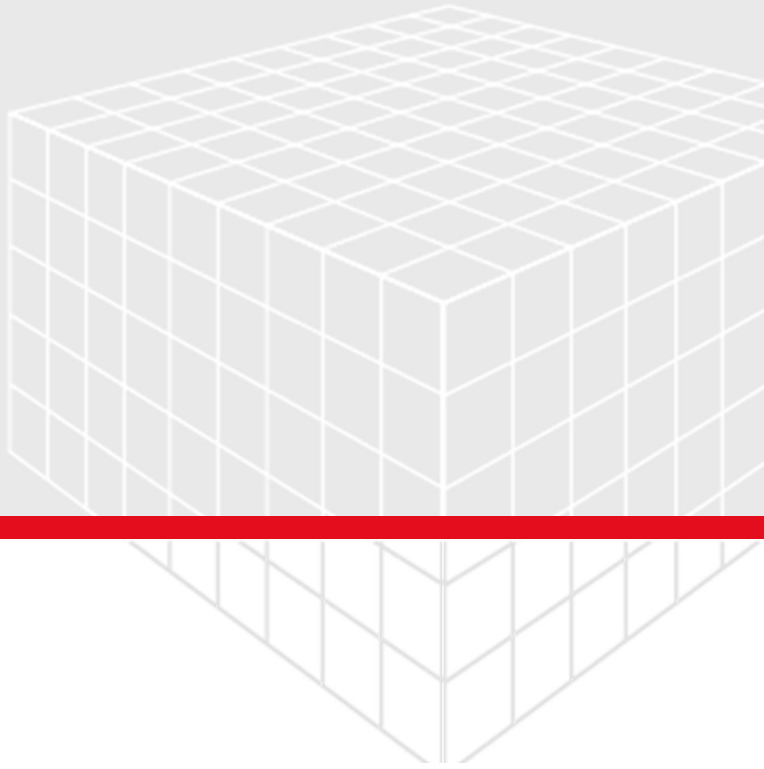
AddiDict

User Guide



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GeoDict

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AddiDict

1 AddiDict

Use AddiDict to simulate mass transport by **ad**vective and **di**ffusive movements. Mass transport can be simulated either for particles, resolved molecules, or a concentration field that represents the molar concentration of a solute. Additionally, AddiDict allows you to simulate adsorption reactions based on the transported molecules or concentration field.

New in GeoDict 2026

- The new Adsorption 112 command has been added, enabling the simulation of solute transport including sorption processes. You can select from several sorption isotherms and specify the associated parameters. Two methodologies are available - a Tracer-based and a Field-based approach - both generating compatible file formats that can be used interchangeably.

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Join the conversation

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

1.1 Theoretical Background

AddiDict simulates how particles or chemical species move and interact within a fluid. Each AddiDict simulation follows these steps:

1. If advection, i.e., transport by moving fluid, is selected as transport mechanism the underlying flow through the medium is computed first. If the flow is laminar, Stokes or Stokes-Brinkman equations can be applied. For higher flow velocities the Navier-Stokes or Navier-Stokes-Brinkman equations should be used.
2. The movement of particles/molecules or a concentration field due to diffusion and/or advection is tracked.
   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.
   Tracking of a concentration field utilizes a continuum-mechanical approach to model the transport phenomena, focusing on a concentration field as the primary variable. The concentration field represents the molar concentration of a solute, which is a dissolved substance within a solvent (the carrying fluid).
3. Adsorption and first order chemical reactions can be computed using either the tracked particles or the concentration field as a basis.

Understand the Theory behind AddiDict Simulations

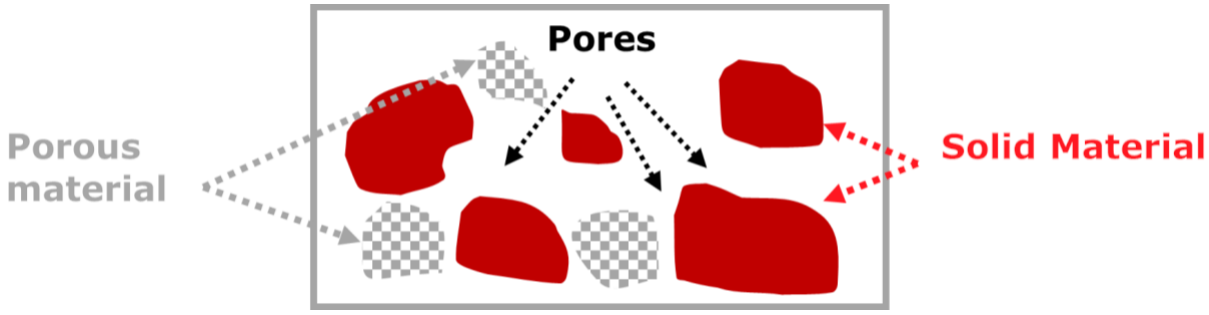
1.1.1 Flow Solver Partial Differential Equations

When advection, i.e., transport via fluid flow, is enabled within an AddiDict simulation setup, the governing flow field through the medium is calculated as the initial step.

For simulations involving slow, laminar flow the Stokes equation is the recommended option. Higher flow velocities require the application of the Navier-Stokes equation. When your structure includes porous material, i.e., regions not fully resolved within the geometry, the

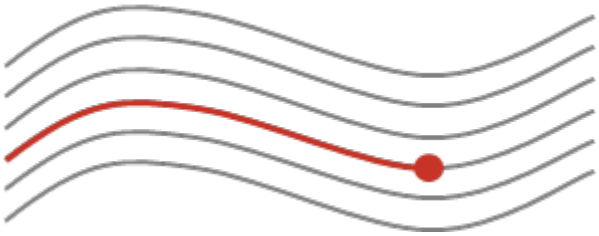
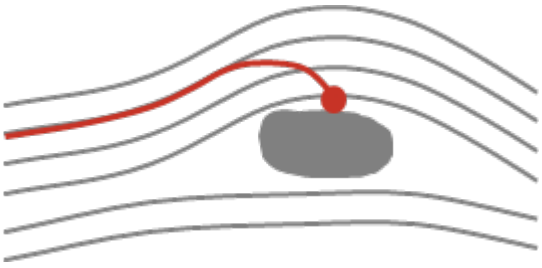
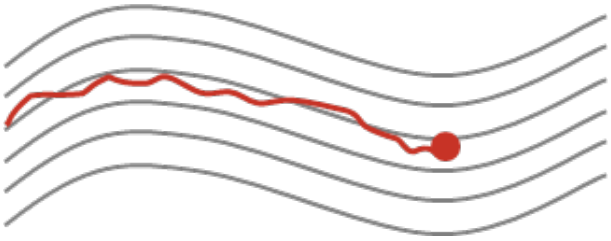
Brinkman term is appended to the flow equations to accurately represent flow behavior within these porous domains. The Brinkman term requires prior specification of the permeability of the porous media. Note that the inclusion of a porous material is a prerequisite for performing Adsorption 112 simulations within AddiDict.

For further documentation regarding the available flow solvers and the underlying partial differential equations, refer to the FlowDict user guide.



1.1.2 Particle Tracking

AddiDict simulates how particles and molecules move through your structure. 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 the streamlines of the flow field
	**Electrostatic effects**. The particles and pore surface can be electrostatically charged. This leads to attraction or repulsion effects.
	**Diffusive (or Brownian) motion**. Particle collisions with fluid molecules lead to small random direction changes.

AddiDict simulates the particle movement by considering these three effects. Electrostatic attraction and/or diffusive motion can be switched off if is known a-priori that these effects have no influence on the mas transport process. Overall, the particle movement is governed by

Particle Momentum = Stokes Drag + External Forces

or, as formula:

$$m\frac{d\vec{v}}{dt} = \gamma\left(\vec{u} - \vec{v} + \sqrt{2D}\frac{d\vec{W}(t)}{dt}\right) + Q\vec{E} + \vec{F} \quad (1)$$

In the friction coefficient

$$\gamma = 6\pi\mu\frac{R}{C_c} \quad (2)$$

the particle radius R is optionally corrected by the Cunningham correction factor,

$$C_c = 1 + \frac{\lambda}{R}\left(1.17 + 0.525 \cdot e^{-0.78\frac{R}{\lambda}}\right) \quad (3)$$

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

$$D = \frac{k_B T}{\gamma} \quad (4)$$

You might disable the simulation of Brownian motion. 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

$$\vec{F} = 0 \quad (5)$$

by default. When you disable electrostatic effects, the electrostatic field $\vec{E}$ is set to zero.

Equations (2), (3), (4), and (5) can be changed through user defined functions, e.g., to include gravity or buoyancy forces in $\vec{F}$.

The used variables and their units are:

Symbol	Unit	Meaning
$\vec{v}$	m/s	particle velocity
$\vec{u}$	m/s	fluid velocity

Symbol	Unit	Meaning
Q	C	particle charge
$\vec{E}$	V/m	electric field

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

k_B	J/K	Boltzmann constant
dW	$\sqrt{s}$	3D Wiener measure
T	K	temperature
D	m^2/s	diffusivity
$\vec{F}$	N	external force

The electrostatic charges are assumed as constant given forces on the solid surface. A constant charge density ξ is assigned on all voxel walls. The electric field

$$E = -\nabla\Phi \tag{6}$$

is determined by solving the Poisson equation for the potential Φ (unit:V)

$$\Delta\Phi = -\frac{\xi}{\varepsilon_0}\int_{\partial G}\delta \tag{7}$$

where ξ is the surface charge density (unit: C/m^2) 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 the 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 electric field E is needed to determine the movement of the particles in equation (1) [6] 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]):

$$Kn = \frac{\lambda}{L} \tag{8}$$

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 $3.0 \cdot 10^{-10}$ m (temperature of 20°C and pressure of 1 bar) and so Knudsen numbers of above 10^{-2} are reached for pores with radii smaller than $3.0 \cdot 10^{-8}$ 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 $6.8 \cdot 10^{-6}$ m. Hence the Cunningham correction will only be relevant for gas flows. The Cunningham correction factor (C_C) is defined as follows:

$$C_C = 1 + \frac{\lambda}{R} \cdot \left(A_1 + A_2 \cdot e^{\frac{-A_3 R}{\lambda}} \right) \tag{9}$$

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

Particle Displacement and Travel Distance

Displacement and travel distance describe two different aspects of a particle's motion.

Displacement is defined as the straight-line distance between a particle's initial position and final position. It depends only on these two points, regardless of the path taken between them.

Travel distance represents the total length of the path the particle follows during its motion. When Brownian Motion influences a particle's movement, it may travel along a highly irregular path. This causes the travel distance to be significantly greater than the displacement.

Molecular Limit

AddiDict can also be used to model the movement of molecules. For molecules, the particle radius R is unknown, and the particle momentum equation cannot be used directly to compute the movement of molecular particles. However, when considering the limit for $R \to 0$ in the particle momentum equation, 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:

$$\vec{u} - \vec{v} + \sqrt{2D}\frac{d\vec{W}(t)}{dt} = 0 \tag{10}$$

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.

1.1.3 Particle Collisions

Particles moving through the fluid phase may collide with solids. In the simulation, such a collision happens when the particle surface (modeled as spherical particle with a given diameter) touches the surface of a grid cell (voxel) that does not allow particles to enter.

When a particle collides with the surface of such a grid cell, it can stick to the current position and become a deposited particle or it can bounce off and continue moving in another direction. This behavior is defined in the **Collision Model**. AddiDict offers three different built-in collision models and the possibility to define your own models.

Caught on first touch

Caught on first touch is the simplest collision model in AddiDict. With this model, the particle sticks to the solid as soon as it touches its surface.

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 its velocity when touching the structure is sufficiently small. The condition on the velocity is

$$v^2 < \frac{H}{4\pi\rho a_0 R^2} \tag{11}$$

where H is the **adhesion** (Hamaker constant), ρ is the particle density, a_0 is the adhesion distance or equilibrium spacing between the particle and the surface (assumed to be the typical value of $4 \cdot 10^{-10}\ \mathrm{m} = 0.4\ \mathrm{nm}$), and R is the particle radius. See Krupp, 1967[158].

Adhesion (Hamaker constant) and, another parameter, **Restitution** need to be fitted in AddiDict.

The restitution parameter determines the amount of kinetic energy conserved during the collision. The restitution value ranges from 0 to 1. If the restitution parameter is set to 1, the collision is perfectly elastic. Then, the particle is reflected with the same velocity 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 0.5 restitution value means that a particle loses half of its velocity in the collision and gets 50% slower.

$$\text{Restitution Coefficient} = \frac{v_2}{v_1} \tag{12}$$

Since the Hamaker model requires the particle diameter as an input, it is only available for finite particle sizes and not for the molecular limit.

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 touches the solid at two different points. The restitution parameter is used in the same way as in the Hamaker model.

Random

Particles may be randomly caught on the surface depending on the given deposition probability.

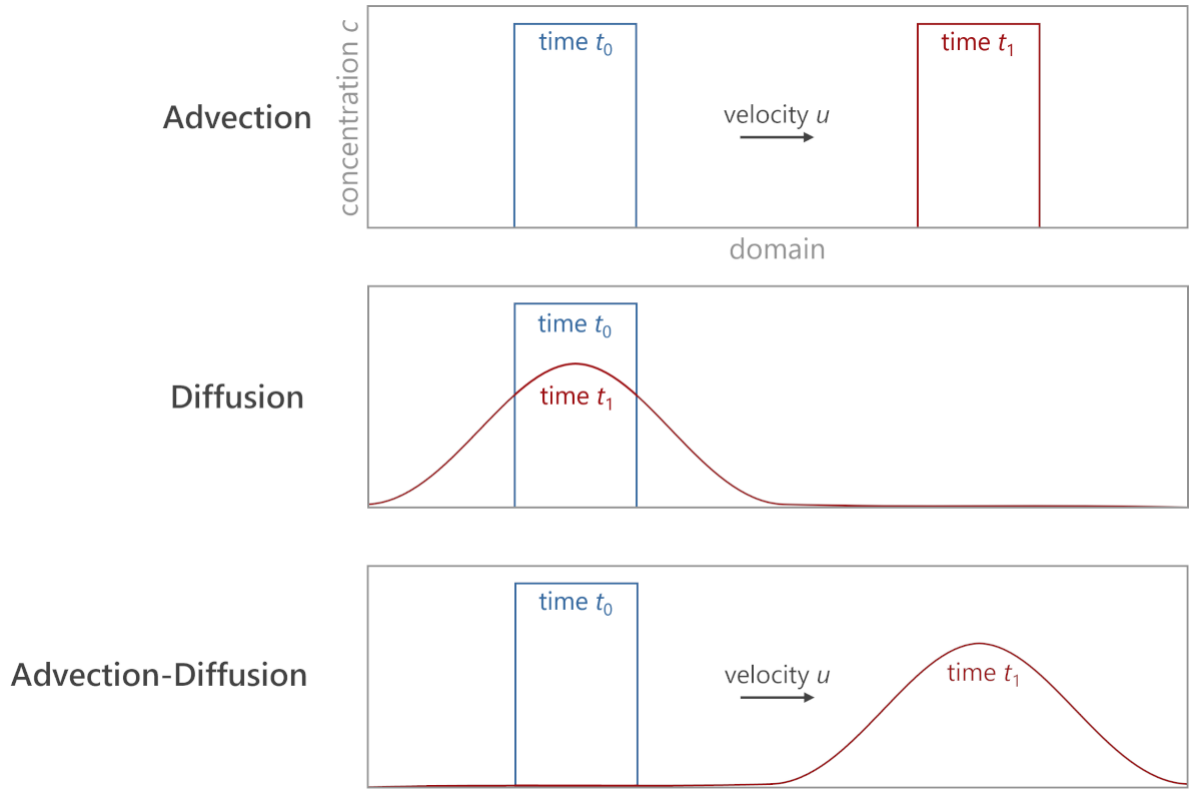
The **Random** collision model is only available for molecules.

User-Defined Collision Models

Additional collision models can be defined in user defined functions.

1.1.4 Transport of Solute Concentration Fields

The **Transport Concentration Field** command employs a continuum-mechanical approach for solute transport, treating the concentration field as the main variable to be solved for. The model can capture both advection, where the flowing solvent fluid carries the solute, and diffusion, driving the solute from regions of higher to lower concentration. The transport of a concentration profile in a one-dimensional example with a constant fluid velocity can be illustrated schematically as follows:



The solution algorithm for solute transport is integrated into the LIR solver, and the flow field required for advection can be computed using LIR, EJ, or SimpleFFT[4] solvers. The key features of the command **Transport Concentration Field** include:

- Stability: no artifacts or oscillations
- Automatic time stepping: you only specify time intervals (time batches)
- Minimal numerical dispersion
- Bound preservation: preventing negative concentration values
- Local mass conservation
- Coverage of the full range of Péclet numbers: from pure diffusion (Pe = 0) to pure advection (Pe = ∞)
- Full compatibility with adaptive grids from the flow computation using the LIR solver

Note! It is possible that over- or undershoots (i.e., concentrations less than zero or greater than the maximum inflow concentration) occur on large, low-porosity structures. This is not caused by the transport solver, but due to the fact that the velocity field is not completely solenoidal (free of divergence). In the continuous case, $\nabla \cdot \vec{u} = 0$ holds. In the discrete case, this only holds up to the solver tolerance. For instance, when $\nabla \cdot \vec{u} > 0$ holds locally (i.e., for a LIR cell), more concentration flows into the cell than it flows out, which creates a local overshoot in c.

Governing Equations

The transport of solute concentration fields is calculated by solving the **Advection – Diffusion** equation:

$$\phi\, \partial_t c + \nabla \cdot (\vec{u}\, c) - \nabla \cdot \left(D_{\text{eff}} \nabla c\right) = 0 \tag{13}$$

The advection – diffusion equation consists of the evolutionary term:

$$\phi\, \partial_t c \tag{14}$$

the advection term:

$$\nabla \cdot (\vec{u}\, c) \tag{15}$$

and the diffusion term:

$$-\nabla \cdot \left(D_{\text{eff}} \nabla c\right) \tag{16}$$

The effective diffusivity is computed by:

$$D_{\text{eff}} = \frac{\phi}{\tau} \cdot D_0 \tag{17}$$

where D_{eff} denotes the effective diffusivity in porous materials, obtained by multiplying the molecular diffusivity D_0 by the porosity ϕ and dividing by the tortuosity τ. For pure fluid voxels, the advection – diffusion equation simplifies, since both the porosity and the tortuosity are equal to one. The simplified equation reads:

$$\partial_t c + \nabla \cdot (\vec{u}\, c) - \nabla \cdot \left(D_0 \nabla c\right) = 0 \tag{18}$$

This simplification is to be understood locally, i.e., voxel-wise (or, if the LIR solver is used, LIR-cell-wise, respectively). The advection - diffusion equation is solved in the union of fluid voxels and porous voxels (containing the active fluid).

Initial and Boundary Conditions

Since the problem is time-dependent, an initial condition for the concentration is required:

$$c = c^0 \tag{19}$$

If advection is considered, the inflow concentration must be prescribed as the inflow boundary:

$$c|_{\Gamma^{\text{in}}} = c^{\text{in}} \tag{20}$$

The inflow boundary Γ^{in} is defined as all boundary points where the velocity vector points inward, i.e., $\{\vec{x} \in \partial\Omega \mid \vec{u}(\vec{x}) \cdot \vec{n} < 0\}$. If advection but no diffusion is considered, the problem is closed and does not require further boundary conditions. If both advection and diffusion are considered, at outflow and no-flow boundaries, homogeneous Neumann conditions are applied:

$$\nabla c \cdot \vec{n} = 0 \tag{21}$$

where $\vec{n}$ is the outward-pointing unit normal. This means that, at the outflow boundary, the diffusive flux is suppressed (homogeneous Neumann condition), while the advective flux remains free to leave the domain. In the case of pure diffusion, $\vec{u} = \vec{0}$ is assumed at all boundaries implying that no inflow or outflow boundaries exist.

Used Variables and their Units

Symbol	Unit	Meaning
$\vec{u}$	m/s	fluid velocity
c	mol/m³	concentration
c^0	mol/m³	initial concentration
c^{in}	mol/m³	inflow concentration
D_0	m²/s	molecular diffusivity

D_{eff}	m^2/s	effective diffusivity
Γ^{in}	m	inflow boundary
t	s	time
ϕ	1	porosity
τ	1	tortuosity

1.1.5 Adsorption

The Adsorption 112 command models adsorption by simulating either tracer particles or a concentration field moving through the structure and interacting with porous voxels. Within the porous active zone, the governing adsorption equations are solved based on the transported concentration and the equilibrium concentration.

Isotherm Models

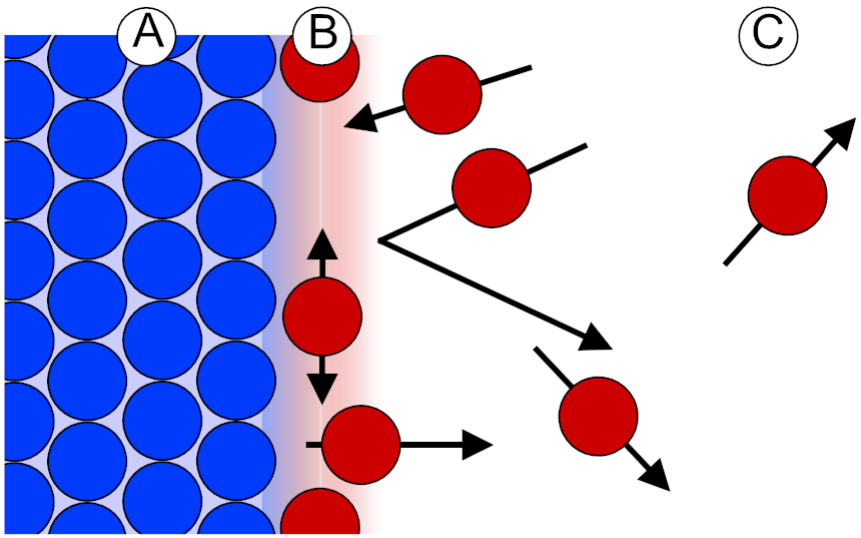
An adsorption isotherm model describes how a **solute** distributes between the liquid or gas phase and the surface of a solid (**adsorbent**) at constant temperature. The adsorbed **solute** is called **adsorbate**. The model mathematically relates the amount of adsorbate to the equilibrium concentration of the solute in the surrounding phase.

Isotherm models are used to characterize adsorption capacity, surface properties, and interaction mechanisms. They help to predict how much solute can be removed under different conditions and are essential for designing and optimizing adsorption processes. Common isotherm models include **Langmuir**, **Freundlich**, and **Toth**, each based on different assumptions about surface behavior and adsorption patterns. Already adsorbed species can detach from the surface and return to the solute phase, making the process reversible. Additionally, the solute is assumed to behave like an ideal gas, and interactions between adsorbates are neglected. The adsorption reaction can be formulated as such:

$$A_{solute} + S \rightleftarrows A_{adsorbate} \tag{22}$$

where A_{solute} is a solute species, S is an adsorbent site, and $A_{sorbent}$ is the adsorbate species.

Below, a schematic representation of the adsorption process is shown. Here, (A) depicts the **adsorbent** surface, (B) indicates the **adsorbate** at the interface, and (C) shows the **solvent** containing the **solute**.



Currently three isotherm models are implemented in the Adsorption command: **Freundlich**, **Langmuir**, and **Toth**. If you require different adsorption isotherm models to accurately simulate your reactions, please contact us to discuss the possibility of implementation.

Langmuir

The **Langmuir** isotherm model describes monolayer adsorption on a surface with a finite number of identical sites, where each site can hold only one solute molecule. Adsorption is reversible, with the adsorption rate proportional to the solute concentration and available sites, and the desorption rate proportional to the amount already adsorbed. This model assumes no interaction between adsorbed molecules and predicts a maximum adsorption capacity when all sites are occupied. For the **Langmuir** model the equilibrium loading of the adsorption sites is calculated by:

$$\varphi(c) = s_{\mathrm{m}} \frac{Kc}{1 + Kc} \tag{23}$$

where c is the concentration (mol/m^3), K is the equilibrium constant (m^3/mol), and s_m is the maximum loading (mol/kg).

Freundlich

The **Freundlich** isotherm model describes adsorption on heterogeneous surfaces with sites of varying adsorption energies and does not assume monolayer coverage or a finite number of identical adsorption sites. When adsorption does not exhibit a strictly bounded capacity, it can be modeled using a power law, where the adsorption rate depends non-linearly on the solute concentration while desorption remains linear. As a result, adsorption increases continuously

with solute concentration. For the **Freundlich** model the equilibrium loading of the adsorption sites is calculated by:

$$\varphi(c) = Kc^m \tag{24}$$

where c is the concentration (mol/m³), K is the equilibrium constant (m³/mol), and m is the empirical exponent.

Tóth

The **Tóth** isotherm model is a modification of the **Langmuir** isotherm that introduces a heterogeneity parameter t to better fit experimental data, especially at low and intermediate pressures. The model reduces to the **Langmuir** equation when the heterogeneity parameter equals one, making it useful for systems that deviate from ideal monolayer adsorption behavior. Here, the equilibrium loading of the adsorption sites is computed from:

$$\varphi(c) = s_{\mathrm{m}} \frac{Kc}{\left(1 + (Kc)^t\right)^{1/t}} \tag{25}$$

where c is the concentration (mol/m³), K is the equilibrium constant (m³/mol), s_{m} is the maximum loading (mol/kg), and t is the Tóth heterogeneity parameter:

$$t = t_0 + c_0/T \tag{26}$$

The calculation of the Tóth heterogeneity parameter requires Tóth coefficients (t_0, c_0) that are valid for given adsorbent/adsorbate pairs and can be derived from experiments or found in literature. Refer to Coker and Knox (2014) [158] for exemplary Tóth coefficients.

Tóth Legacy

The **Tóth Legacy** isotherm model uses a different definition and was available in the Adsorption GeoApp in GeoDict 2025. To allow you to continue using this definition it is included as a legacy option in GeoDict 2026. The **Tóth Legacy** model is defined as:

$$\varphi(c) = \frac{ac}{\left(1 + (bc)^t\right)^{1/t}} \tag{27}$$

with

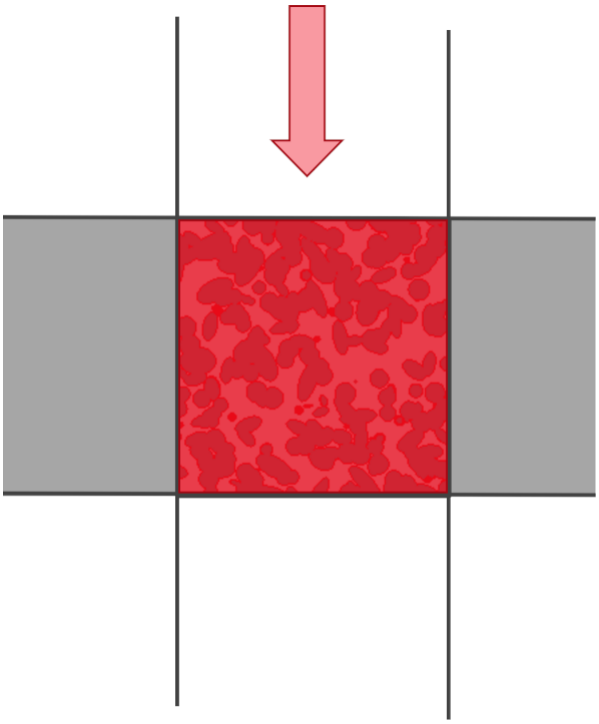
$$a = a_0 \exp(E/T) \tag{28}$$

$$b = b_0 \exp(E/T) \quad (29)$$

Here further Tóth coefficients (a_0, b_0, E) are required. Refer to Coker and Knox (2014)[158] for exemplary Tóth coefficients.

