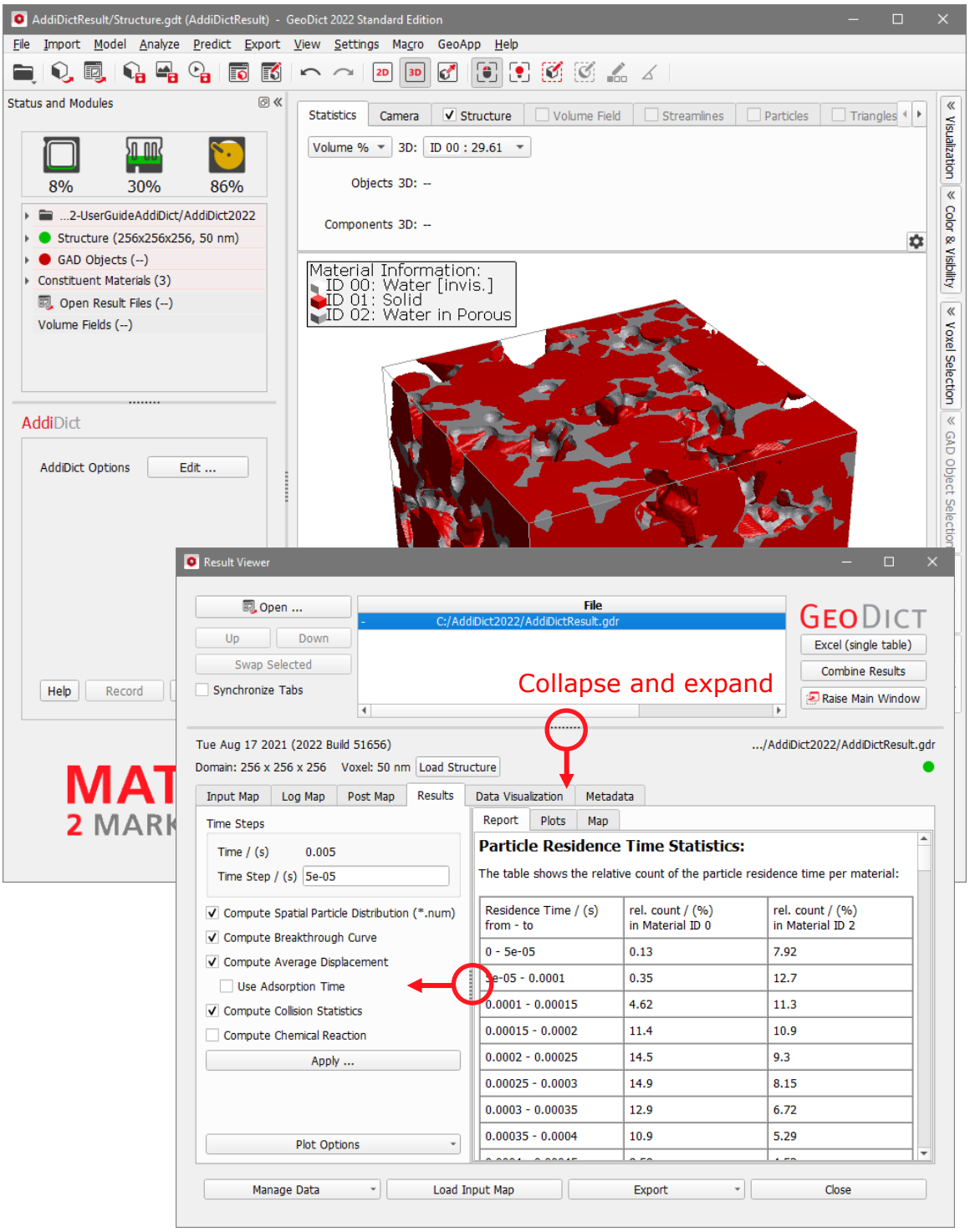
EQUATIONS & REFERENCES



On the tab **Equations & References**, the equations solved for fluid flow and particle tracking are shown. Variables and constants used in the equations are listed, together with their physical units. Additionally, some references for the equations are shown on this tab.

ADDIDICT COMPUTATIONS RESULT FILE

After the selected solver has finished, the result file (*.gdr) is saved in the project folder and a Result Viewer of the GeoDict result file opens automatically.



The first entry on top shows the path and the **Result File Name** previously entered in the **AddiDict Options** dialog box. The result file is accessible at any time by selecting **File → Open Results (*.gdr)...** from the Menu bar. Several AddiDict result files, corresponding to different studies, can be opened simultaneously in the Result Viewer to simplify comparison of computational results.

The box in the upper portion of the **Result Viewer** can be collapsed (and expanded) by pulling up (or down) the dotted line under the box.

The same applies to the left panel of the **Results** tab, which can be collapsed (and expanded) by pulling left (or right) the dotted line between the post-processing options and the **Results** – **Report** subtab.

The green or red dot in the upper right corner indicates if the .gdr file currently shown in the Result Viewer contains results for the structure showing in the **Visualization** area or not. The dot is red if a different structure or no structure at all is loaded. When two files in the Result Viewer have green dots, it indicates that both result files correspond to the structure shown in the **Visualization** area but are from two different simulations with AddiDict.

As usual for all GeoDict result files, several buttons for further processing are available at the bottom of the **Result Viewer**.

- **Manage Data**:
  - **Clean-Up/Pack**: Zip the information contained in the result folder or clean-up the result folder.
  - **Rename:** Change the name of result file and result folder.
- **Load Input Map**: Reload solver options and material parameters used for the computation of the results. After loading, these parameters are available in the AddiDict dialog box.
- **Export:** Export the results for postprocessing with another tool
  - **Excel (generic)**: Export the information of the section ResultMap of the GeoDict result file to Microsoft Excel®. You can analyze computation results in Microsoft Excel® using GeoDexcel provided with GeoDict. See the GeoDexcel handbook for more information.
  - **Excel (generic) – Python**: Export the information to an .xlsx Excel file in the same way as with **Excel (generic)** but using a Python script. This export does not need an Excel installation and can therefore also be used on Linux systems.
  - **Matlab**: Open Matlab® if an installation and license is available, change to the project folder, and load the result file with GeoLab. See the GeoLab handbook for more information.
  - **Store As Html**: Export the information shown in the **Results** tab to a html file.
  - **Save Plots**: Export all plots to the GeoDict result folder.
  - **Input Map as Python**: Export the solver options and material parameters used for the computation, together with the computation command to a Python file. This file can be executed as a GeoDict macro to rerun the computation, see the Automation handbook for more detailed information.

With the **Combine Results** button on the upper right part of the Result Viewer, results of several simulations can be combined to one .gdr file and visualized together in the Result Viewer. More details can be found in the GeoDict Result Viewer documentation.

RESULTS

The information contained in the GeoDict result file (*.gdr) is accessed through six tabs in the Result Viewer.

The computational results are shown under the **Results** tab, and can be loaded for visualization in the **Data Visualization** tab.

The other four tabs (**Input Map**, **Log Map**, **Post Map** and **Metadata**) display additional information about the computation. See more information from page 65 on.

RESULTS – REPORT

The Result Viewer dialog pops up at the end of the computation showing the **Results – Report** subtab.

The content of the **Report** and the **Plots** subtabs is determined by the choices made in the left panel of the **Results** tab. After changing the values there and clicking **Apply...** a new report is generated. The chosen values are automatically stored in the *.gdr file. When the file is opened again later, it shows the last choice of post-processing parameters.

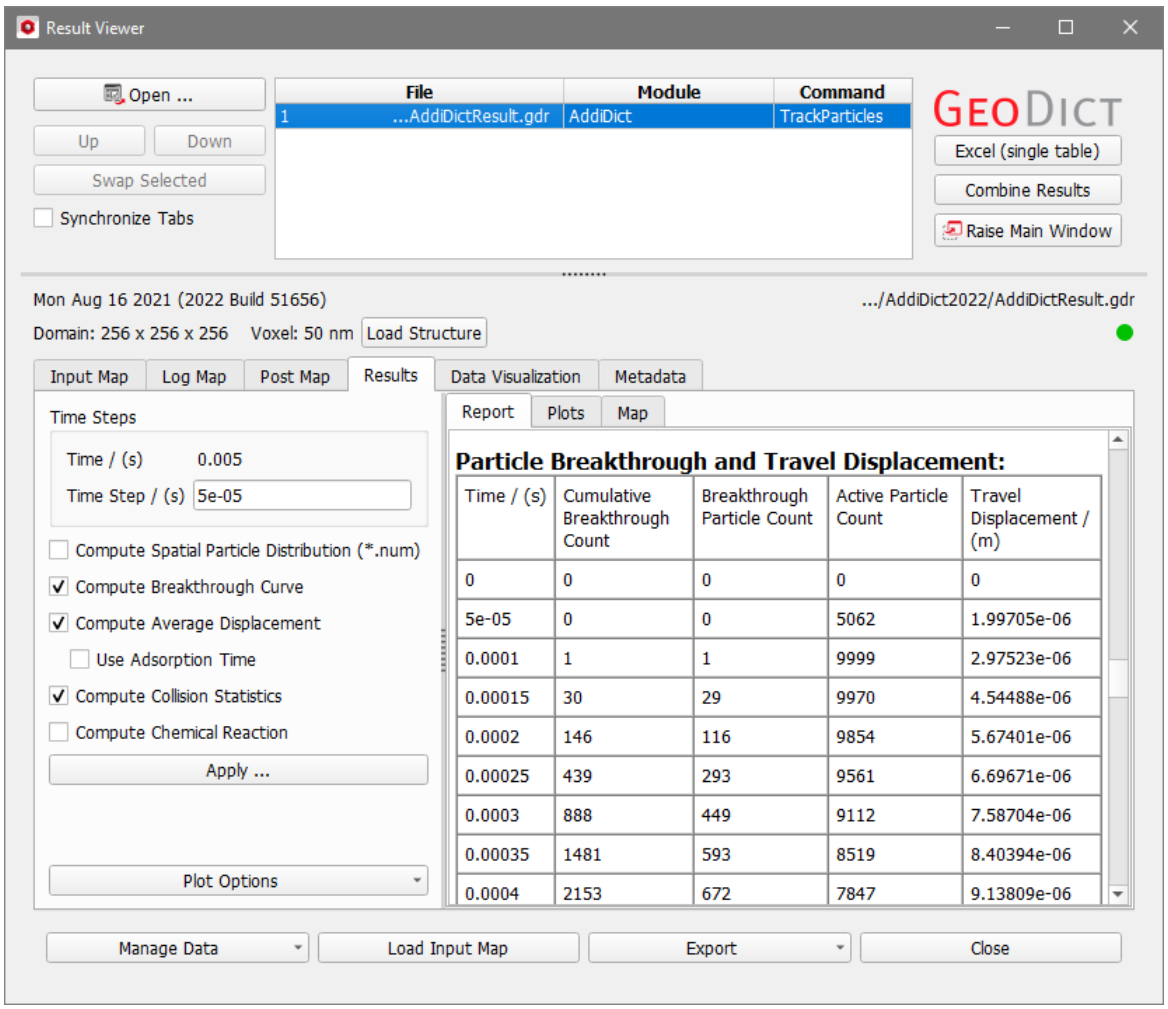
The **Time** value shows the final time of the simulation run. By changing the **Time Step**, the user can choose at which times the particle positions are evaluated, i.e., how many rows appear in the tables shown in the report.