Adsorption Rate Models

In the **Adsorption** command, the adsorbent is always represented by a porous material with unresolved porosity. Adsorption then occurs on internal interfaces in this unresolved adsorption zone.



The amount of available adsorption sites is given as a maximum loading s_{m} under the defined equilibrium conditions. Inside the porous zone the solute can loose or gain concentration c, while the porous voxel of the adsorbent gains or looses the corresponding adsorbate loading s. Here, the adsorption speed is defined by the solute concentration and the number of free adsorption sites on the adsorbent surface. The desorption speed is determined by already occupied number of adsorption sites.

Linear Driving Force

The **Linear Driving Force** model represents the net reaction rate as directly proportional to the deviation from equilibrium. It reflects the concept that sorption moves toward equilibrium, with the rate depending on how far the current adsorbed amount is from the equilibrium

value. The rate is positive when net adsorption occurs, negative during net desorption, and zero when the system reaches equilibrium.

Using the rate constant k_{ldf}, the selected isotherm equation $\varphi(c)$, and the current loading inside the voxel the local reaction rate R (mol m^{-3} s^{-1}) can be calculated according to:

$$R(c,s) = k_{\mathrm{ldf}}\left(\varphi(c) - s\right) \tag{30}$$

1.1.6 First Order Chemical Reactions

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.

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

$$\frac{-d[A]}{dt} = k \cdot [A] \tag{31}$$

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

$$t_{1/2} = \frac{\ln(2)}{k} \tag{32}$$

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

$$[A]_t = [A]_0 \cdot e^{-kt} \tag{33}$$

1.2 Track Particles & Molecules

Use **Track Particles & Molecules** to simulate the movement of finite-sized particles or point-like molecules through a structure.

Particles or molecules can move through the structure via advection driven by fluid flow and/or diffusion governed by a specified diffusivity. Additionally, particles and molecules can interact with solid surfaces and porous materials.

The Track Particles & Molecules command

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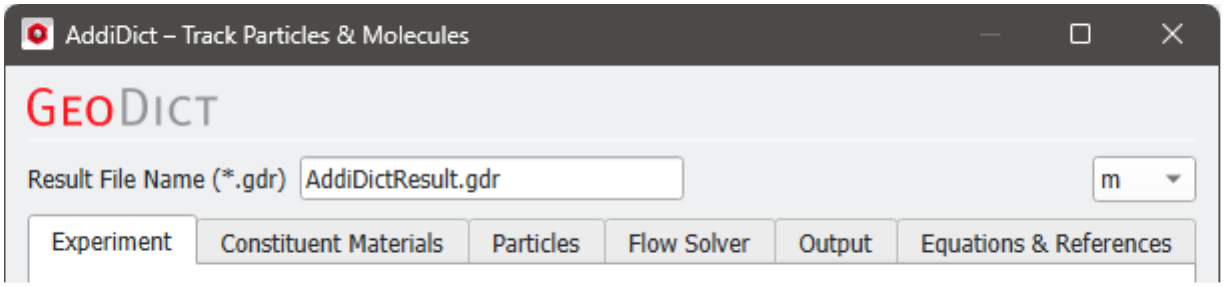
  See selected exemplary simulations.

1.2.1 Options

Select **Track Particles & Molecules** from the pull-down menu and click the **Option**'s **Edit** button to open a dialog to enter or edit the simulation options. Choose a **Result File Name** for the result file (*.gdr) fitting to your current project.



The track particles & molecules simulation parameters are organized under the tabs: **Experiment**, **Constituent Materials**, **Particles**, **Flow Solver**, and **Output**. The **Equations & References** tab gives a summary of the used equations and symbols which are explained in more detail in this user guide.

Tabs of the Track Particles & Molecules dialog

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  Define flow and transport conditions.
- Constituent Materials 24
  Define the temperature and materials in your structure.
- Particles 26
  Select particle sizes and their start positions. Set all parameters that govern the particle motion and define interaction models.
- Flow Solver 45

Tabs of the Track Particles & Molecules dialog

Select the flow solver, set the stopping criteria, and define the computational resources.

- Output 57
  Define multiple output options.

Experiment

The **Experiment** tab is organized in the following sections:

Transport Mechanisms

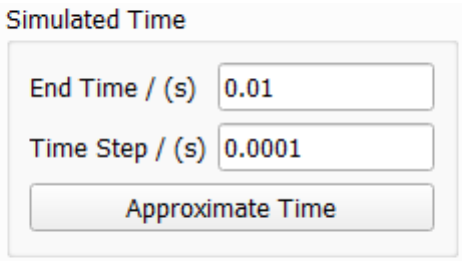
Select the **Transport Mechanism** by checking the **Advection** and/or **Diffusion** boxes in the upper left part of the **Experiment** tab.

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 the particle momentum equation 6.

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 this case the Flow Boundary Conditions 22 and the Flow Solver 45 tab are set to inactive.

Simulated Time

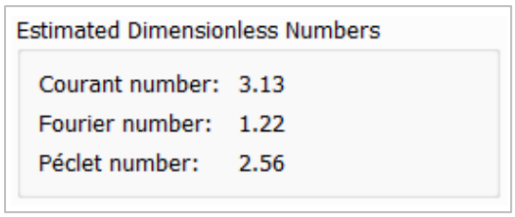
In the **Simulated Time** panel, the simulated **End Time** can be given. At each **Time Step**, the particle positions are evaluated for their spatial distribution, their breakthrough curve, and their residence times.



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 22 panel), most particle trajectories will pass through the whole geometry and a full breakthrough curve is computed. This works only if the advection is the dominant transport process. The **Time Step** value is automatically set to be 1% of the **End Time**.

Estimated Dimensionless Numbers

In this panel, three **Dimensionless Numbers** are automatically estimated based on the entered parameter values, provided a structure is loaded. They give you an idea of how strongly advection and diffusion contribute to transport *before* the simulation is started. After the simulation, more precise values are listed in the report.



The **Courant number** Co quantifies the extent to which particles, molecules, or concentration fields are transported through the structure by advection during the simulation. For instance, if $\mathrm{Co} = 0.5$, then the solute (particles, molecules, or the concentration field) is advectively transported by the flowing solvent across half of the domain. The Courant number is defined as:

$$\mathrm{Co} = \frac{V\,T}{L} \tag{34}$$

where V is the characteristic velocity estimated from the flow boundary conditions, T is the simulation time (which equals the **End Time**, given that the initial time is zero), and L is the length of the structure in the through direction.

In contrast, the **Fourier number** Fo quantifies the extent to which the solute (particles, molecules, or the concentration field) is transported through the structure by diffusion during the simulation. The Fourier number is defined as:

$$\mathrm{Fo} = \frac{D\,T}{L^2} \tag{35}$$

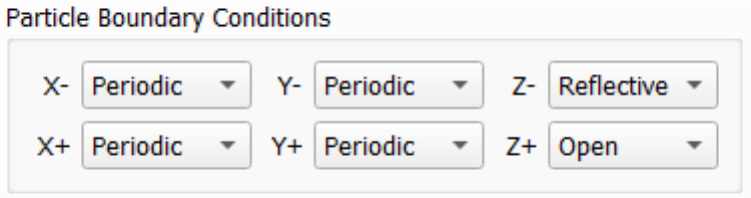
where D is the characteristic diffusivity, taken as the maximum effective diffusivity across all existing materials.

Finally, the **Péclet number** Pe is the ratio of advective transport to diffusive transport. A Péclet number of infinity implies purely advective transport, whereas a value equal to zero corresponds to purely diffusive transport. The Péclet number is defined as:

$$\mathrm{Pe} = \frac{V\,L}{D} = \frac{\mathrm{Co}}{\mathrm{Fo}} \tag{36}$$

Particle Boundary Conditions

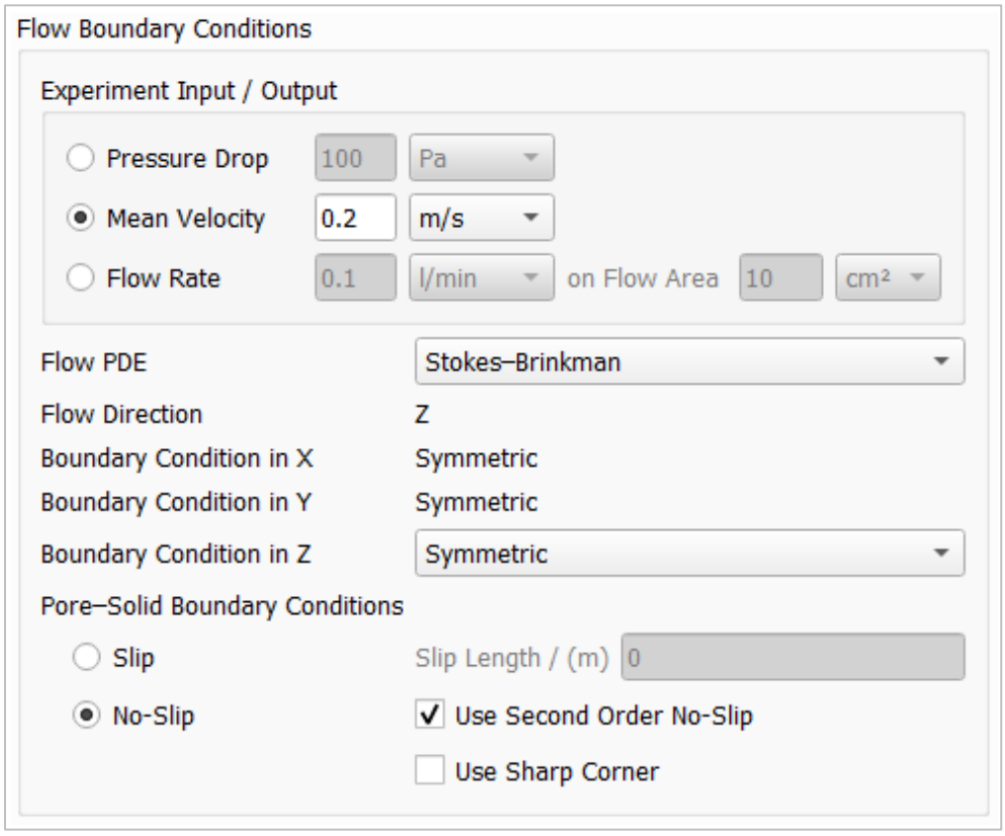
In the **Particle Boundary Conditions** panel, the user can choose what happens when a particle arrives at the domain boundary. This can be done individually for each of the six domain sides. In the **Periodic** case, a particle that leaves through one side of the domain, enters on the opposite side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



Flow Boundary Conditions

In the **Flow Boundary Conditions** panel, either the **Pressure Drop**, the mean flow **Velocity**, or the **Flow Rate** can be defined. Note that this part of the dialog is accessible only if Simulate Advection 20 is selected.

Important! In AddiDict, the fluid flow and transport is always computed in **Z-direction**. If another direction is required, the 3D model can be rotated with ProcessGeo prior to using AddiDict.



From the **Flow PDE** menu, you can specify the equations to be solved for computing the fluid flow field. The flow field is required to simulate the particle movements and trajectories or transport of the concentration field. (Navier-)Stokes equations describe fluid flow in structures containing only solid materials and pores. (Navier-)Stokes-Brinkman equations describe the flow through structures containing porous materials, solids, and pores. Use the Stokes equation when fluid velocities are slow or the viscosities are high, i.e., at low Reynolds numbers. The Navier–Stokes equation should be used for high fluid velocities when inertial effects cannot be neglected.

Note! The **Adsorption** command always requires (Navier-)Stokes-Brinkman equations since the Adsorbent needs to be defined as porous solid.

The used flow boundary conditions in **X** and **Y** direction are reported. For the **Track Particles & Molecules** command 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 leads to **Symmetric** flow boundary conditions.
- **Periodic** particle movement requires **Periodic** flow boundary conditions.

For the **Transport Concentration Field** and **Adsorption** commands the boundary conditions in **X** and **Y** direction are fixed to **Symmetric**.

The boundary condition in **Z** direction, can be **Periodic**, **Symmetric**, or **VinPout**. Please refer to the FlowDict user guide for more details. For the **Track Particles & Molecules** command, using the Stokes(-Brinkman) equation only allows for using **Periodic** or **Symmetric** boundary conditions, while the Navier-Stokes(-Brinkman) equation uses the **VinPout** 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. The default **Slip Length** of zero corresponds to a flow velocity of zero along the solid surface. 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, e.g., for gases when the mean free path is comparable to the pore size. The same slip length must be set for all materials in the structure. Find more details on the **Slip Length** here.

For the **No-Slip** boundary condition two additional options are available:

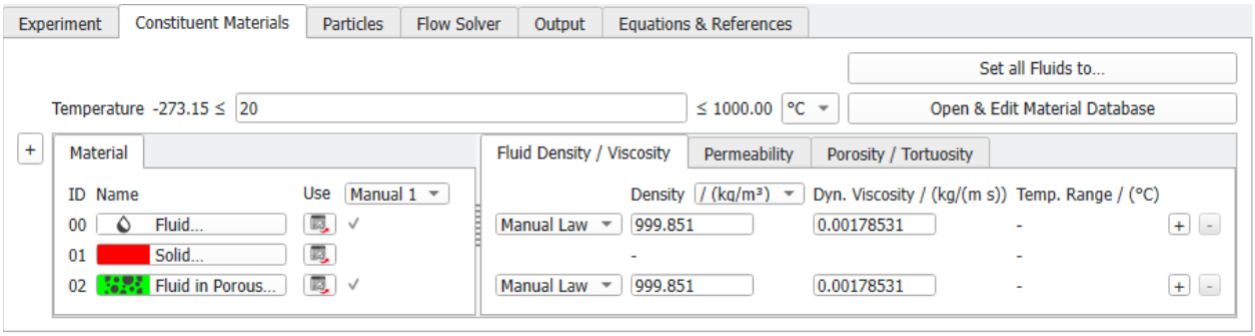
- **Use Second Order No-Slip** (default): This option sets the tangential velocity to zero at the center of the voxel surfaces and use a second order approximation of the velocity field.
- **Use Sharp Corner**: This option sets the tangential velocity to zero at the voxel corners.

Find more details on these settings in the FlowDict user guide.

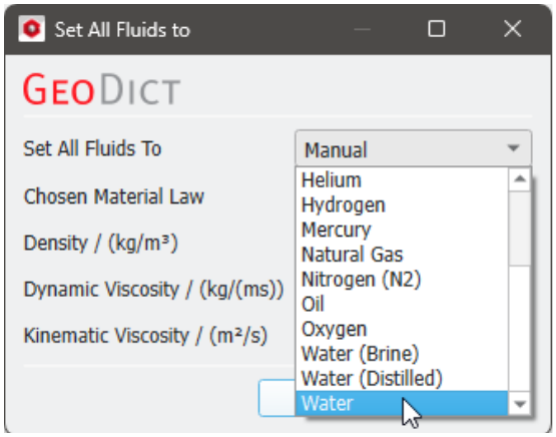
Constituent Materials

Define the materials in the structure and their properties in the **Constituent Materials** tab.

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.



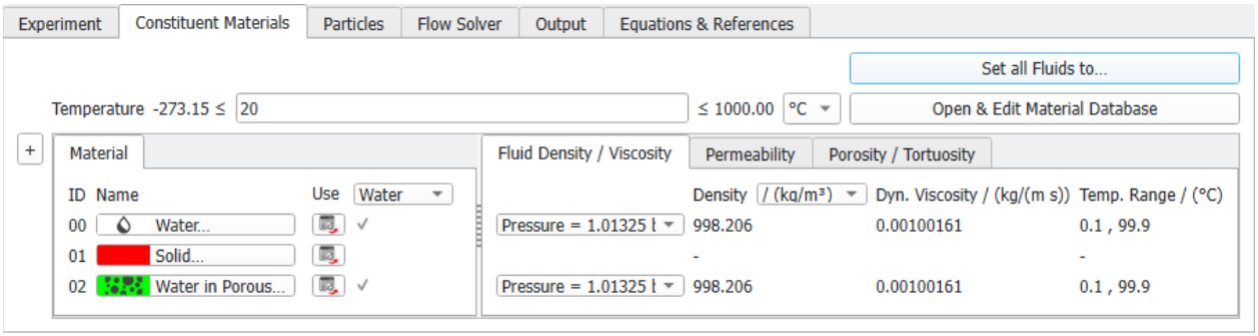
The fluid flowing through all pore and porous materials can be set by clicking **Set all Fluids to** and selecting it from the pull-down menu.



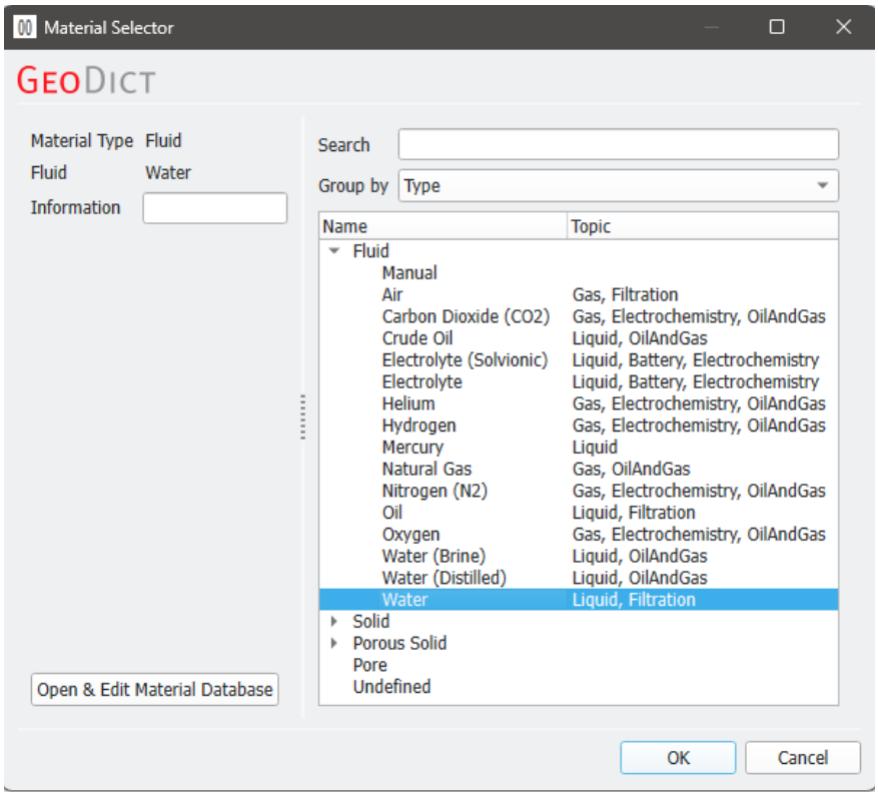
If one of the predefined fluids is used, the values for **Density**, **Dynamic Viscosity**, and **Kinematic Viscosity** are taken from the material database and are dependent on the given **Temperature** value. If **Manual** is chosen, you can enter these values manually.

Any values entered manually, e.g., those for a special type of oil, can also be added to the Material Database. Find more information on editing, expanding, and using the material database in the respective user guide.

As soon as you define 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 ID 02. The density and the dynamic viscosity of this fluid, at the selected temperature range, is shown under the **Fluid Density/Viscosity** subtab.



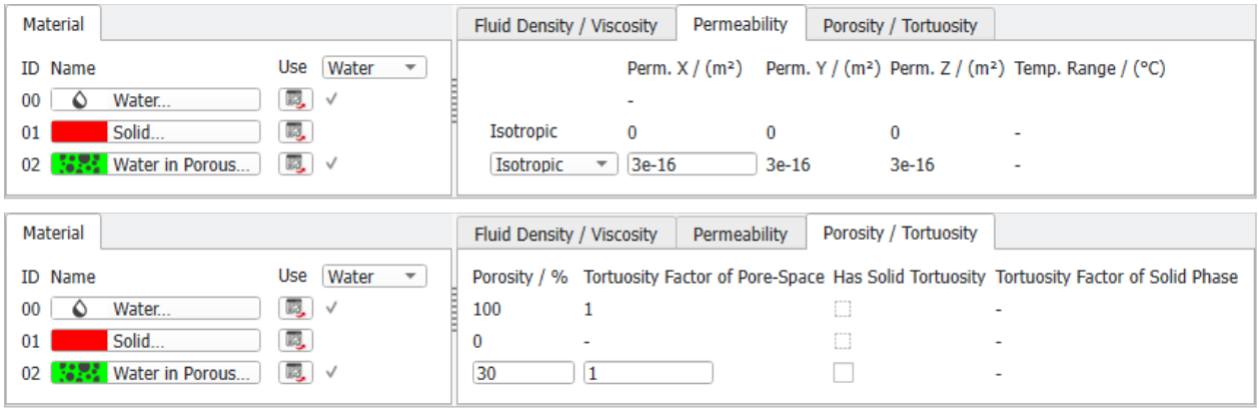
All materials assigned to the material IDs, which fall into one of the material categories (pore, porous or solid), can be selected individually through the **Material Selector** dialog, by clicking on the material's buttons. Fluid flow can occur only in pores and in porous materials.



For porous materials, also the information about the permeability needs to be defined in the **Permeability** subtab. If the **Pass Through Model Reflection Probability** should be selected for a porous material and the reflection probability 38 is not selected manually, the porosity of a porous material needs to be defined on the **Porosity** subtab. The porosity is also required to compute the effective diffusivities. Together with the **Tortuosity Factor of Pore-Space** the effective diffusivity of a porous material is computed:

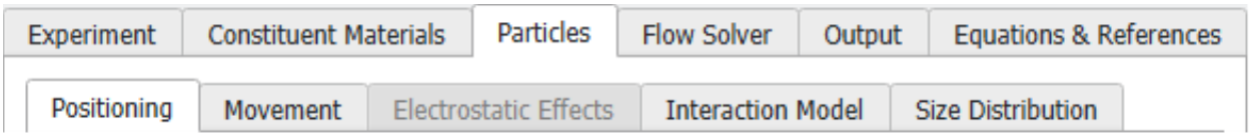
$$D_{eff} = D_0 \frac{\phi}{\tau} \tag{37}$$

where D_0 is the diffusivity in the pore space that is defined under the Particles - Size Distribution 45 tab, ϕ is the entered porosity, and τ is the entered tortuosity.



Particles

Under the **Particles** tab, five sub-tabs are available for **Positioning**, **Movement**, **Electrostatic Effects**, **Interaction Model** and **Size Distribution**.



Particles Subtabs

- Positioning 26
  Define initial and end position of the particles.
- Movement 34
  Control particle movement.
- Electrostatic Effects 35
  Apply electrostatic effects to the particles and materials.
- Interaction Model 37
  Define properties of the particles as well as their interaction with solid and porous materials.
- Size Distribution 42
  Define a particle size distribution and various other size dependent properties.

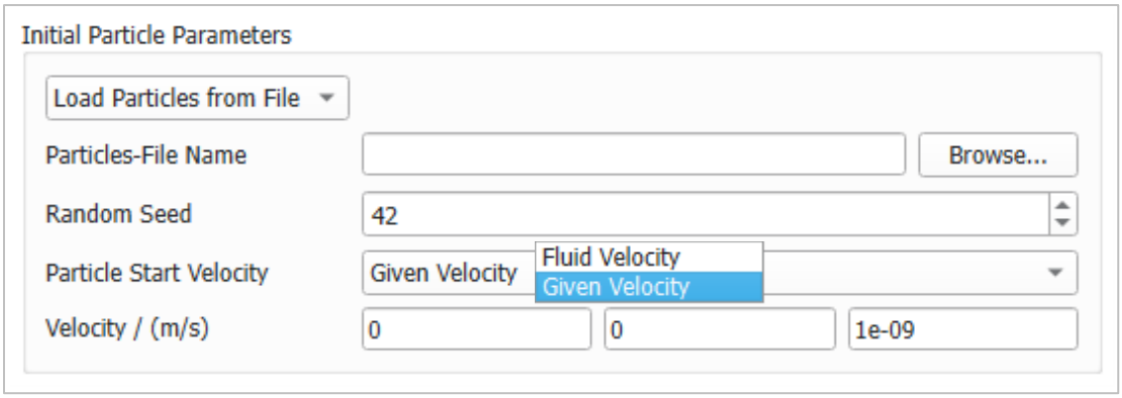
Positioning

Initial particle parameters

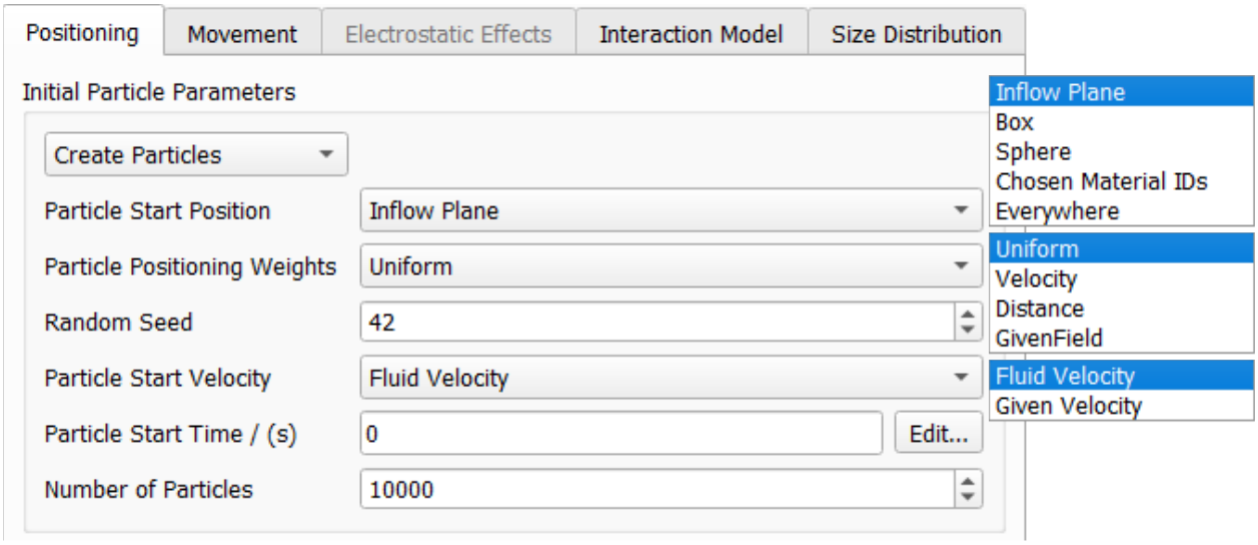
For the **Initial Particle Parameters**, either choose to **Create Particles** according to the options below or **Load Particles from File**.