To create an updated report, GeoDict reads the particle positions from the stored particle trajectory file. Bear in mind, that this file does not necessarily contain every intermediate position of the particles. Trajectories are only stored with the precision defined in the **Output** tab of the **AddiDict Options** dialog. Because the option **Write at Given Time Steps** in the output tab is always selected, it is guaranteed that the position of each particle is stored for the originally selected time steps. When the time steps chosen in the post-processing are not a subset of the original time steps, particle positions are interpolated, which might cause some loss of accuracy.

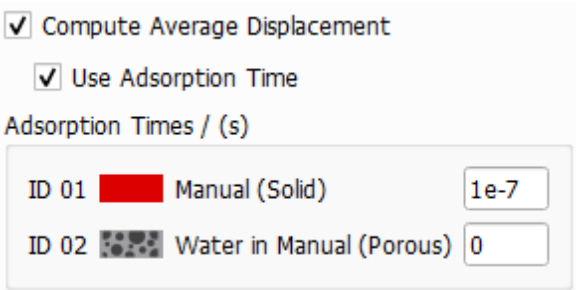
If the **Compute Spatial Particle Distribution (*.num)** box is checked, a particle concentration file is created for each **Time Step**. The user can load and visualize those files through the **Data Visualization** tab.

If the **Compute Breakthrough Curve** box is checked, the **Cumulative Breakthrough Count**, the **Breakthrough Particle Count** and the **Active Particle Count** columns are shown in the report for **Particle Breakthrough and Travel Displacement**. A **Breakthrough Curve** plot is added to the **Plots** subtab. The column Cumulative Particle Count shows at each time step the total number of particles that left the simulation domain until this time step. The column Particle Count lists the number of particles that left in each time step.

If the **Compute Average Displacement** box is checked, the **Travel Displacement** column is shown additionally in the report, and a Travel Displacement curve is added to the **Plots** subtab.



Check **Use Adsorption Time** and define an adsorption time for each solid or porous material to consider short-time adsorption in the Travel Displacement curve. This option has no effect on the Travel Displacement values shown in the tables under the **Report** subtab but will influence the calculation of particle diffusivities.



If particle movement by diffusion only is simulated (box **Simulate Advection** unchecked on the **Experiment** tab in the AddiDict options dialog), additionally the diffusivity is computed from the particle distances travelled and shown under the **Report** subtab.

The **Particle Diffusivity** is the diffusivity of each particle moving through the structure.

The **Effective Diffusivity** is the overall diffusivity of the structure. It takes into account that due to the microstructure, particles starting from somewhere outside of the computational domain will not all enter the structure.

The **Particle Diffusivity (with Adsorption)** is the diffusivity if an adsorption time is set for one or several materials.

Diffusion Parameters:

Average Displacement: 1.22152e-05 m
Average Displacement with Adsorption: 8.21881e-06 m
Average Shift X: 1.24785e-07 m
Average Shift Y: 3.39731e-07 m
Average Shift Z: -5.81937e-06 m
Isotropic Particle Diffusivity: 6.38068e-09 (m^2/s)

Particle Diffusivity / (m²/s)

7.98434e-09	-1.40431e-10	-3.6522e-11
-1.40431e-10	**5.85726e-09**	-2.32977e-10
-3.6522e-11	-2.32977e-10	**5.30045e-09**

Rel. std. dev. of particle diffusivities: (2.06 1.83 1.12) %

Effective Diffusivity / (m²/s)

3.19932e-09	-5.62707e-11	-1.46343e-11
-5.62707e-11	**2.347e-09**	-9.33539e-11
-1.46343e-11	-9.33539e-11	**2.12389e-09**

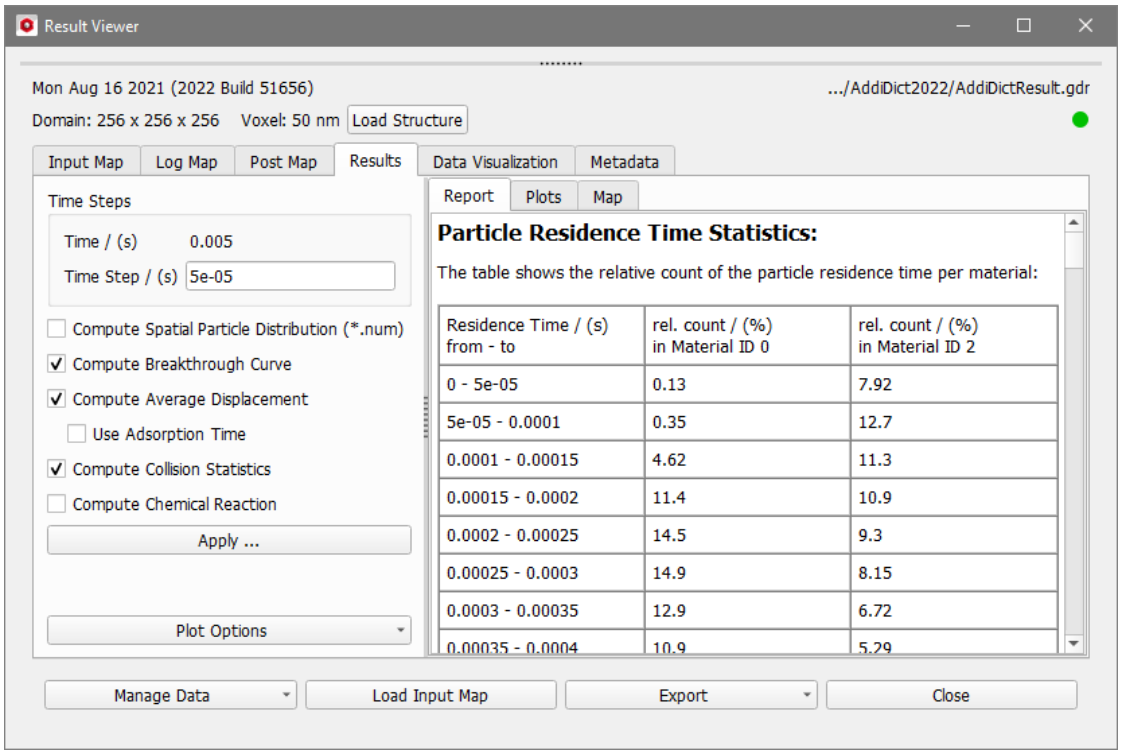
This is the particle diffusivity multiplied with the global porosity.

Particle Diffusivity (with Adsorption) / (m²/s)

5.37213e-09	-9.44868e-11	-2.45732e-11
-9.44868e-11	**3.94096e-09**	-1.56755e-10
-2.45732e-11	-1.56755e-10	**3.56632e-09**

The Diffusivity was multiplied by a factor of 0.672834 due to Adsorption of particles.

To evaluate the residence time in the different materials, check **Compute Collision Statistics**. The table **Particle Residence Time Statistics** in the **Report** subtab is created with columns showing the percentage of particles with specific residence times in each of the materials. A **Residence Time** plot is created on the **Plots** subtab.



The table **Particle Collision Statistics** is shown additionally below the **Particle Residence Time Statistics** table. It shows the mean residence time of particles for each material, together with the mean number of collisions with this material, the mean number of entries to this material and the percentage of particles trapped in this material.

In the example shown, the mean value of particle collisions with the solid material with material ID01 is 3622.46. Since it is a solid material, particles cannot enter the material and the residence time in this material is 0.

Report | Plots | Map

Particle Collision Statistics:

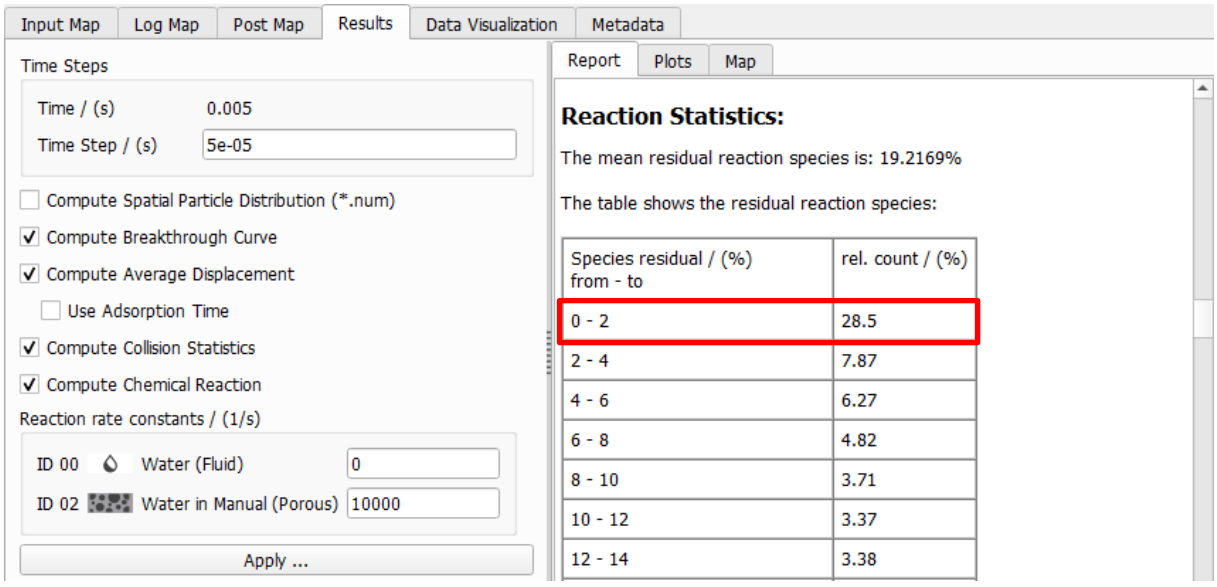
The table shows the mean values for a single particle:

Material ID	Residence Time / (s)	Collisions	Entries	Trapped / (%)
0	0.00034843	0	439.898	0
1	0	3622.46	0	0
2	0.000327159	1074.69	434.878	0

For the porous material with ID02, a reflection probability was defined for the particles. Due to this reflection probability, particles can enter the material, or are reflected at the boundary. The mean value for residence time, collisions and entries are non-zero. Dependent on the collision model with solid or porous material, particles can also be trapped in a material. If this is the case, the percentage of trapped particles is reported in the last column of the table.