To **Load Particles from** a **File**, browse, select, and open an existing *.gpp (GeoDict particle parameters) file. This file may origin from a previous AddiDict simulation or can be generated using GeoDict's Python API. See the Automation user guide for further information. Additionally, you can define a **Random Seed** and the **Particle Start Velocity**. 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.



When you select **Create Particles**, the parameters for the creation of the particles can be defined in detail.

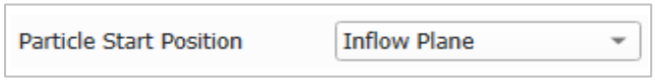


Particle Start Position

Select one of the following **Particle Start Position** types. The default start position is the Inflow Plane.

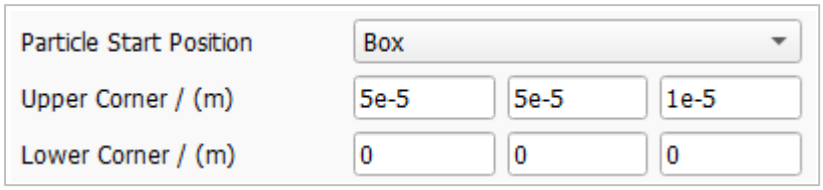
Inflow Plane

If **Inflow Plane** is chosen as **Particle Start Position**, the particles start at the inflow boundary which is always the Z- domain boundary.



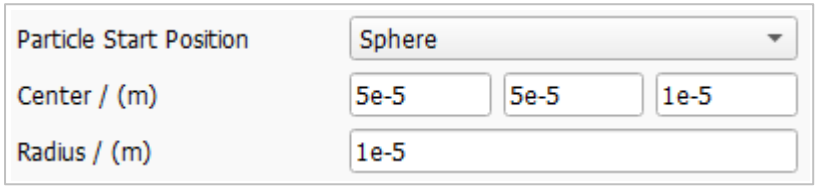
Box

If **Box** is chosen as **Particle Start Position**, two opposite corners of a rectangular box must be defined. All particle start positions will then be inside of this box.



Sphere

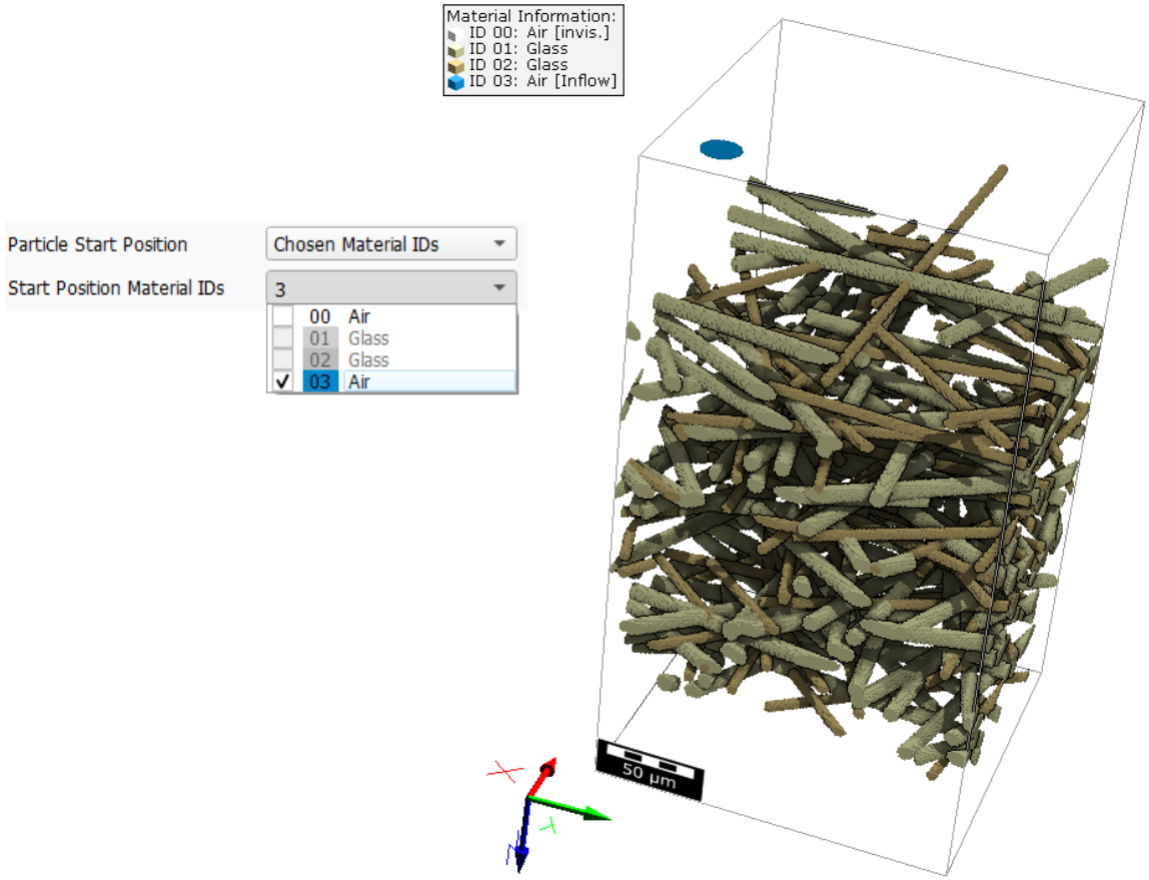
If **Sphere** is chosen as **Particle Start Position**, the center and radius of the sphere must be defined. All particle start positions will then be inside of this sphere.



Chosen Material ID

An arbitrary location can be set by selecting **Chosen Material IDs** as **Particle Start Position.**

For example, by using GadGeo, various objects can be added into the inflow area. Those objects can be assigned to the same fluid material as the surrounding pore space, so they only serve as markers of a certain area (see picture below).



If this area ID is now chosen as **Start Position Material ID**, all particles start in this area. It is possible to mark several areas in this way and/or to choose several IDs as starting areas.

Everywhere

If **Everywhere** is chosen as **Particle Start Position**, particles may start everywhere in the pore space of the structure. .

Particle Positioning Weights

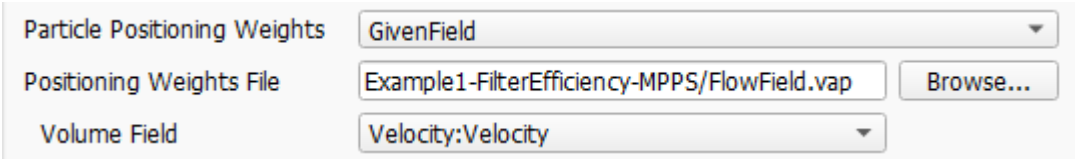
Particle start positions are scattered randomly inside the defined **Particle Start Position** area or volume.

By default, those positions are uniformly distributed. Be aware that a spatially **Uniform** placement in the inlet will lead to an increased particle concentration in areas with low fluid velocity, e.g., in proximity to a surface or a walls.

If **Velocity** is selected, the starting probability is based on the local fluid velocity. Selecting this option will lead to a uniform particle concentration in the inflow.

If **Distance** is selected, the starting probabiliy is based on the distance from the next solid object. This will lead to higher particle numbers in the core flow, while there will be less particles starting next to the surface.

With **GivenField**, it is possible to load an arbitrary 3D field of scalar values to define the starting probability. For example, it is possible to load the flow field of a previous computation and select the velocity or one of its components.



Random Seed

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.

Particle Start Velocity

Select either **Fluid Velocity** (the default option, which was used until GeoDict 2025) or **Given Velocity** as the **Particle Start Velocity**.

With the first option, particles begin moving with the fluid velocity at their start position.

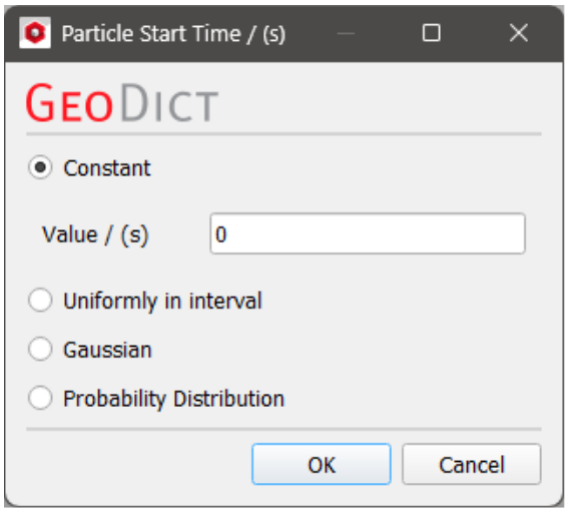
With the second option, all particles start with the same user-defined velocity.

Particle Start Time

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 one of these distributions: **Uniformly in interval**, **Gaussian**, or an arbitrary **Probability Distribution**.

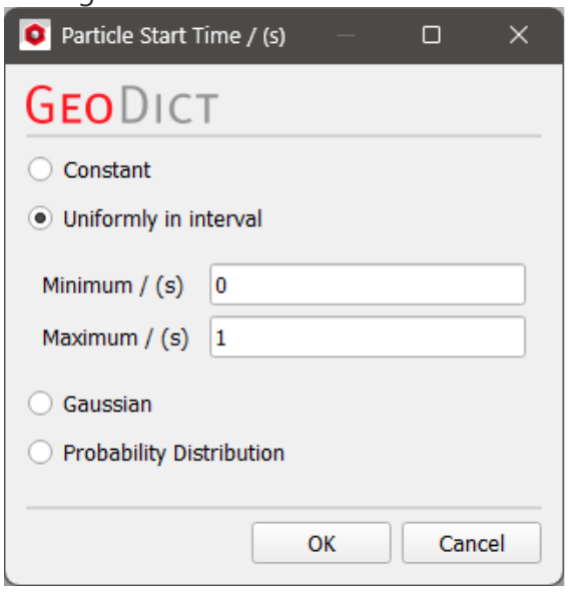
Constant

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



Uniformly in interval

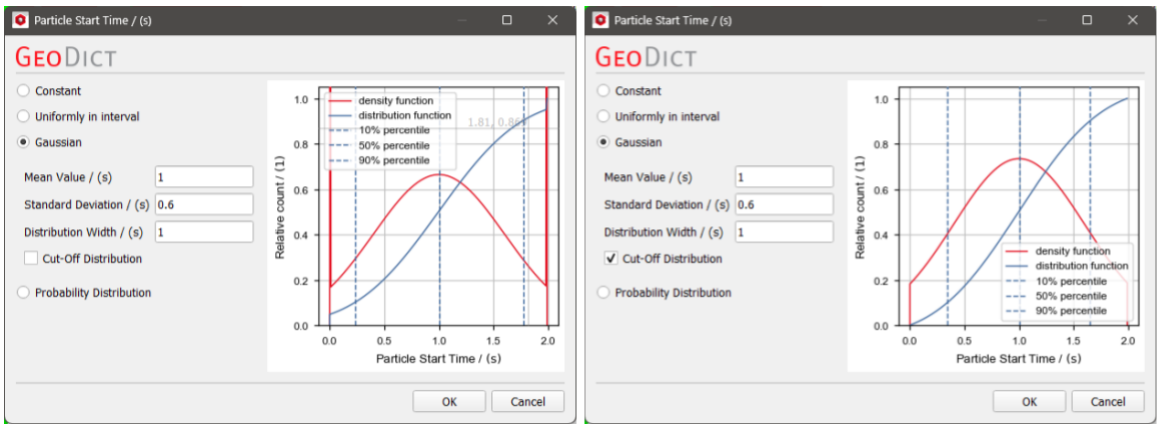
Particles can be released **Uniformly in interval** by specifying the beginning and ending of the time interval.



Gaussian

For particles to be released following a **Gaussian** distribution, define the **Mean Value**, the **Standard Deviation**, and the **Distribution Width** of the distribution. The particle

release times are centered on the **Mean Value** and 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 1 means that release time values may deviate only from -1 s to +1 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 1 s and a distribution width of 2 s would lead to an error message appearing, as the time could reach a value less than zero.
Check **Cut-Off Distribution** to restrict the start times selected by the random number generator to the interval defined by the distribution bounds. Otherwise, random numbers outside of this interval are set to the distribution bounds.

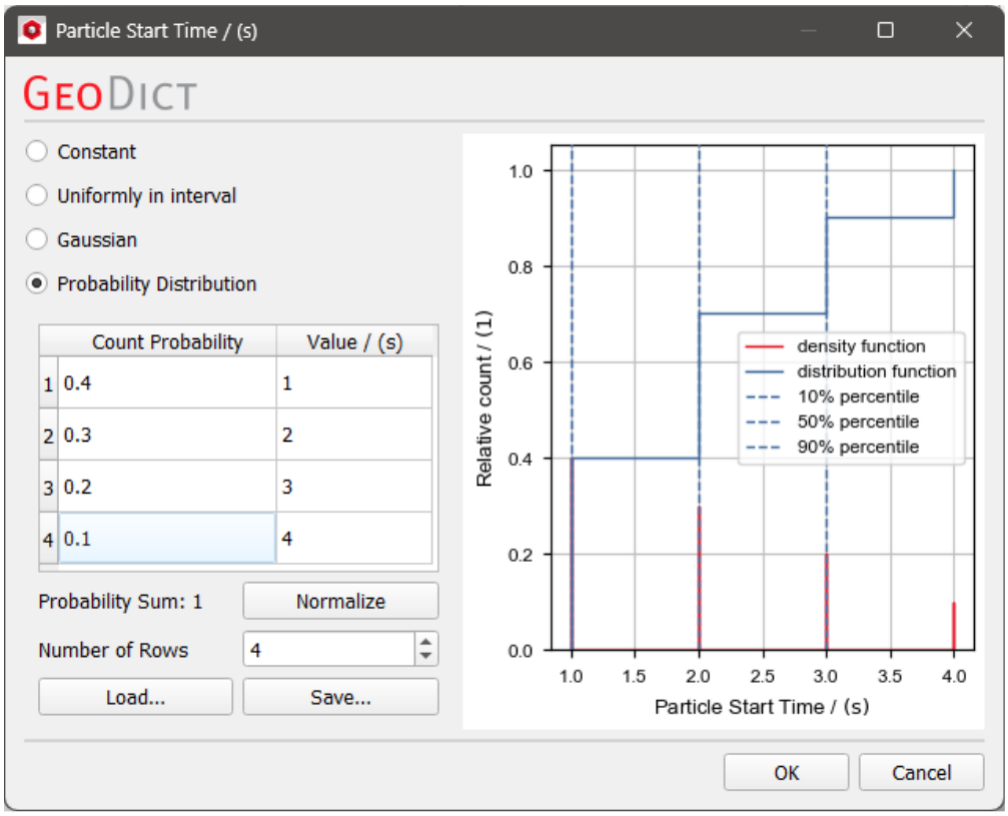


Probability Distribution

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 **Probability Sum** of all **Count Probabilities** defined in the table needs to be equal to one. Use the **Normalize** button to scale the **Count Probabilities** accordingly. 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 you to load a previously defined probability distribution and save the

current one for later use.



Number of Particles

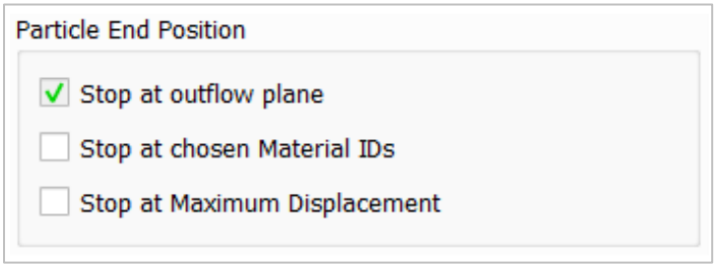
The **Number of Particles** determines the number of particles inserted into the geometry over the entire simulation period.

Particle End Position

Three options are available for the **Particle End Position**:

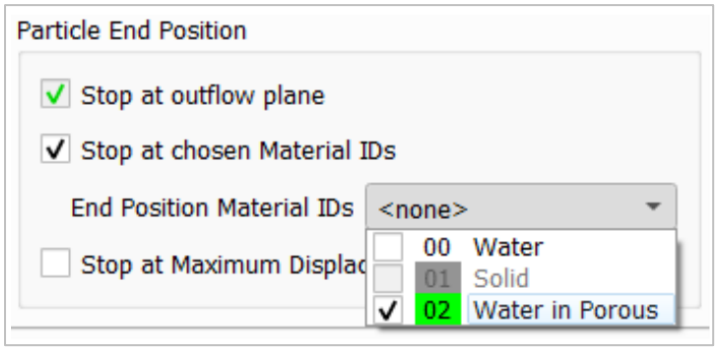
Stop at Outflow Plane

Particles always leave the simulation when they leave the computational domain at a defined **Outflow Plane**.



Stop at chosen Material IDs

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.

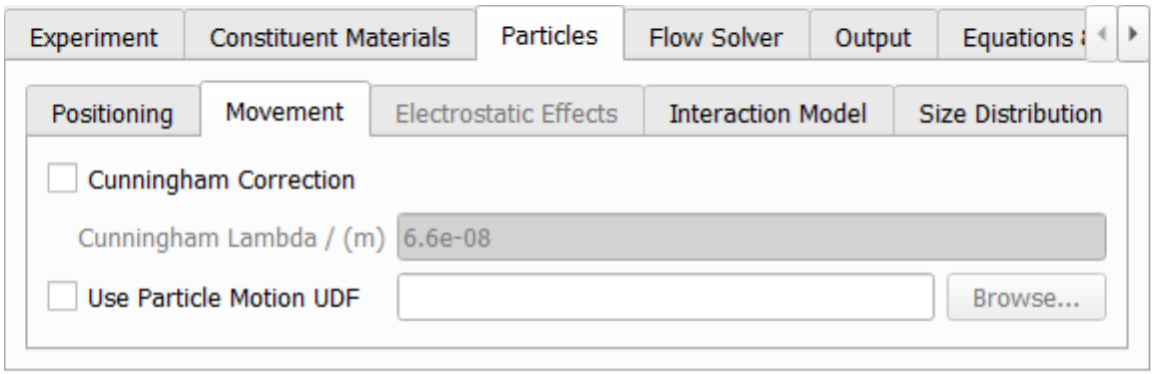


Stop at Maximum Displacement

Particles can stop moving and leave the simulation if the Particle Displacement[8] is larger than a predefined maximum value. This option can be used to, e.g., 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 using periodic boundary conditions.

Movement

In the **Movement** subtab of the **Particles** tab, the particle movement is controlled by changing the terms of the governing particle momentum[6] equation.



Checking Cunningham Correction[6] activates the corresponding correction method and adjusts the drag force. 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.

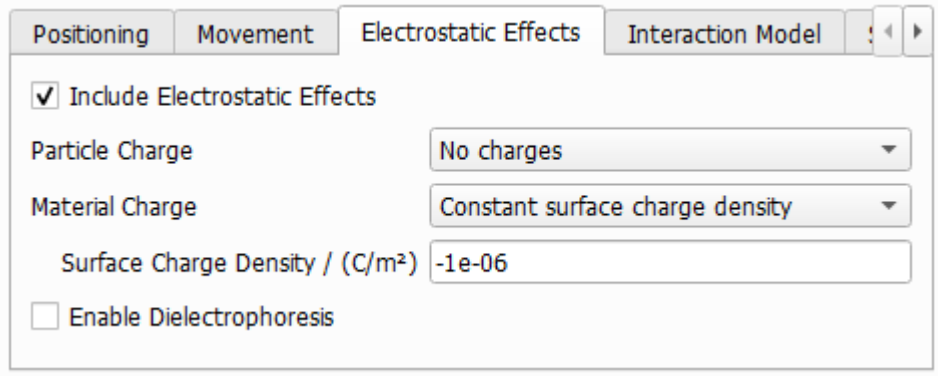
With the **Use Particle Motion UDF** option, you can replace the equations for the friction coefficient, external forces, and diffusion by your own equations. When **Use Particle Motion UDF** is checked, the formulas in the (modified) UDF file are used for all four formulas in the AddiDict simulation instead of the built-in equations. For details on how to modify and compile user defined functions, refer to the description in the FilterDict user guide.

In case molecule movement is simulated, only the option **Use Particle Motion UDF** is available in the **Movement** tab.

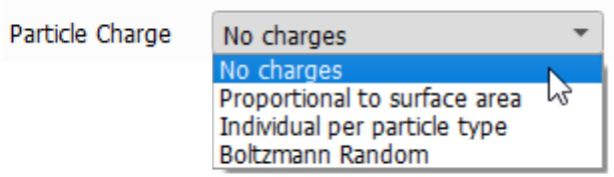
Electrostatic Effects

Important! This tab is only available if there are no porous materials present in the 3D structure.

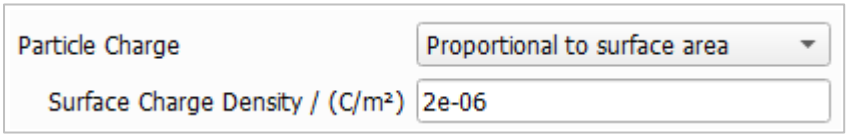
Check **Include Electrostatic Effects** to simulate electrostatic effects between solids and particles in the fluid.



Particle Charge



If electrostatic effects are negligible, set **Particle Charge** to **No charges**.



Select **Proportional to surface area** and enter a **Surface Charge Density** to set the value of Q in equation (1) to the product of the entered **Surface Charge Density** and the particle surface area.

Select **Individual per particle type** to enter an individual particle charge for each particle type or size. In this case Q in equation (1) is the entered particle charge. Enter the desired values

in the **Particle Charge [C]** column that is automatically added to the table under the Size Distribution 45 subtab.

If **Boltzmann Random** is chosen, particle charges follow a normal distribution with mean value 0 and standard deviation

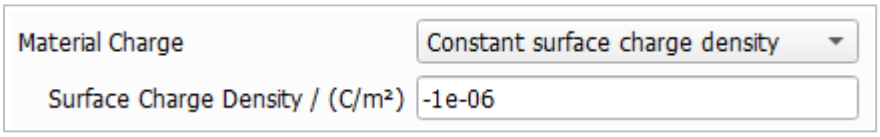
$$\sigma = \frac{\sqrt{2\pi d \varepsilon_0 k_B T}}{e} \tag{38}$$

where d denotes the particle diameter, ε_0 the dielectric constant, k_B the Boltzmann constant, T the temperature and e the electron charge.

Note! Electrical charges appear only as multiples of the elementary electric charge. Since GeoDict 2025, the **Boltzmann Random** distribution is therefore discretized into elementary electric charges. For large particles, this approaches a normal distribution of charge values, whereas small particles are mostly uncharged or carry just a single positive or negative charge.

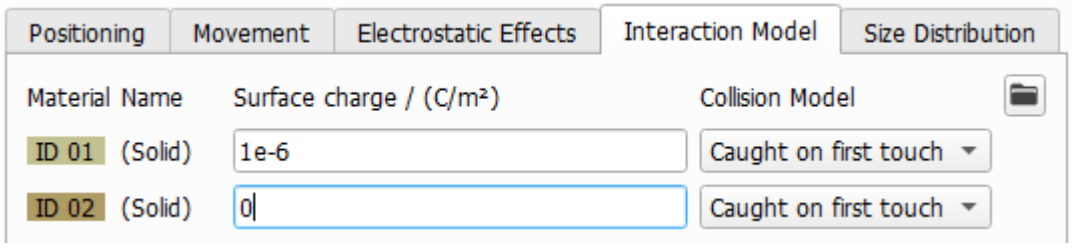
Material Charge

Select **Constant surface charge density** and set the **Surface Charge Density** (C/m^2), which corresponds to ξ in equation (7) 7.



This charge density is applied to all solid material surfaces.

Select **Individual per material ID** to set different surface charge densities for different material IDs. If selected, an additional column **Surface Charge (C/m^2)** appears on the Interaction Model tab 37. Enter the surface charge density of each material ID there.



The charges are given 'per surface area', therefore it is of special importance how the surface area is taken into account in the simulation. GeoDict uses a voxel grid. When simply applying the surface charge to each voxel surface, the overall charge would be overestimated, because the sum of all voxel surfaces overestimates the true surface area of the material. Therefore, the given surface charge density is corrected by the ratio between the computed surface area of

the material (see the Estimate Surface Area command in the MatDict user guide) and the sum of the voxel surfaces.

Note! Until GeoDict 2022, particles and solid were assumed to have opposite charges. Entering positive surface charge values for solid and particles lead to the solid attracting the particles. This was unintuitive and did not reflect the correct physics.

Therefore, since GeoDict 2023, it is no longer assumed that particles and solid have opposite charges. Entering opposite sign charge values (e.g., 5e-7 C/m² as surface charge and -6e-7 C/m² as material charge) for solid and particles leads to the solid attracting the particles.

Enable Dielectrophoresis

Dielectrophoresis is a phenomenon in which a force $\vec{F}$ is exerted on a particle when it is subjected to a non-uniform electric field $\vec{E}$. This force does not require the particle to be charged. All particles exhibit dielectrophoretic activity in the presence of electric fields.