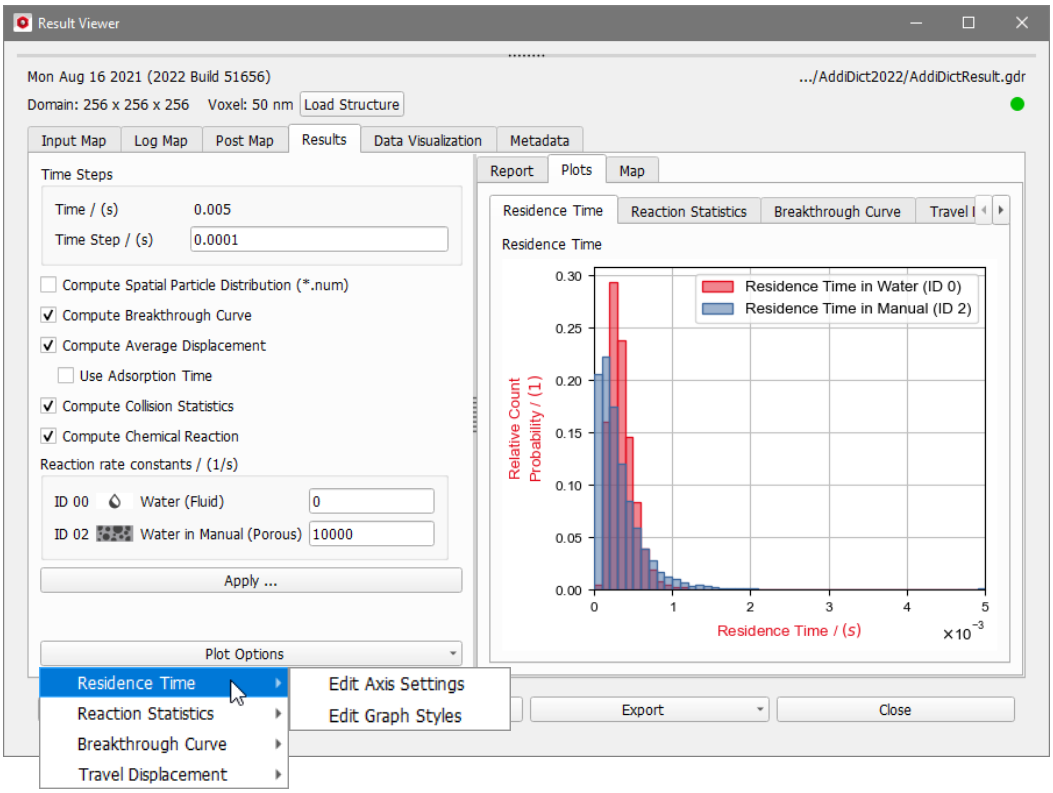
To compute chemical reactions of first order based on the residence times in the different materials, check **Compute Chemical Reaction** and enter a reaction rate constant for each pore or porous material. Dependent on the reaction rate constant and the residence time of the particles in a material, the residual of each particle species is computed based on the formula $-\frac{dA}{dt} = kA$. The half-life of a particle species, i.e., the time necessary for half of the particles to react is $t_{1/2} = \frac{\ln(2)}{k}$, see also page 15.

The table **Reaction Statistics** is created on the **Report** subtab, and a **Reaction Statistics** plot on the **Plots** subtab. Both contain the histogram data with the relative particle count for specific residuals of the particles. In the example shown above, for nearly 30% of the particles, only up to 2% remain that have not reacted yet.



Results – Plots

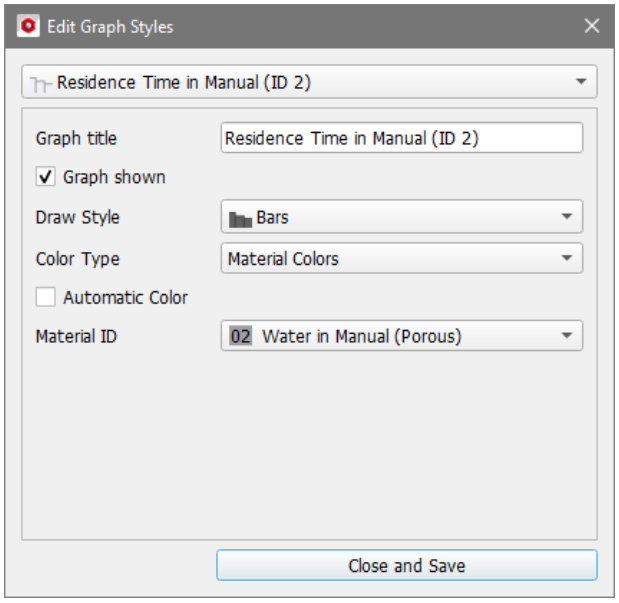
Under the **Plots** subtab, the **Residence Time** shows how long particles are located in each pore and porous material. This plot is created if **Compute Collision Statistics** is checked in the left panel. In the example shown here, around 29% of the particles are in the pore part of the structure (Water, ID 0) for between 2e-04 s and 3e-04 s.



Click the button **Plot Options** to change the settings of the graphs for the residence time plot as well as for the other plots.

With **Edit Axis Settings**, scaling, label and ticks of the axis as well as font size and legend placement can be selected.

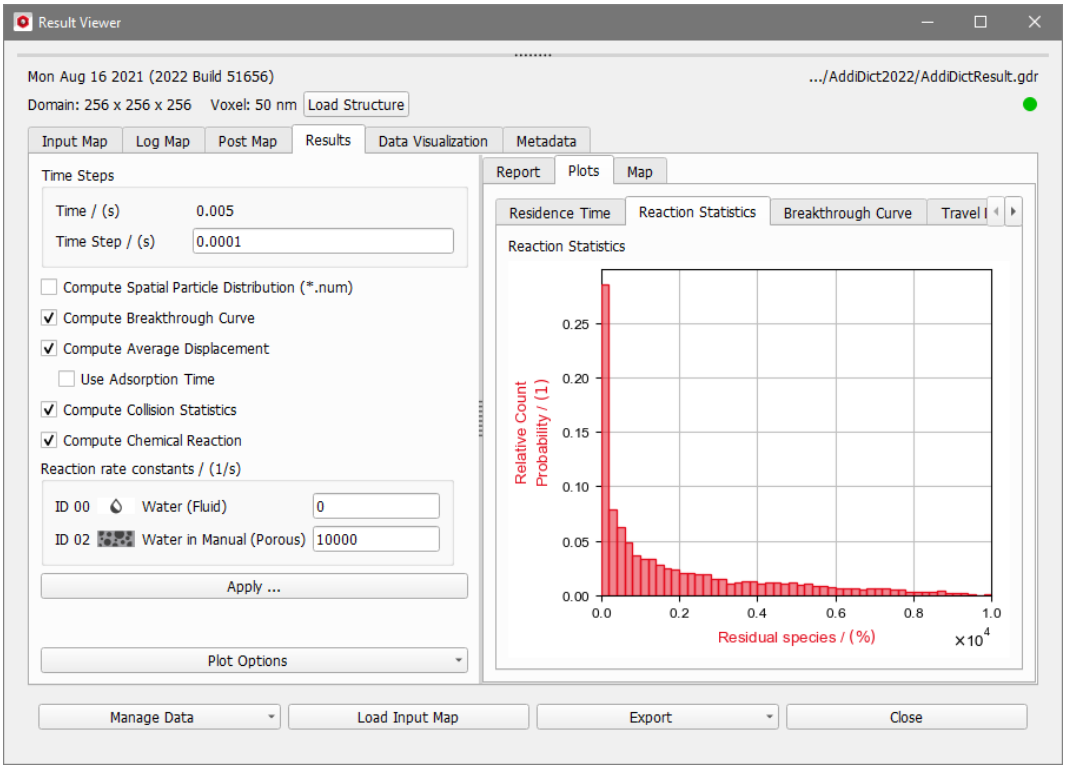
With **Edit Graph Styles**, title, style and color can be defined for each graph shown in the plot. E.g., select **Color Type Material Colors**, to select the same colors for the bars in the histogram as for the structure shown in the Visualization Area.



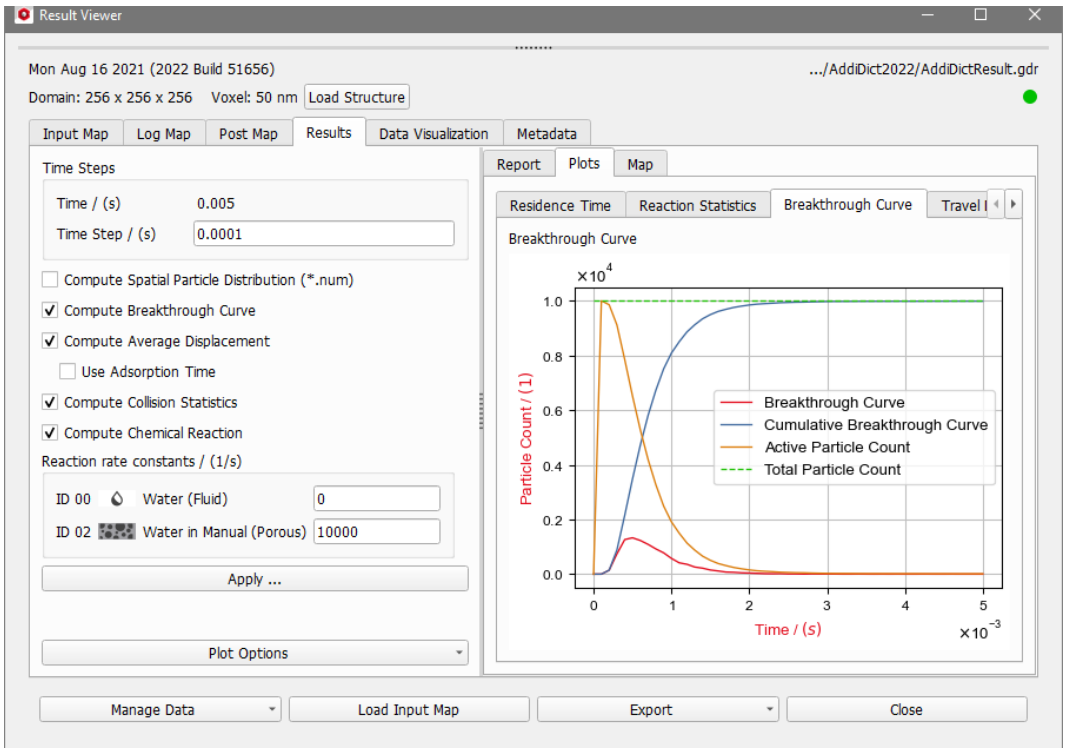
By a right mouse click in the plot, axis and graph settings can be accessed as well and the image or data can be saved. More details on changing plot settings, are available in the Result Viewer handbook.

A histogram of the Reaction Statistics of the chemical reactions is shown if **Compute Chemical Reactions** is checked in the left panel and reaction rate constants are defined for one or several materials.

In the example shown here, for nearly 30% of the particles only up to 2% have not reacted yet and remain in the structure.



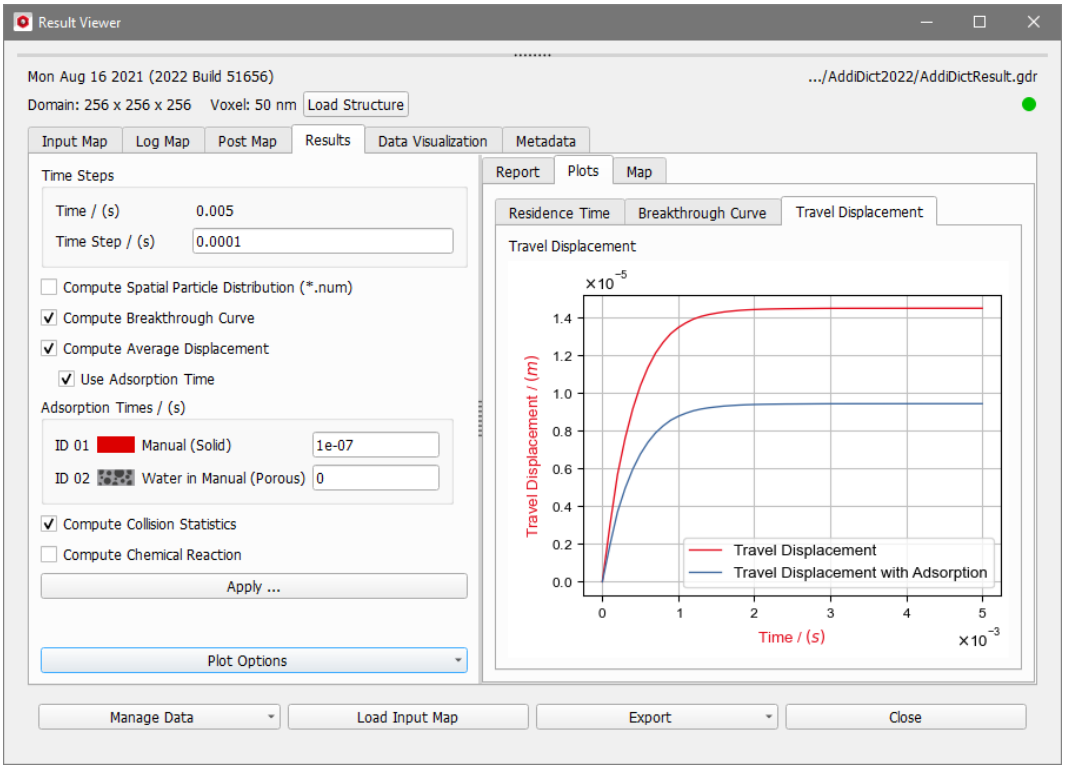
If the **Compute Breakthrough Curve** box is checked in the left panel, the **Breakthrough Curve** as a graph of the changes in **Particle Count** is shown over **Time.** The graph is a plot of the values listed in the table under the **Report** subtab in the columns Particle Count, Cumulative Particle Count and Active Particle Count.