When dielectrophoresis is enabled, the force $\vec{F}$ in equation (1) [6] is computed as

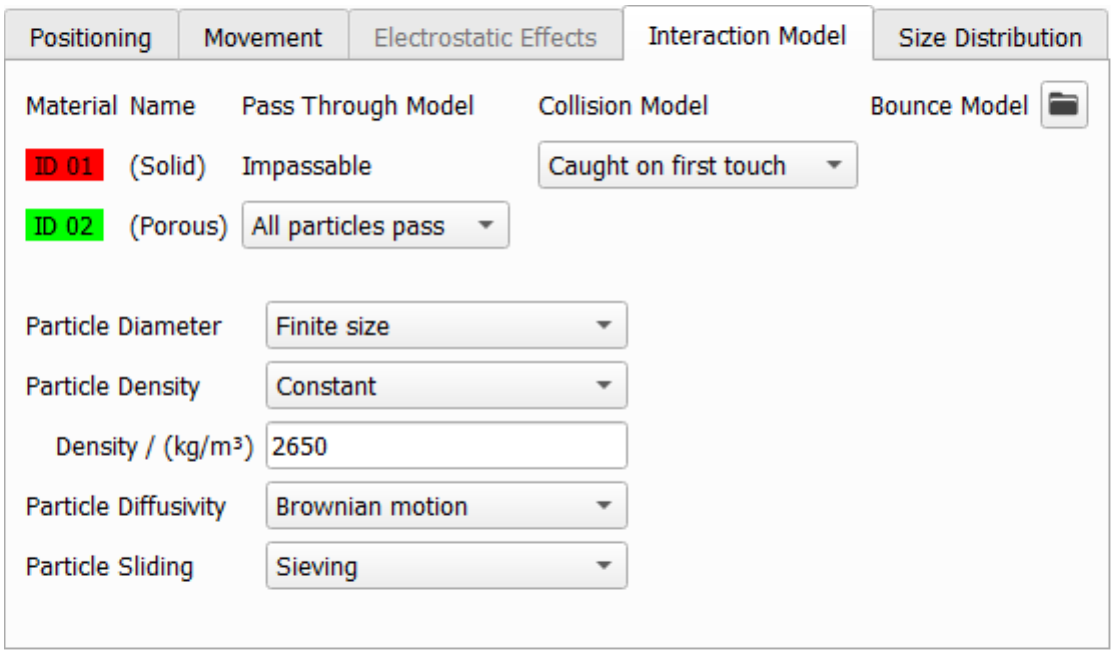
$$\vec{F} = 2\pi R^3 \varepsilon_m \left(\frac{\varepsilon_p - \varepsilon_m}{\varepsilon_p + 2\varepsilon_m} \right) \nabla |\vec{E}|^2 \quad (39)$$

Here, ε_p is the relative permittivity of the particles, ε_m is the relative permittivity of the fluid, and R is the particle radius. $\nabla|\vec{E}|$ denotes the gradient of the electric field and dictates the direction of the dielectric force.

Switch on this effect by marking the check box, and enter the relative permittivity values ε_m and ε_p in the dialog:

Interaction Model

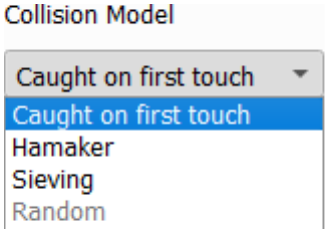
Under the **Interaction Model** subtab, properties of the particles as well as their interaction with the solid and porous materials, available in the structure, are defined. The choice of parameters under this subtab affects the entries and columns shown in the table under the Size Distribution [42] subtab.



Pass Through and Collision Models

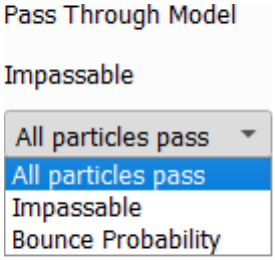
For all materials in the model, a **Pass Through Model** and a **Collision Model** must be defined. It depends on the choice of the **Pass Through Model** whether a **Bounce Model** needs to be selected as well.

Solid materials are always **Impassable** for particles, and for them, one of the collision models **Caught on first touch**, **Hamaker**, **Sieving** and **Random** can be chosen. The **Hamaker** model can only be selected for particles with finite size diameter, while **Random** can only be chosen for molecules. Additional columns appear in the table under the Size Distribution 42 subtab when **Hamaker** (columns Restitution and Adhesion), **Sieving** (column Restitution), or **Random** (column Deposition Probability) 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 at the top right of this tab. UDFs are more commonly used for filter simulations. Thus, more details can be found in the FilterDict user guide.

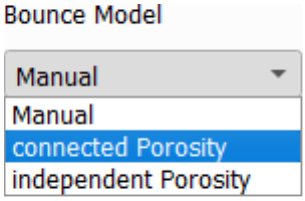
For porous materials, one of three **Pass Through Models** can be selected:



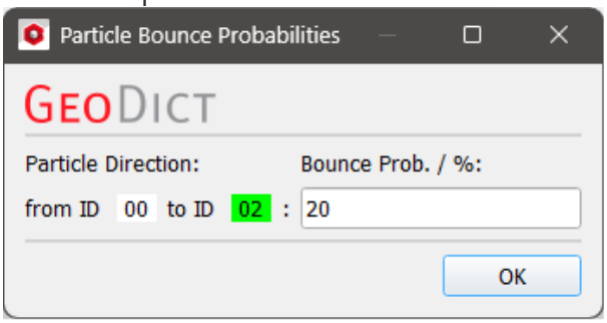
- When set to **All particles pass**, particles can move through the material. In that case, no **Collision Model** can be selected.
- Choosing **Impassable** sets the material to be treated as a solid material and particles cannot enter.
- When **Bounce Probability** is selected, part of the particles can enter the porous material, while others collide with the material. Here the expected behavior of a fully resolved porous materials is simulated. The part of the particles that enter the material are the particles that hit the porous material at a pore. The part of the particles that collide with the material are the particles that hit the solid. This option should only be chosen if the particles are smaller than the pore sizes of the porous material, i.e., they can enter the material. The percentage of the particles that enter the material, depends on the choice of the **Bounce Model**.

Bounce Models

For the **Bounce Model** three different options are available:



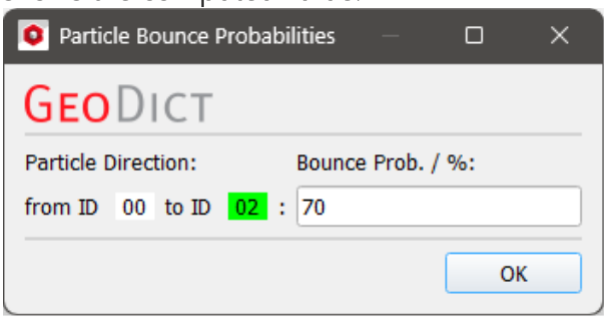
- Select **Manual** to define the probability of a particle to be reflected at the interface between pore space and porous material by clicking the **Edit** button. In the example shown, the probability of a particle to be reflected, if it reaches the interface between the pore space (ID 00) and the porous material (ID 02), is **20%**. Vice versa the probability that the particle enters the porous material is 80%.



- For **Connected Porosity**, the bounce 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 $porosity_{from}$ - $porosity_{to}$ / $porosity_{from}$.

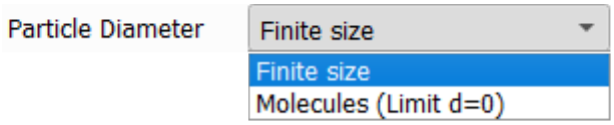
If the particle is moving from a region with low porosity to one with higher porosity, it will never be reflected, i.e., the reflection probability is always kept between 0% and 100%. This **Bounce Model** should be selected when you have materials with different porosities, i.e., pores that are connected and change only their width at the interface between materials. The porosity value(s) of the porous material(s) need to be set correctly on the Constituent Materials 24 tab.

- 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. The porosity value(s) of the porous material(s) need to be set correctly on the tab Constituent Materials 24.
  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 computed value.



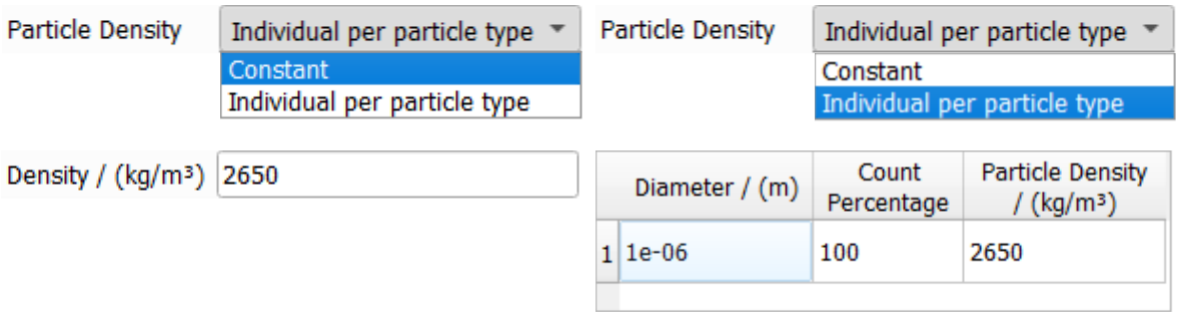
Particle Diameter

For the **Particle Diameter** two options are available. If **Finite Size** is set for the **Particle Diameter**, the momentum equation 6 is solved to model the particle movement. For **Molecules (Limit d=0)** the simplified movement equation 9 is solved. In this case, no **Particle Density** value has to be entered, **Particle Charges** are set to zero (i.e., the subtab Electrostatic Effects 35 becomes inactive), and **Diffusivities** have to be defined individually per particle type in the Size Distribution 45 subtab.



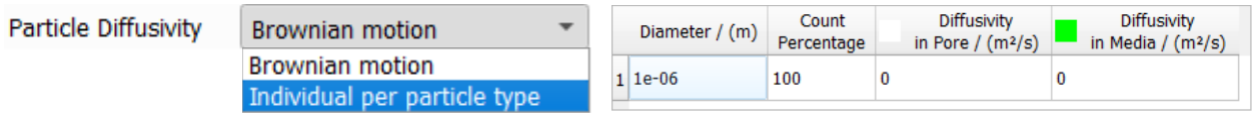
Particle Density

For finite sized particles, a **Particle Density** has to be entered. 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** disappears and individual density values have to be entered in the Size Distribution 44 subtab.



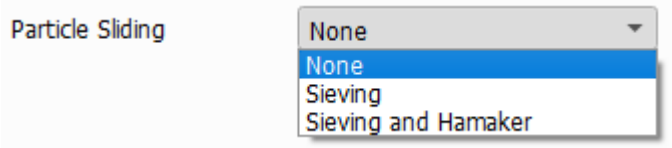
Particle Diffusivity

For **Particle Diffusivity**, you can choose between **Brownian Motion** and **Individual per particle type**. For **Brownian motion**, the diffusivity coefficient is computed following the equation described in the theoretical background 6. For **Individual per particle type**, the value of *D* must be entered under the Size Distribution 45 subtab for each particle type. 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 porous materials. 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 **Bounce Probability**.



Particle Sliding

Particles that collide with the surface loose some of their energy if the restitution factor is smaller than 1. In certain pore geometries, the flow may move a particle very close to a pore surface. This causes many consecutive hits, and repeatedly applying the restitution factor will stop the particle's motion. This behavior is often undesired, and it may overestimate the filter efficiency when combining a **Sieving** collision model with a relatively low restitution value.

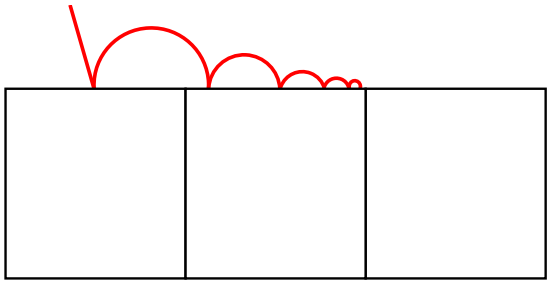
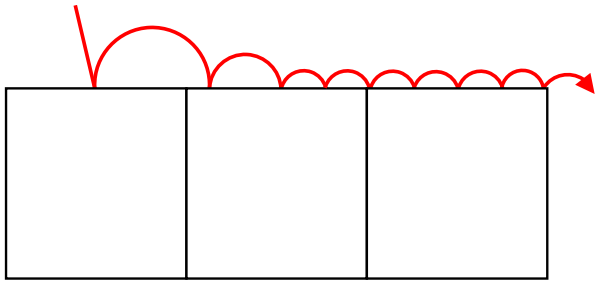


When **Sieving** is selected in the drop-down menu, all **Sieving** particle-wall collisions are modified, when **Sieving and Hamaker** is selected, all **Sieving** particle-wall collisions are modified and all **Hamaker** particle-wall collisions are modified. **Caught on First Touch** particle-wall collisions are not modified.

Enabling **Particle Sliding** for the **Sieving** or **Hamaker** collision models enlarges the tangential restitution factor when a particle hits a surface in a location that lies close to the last surface collision.

The first bounce on the wall is always treated the same, independent whether particle sliding is

active or not: A particle arrives with a certain velocity, loses energy on impact, and bounces back again. The strength of the bounce-back is controlled with the given **Restitution**. When particle sliding is active, further impacts near the first hit are treated differently: Only the momentum perpendicular to the wall is reduced. The velocity along the wall is not reduced further, so in this direction the restitution is equal to 1. This means that particle movement along the wall is no longer slowed down. The normal restitution remains unchanged. In effect, the particle will slide along the surface.

Without particle sliding:	With particle sliding
• energy lost at every collision • particle caught on surface	• energy conserved after some hits • particle moves along surface
	

In setups where particles are sieved by filter materials having pores of well-defined sizes (e.g., in meshes, nets or weaves), selecting particle sliding has a great influence on the computed filter efficiency and pressure drop and it is recommended to select this option.

In setups where particles are mainly caught by adhesion or where the filter material consists of irregular pores of many different sizes (e.g., nonwovens), the choice of the particle sliding model has little to no effect on the simulation results.

Size Distribution

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

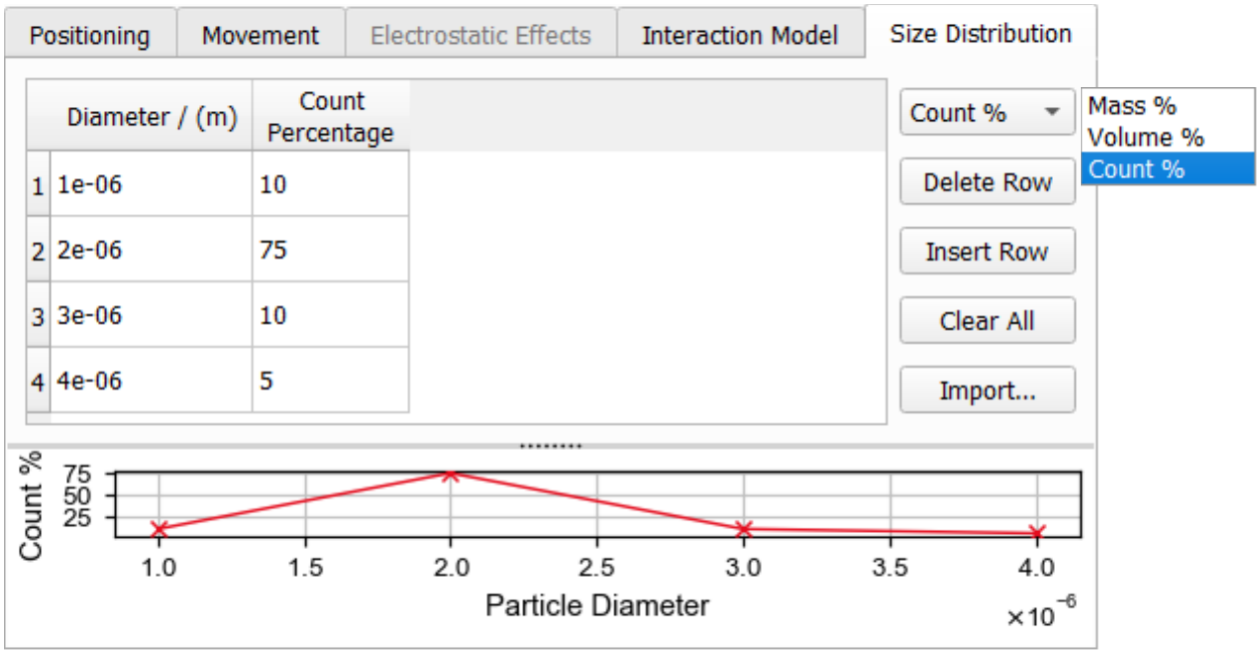
For the default settings of

- **Finite Size** as **Particle Diameter**
- **Constant** as **Particle Density**
- **Caught on first touch** as **Collision Model**
- **Brownian Motion** as **Particle Diffusivity**

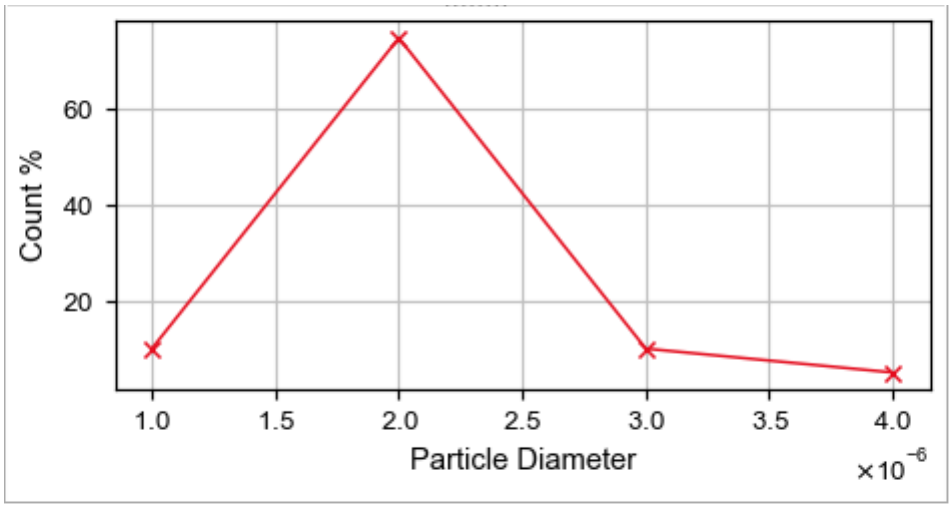
only two columns are available.

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**, **Volume**, or total number of particles (**Count**), that can be selected to the right of the table.



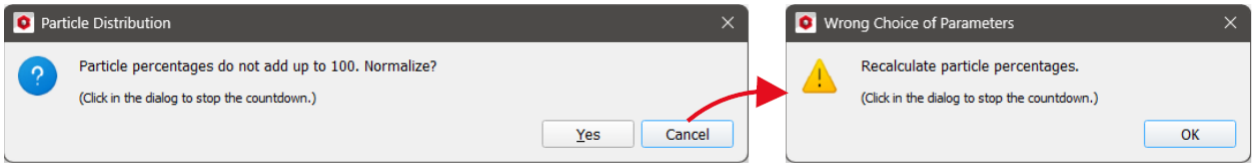
Below the size distribution table, a graphical presentation of the particle size distribution is displayed, if particles with **Finite Size** are selected. The graph is automatically updated after changes in the table. The x-axis shows the **Particle Diameter**, and the y-axis the **Mass**, **Count**, or **Volume** percentage. Right-click the plot to store the graph as a *.txt file, to save the graph as image, to copy the values to the clipboard, or to edit the plot settings.



To the right of the size distribution table multiple buttons are available:

- Clicking **Delete Row** 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. Percentages in the *.txt file are always considered as count percentages. You can save your current settings in the size distribution table by changing the displayed values to **Count %** and saving the graph as text file. It is possible to load the text file into the dialog for other simulations.

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



Additional columns appear under the **Size Distribution** subtab, depending on the user choices under the Interaction Model 37 and Electrostatic Effects 35 subtabs.

Molecules

If **Molecules (Limit d=0)** 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**).

Particle Density

Selecting **Individual per particle type** for the **Particle Density** causes the **Particle Density (kg/m³)** column to appear.

Diameter / (m)	Count Percentage	Particle Density / (kg/m³)

Collision Models

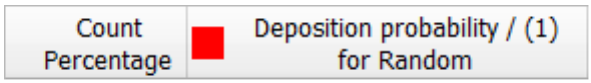
Dependent on the choice for the solid and porous material IDs collision models, an individual column for each material ID may appear. After choosing **Caught on first touch**, no additional columns appear. When choosing the **Hamaker** collision model for a material, the columns **Restitution** and **Adhesion** appear. In the case of **Sieving** and particles of finite size, only the **Restitution** column appears.

Diameter / (m)	Count Percentage	Restitution (in [0,1]) for Hamaker	Adhesion / (J) for Hamaker	Restitution (in [0,1]) for Sieving

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

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.

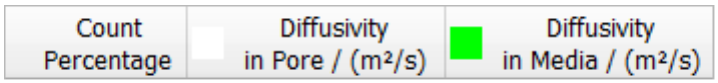
When choosing **Random** as collision model, a column for the **Deposition Probability** appears.



The **Deposition Probability** defines the probability of trapping a particle when it hits a solid or porous material.

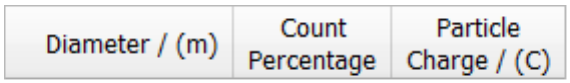
Diffusivity

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



Particle Charge

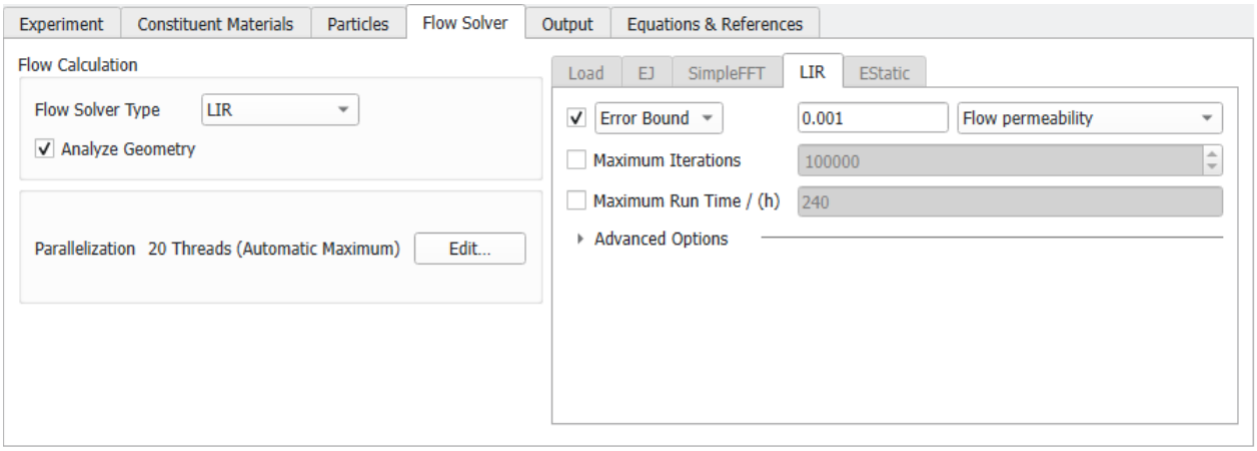
Choosing **Individual per particle type** for the **Particle Charge** in the Electrostatic Effects subtab adds a column for the **Particle Charge**.



Flow Solver

Under the **Flow Solver** tab, the settings for the flow solver used in the AddiDict simulation can be chosen and its parameters can be defined. The tab is subdivided into three panels for **Flow Calculation**, **Parallelization**, and **Solver Settings**.

Important! 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.

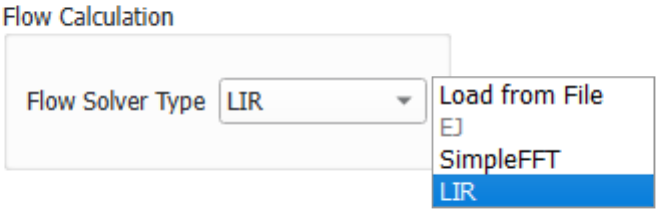


Flow Solver Panels

- Flow Calculation 46
  Choose the flow solver.
- Parallelization 47
  Define the used computational resources.
- Solver Settings 49
  Learn more about stopping criteria and advanced settings.

Flow Calculation

In the **Flow Calculation** panel on the top left, select the **Flow Solver Type** to be used for solving the chosen partial differential equations from the pull-down menu (EJ, SimpleFFT, or LIR). EJ cannot be selected for solving Brinkman equations.



It is also possible to choose **Load from file** to import the result file (*.gdr) 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.

Checking **Analyze Geometry** performs an analysis of the geometry before the solver computations.

If no percolation path through the structure is found, the partial differential equation does not need to be solved, and a permeability of 0.0 is directly reported as the solution.

Furthermore, the solver operates on the whole structure, regardless of which parts are connected or unconnected. However, unconnected components are not transport relevant, thus

the effort of solving in these parts is not necessary.

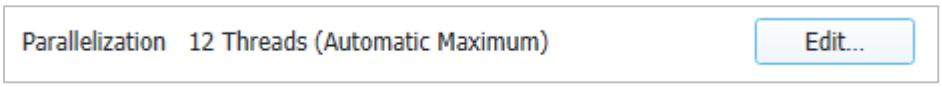
For these reasons, a geometrical analysis is routinely run to determine whether a through path exists. After the analysis is finished, unconnected components are removed from the computational grid.

This may speed up the computations but requires some time for the geometrical analysis, especially for very large structures. So if you know beforehand that there are no unrelevant parts or that the structure has been processed to eliminate them, the geometry analysis can be switched off by unchecking **Analyze Geometry**.