The **Travel Displacement** curve is shown when the **Compute Average Displacement** box is checked. The displacement of each particle is computed as the straight distance between its starting position and its final position at a given time.

The displacement should not be confused with the distance that each particle travels along its trajectory, which might be a lot longer due to the zig-zag movement caused by diffusion.

If the box **Use Adsorption Time** is checked in the left panel, an additional curve is shown in the plot, with travel displacements adjusted according to the defined adsorption time(s).

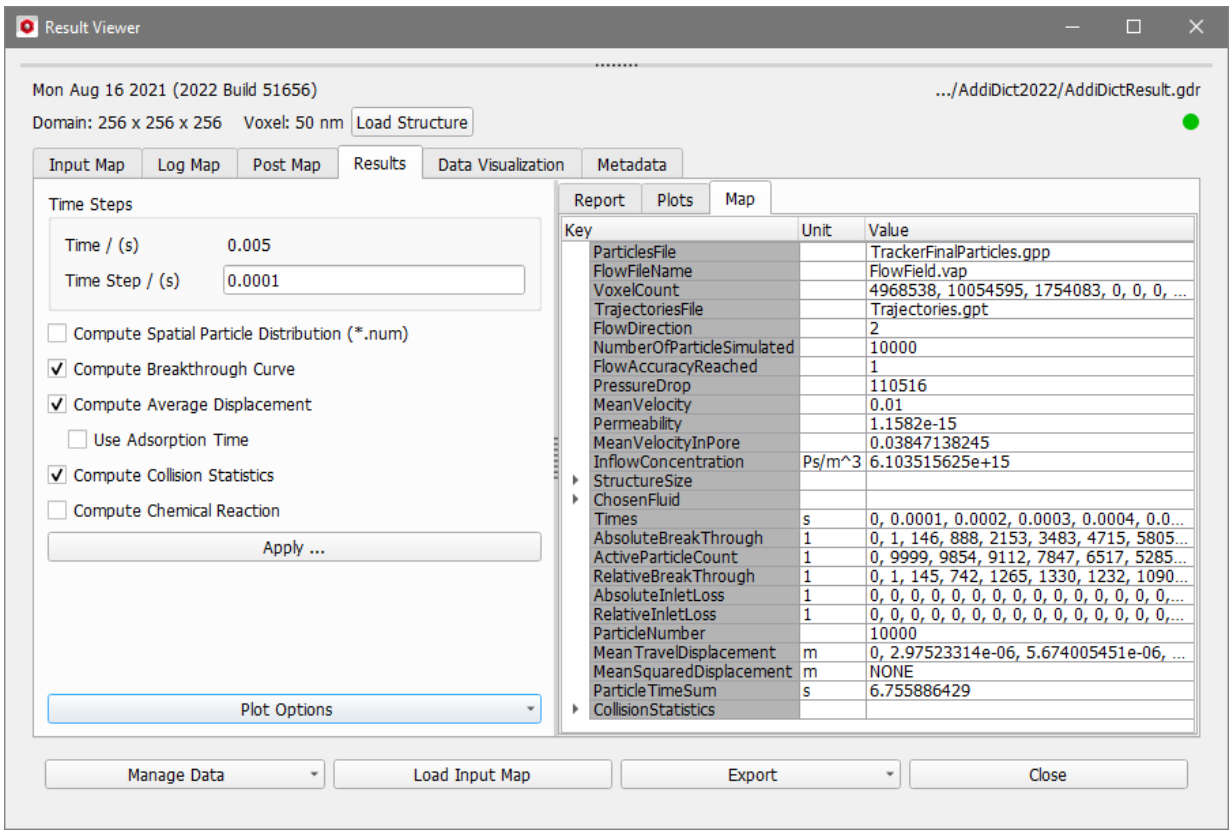


Properties of the axis and graphs can be modified for all plots in the same way as for the Residence Time plots, see page 50.

Results – Map

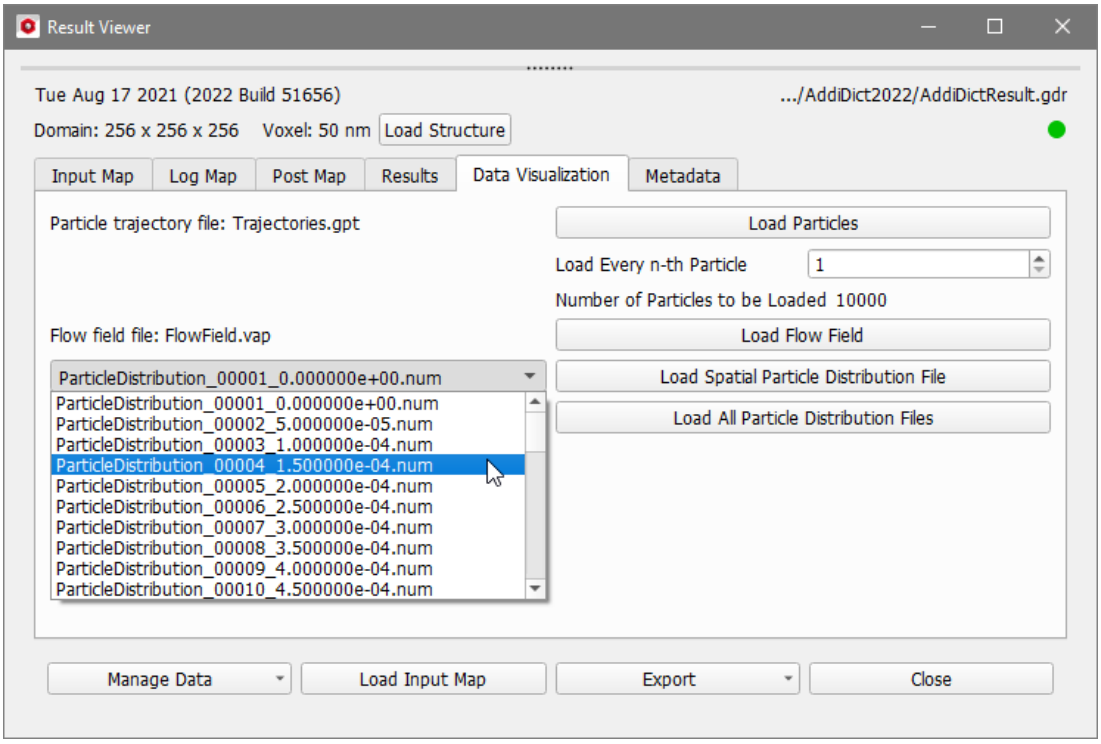
The **Results - Map** subtab gives access to the computed values as well as to solution file names. Especially, it contains all values shown in the **Report** subtab and plotted in the **Plots** subtab.

When changing the **Time Step** value, and clicking **Apply...** in the left panel, some results stored in the map are recomputed. Recomputed results are automatically stored in the .gdr file.


Result Viewer
Mon Aug 16 2021 (2022 Build 51656)
.../AddiDict2022/AddiDictResult.gdr
Domain: 256 x 256 x 256
Voxel: 50 nm
Load Structure
Input Map
Log Map
Post Map
Results
Data Visualization
Metadata
Time Steps
Time / (s) 0.005
Time Step / (s) 0.0001
Compute Spatial Particle Distribution (*.num)
Compute Breakthrough Curve
Compute Average Displacement
Use Adsorption Time
Compute Collision Statistics
Compute Chemical Reaction
Apply ...
Plot Options
Report
Plots
Map
Key
Unit
Value
ParticlesFile TrackerFinalParticles.gpp
FlowFileName FlowField.vap
VoxelCount 4968538, 10054595, 1754083, 0, 0, 0, ...
TrajectoriesFile Trajectories.gpt
FlowDirection 2
NumberOfParticleSimulated 10000
FlowAccuracyReached 1
PressureDrop 110516
MeanVelocity 0.01
Permeability 1.1582e-15
MeanVelocityInPore 0.03847138245
InflowConcentration Ps/m^3 6.103515625e+15
StructureSize
ChosenFluid
Times s 0, 0.0001, 0.0002, 0.0003, 0.0004, 0.0...
AbsoluteBreakThrough 1 0, 1, 146, 888, 2153, 3483, 4715, 5805...
ActiveParticleCount 1 0, 9999, 9854, 9112, 7847, 6517, 5285...
RelativeBreakThrough 1 0, 1, 145, 742, 1265, 1330, 1232, 1090...
AbsoluteInletLoss 1 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,...
RelativeInletLoss 1 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,...
ParticleNumber 10000
MeanTravelDisplacement m 0, 2.97523314e-06, 5.674005451e-06, ...
MeanSquaredDisplacement m NONE
ParticleTimeSum s 6.755886429
CollisionStatistics
Manage Data
Load Input Map
Export
Close

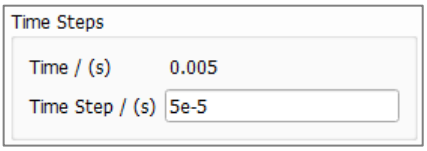
DATA VISUALIZATION

The **Data Visualization** tab enables the user to load the fluid flow field, the particle trajectories, or the spatial particle distribution for 3D visualization in the Visualization area of the GeoDict GUI.



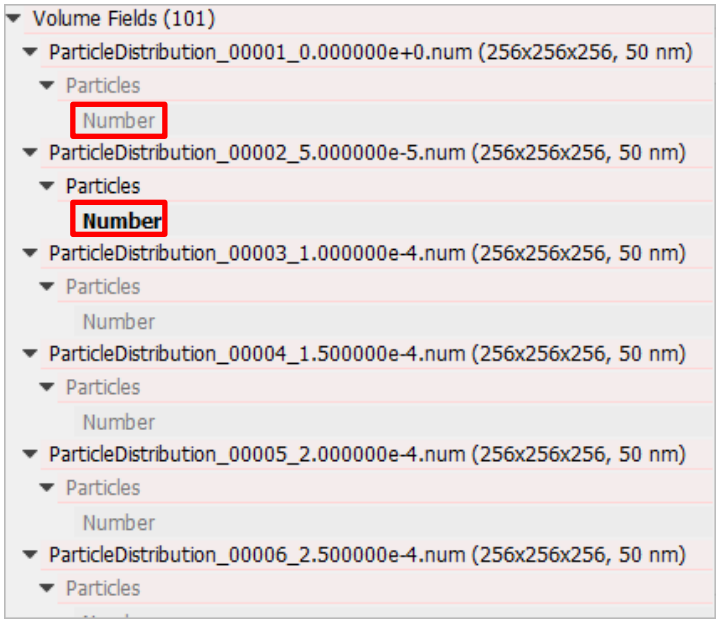
- **Load Particles** loads the particle data and allows displaying the particles and their trajectories. The number of particles to be loaded is shown and the user can select to load only part of them by specifying the value of **Load Every n-th Particle**.
- **Load Flow Field** loads the results of the fluid flow simulation, saved in the file **FlowField.vap** in the result folder.
- **Load Spatial Particle Distribution File** loads a field of particle numbers, which contains the particles per voxel at a certain point in time. The file name consists of an index number with 5 digits and the time step value in scientific notation. Those files are available if the **Compute Spatial Particle Distribution** box in the **Results** tab is checked, and there is a .num file available for each time step.