Parallelization

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

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



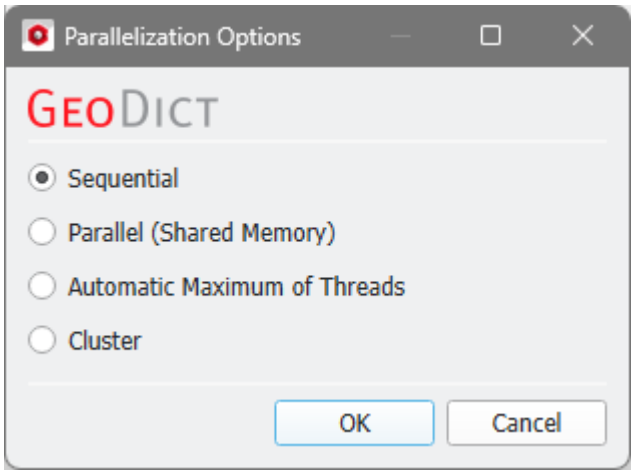
The parallelization of the solvers is done with two technical methods: **MPI Parallelization** or **Thread parallelization**. The following table shows the support of both parallelization methods:

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

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

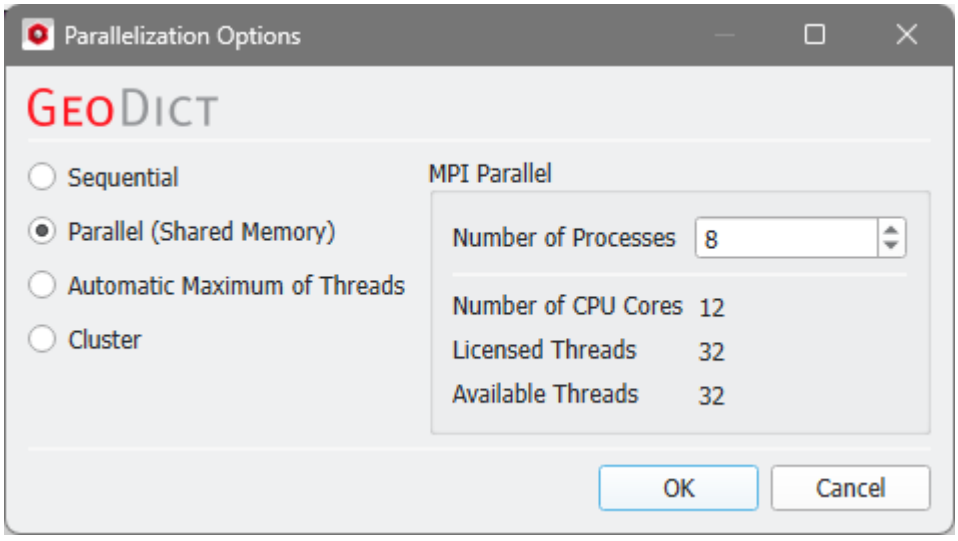
Sequential

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



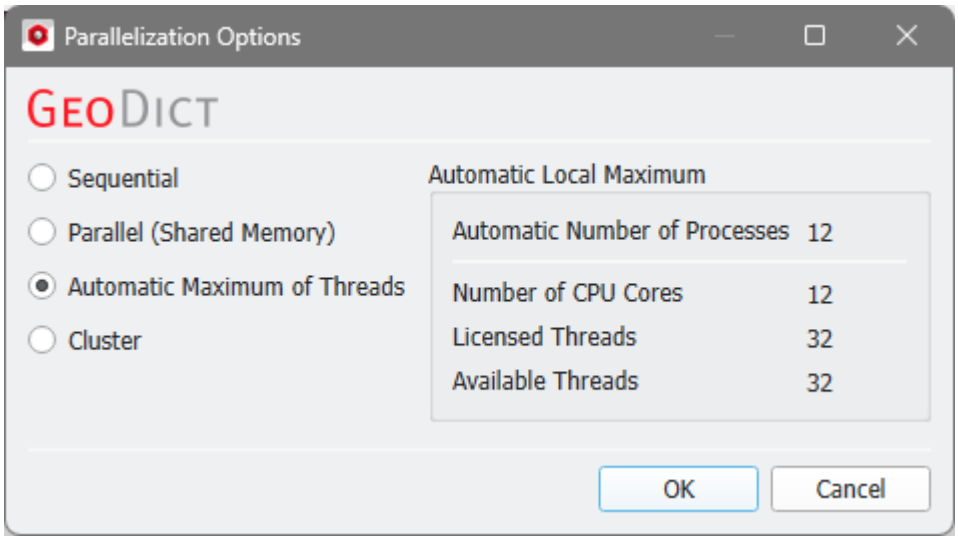
Parallel (Shared Memory)

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



Automatic Maximum of Threads

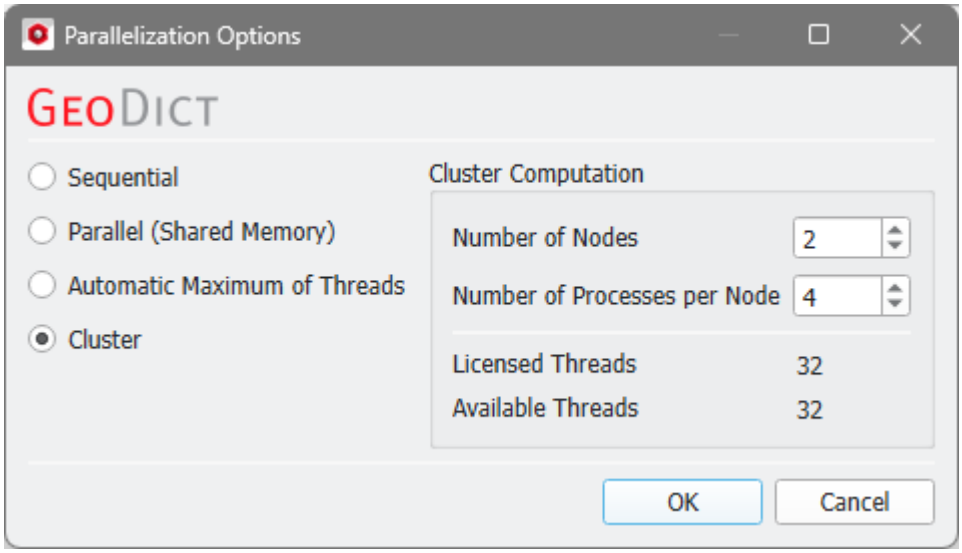
If **Automatic Maximum of Threads** is selected, the number of parallel processes is automatically selected for optimal speed, based on the CPU cores and licensed parallel processes.



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

Cluster

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



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

Solver Settings

Stopping Criteria

The equations are solved by an iterative approach.

Iterative Solver

The basic idea of an iterative method is to

1. Start with some initial guess for the unknown values
2. Improve the current values in each iterative step
3. Repeat the iterative process until one of the stopping criteria is reached.

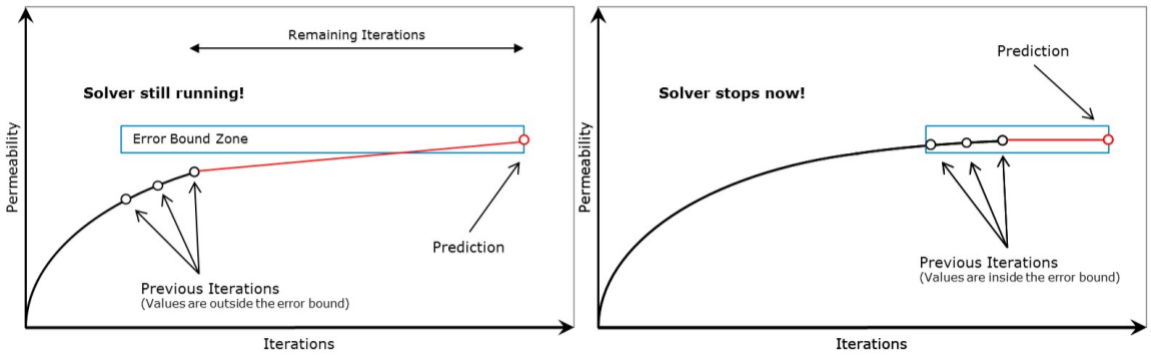
The iterative process is controlled by setting the values and activation for **Error Bound, Tolerance, Residual**, **Maximal Iterations**, and **Maximal Run Time (h**). The stopping criteria apply for each computational direction individually.

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

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

Error Bound

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



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

Tolerance

The **Tolerance** stopping criterion looks for stagnation of the method when the process

becomes stationary, i.e., the improvement in the permeability value becomes extremely small from iteration to iteration.

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

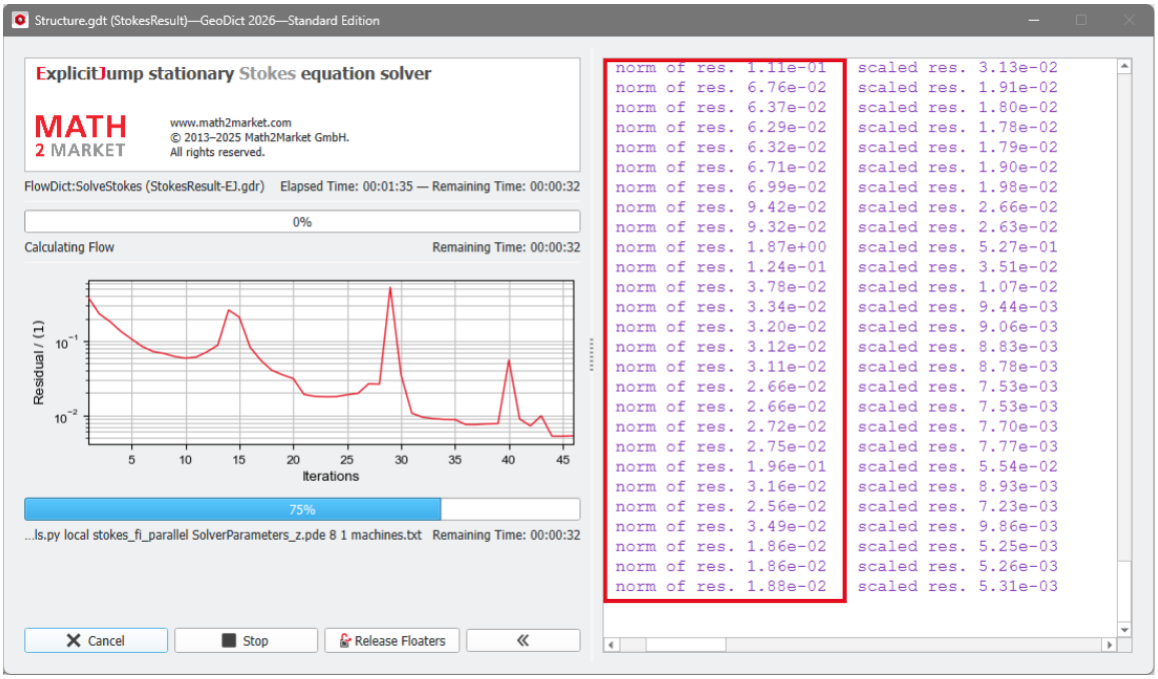
$$\max_{i\in[1,100]} \frac{x_c - x_{c-i}}{x_{c-i}} < \text{tolerance} \tag{40}$$

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

Residual

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

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



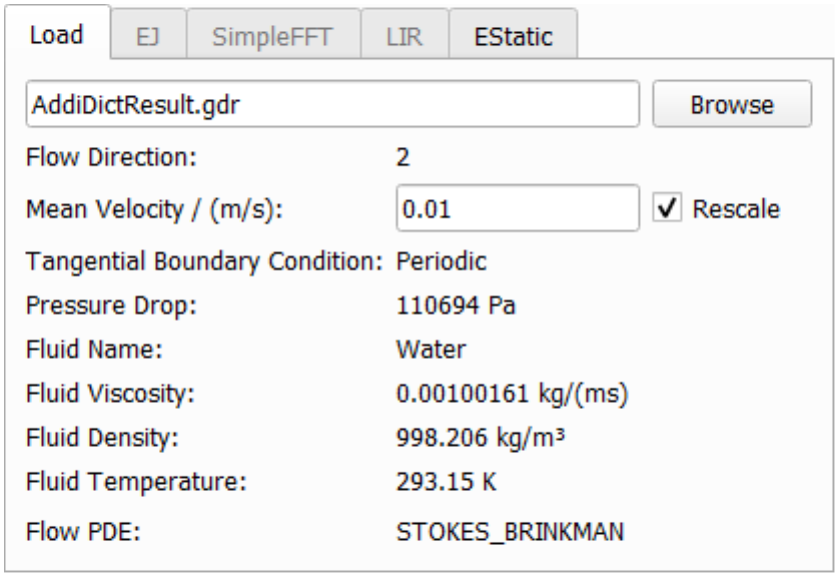
The recommendation to choose **Tolerance** or **Residual** for the **EJ** solver is based on the structure's porosity. Both give similar results for highly porous structures. For dense

structures, if using the Schur Complement **Residual**, the relative norm of the residual may be small even though the correct permeability has not been reached. So, when in doubt, use the **Tolerance** criteria – the default option.

Additional Settings

Load

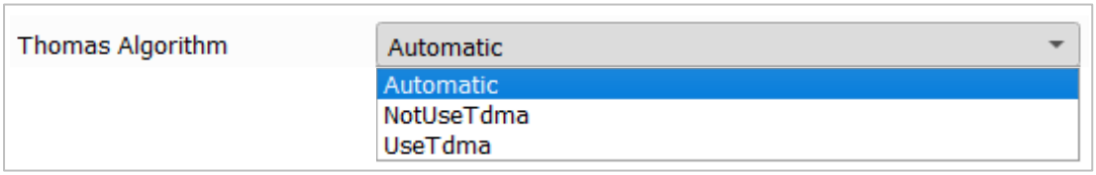
If **Load from File** has been selected from the **Flow Solver Type** menu in the **Flow Calculation** panel, choose a GeoDict result file of a previously run computation. Some information about the computation is shown. The mean velocity of the computation can be rescaled to another one by checking **Rescale** and editing the mean velocity.



SimpleFFT

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

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



If **Automatic** is selected, the SimpleFFT solver decides if **Tdma** will be used, regarding

the porosity of the structure. Thus, **Tdma** is used if the porosity is high. For most cases it is recommended to choose **Automatic**.

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

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

For more information about the Thomas algorithm see here.

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

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

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

LIR

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

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

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

The **Multigrid Method** (see, e.g., Wesseling, 2004) was introduced to speed-up the computation and reduce the runtime significantly. The main idea of **Multigrid** is the

usage of multiple coarser adaptive grids to speed up convergence behavior but requires only little more memory.

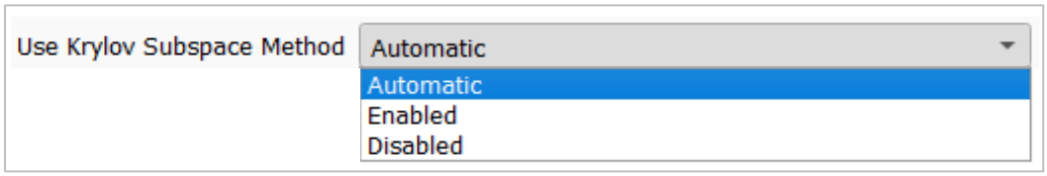
The method is available to solve the Stokes and Stokes–Brinkman equations as well as for solving mechanics, diffusion, thermal, and electrical conduction and is enabled by default.

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

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

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

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

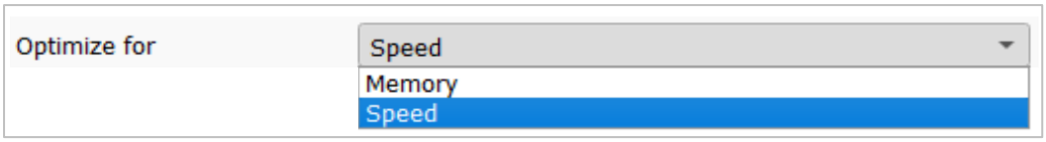


Note! In case that the Krylov subspace method (BICGStab) is used, the **Relaxation** may also be adapted automatically.

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

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

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.

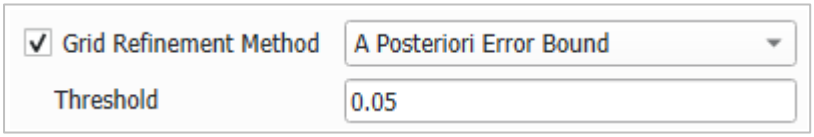
The default option is **LIR-Tree** and should always be used. The solver uses an adaptive grid structure called LIR-tree and needs up to 10 times less runtime and memory compared to the **Regular Grid** option.

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

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

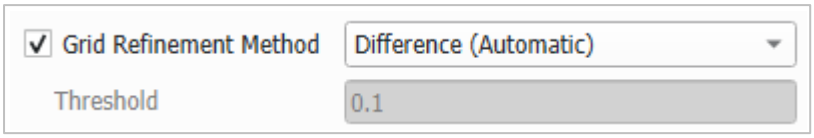
Select one of the three available refinement methods from the drop-down menu.

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

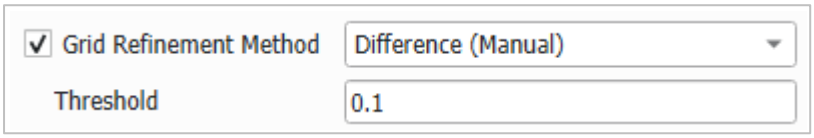


Choosing **Difference (Automatic)** leads to computational cells being split when the difference in values between neighboring cells exceeds a certain **Threshold**. The solver automatically chooses all internal parameters based on the structure and simulation settings. For this option, cells are split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

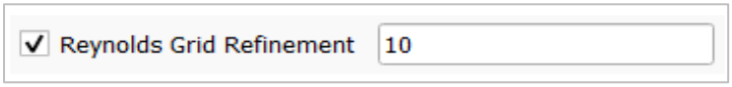
Threshold multiplied by the maximum gradient, where the threshold is determined automatically.



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



Activate **Reynolds Grid Refinement** to use the local Reynolds number (Re) for adaptive grid refinement.



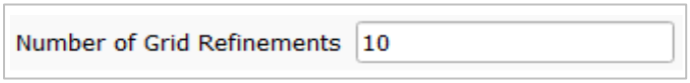
A grid cell is split if the local Reynolds number, i.e., the ratio between inertial and viscous forces exceeds the given threshold. The Reynolds number is defined as:

$$\mathrm{Re} = \frac{\rho \mathrm{u} \mathrm{L}}{\mu} \quad (41)$$

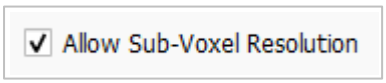
Reynolds Number

where ρ is the density of the fluid (SI units: kg/m^3), u is the velocity of the fluid (m/s), μ is the dynamic viscosity of the fluid (Pa·s or N·s/m^2 or kg/m·s), L is a characteristic length (m). For the local Reynolds number, the size of the grid cell is used for the characteristic length.

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



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



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

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

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

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

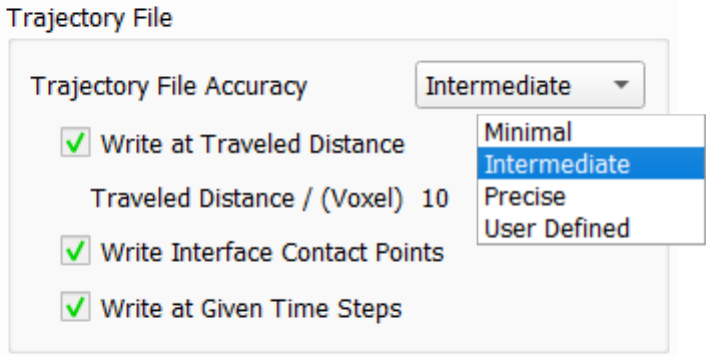
EStatic

The **EStatic** subtab is only active when **Include Electrostatic Effects** has been checked previously under the **Electrostatic Effects** subtab. 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 the corresponding equation[7] for more details.

Output

Trajectory File

In the **Trajectory File** panel, you can set how accurately the particle trajectories are stored. These settings strongly influence 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**.



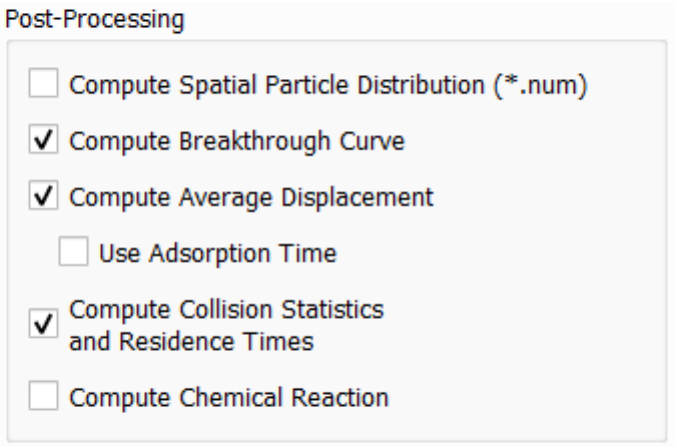
The **Write at Given Time Steps** option is always checked. This causes the particle positions to be stored at the time steps defined in the Experiment 20 tab.

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

Post-Processing

In the **Post-Processing** panel, you 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 these settings at any time after the computation, and then a modified report will be created. Refer to the Results - Report 59 section for more details.

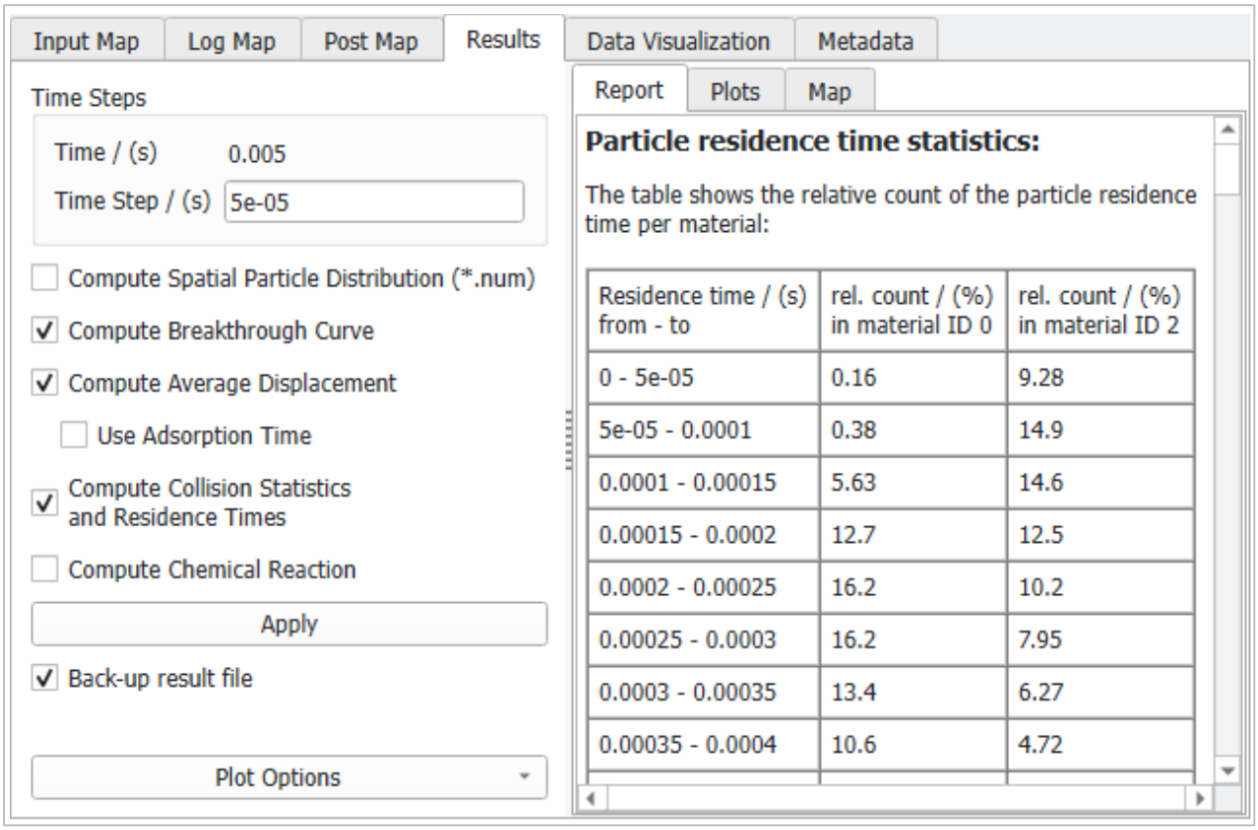


1.2.2 Results

After the **Track Particles & Molecules** simulation is completed, the resulting files are saved in the project folder and a **Result Viewer** with the GeoDict result file opens automatically. The created GeoDict result file (*.gdr) contains six tabs. The computational results are shown under

the **Results** tab, and can be loaded for visualization via the **Data Visualization** tab. The other four tabs (**Input Map**, **Log Map**, **Post Map** and **Metadata**) display additional information about the computation.

Find more details on the general functionalities in the Result Viewer user guide.



Track Particles & Molecules Results

- Report 59
  See the computed results.
- Plots 64
  View result plots.
- Data Visualization 68
  Load results for a graphical visualization.

Report

The content of the **Report** subtab is determined by the choices made in the left panel of the **Results** tab. Change the values and settings therein and click **Apply** to generate an updated report. 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. Select **Back-up result file** in the left panel to save a copy of the current *.gdr file before modification. The back-up file will be located in the result folder and gets the file name *AddiDictResult.gdr.bck##* as an example for the default result file name *AddiDictResult.gdr*.

The main results of a **Track Particles & Molecules** simulation are statistics on the particle movement such as residence times, collisions with solids, or breakthrough and displacement.

If only diffusion is simulated, i.e., **Simulate Advection** is unchecked in the Experiment 20 tab, the diffusivity is computed from the particle distances traveled. The **Particle diffusivity** is the diffusivity of all particles 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 61 is set for one or several materials.

Diffusion parameters:

Average Displacement: 1.13002e-05 m
Average Displacement with Adsorption: 7.59277e-06 m
Average Shift X: -1.07374e-07 m
Average Shift Y: 3.29646e-07 m
Average Shift Z: -5.86475e-06 m

Particle diffusivity D_p / (m^2/s)

5.694e-09	-1.003e-10	9.6e-11
-1.003e-10	**4.774e-09**	-2.651e-10
9.6e-11	-2.651e-10	**5.417e-09**

Isotropic particle diffusivity: **5.29513e-09 m^2/s**
Rel. std. dev. of particle diffusivities: (1.5 1.49 1.12) %

Effective diffusivity D_{eff} / (m^2/s)

2.282e-09	-4.018e-11	3.847e-11
-4.018e-11	**1.913e-09**	-1.062e-10
3.847e-11	-1.062e-10	**2.171e-09**

Particle Diffusivity (with Adsorption) / (m^2/s)

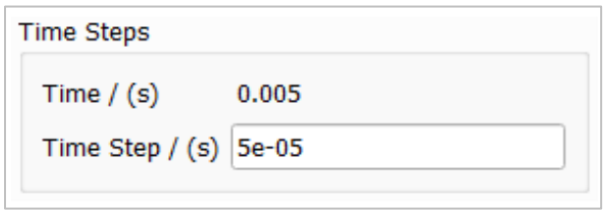
3.82608e-09	-6.73687e-11	6.45013e-11
-6.73687e-11	**3.20783e-09**	-1.78119e-10
6.45013e-11	-1.78119e-10	**3.63972e-09**

The Diffusivity was multiplied by a factor of 0.671915 due to Adsorption of particles.

Post-Processing Parameters

Time Steps

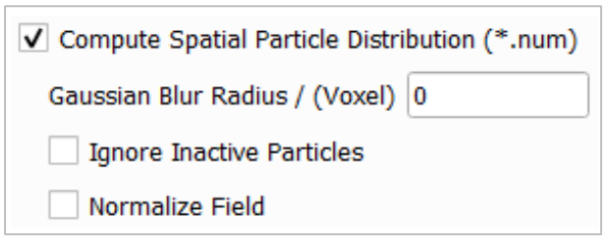
The **Time** value shows the final time of the simulation run. By changing the **Time Step**, the user can choose at which times the particle positions are evaluated, i.e., how many rows appear in the tables shown in the report. To create an updated report, GeoDict reads the particle positions from the 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 57 tab. 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.



Compute Spatial Particle Distribution (*.num)

When the **Compute Spatial Particle Distribution (*.num)** box is checked, a particle concentration file is created for each **Time Step**. You can load and visualize these files through the **Data Visualization** tab. It is possible to modify the created particle concentration file. When **Compute Spatial Particle Distribution (*.num)** is selected, the following options are enabled:

- **Gaussian Blur Radius / (Voxel)**: Choose a voxel number larger than 0 to blur the particle distribution fields with a Gaussian kernel of the given size.
- **Ignore Inactive Particles**: Check this option to ignore particles not moving anymore in the particle distribution field.
- **Normalize Field**: Check this option to normalize the mean of the particle distribution field to the inflow concentration.