  In the shown example, there are 101 files available from index 00001 at time 0.0 to index 00101 at time 0.005 with intermediate time steps each 0.00005 (5e-05) seconds.



- **Load All Particle Distribution Files** loads all .num files with spatial particle distribution available and lists them under Volume Fields in the left part of the GUI. The spatial particle distribution of each file can be accessed by double clicking **Number**.

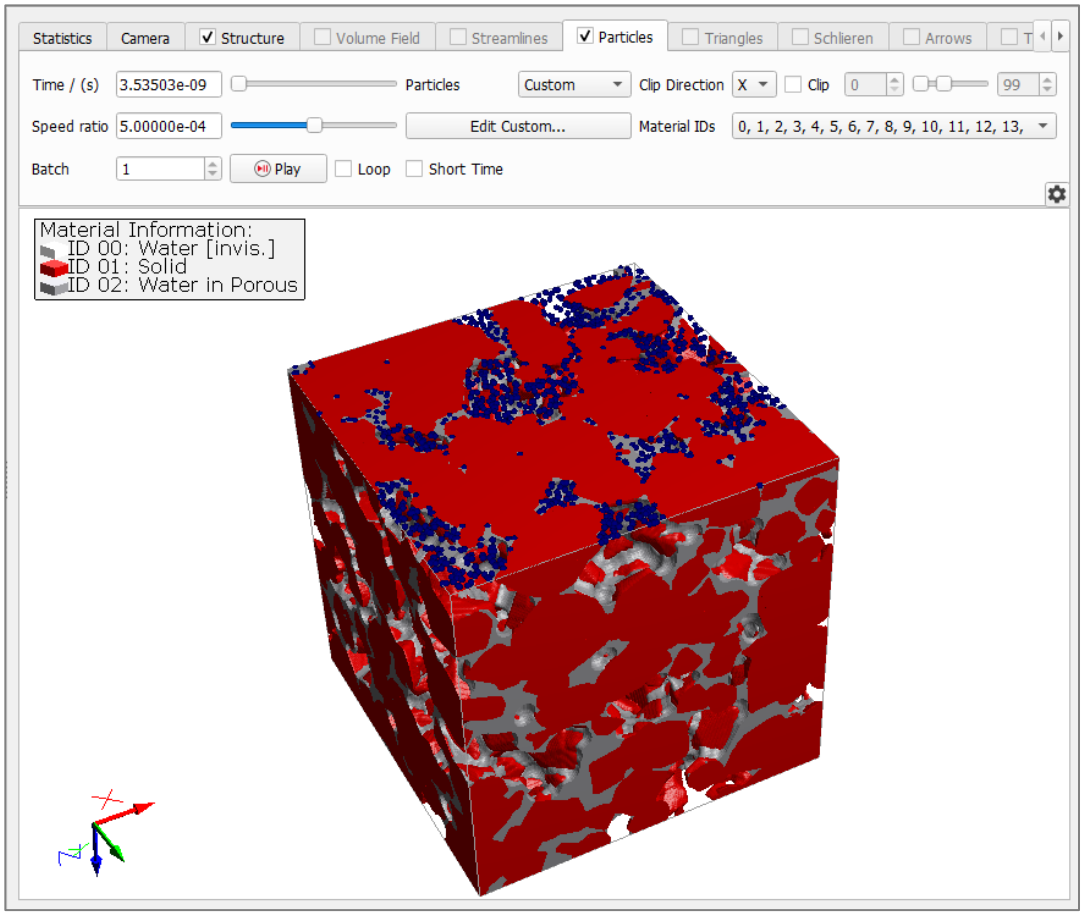
  The distribution is loaded and visualized in the Visualization Area of the GUI. The files already loaded once appear in black in the list and can be accessed much faster since they are kept in memory.



VISUALIZATION OF PARTICLES

The computed particle trajectories can be loaded directly by clicking **Load Particles**. In the example shown here, every 10th particle of the 10,000 simulated particles, was loaded.

The structure model with the particles at their start position appears in the Visualization area of the GeoDict GUI. In the Visualization panel, directly above it, parameters for the visualization of the particles during the transport simulation are selectable under the **Particles** tab.



Sliders for **Time** and **Speed ratio** control the visualization of particle movement. Moving the slider or directly entering a **Time** allows displaying the particles at a particular point in time.

The **Speed ratio** controls the visualization speed by entering values directly or by moving the slider. Low values of **Speed ratio** result in the transport process being shown in slow motion, whereas high values lead to faster motion.

The animation of the particles starts by clicking **Play.** The **Time** slider does not return to zero when the animation has finished and has to be set to the initial value to restart the animation. Checking **loop** makes the animation play endlessly.

Checking **Short Time** adapts the visualization **Time** to the period when the majority of particles move. This option cuts off the final part of a simulation where only a few particles move at probably very low velocities and no changes are visible.

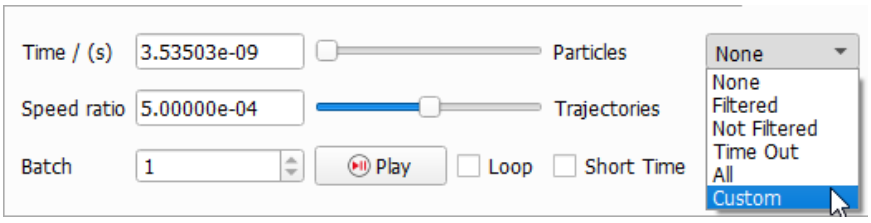
The **Particles** pull-down menu can be set to:

- **None** to fade out all particles,
- **Filtered** to show only the particles that remain attached to the solid,
- **Not Filtered** to show only the particles that went through the structure,
- **Time Out** to display only particles that were still moving at the end of the simulation,
- **All** to show the particles caught in the structure and those that went through it, or
- **Custom**.

Sometimes it is useful to switch off the visualization of the structure by selecting **View** and uncheck **Structure** in the menu bar or to uncheck the **Structure** tab above the Visualization Area. The structure model is still present, but not visible.

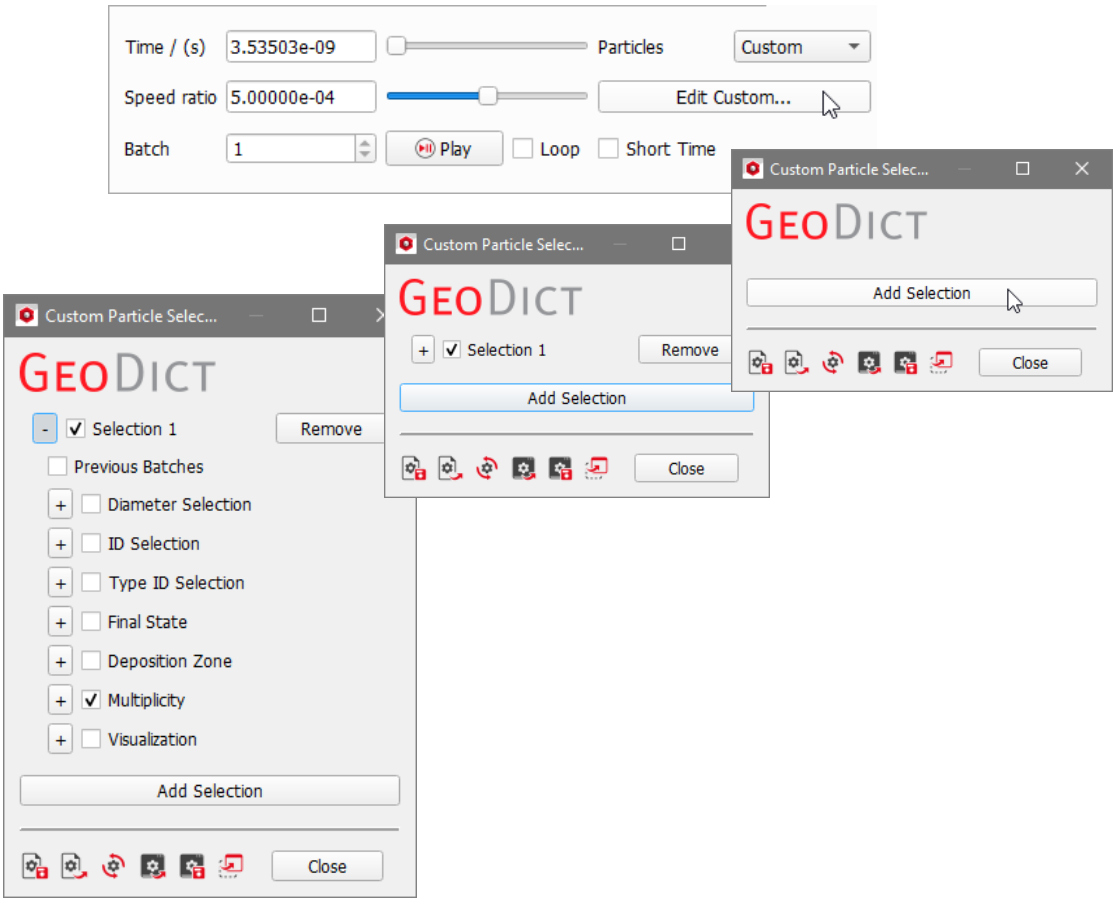
Particle visualization is identical in the modules FilterDict and AddiDict. However, since the functions implemented in AddiDict and FilterDict are not completely identical, some of the options available have no effect or are not that useful for AddiDict result visualization.

In AddiDict simulations, typically no particles are filtered, such that the best visualization option is to choose **Custom**. However, if particles stick to a solid or porous material due to the collision model, they are shown as filtered ones.



If **Custom** is chosen for the visualization of the particles, user-defined visualization settings can be defined by clicking the **Edit Custom...** button. Clicking **Add Selection** generates **Selection 1**.

Clicking + at the left of **Selection 1** opens the options: **Previous Batches**, **Diameter Selection**, **ID Selection**, **Type ID Selection**, **Final State**, **Deposition Zone**, **Multiplicity**, and **Visualization**.



Parameters for all these options are accessed by clicking on their [+] symbol. **Previous Batches** is a FilterDict-only option, since in AddiDict always one batch is computed only.