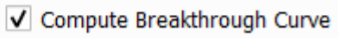


Compute Breakthrough Curve

When the **Compute Breakthrough Curve** box is checked, new columns are added to the **Particle breakthrough and travel displacement** table:

- **Cumulative particle count** shows at each time step the total number of particles that left the simulation domain until this time step.
- **Breakthrough particle count** lists the number of particles that left in each time step.
- **Active particle count** gives the number of particles that remain in the structure in this time step.

Additionally, a Breakthrough curve 66 plot is added to the **Plots** subtab.

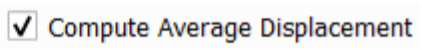


Particle breakthrough and travel displacement:

Time / (s)	Cumulative breakthrough count	Breakthrough particle count	Active particle count
0	0	0	0
5e-05	0	0	5021
0.0001	0	0	10000
0.00015	20	20	9980

Compute Average Displacement

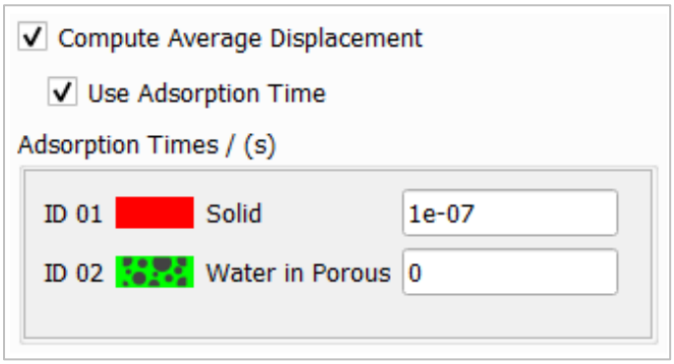
If the **Compute Average Displacement** box is checked, the **Travel displacement** column is shown additionally in the report, and a Travel Displacement curve[67] is added to the **Plots** subtab.



Particle breakthrough and travel displacement:

Time / (s)	Travel displacement / (m)
0	0
5e-05	1.93014e-06
0.0001	2.86532e-06
0.00015	4.4244e-06

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. On the Plots[64] subtab, two **Travel Displacement** curves, with and without adsorption are plotted.



Compute Collision Statistics and Residence Times

To evaluate residence times in the different materials, check **Compute Collision Statistics and Residence Times**. 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. Additionally, a Residence time[64] plot is created on the **Plots** subtab.

Compute Collision Statistics and Residence Times

Particle residence time statistics:

The table shows the relative count of the particle residence time per material:

Residence time / (s) from - to	rel. count / (%) in material ID 0	rel. count / (%) in material ID 2
0 - 5e-05	0.16	7.46
5e-05 - 0.0001	0.33	12.6
0.0001 - 0.00015	4.34	12
0.00015 - 0.0002	11.1	11.5

The **Particle collision statistics** table is shown 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 here, the mean value of particle collisions with the solid material with material ID 1 is 3569.49. Since it is a solid material, particles cannot enter the material and the residence time in this material is 0. For the porous material with ID 2, 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.

Particle collision statistics:

The table shows the mean values for a single particle:

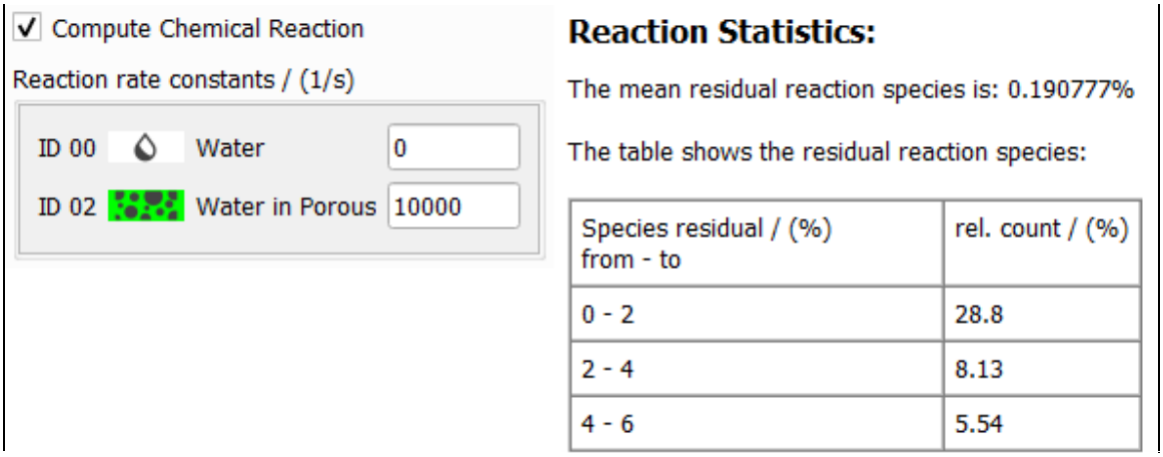
Material ID	Residence time / (s)	Collisions	Entries	Trapped / (%)
0	0.000353492	0	450.551	0
1	0	3535.81	0	0
2	0.000329022	1093.69	450.366	0

Compute Chemical Reaction

To compute chemical reactions of the first order based on the residence times in the different materials, check **Compute Chemical Reaction** in the left panel 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 18 described in the theoretical background.

The table **Reaction Statistics** is created on the **Report** subtab, and a Reaction Statistics 65 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 here, for nearly 30% of the particles, only up to 2% remain that have not reacted yet.



Species residual / (%) from - to	rel. count / (%)
0 - 2	28.8
2 - 4	8.13
4 - 6	5.54

Plots

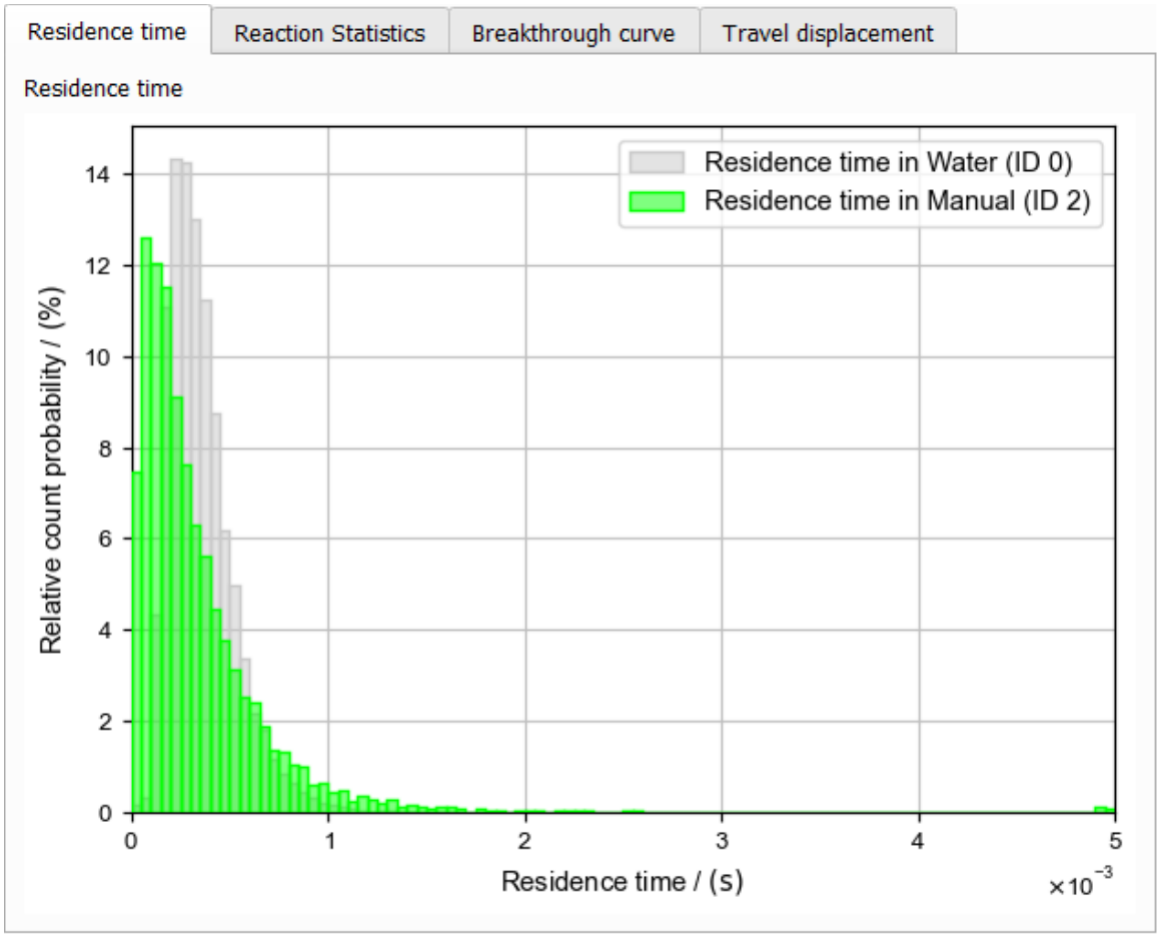
Under the **Plots** subtab multiple plots are available depending on the choices made in the post-processing of the Results 59 tab.

Properties of the axis and graph can be modified for all plots. Click the button **Plot Options** or right click the graph to access the settings menus. With **Edit Axis Settings**, scaling, labels and ticks of the axis as well as font sizes and legend placement can be selected. With **Edit Graph Styles**, title, style and color can be defined for each graph shown in the plot. In the menu that appears after right clicking the graph the data contained in the plot can be saved as well. More details on changing plot settings, are available in the Result Viewer user guide.

Modifications in the plots due to changes in the post-processing options in the left panel are also changed in the GeoDict result file *(.gdr). Check **Back-up result file** in the left panel to save a copy of the current *.gdr file before modification. The back-up file will be located in the result folder and gets the file name *AddiDictResult.gdr.bck##* as an example for the default result file name *AddiDictResult.gdr*.

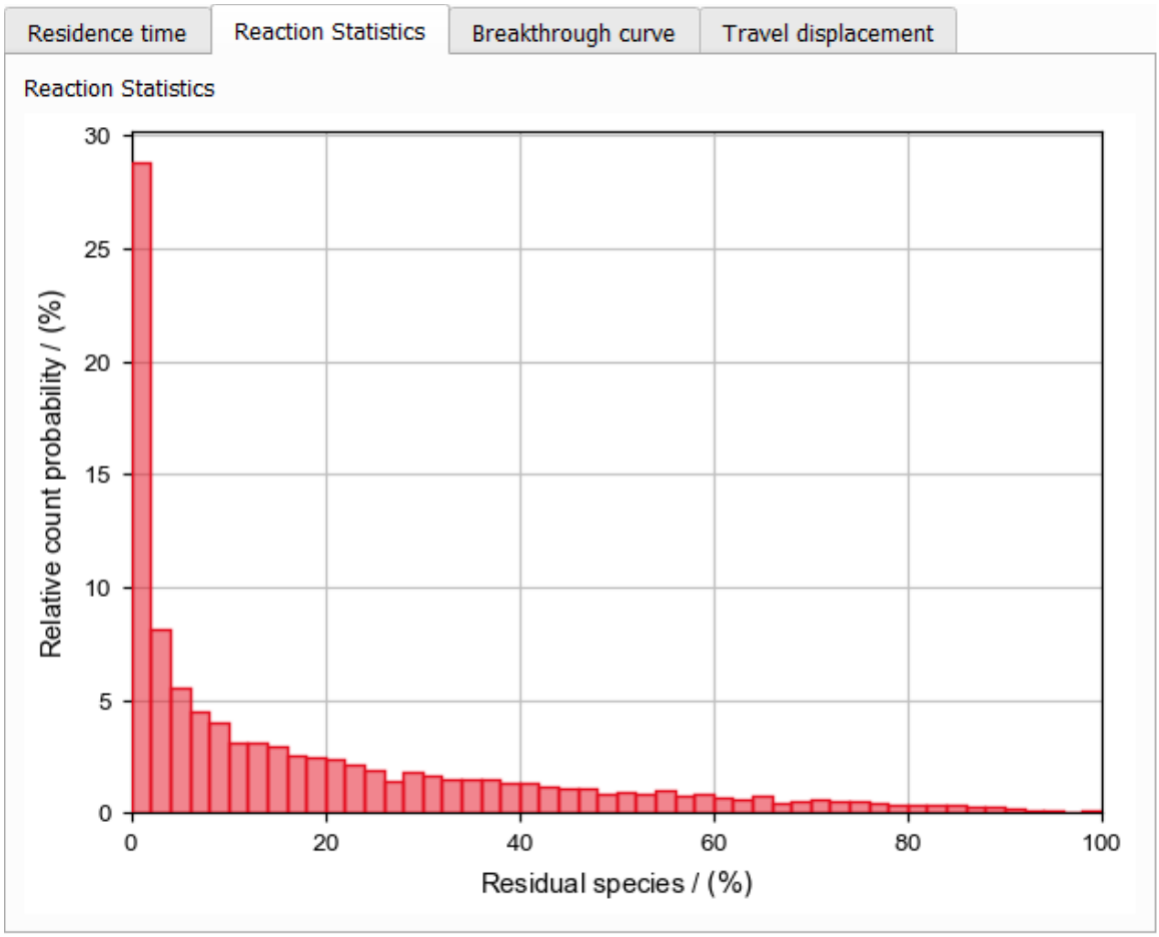
Residence time

The **Residence time** plot shows how much time particles spend in each pore and porous material. This plot is created if Compute Collision Statistics and Residence Times 62 in the **Report** subtab is selected. In the example shown here, ~14% of the particles are in the pore part of the structure (Water, ID 0) between $2e^{-04}$ s and $3e^{-04}$ s.



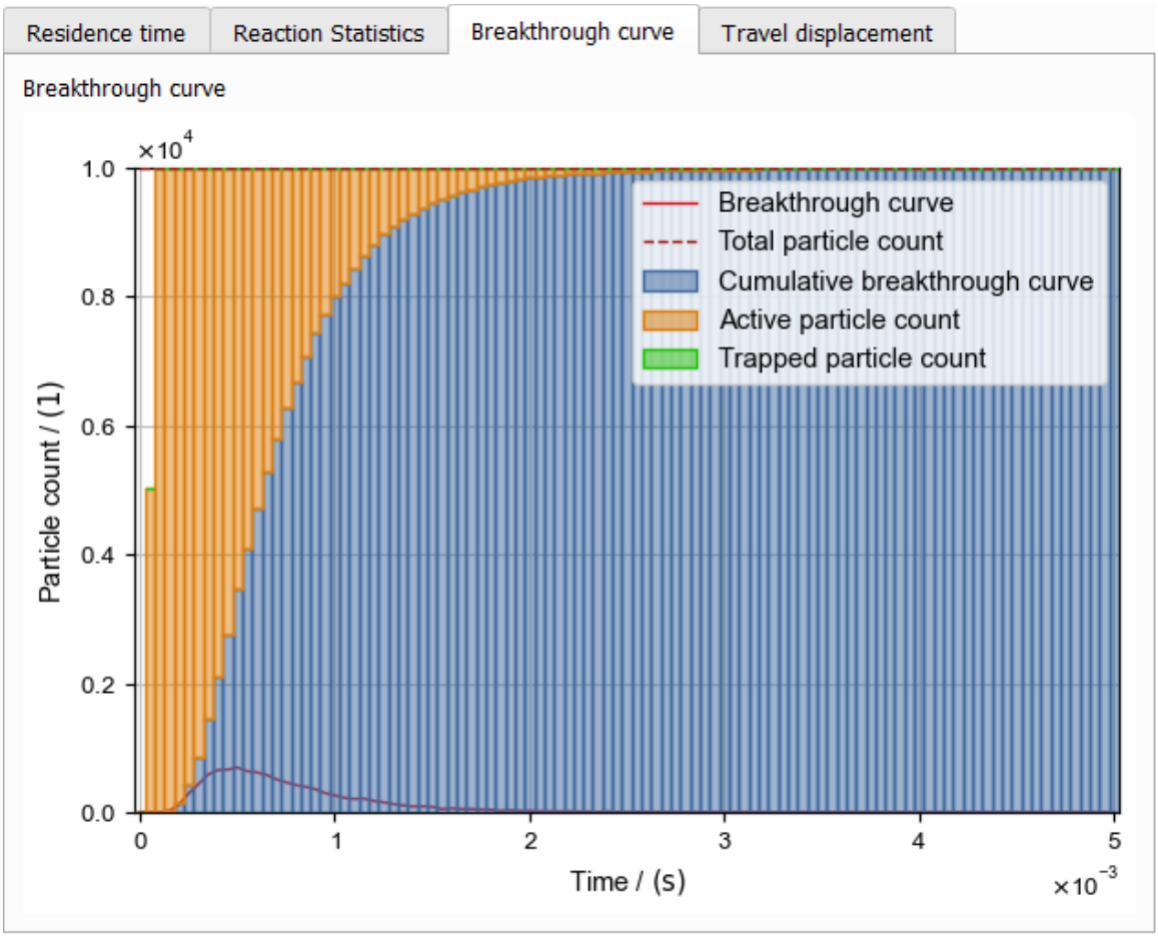
Reaction Statistics

A histogram of the **Reaction Statistics** of the chemical reactions is shown if Compute Chemical Reaction is checked 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 yet reacted and remain in the structure.



Breakthrough curve

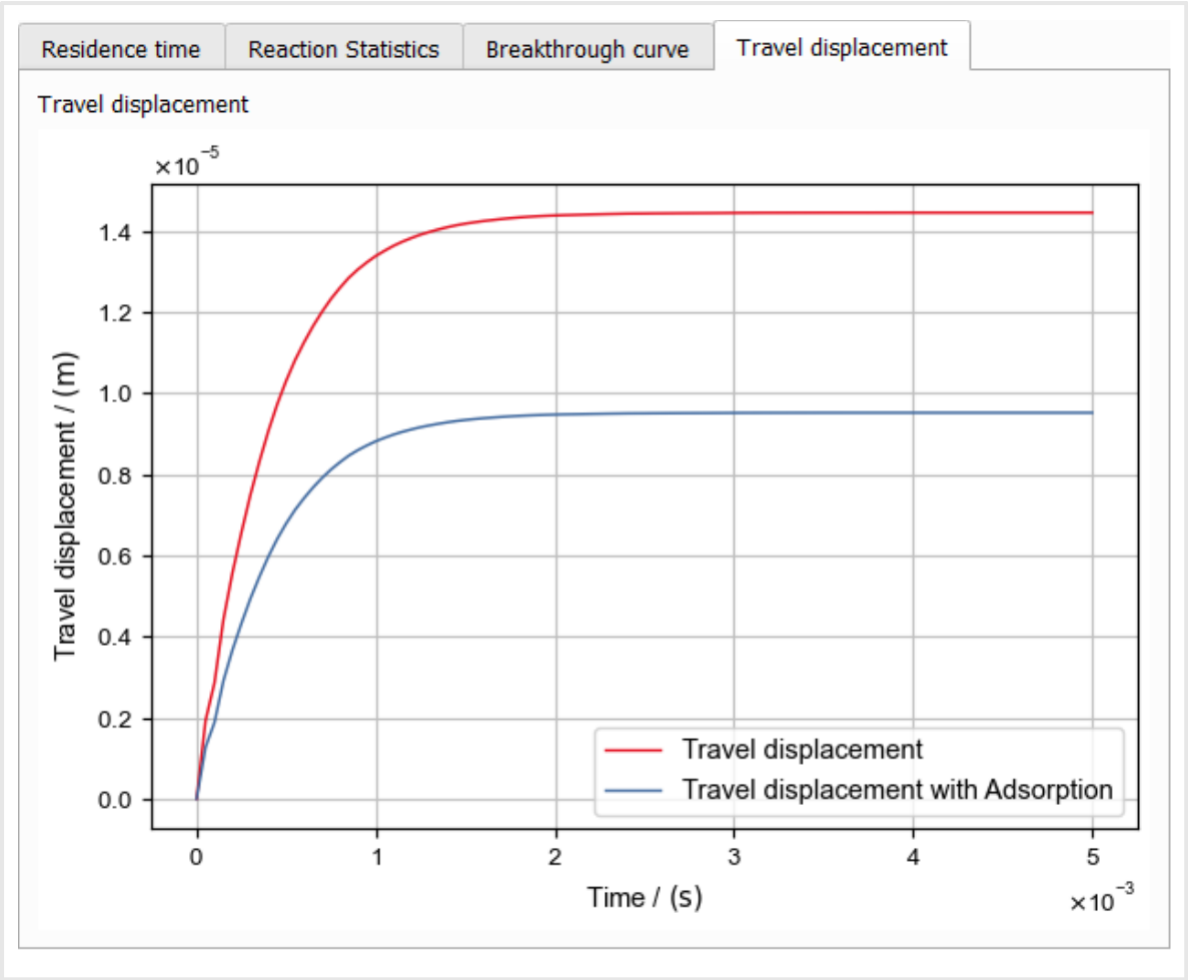
If the Compute Breakthrough Curve 61 box is checked, the **Breakthrough Curve** is shown as a graph over time. The graph shows additionally the values of the **Cumulative breakthrough curve**, the **Active particle count** and the **Trapped particle count** values listed in the table under the Report 59 subtab.



Travel displacement

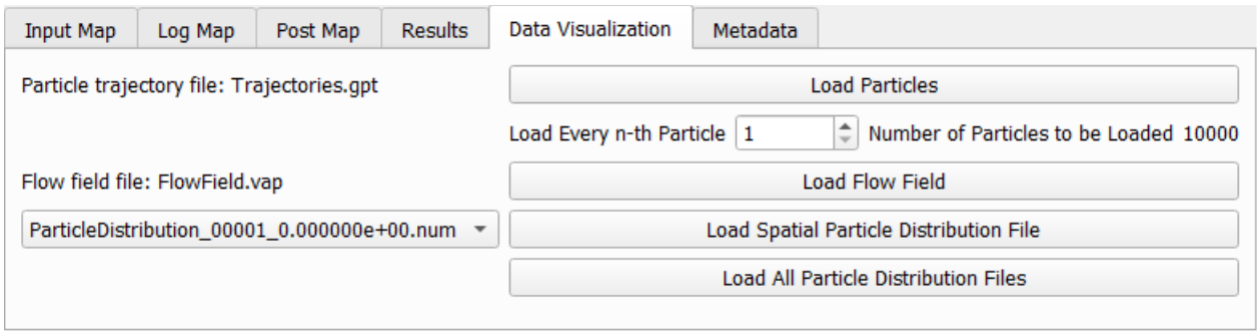
The **Travel Displacement** curve is shown when the Compute Average Displacement box is checked. The displacement of each particle is computed as the straight distance between its starting position and its final position at a given time. The displacement should not be confused with the distance that 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, an additional curve is shown in the plot, with travel displacements adjusted according to the defined adsorption time(s).



Data Visualization

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



Load Particles

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**.

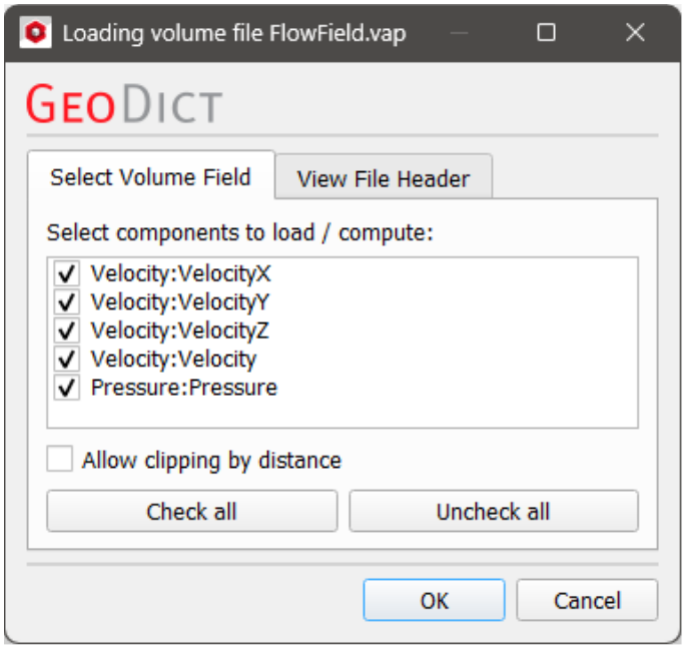
After loading, the structure model with the particles at their start position appears in the **Visualization area** of GeoDict. In the **Visualization panel**, directly above it, parameters for the visualization of the particles during the transport simulation are selectable under the **Particles** tab. Find further details on how to visualize particles in GeoDict in the Visualization user guide

Load 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 File** 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.

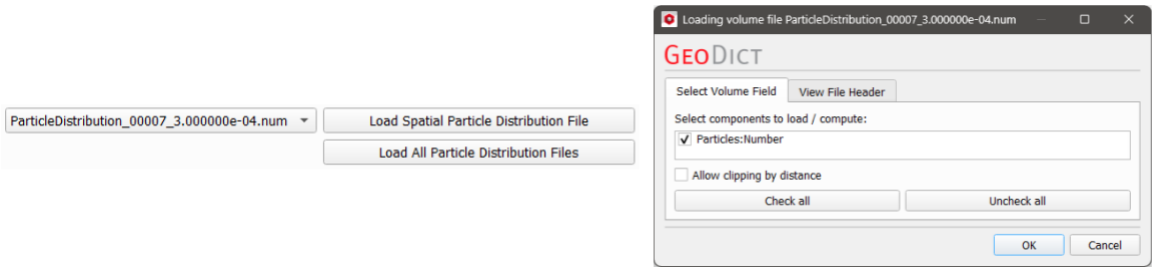
Click **Load Flow Field** and, in the opening dialog, select the desired components of the flow field to be shown. Click **OK**. The options available for the visualization of the flow field are the same as in FlowDict, SatuDict, or FilterDict. A detailed description of the visualization options can be found in the FlowDict user guide.



Load Spatial Particle Distribution File

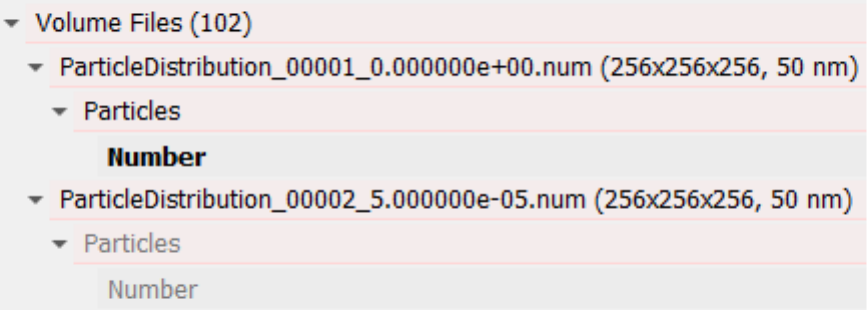
When the Compute Spatial Particle Distribution (*.num) box is checked under the **Output** tab or in the post-processing options of the Results tab, *.num files are created during the post-processing. These files can be imported for visualization by clicking **Load Spatial Particle Distribution File** or **Load All Particle Distribution Files** under the **Data Visualization** tab.