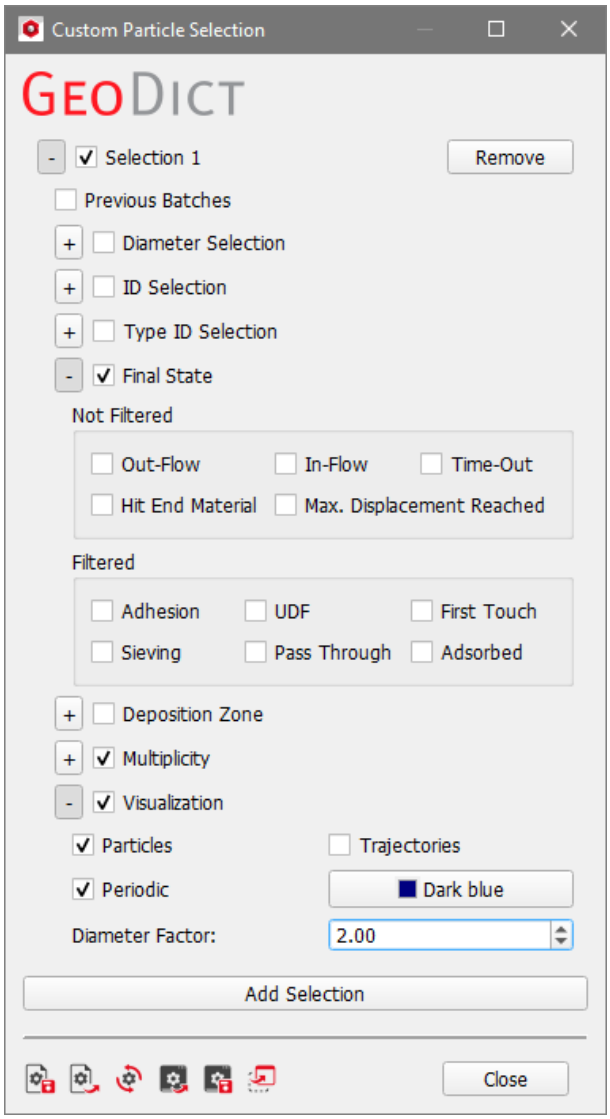
Checking **Diameter Selection** limits the visualized particles to those with a particle diameter in the range specified by min and max. If **Molecules** was chosen as **Particle Diameter** in the AddiDict options dialog (see page 31), no particles will be shown once a diameter selection is active, because no diameter is defined for each particle.

The **ID Selection** does basically the same as the Diameter Selection, merely picking out particles based on their individual particle number rather than their diameter.

The **Type ID Selection** picks out particles based on their type. Each row of the size distribution table (see page 33) defines one particle type, so the number of type IDs corresponds to the number of rows in the table.

Final State enables the visualization of particles that obtained a particular state at the end of the simulation.

In the **Not Filtered** panel, particles that did not get attached to a solid or porous medium are selected as follows:



- **Out-Flow** denotes particles that left the computational domain via the fluid outflow region.
- **In-Flow** designates particles that left the computational domain via the fluid inflow region.
- **Time-Out** identifies all particles that do not stick to a solid or porous medium and did not leave the computational domain via the inflow or outflow, i.e., slow particles that were still moving at the end of the simulation.
- **Hit End Material** denotes all particle that stopped moving since they reached a voxel with a material that was defined as particle end position (see page 26).
- **Max. Displacement reached** identifies all particles that reached the maximum displacement defined as particle end position (see page 27).

The **Filtered** panel contains the options for particles that became attached to a solid or porous medium during simulation.

- **Adhesion** denotes particles that stick to a medium due to the Hamaker collision model.
- **UDF** designates particles that are attached to a solid or porous medium due to a user defined collision model.
- **First Touch, Sieving** or **Adsorbed** identifies particles that stick to a solid or porous medium due to the collision model Caught on First Touch, Sieving resp. Adsorption.
- **Pass Through** denotes particles that were filtered while passing through a porous medium. This is a FilterDict-only option.

The **Deposition Zone** defines a location in the computational domain where the particles have to be situated at the end of the simulation to be eligible for visualization. This zone is delimited by the min / max coordinates of the Cartesian direction in which fluid flow occurs, i.e., the z-axis.

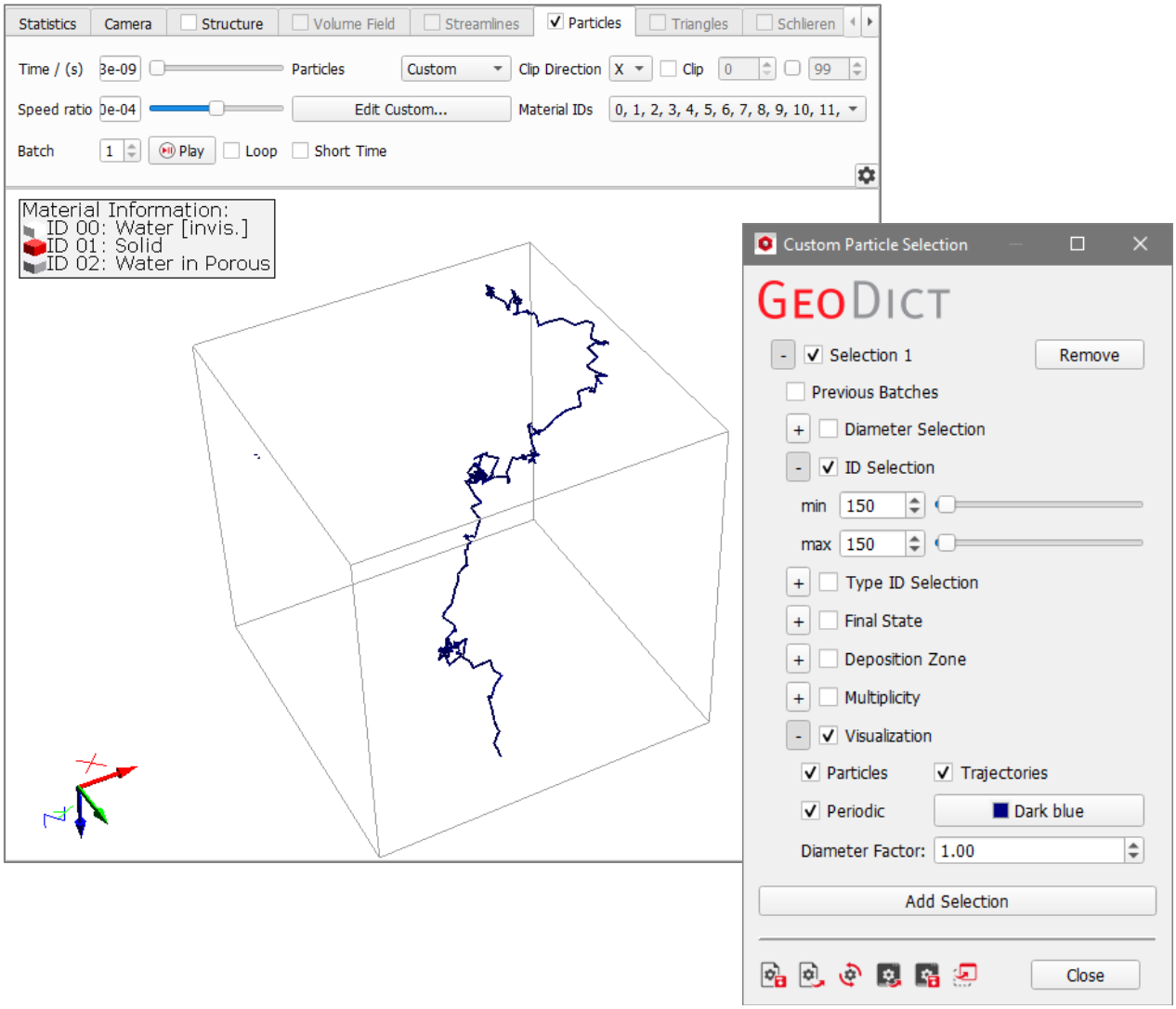
Multiplicity is again a FilterDict-only option.

Under **Visualization** the user may choose how the particle selection made above is visualized. Checking **Particles** displays all particles that conform to the previously set options. Checking **Trajectories** displays the trajectories of all particles that conform to the previously set options.

Checking **Periodic** enables periodic boundaries for the display of particle movement and trajectories. The default color **Green** for the particles, can be changed to another color (e.g. dark blue) through the button.

The **Diameter Factor** scales the particle sizes relative to their original size for visualization purposes and enables the display of particles that are nominally below the visibility of the visualization settings. The diameter of all particles moving in the simulation artificially grows by this factor when visualizing them. If **Molecules** was chosen for **Particle Diameter** (see page 31) under the **Particles – Interaction Model** subtab, the particles are visualized with a default diameter of 1 voxel.

The following is an example of the visualization obtained by choosing the indicated settings in the **Custom Particle Selection** dialog. The visualization of the structure has been turned off as indicated above on page 56. The visualization area shows the domain (with the structure model turned off) and, in it, the trajectory of the particle with ID 150 going through the structure.



It is possible to add several selections by clicking the **Add Selection** button. This allows to plot different selections of particles (for example, by ID Selection or by Type ID Selection, etc.) in different colors.

Selections can be removed by clicking the button **Remove** on the right of a selection.

CREATING VIDEOS OF THE PARTICLE MOVEMENT

The visualization of the particles' movement can be saved as a movie in MPEG, MP4, or MKV format when selecting **File** → **Save Video as ...** or clicking the  icon in the toolbar.

In the **Create Video** dialog, click **Generate Video** for **Particle Animation** in the tab **3D**.

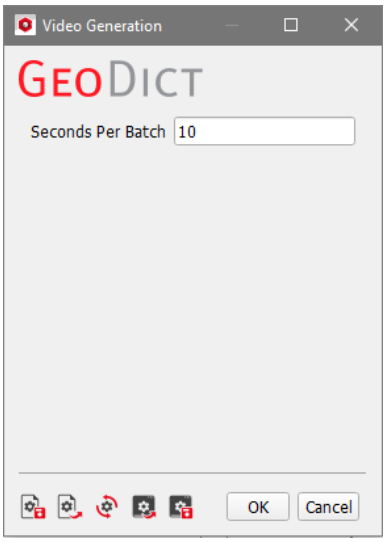
In the **Save Video** dialog, define a **Result File Name**, select the **Video Format** (mpg, mp4, mkv or Images) and the **Image Resolution**. For mpg and mkv, select the **Video Quality** as well. Set the value for the number of frames per second in **Frames per Second**.

Check **Keep Images** if the individual frames should be saved and not only the complete video. Check **Unroll as Python** to save the video generation as unrolled python script, to make modifications that are not directly possible with the video dialog.

Clicking **OK** opens the **Video Generation** dialog to select the time per batch in seconds. This again is a FilterDict option. In AddiDict only one batch is computed, i.e.,

the number in seconds per batch entered here defines the complete length of the video.

Clicking **OK** activates the creation of the video with the parameters set in the visualization area.