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 **Name_TimeStep_AbsoluteSimulationTime.num**. For example, the file *AddiDictResult_00007_3.000000e-04.num* corresponds to the time step 7 of the simulation, which was reached at t=0.3 milliseconds.

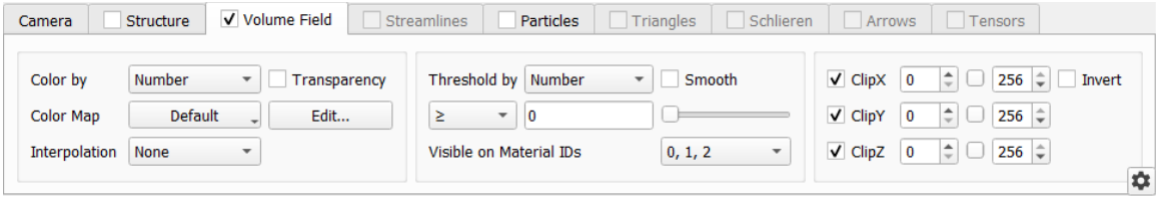


After choosing the *.num file, click **Load Spatial Particle Distribution File** and, in the **Loading volume file** dialog, keep the only option shown, **Particles:Number**. Click **OK**. The fields from other time steps can be loaded at any time by going back to the **Result Viewer**, choosing a new time step *.num file, and clicking **Load Spatial Particle Distribution File**.

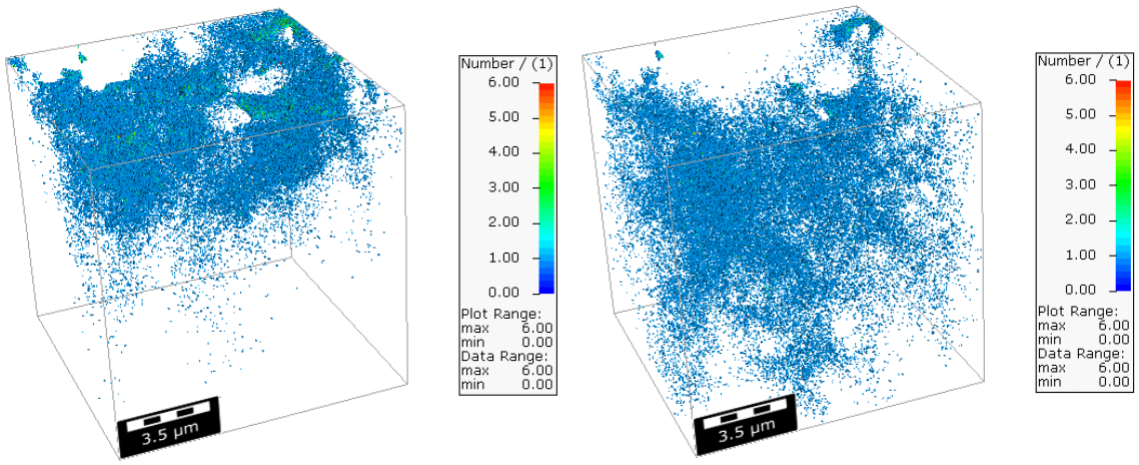
To access the fields from all time steps, choose **Load All Particle Distribution Files**. All *.num files with spatial particle distribution available are listed under Volume Fields in the left part of the GUI. The spatial particle distribution of each file can be accessed by double clicking **Number**. 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**). Additionally, under the **Volume Field** tab, select **None** for **Interpolation** and uncheck **Smooth** for **Threshold by**.



The **Threshold By** pull-down menu, with the entry **Number** for each of the *.num files (same 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.

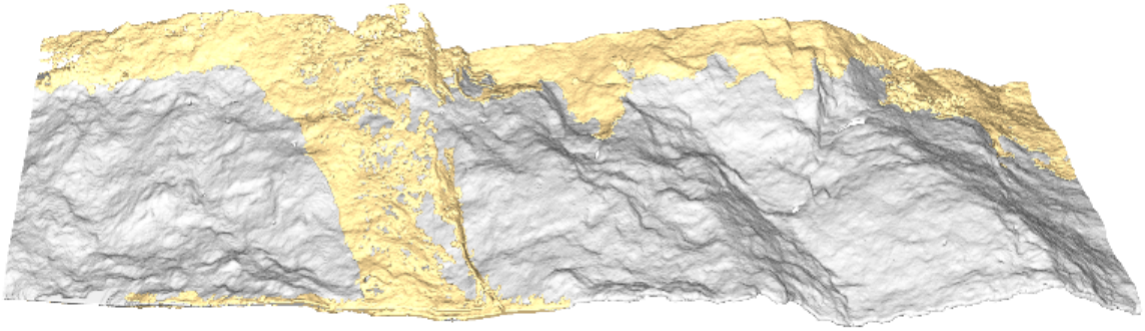


1.2.3 Examples

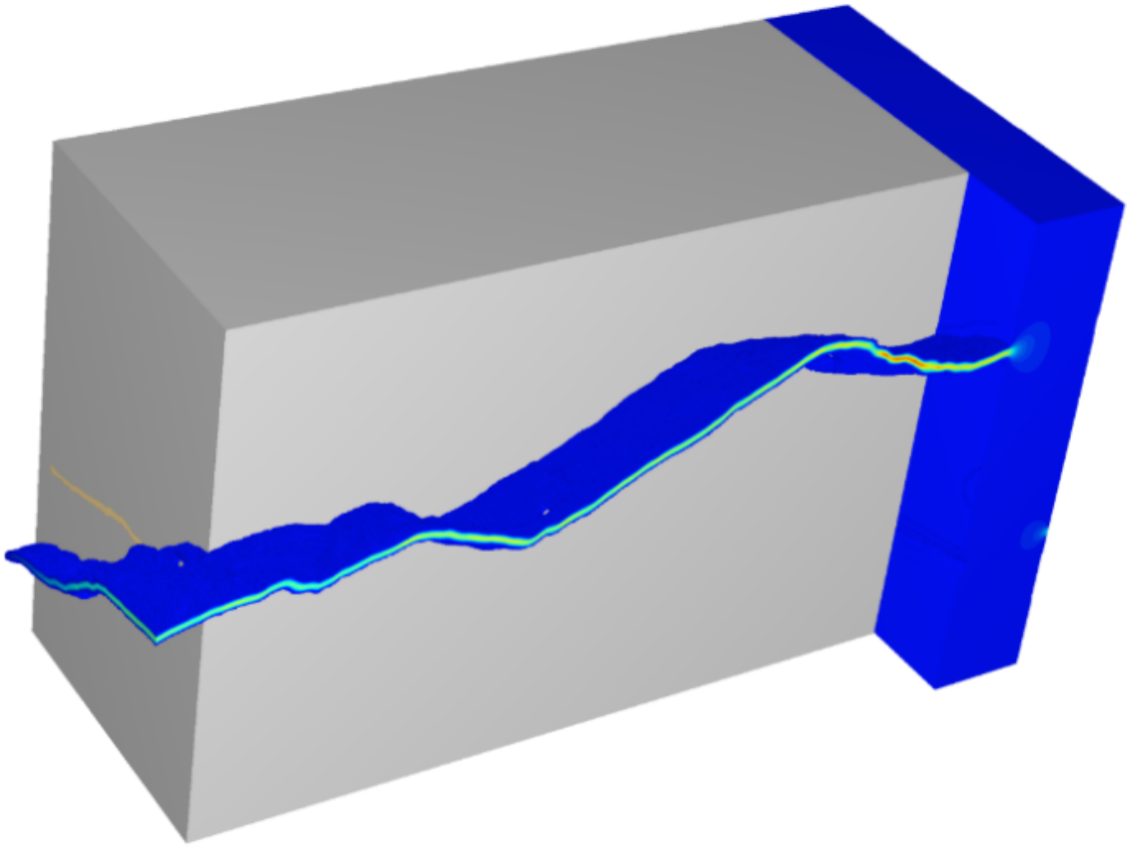
Transport of Particles in Fractured Rock

An example of a particle simulation with GeoDict is the experimental and numerical examination of the transport of particles in a fractured rock (Glatt et al., 2011)[158]. Here, three figures from the simulation are shown:

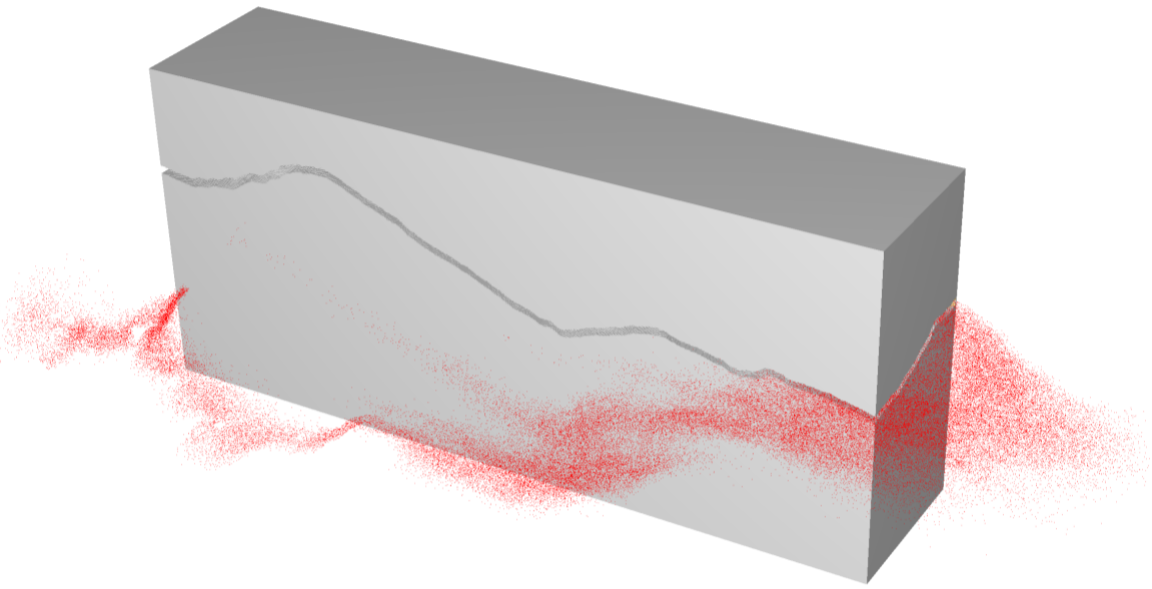
1. The 3D fracture geometry,



2. The water velocity computed in the fracture,



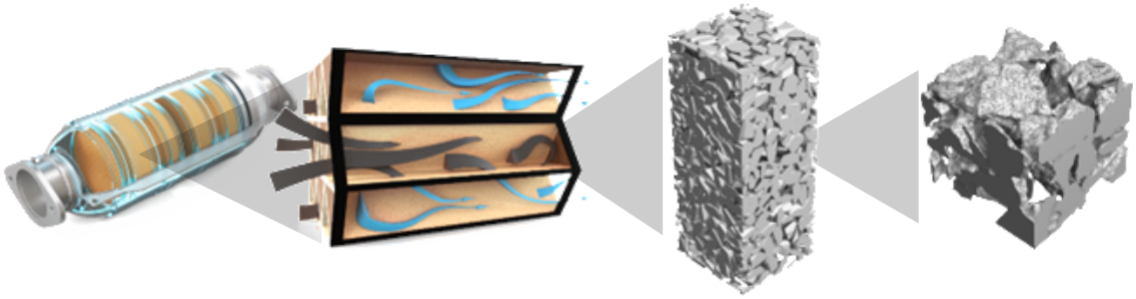
3. And a visualization of the particles from the transport simulation.



Simulation of Catalytic Converters

Modeling exhaust treatment bears many challenges at 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.



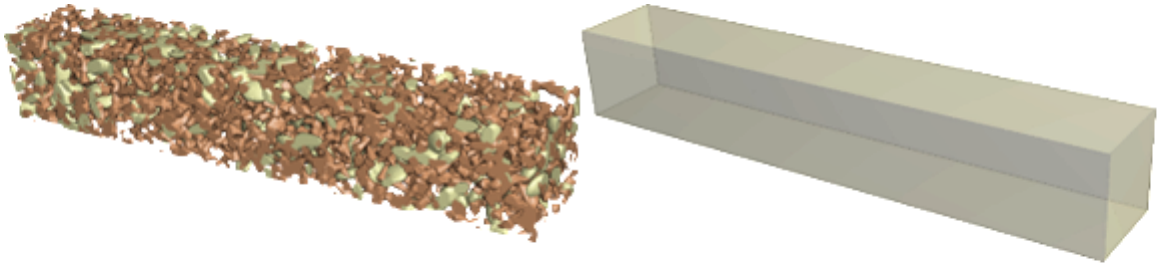
GeoDict provides the possibility to simulate on all these scales and to determine the relevant parameters for the upscaling.

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

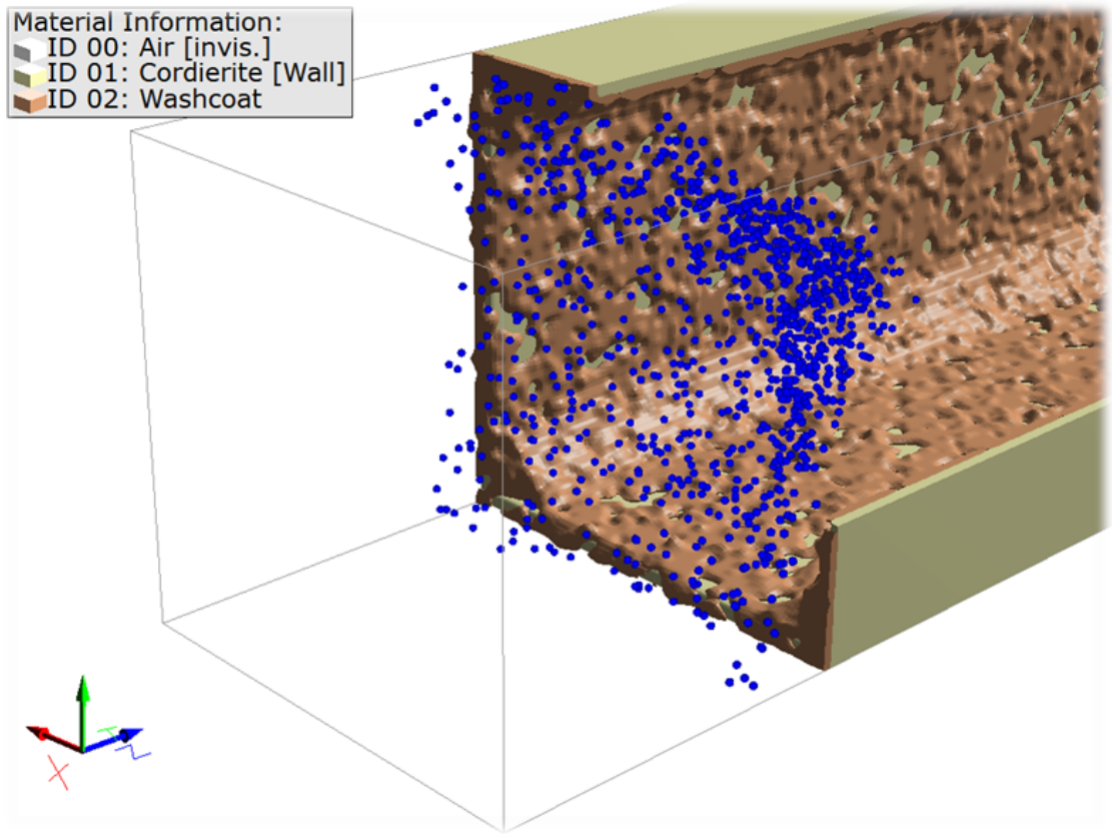
- Providing residence times in all pore and porous materials.
- Computing first order reactions.
- Simulate slip flow with improved molecule tracking near surfaces.
- Model reflection probability for porous media.
- Simulate effective molecule diffusivity.
- Simulate the influence of short-time adsorption on surfaces.
- Provide the possibility of choosing a maximal displacement as particle end position.

To simplify modeling and simulation of catalytic converters:

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 the effective diffusivity 60 for details. This allows to simulate the behavior on a larger scale but with the correct diffusivity of the microstructure.

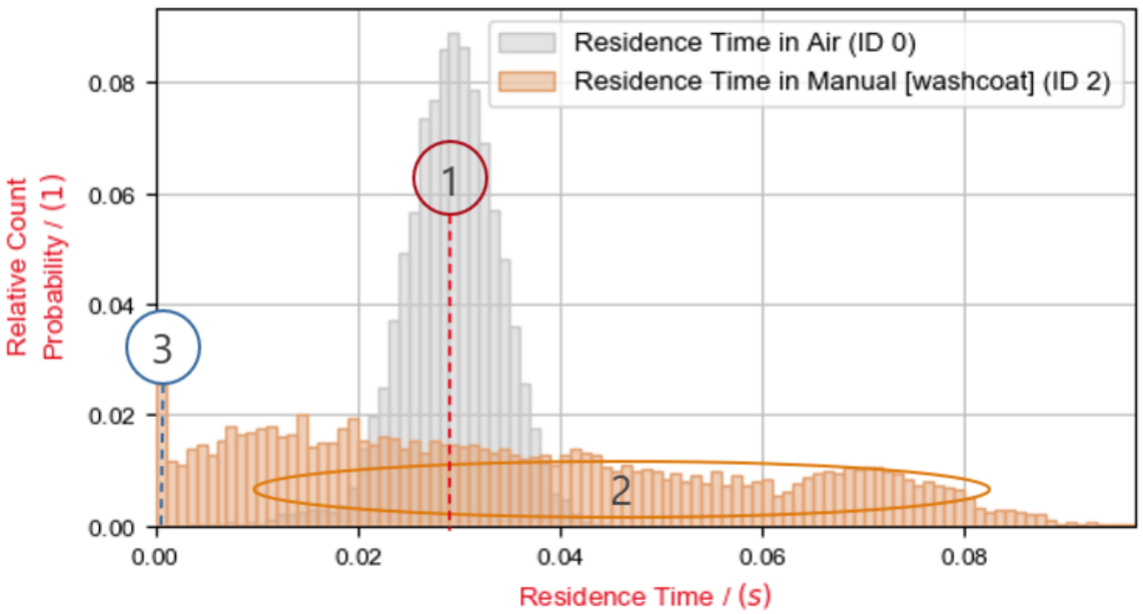


Model the wash coat layer of a channel as porous material. A reflection probability 38 for this material that defines the probability that molecules enter the wash coat layer can be defined.



AddiDict tracks the molecules on their way through the channel. Evaluate the residence time 64 of the molecule trajectories in each material, to investigate how long the molecules stay in the reaction zone (the wash coat layer). In the example shown here, the following behavior of the molecules can be observed from the residence times:

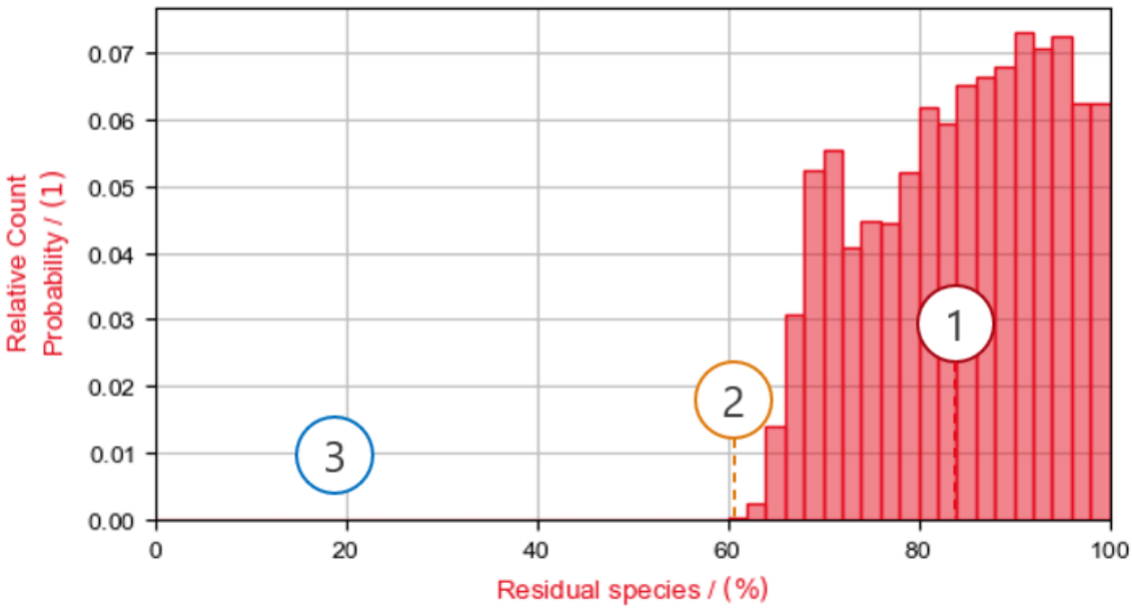
1. All molecules spent between 0.02 s and 0.04 s in air in the channel.
2. The time spent in the wash coat layer is very different for individual molecules.
3. Some molecules have not spent any time in the wash coat at all.



Finally, the residence times can be used to compute chemical reactions[65] of first order in the AddiDict post-processing, by defining reaction rate constants. In the example here, the following behavior can be observed:

1. On 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[34] as particle end position.

1.3 Transport Concentration Field

Use **Transport Concentration Field** to simulate and analyze how solute concentration fields evolve within a structure over time.

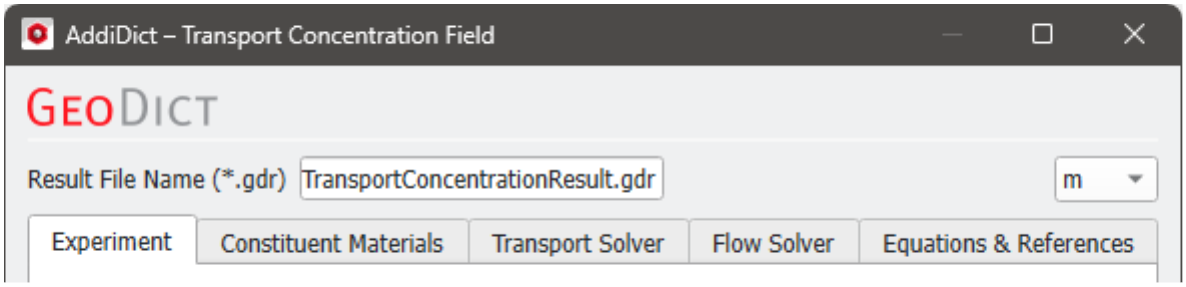
This feature models the movement of dissolved substances driven by advection (transport caused by fluid flow), diffusion (movement from regions of high concentration to low concentration), or a combination of both processes. It enables you to study how concentration gradients develop, spread, and interact with the surrounding geometry, helping you better understand mass transport behavior within complex systems.

The Transport Concentration Field command

- Options 77
  Understand the input parameters.
- Results 102
  View the simulation results.

1.3.1 Options

Select **Transport Concentration Field** from the pull-down menu and click the **Option**'s **Edit** button to open a dialog to enter or edit the simulation options. Choose a **Result File Name** for the result file (*.gdr) fitting to your current project.



The transport concentration field simulation parameters are organized under the tabs: **Experiment**, **Constituent Materials**, **Transport Solver**, and **Flow Solver**. The **Equations & References** tab gives a summary of the used equations and symbols which are explained in more detail in this user guide.

Tabs of the Transport Concentration Field dialog

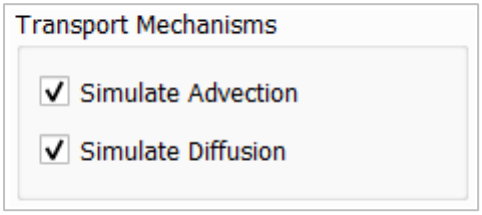
- Experiment 78
  Define flow and transport conditions.
- Constituent Materials 82
  Define the temperature and materials in your structure.
- Transport Solver 85
  Set up the transport solver, set the stopping criteria, and define the computational resources.
- Flow Solver 91
  Select the flow solver, set the stopping criteria, and define the computational resources.

Experiment

The **Experiment** tab is separated into five panels:

Transport Mechanisms

Select one or both of the **Transport Mechanisms** by checking the **Advection** and/or **Diffusion** boxes in the upper left part of the **Experiment** tab.

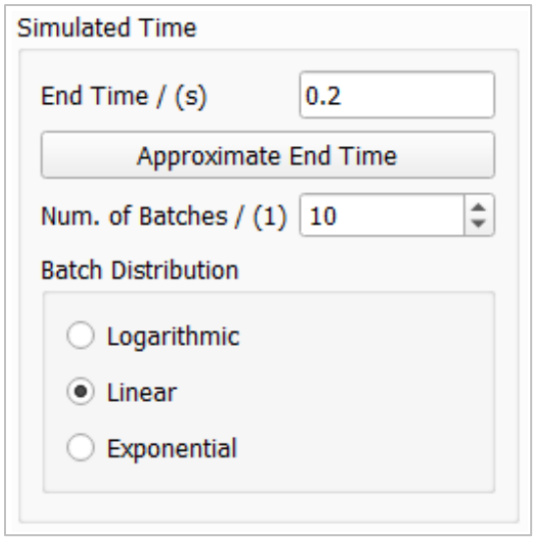


Check **Simulate Diffusion** to activate the computation of transport by diffusion. If the button is unchecked, the diffusivity is set to $D_0 = 0$ in the advection-diffusion equation 12.

Check **Simulate Advection** to activate the computation of advective transport due to the fluid flow. If unchecked, the velocity of the fluid is zero, i.e. $\vec{u} = \vec{0}$ in the advection-diffusion equation 12, and therefore, the concentration field is transported by diffusion only. In this case, the Flow Boundary Conditions 81, the Flow Solver 91 tab, and the Inflow Concentration 80 are set inactive.

Simulated Time

In the **Simulated Time** panel, the physical **End Time** of the simulation can be specified. The initial time is always zero. By clicking the **Approximate End Time** button, the **End Time** is automatically determined such that, for the specified average fluid velocity (defined in the Flow Boundary Conditions 81 panel by **Mean Velocity** or by **Flow Rate**), most of the solute passes through the entire structure and a complete breakthrough curve is computed. When it is unclear how to choose the **End Time**, it is highly recommended that the **Approximate End Time** is used before starting the simulation. The approximation works best for high Péclet 80 numbers, i.e., when advection dominates the transport.