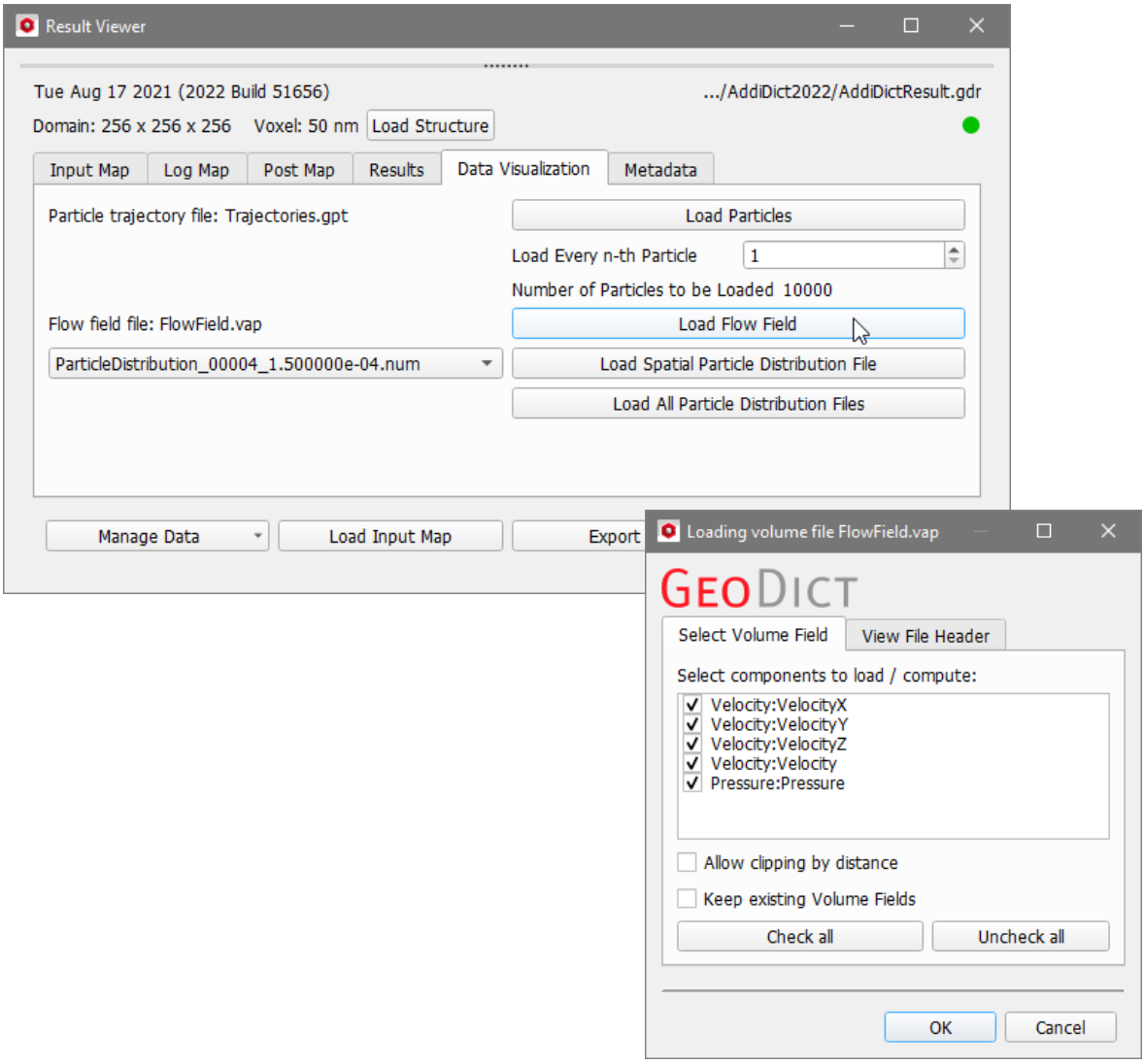


VISUALIZATION OF FLOW FIELD

The computed results for the flow field can be loaded directly from the result file by clicking **Load Flow Field** under the **Data Visualization** tab. It can also be loaded by clicking **File → Load Volume Field...** in the Menu bar and selecting the file FlowField.vap in the result folder.

If previously the movement of particles was visualized, uncheck the **Particles** tab, unless visualizing particles simultaneously with the flow field is explicitly desired.

Click **Load Flow Field** and, in the opening dialog box, select the desired components of the flow field to be shown. Click **OK**.



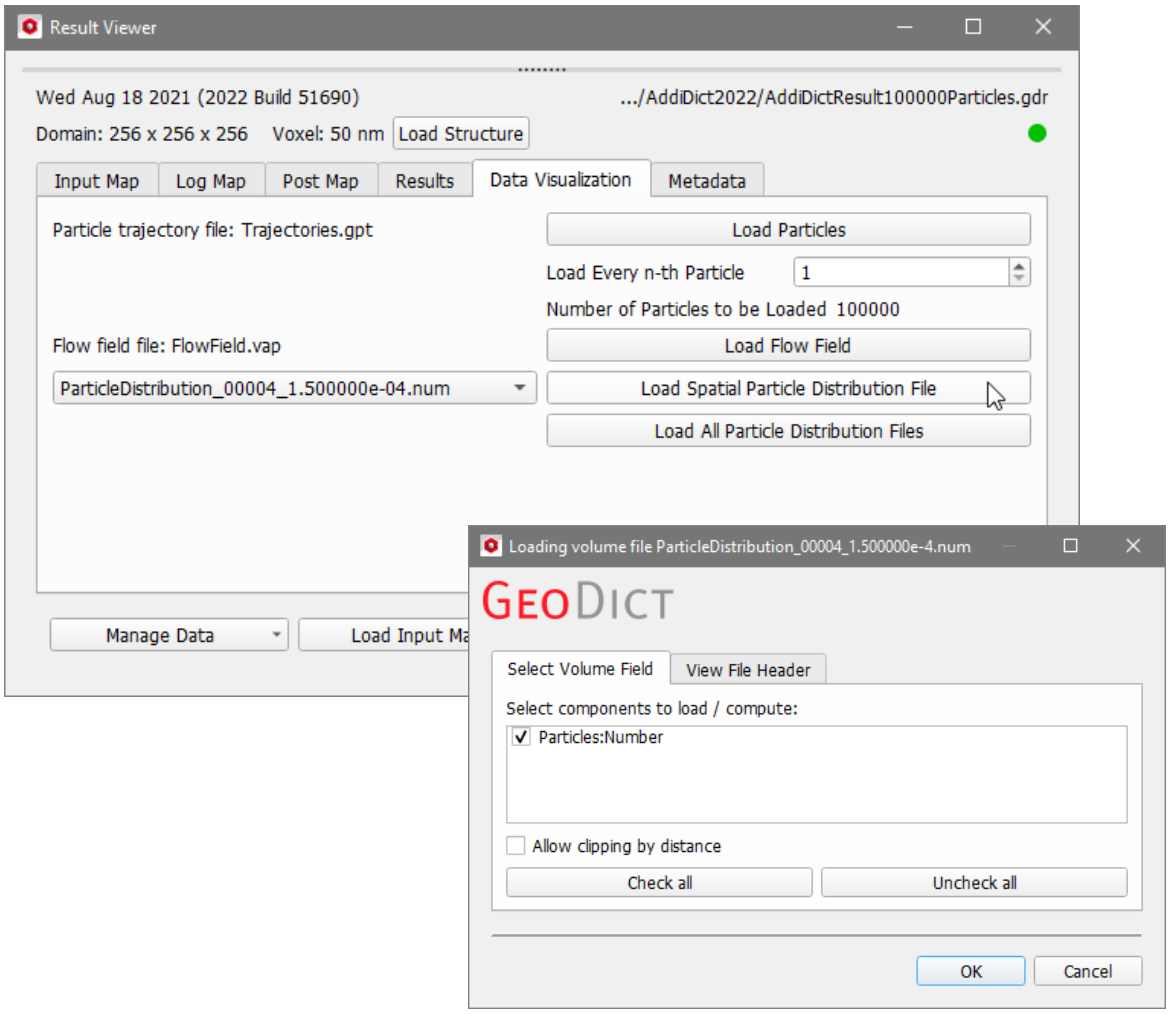
The options available for the visualization of the flow field are the same as in FlowDict, SatuDict, or FilterDict.

A detailed description of the visualization options can be found in the FlowDict handbook of this User Guide, in the section **Flow Visualization**.

Visualization of Spatial Particle Distribution

If the **Compute Spatial Particle Distribution (*.num)** box had been checked under the **Output** tab (see page 42), *.num files were created during the post-processing. These files can be imported for visualization by clicking **Load Spatial Particle Distribution File** or **Load All Particle Distribution Files** under the **Data Visualization** tab of the Result Viewer.

In a *.num file, the number of particles present in a voxel at a given time step is stored. Before importing, the user must choose the time step of interest from the pull-down menu to the left of the **Load Spatial Particle Distribution File** button. The names displayed are formatted as **Result File Name_time step_absolute simulation time.num**. For example, the file *AddiDictResult_00004_1.500000e-04.num* corresponds to the time step 4 of the simulation, which was reached at t=0.15 milliseconds.

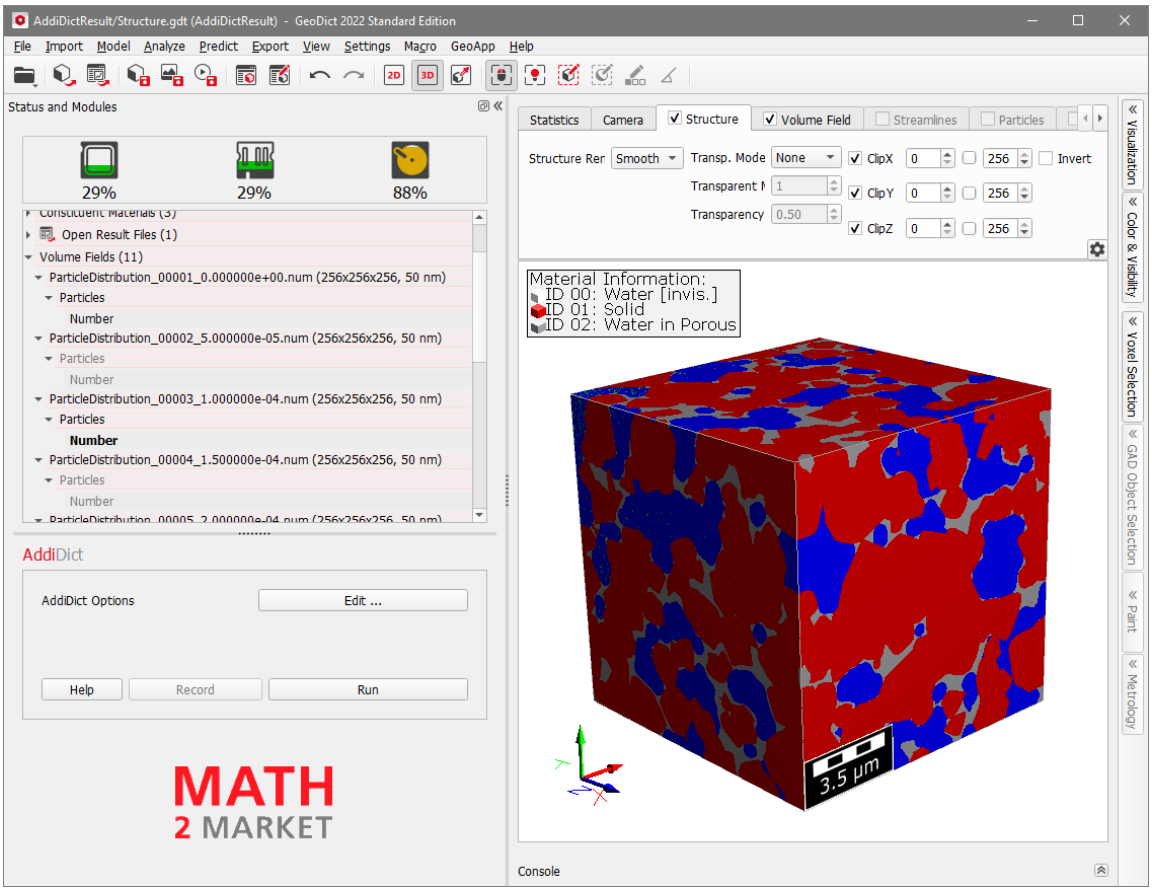


After choosing the *.num file, click **Load Spatial Particle Distribution File** and, in the **Loading volume file** dialog, keep the only option shown, **Particles:Number**. Click **OK**.

The fields from other time steps can be loaded at any time by going back to the Result Viewer, choosing a new time step *.num file, and clicking **Load Spatial Particle Distribution File**.

To access the fields from all time steps, choose **Load All Particle Distribution Files**.

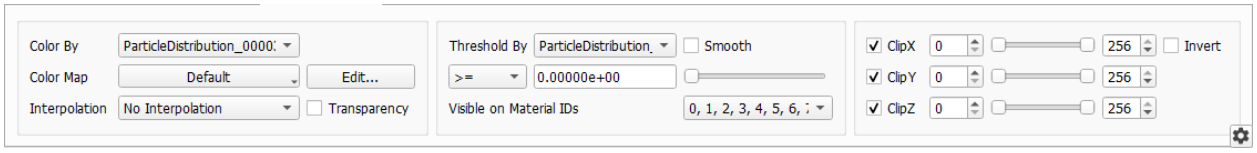
All *.num files with spatial particle distribution available are listed under Volume Fields in the left part of the GUI. The spatial particle distribution of each file can be accessed by double clicking **Number**. Files already loaded are shown in black in the list and can be accessed much faster since they are kept in memory, other files are shown in gray in the list.



The initial default visualization after loading a spatial particle distribution must be optimized by modifying the parameters under the **Volume Field** tab in the **Visualization panel**, above the Visualization Area.

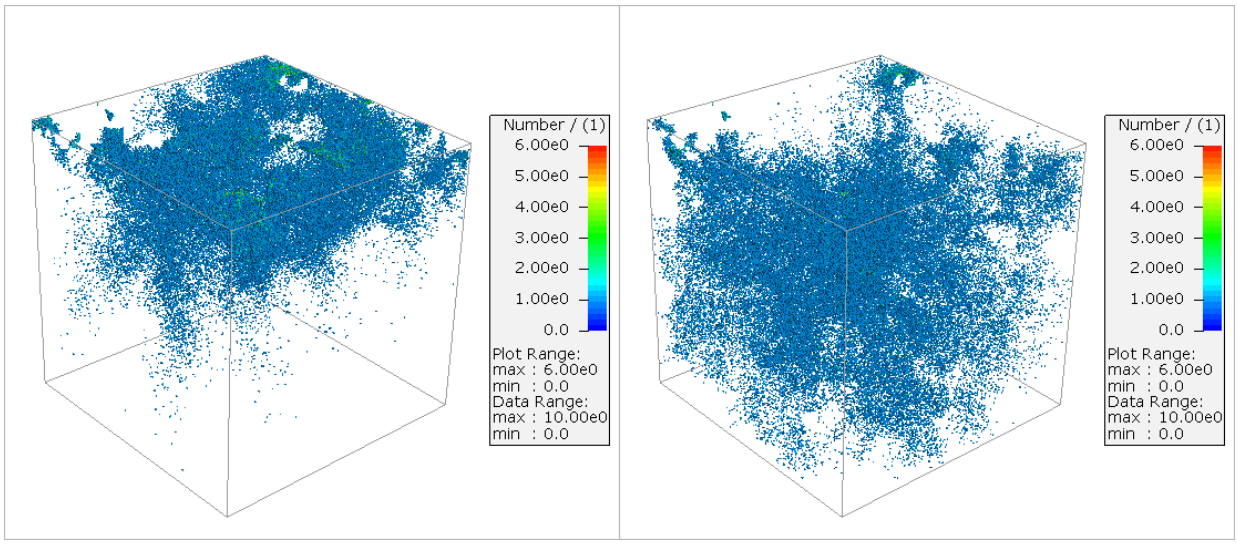
First, it might be useful to turn off the visualization of the structure model (**Structure**), as shown on page 56.

Additionally, under the **Volume Field** tab, select **No Interpolation** for **Interpolation** and uncheck **Smooth** for the **Threshold**.



The **Threshold By** pull-down menu, with the entry Number for each of the *.num files (as it is also for **Color By**) allows a clipping related to the data range. Move the slider, or enter directly e.g. 1, to make the clipping value larger than the default zero and see the locations where the number of particles at the selected time step is equal or above 1, corresponding to the clipping mode (>=). In this case, only the voxels that contain 1 or more particles are visible.

For example, the following visualization of spatial particle distribution is obtained when loading the field at time steps 3 and 7 and after setting the clipping to 1. For this visualization the computation was done with 100.000 particles.



Input Map

The **Input Map** tab contains all input parameters entered in the AddiDict Options dialog. Those values can be loaded back into the AddiDict Options dialog by clicking **Load Input Map** at the bottom of the Result Viewer.

Log Map

The **Log Map** stores information about the computational costs (runtimes, memory usage, number of iterations needed by the solvers) and the used hardware. This information is mainly needed for benchmarking.

Post Map

The **Post**(-Processing) **Map** stores information about the shown plots and the result report in the **Results** tab.

Metadata

Here, the user may edit the description stored with the result file (*.gdr file) and add his/her own parameter list to the result file.

These parameters may be used in Excel (GeoDexcel) or Matlab (GeoLab) to identify the results.

APPENDIX: USER-DEFINED FUNCTIONS

Three different types of user defined functions (UDF) are used in AddiDict:

- The **Particle motion UDF**, to change the equations that describe the particle motion.
- The **Collision UDF**, to define collision models in addition to the in-built models (Caught on First Touch, Sieving, Hamaker and Adsorption).
- The **User Data UDF** can be used in combination with one of the other UDF types. It allows to attach additional data to a particle, which can be used and modified during the simulation.

During the first startup, GeoDict copies a number of sample UDFs into the user's directory at:

- /home/*username*/.geodict2022/UDF/ (Linux)
- C:\Users*username*\GeoDict2022\UDF\ (Windows).

These files contain Particle Motion UDFs:

- ParticleMotionUDF-Standard.cpp
- ParticleMotionUDF-Gravity.cpp
- ParticleMotionUDF-GravityPlusBuoyancy.cpp

These files contain Collision UDFs:

- CollisionUDF-Count.cpp
- CollisionUDF-Hamaker.cpp

The files UDFUserData.h and UDFUserData.cpp can be used to define and initialize a user defined struct.

GeoDict does not compile the source code (*.cpp) automatically. Therefore, the user has to compile the UDF before using it in GeoDict, as described below.

Here, we describe only the usage of Particle motion UDF, since they are more often used in AddiDict. Details about using Collision UDFs and User Data UDFs can be found in the appendix of the FilterDict handbook of the user guide.

PARTICLE MOTION UDF

The Particle Motion UDF allows changing the equations (6), (7), (8)and (9) of page 10:

$$\gamma = 6\pi\mu \frac{R}{C_C} \qquad (6)$$

$$C_C = 1 + \frac{\lambda}{R}\left(1.17 + 0.525e^{-0.78\frac{R}{\lambda}}\right) \qquad (7)$$

$$D = \frac{k_B\, T}{\gamma} \qquad (8)$$

$$\vec{F} = 0 \qquad (9)$$

This UDF contains three functions: `udf_friction()`, `udf_diffusivity()`, and `udf_force()`.

The first function contains the definition of the Cunningham correction and returns γ. The second function returns D. The last function returns the external force $\vec{F}$.

As an example, the file **ParticleMotionUDF-Standard.cpp** shows the formulas as implemented in GeoDict:

```
// returns friction coefficient in [kg/s]
double udf_friction(const InputData_UDF& d) {

  /* Compute the Cunningham corrected Stokian friction
     coefficient of a moving spherical particle
  */

  double lambda = d.meanFreePath;  // [m]

  double cunningham = 1.0 + lambda / d.particleRadius *
    (1.17 + 0.525 * exp(-0.78 * d.particleRadius / lambda) );
  double dynViscosity = d.kinematicViscosity * d.fluidDensity;

  double g = 6.0 * M_PI * dynViscosity * d.particleRadius / cunningham;

  return g;
}

// returns diffusivity in [m^2/s]
double udf_diffusivity(const InputData_UDF& d, const int materialID) {

  double gamma = udf_friction(d);

  return 1.3806485e-23 * d.temperature / gamma;
}
```

Another example is the file **ParticleMotionUDF-Gravity.cpp**, where f is used to model gravity:

```
// returns external force in [N]
void udf_force(double* f, const InputData_UDF& d) {

  f[0] = 0;
  f[1] = 0;
  // gravity in z-direction
  double g = 9.81;  // [m/s^2]
  f[2] = g * d.particleMass;
}
```

To include e.g. gravity and buoyancy, the function can be changed to:

```
// returns external force in [N]
void udf_force(double* f, const InputData_UDF& d) {

  f[0] = 0;
  f[1] = 0;
  double g = 9.81;  // [m/s^2]
  double buoyancy = g * 4.0/3.0 * M_PI * pow(d.particleRadius,3) * d.fluidDensity;
  double gravity = g * d.particleMass;
  f[2] = gravity - buoyancy;
}
```

The input data struct `InputData_UDF` is defined in the **ParticleMotionStructs.h** header file which can be found in the `include` folder and contains the following data:

```
struct InputData_UDF{
  double particleRadius;     // [m]
  double particleDensity;    // [kg/m^3]
  double particleMass;       // [kg]

  double kinematicViscosity; // [m^2/s]
  double fluidDensity;       // [kg/m^3]
  double meanFreePath;       // [m]
  double temperature;        // [K]

  // Those parameters are only available in the force() function:
  double position[3];        // [m]
  double eStatic[3];         // [V/m]

  void * userData;
};
```

The two parameter vectors `position` and `eStatic` may only be used inside of the udf_force() function. The functions udf_friction() and udf_diffusivity() are called by GeoDict only once when the particle is initialized, and not while the particle trajectory is computed. Therefore, when these functions are called, those parameters do not contain any meaningful information.

Modifying and compiling User Defined Functions

in Linux

The simplest way to work with UDFs is as follows:

1. change into the UDF directory with:
   ```
   cd ./geodict2022/UDF
   ```
2. copy one of the sample files. For example:
   ```
   cp ParticleMotionUDF-Standard.cpp MyParticleUDF.cpp
   ```
3. open **MyParticleUDF.cpp** in a text editor of your choice (emacs, kwrite, vi…).

The code must be compiled after making all needed changes. For this, the compile.sh script can be used:

```
./compile.sh MyParticleUDF.cpp
```

This script creates the runtime library **MyParticleUDF.so**, that can be used by GeoDict.

Requirements	gcc-c++ compiler and libraries installed

in Windows

To compile the three UDF files delivered with GeoDict, open **AddiDictUDF.sln** with Visual Studio 2013 (or later) and build the solution.

Alternatively, you can run compilex.bat from the Visual Studio command prompt (x64). This creates three runtime library files that can be used in AddiDict: ParticleMotionUDF-Standard.dll, CollisionUDF-Count.dll, and CollisionUDF-Hamaker.dll.

To create additional UDFs, add them as additional projects to your solution. The simplest way to do that is to create a copy of an existing .cpp and .vcxproj file first. For example,

1. create **MyParticleUDF.cpp** as a copy of **ParticleMotionUDF-Standard.cpp** and **MyParticleUDF.vcxproj** as a copy of **ParticleMotionUDF-Standard.vcxproj**.
2. open the **AddiDictUDF.sln** solution in Visual Studio
3. add the existing project **MyParticleUDF.vcxproj**.

This project now still contains the old file **ParticleMotionUDF-Standard.cpp**. Therefore, remove this file from the project and, instead, add the existing item **MyParticleUDF.cpp** to the project. Then rebuild the project in Visual Studio or run compilex.bat to create the runtime library files.

Requirements	Microsoft Visual Studio 2013 (or later) installed

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

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