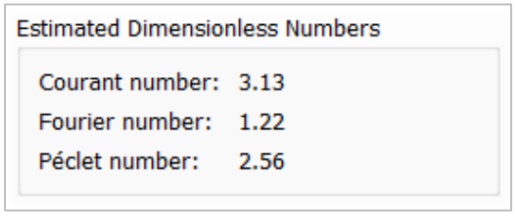


The simulation time can be divided into intervals (so-called "time batches"), after which the concentration field and other information is written to disk. Define the **Number of Batches**. Depending on which time period should be more finely resolved, one of the following options can be chosen:

- **Logarithmic**: Time batches are large close to zero and small close to the end time.
- **Linear**: All time batches have the same size.
- **Exponential**: Time batch sizes are small close to zero and large close to the end time. This option is useful for scenarios that approach a stationary state.

Estimated Dimensionless Numbers

In this panel, three **Dimensionless Numbers** are automatically estimated based on the entered parameter values, provided a structure is loaded. They give you an idea of how strongly advection and diffusion contribute to transport *before* the simulation is started. After the simulation, more precise values are listed in the report.



The **Courant number** Co quantifies the extent to which particles, molecules, or concentration fields are transported through the structure by advection during the simulation. For instance, if $\mathrm{Co} = 0.5$, then the solute (particles, molecules, or the concentration field) is advectively transported by the flowing solvent across half of the domain. The Courant number is defined as:

$$\mathrm{Co} = \frac{V\,T}{L} \tag{42}$$

where V is the characteristic velocity estimated from the flow boundary conditions, T is the simulation time (which equals the **End Time**, given that the initial time is zero), and L is the length of the structure in the through direction.

In contrast, the **Fourier number** Fo quantifies the extent to which the solute (particles, molecules, or the concentration field) is transported through the structure by diffusion during the simulation. The Fourier number is defined as:

$$\mathrm{Fo} = \frac{D\,T}{L^2} \tag{43}$$

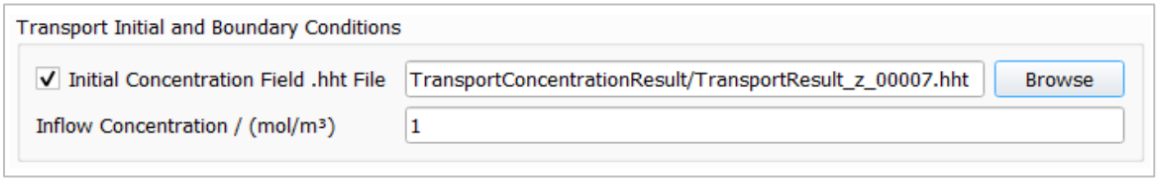
where D is the characteristic diffusivity, taken as the maximum effective diffusivity across all existing materials.

Finally, the **Péclet number** Pe is the ratio of advective transport to diffusive transport. A Péclet number of infinity implies purely advective transport, whereas a value equal to zero corresponds to purely diffusive transport. The Péclet number is defined as:

$$\mathrm{Pe} = \frac{V\,L}{D} = \frac{\mathrm{Co}}{\mathrm{Fo}} \tag{44}$$

Transport Initial and Boundary Conditions

In the **Transport Initial and Boundary Conditions** panel, the initial concentration distribution in the structure and the **Inflow Concentration** can be defined. **Inflow Concentration** is only available if Simulate Advection 78 is checked as otherwise the inflow boundary is not available.



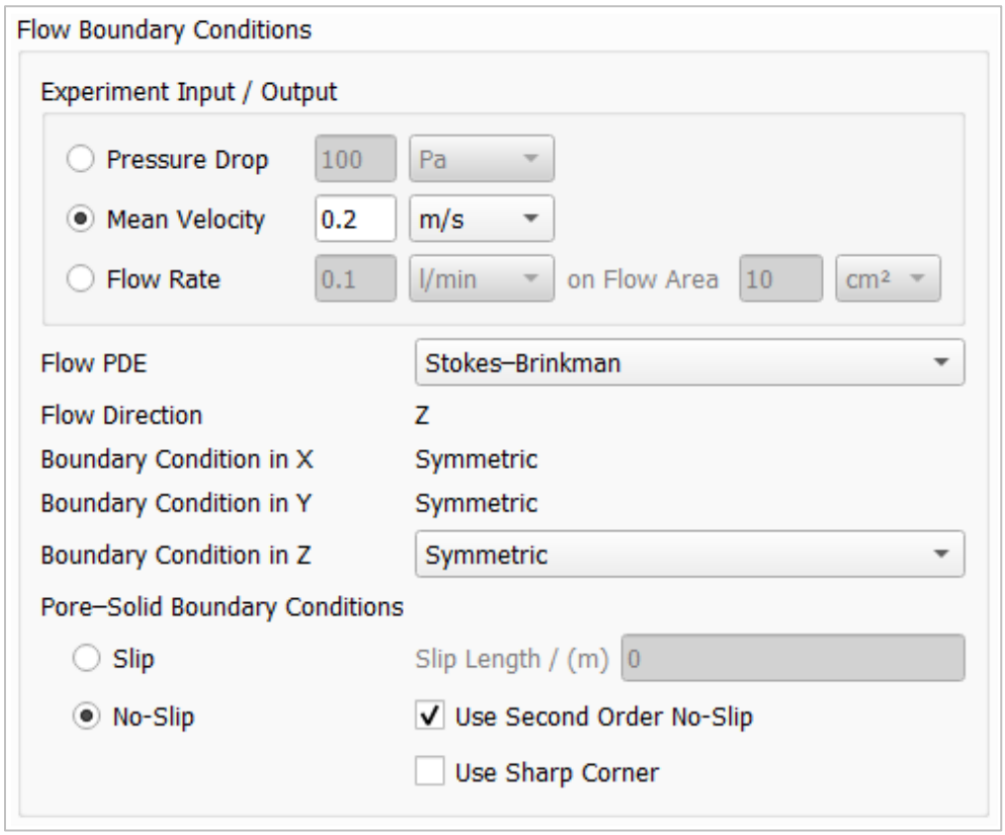
When the check box next to **Initial Concentration Field .hht File** is checked, a concentration field can be loaded by clicking **Browse**. Through this option, an initial distribution of the solute in the structure can be defined. For each time batch 78, AddiDict automatically generates a *.hht file, so the output of a previous transport simulation can easily serve as the input for subsequent runs. Alternatively, *.hht files can be manipulated with Python scripting.

Under the **Inflow Concentration**, a concentration value that represents the amount of solute carried into the structure by the inflowing solvent fluid can be set. Currently, the distribution of one solute species can be simulated in a **Transport Concentration Field** simulation at a time.

Flow Boundary Conditions

In the **Flow Boundary Conditions** panel, either the **Pressure Drop**, the mean flow **Velocity**, or the **Flow Rate** can be defined. Note that this part of the dialog is accessible only if Simulate Advection 78 is selected.

Important! In AddiDict, the fluid flow and transport is always computed in **Z-direction**. If another direction is required, the 3D model can be rotated with ProcessGeo prior to using AddiDict.



From the **Flow PDE** menu, you can specify the equations to be solved for computing the fluid flow field. The flow field is required to simulate the particle movements and trajectories or transport of the concentration field. (Navier-)Stokes equations describe fluid flow in structures containing only solid materials and pores. (Navier-)Stokes-Brinkman equations describe the flow through structures containing porous materials, solids, and pores. Use the Stokes equation when fluid velocities are slow or the viscosities are high, i.e., at low Reynolds numbers. The Navier–Stokes equation should

be used for high fluid velocities when inertial effects cannot be neglected.

Note! The **Adsorption** command always requires (Navier-)Stokes-Brinkman equations since the Adsorbent needs to be defined as porous solid.

The used flow boundary conditions in **X** and **Y** direction are reported. For the **Track Particles & Molecules** command 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 leads to **Symmetric** flow boundary conditions.
- **Periodic** particle movement requires **Periodic** flow boundary conditions.

For the **Transport Concentration Field** and **Adsorption** commands the boundary conditions in **X** and **Y** direction are fixed to **Symmetric**.

The boundary condition in **Z** direction, can be **Periodic**, **Symmetric**, or **VinPout**. Please refer to the FlowDict user guide for more details. For the **Track Particles & Molecules** command, using the Stokes(-Brinkman) equation only allows for using **Periodic** or **Symmetric** boundary conditions, while the Navier-Stokes(-Brinkman) equation uses the **VinPout** 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. The default **Slip Length** of zero corresponds to a flow velocity of zero along the solid surface. 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, e.g., for gases when the mean free path is comparable to the pore size. The same slip length must be set for all materials in the structure. Find more details on the **Slip Length** here.

For the **No-Slip** boundary condition two additional options are available:

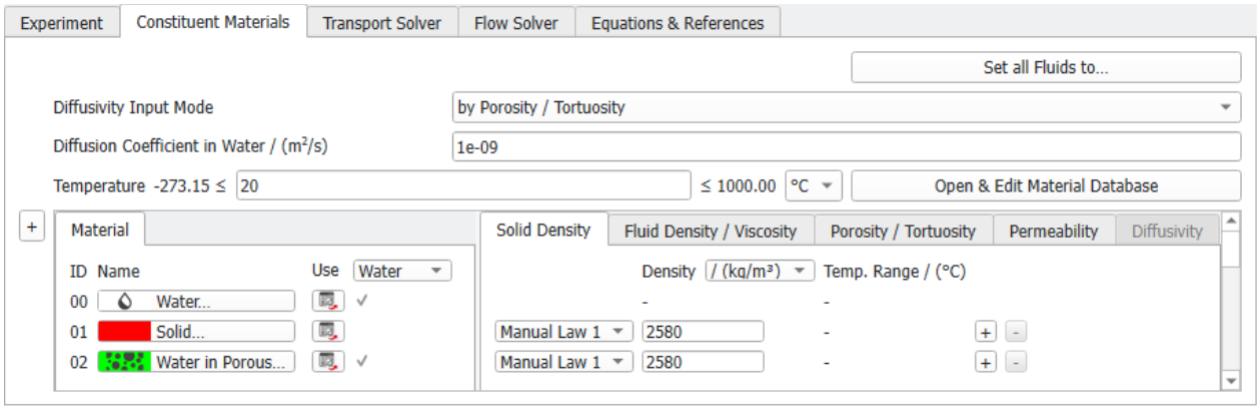
- **Use Second Order No-Slip** (default): This option sets the tangential velocity to zero at the center of the voxel surfaces and use a second order approximation of the velocity field.
- **Use Sharp Corner**: This option sets the tangential velocity to zero at the voxel corners.

Find more details on these settings in the FlowDict user guide.

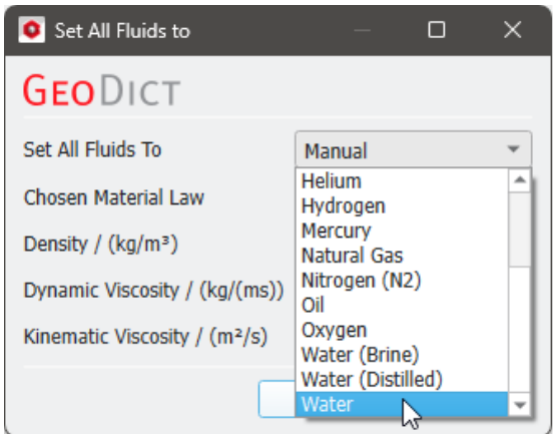
Constituent Materials

Define the materials in the structure and their properties in the **Constituent Materials** tab.

The **Temperature** 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.



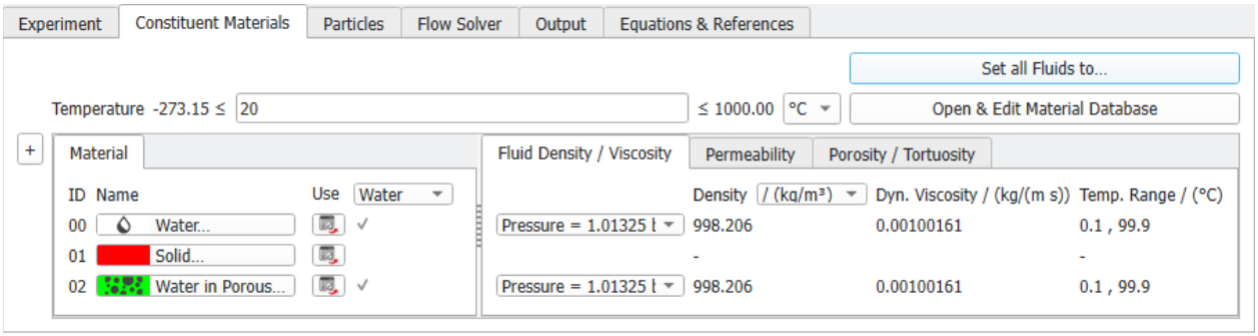
The fluid flowing through all pore and porous materials can be set by clicking **Set all Fluids to** and selecting it from the pull-down menu.



If one of the predefined fluids is used, the values for **Density**, **Dynamic Viscosity**, and **Kinematic Viscosity** are taken from the material database and are dependent on the given **Temperature** value. If **Manual** is chosen, you can enter these values manually.

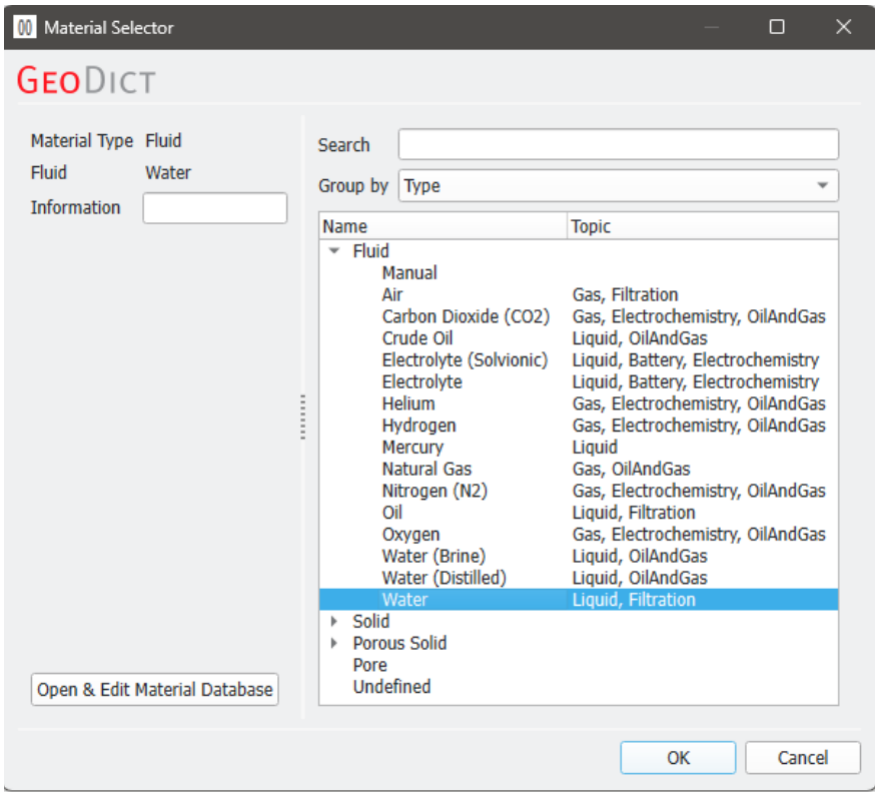
Any values entered manually, e.g., those for a special type of oil, can also be added to the Material Database. Find more information on editing, expanding, and using the material database in the respective user guide.

As soon as you define 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 ID 02. The density and the dynamic viscosity of this fluid, at the selected temperature range, is shown under the **Fluid Density/Viscosity** subtab.



All materials assigned to the material IDs, which fall into one of the material categories (pore,

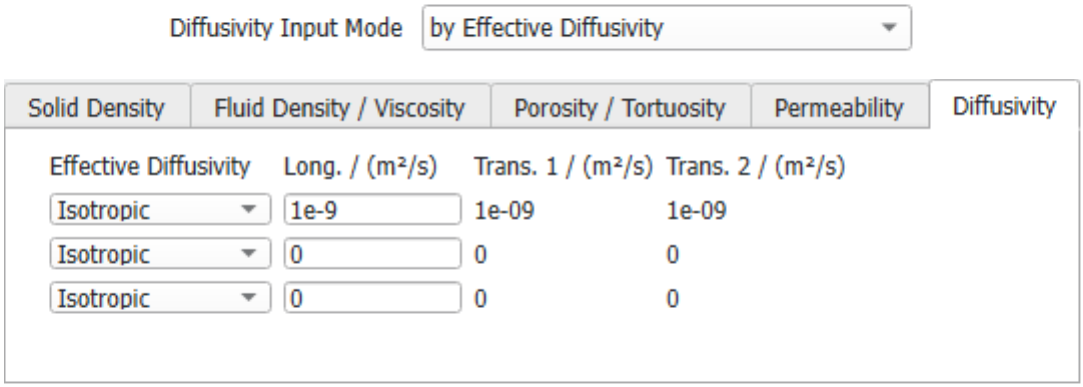
porous or solid), can be selected individually through the **Material Selector** dialog, by clicking on the material's buttons. Fluid flow can occur only in pores and in porous materials.



Under the **Constituent Materials** tab the effective diffusivity of the solute in the fluid and porous materials needs to be defined. Here two options are available for the **Diffusivity Input Mode**:

by Effective Diffusivity

Select the option **by Effective Diffusivity** to activate the **Diffusivity** subtab in the bottom right of the dialog. In this subtab the **Effective Diffusivity** D_{eff} can be set for all materials manually.



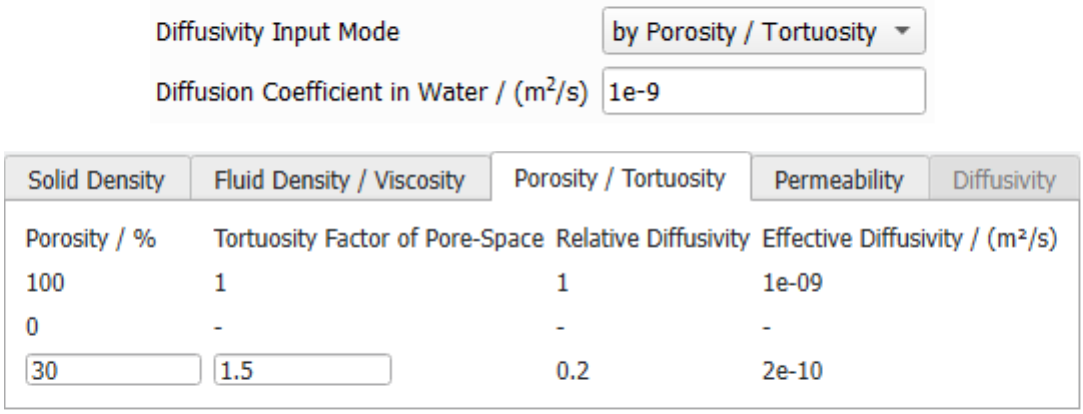
by Porosity/Tortuosity

Select **by Porosity/Tortuosity** to activate the field for the **Diffusion Coefficient in**

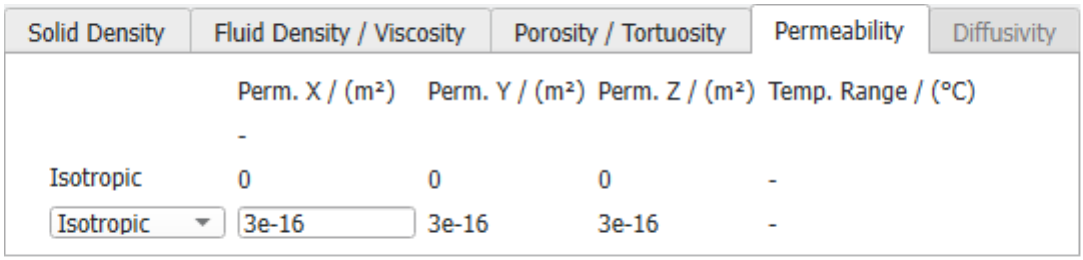
Fluid and the **Porosity / Tortuosity** subtab in the bottom right of the dialog. In the field for the **Diffusion Coefficient in *Fluid*** the diffusion coefficient D_0 for the solute in the fluid material in the structure needs to be provided, e.g., for solute in water. This value is automatically set as effective diffusivity for the fluid material. Under the **Porosity / Tortuosity** subtab the porosity ϕ and the tortuosity τ for each porous material need to be defined. These values are used to calculate the relative (D_{rel}) and effective (D_{eff}) diffusivity for each porous material:

$$D_{\mathrm{rel}} = \frac{\phi}{\tau} \tag{45}$$

$$D_{\mathrm{eff}} = D_{\mathrm{rel}} \cdot D_0 \tag{46}$$

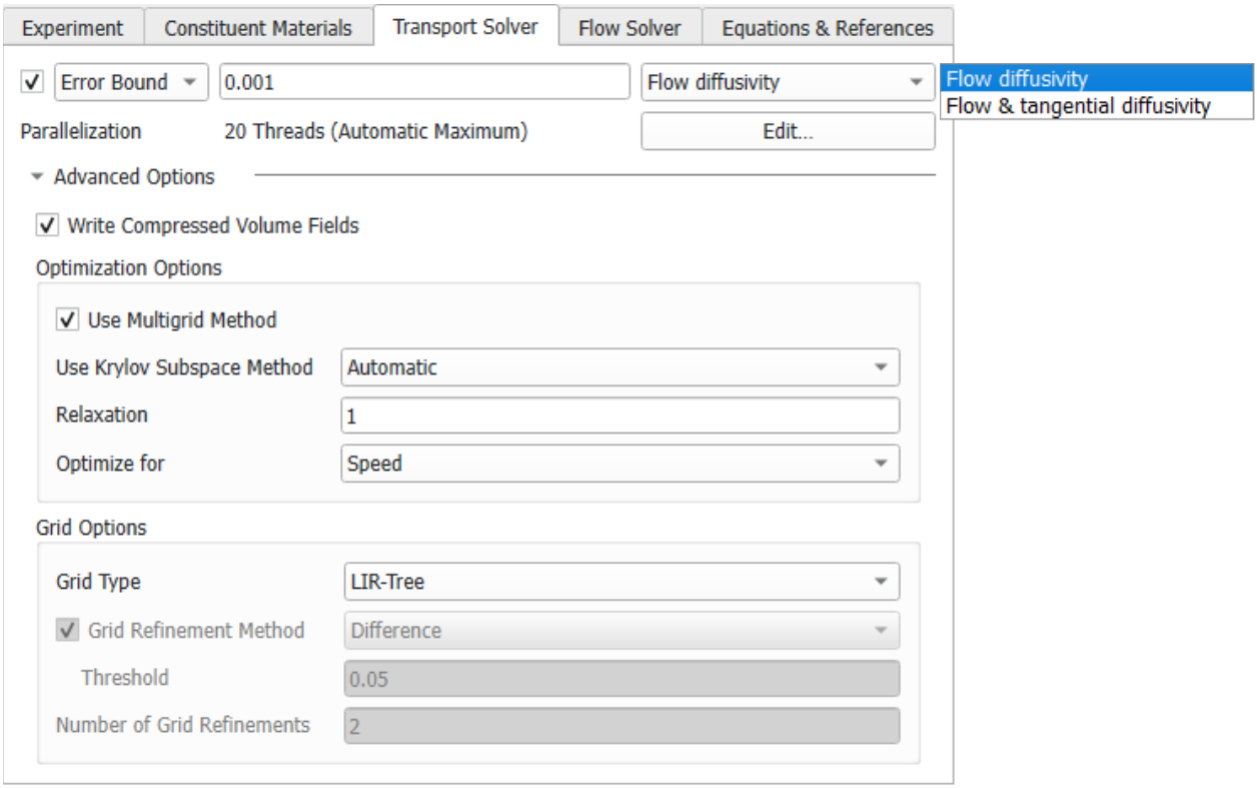


For porous materials, their permeability needs to be defined on the **Permeability** subtab.



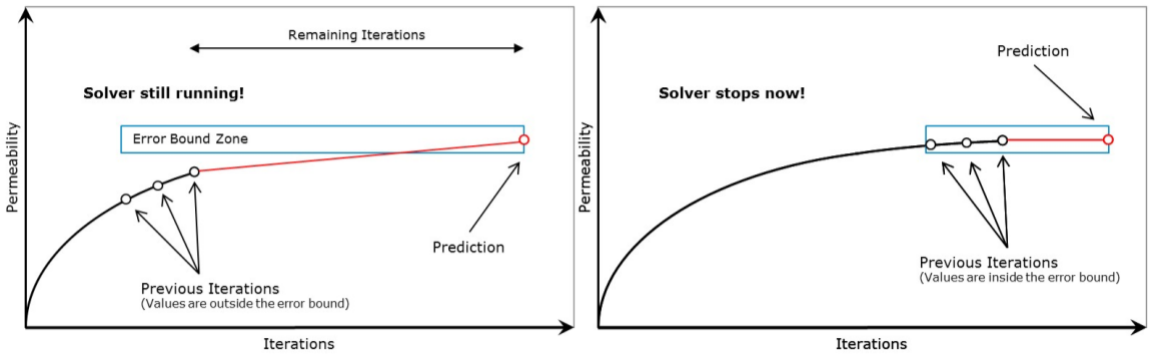
Transport Solver

Under the **Transport Solver** tab, several options regarding the solver for the transport of the concentration field are available. The solution algorithm for concentration field transport is integrated into the LIR solver only.



Stopping Criterion

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



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

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

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

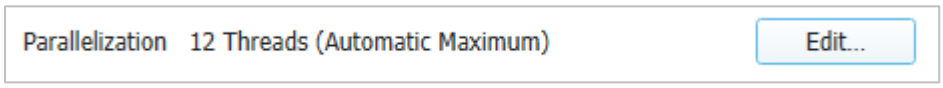
$$\max_{i\in[1,100]} \frac{x_c - x_{c-i}}{x_{c-i}} < \text{tolerance} \tag{47}$$

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

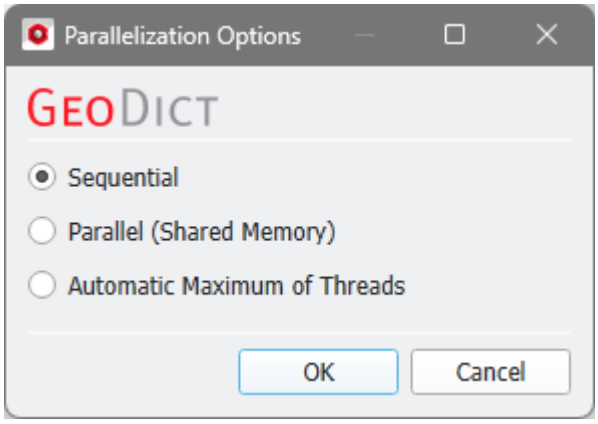
Parallelization

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

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

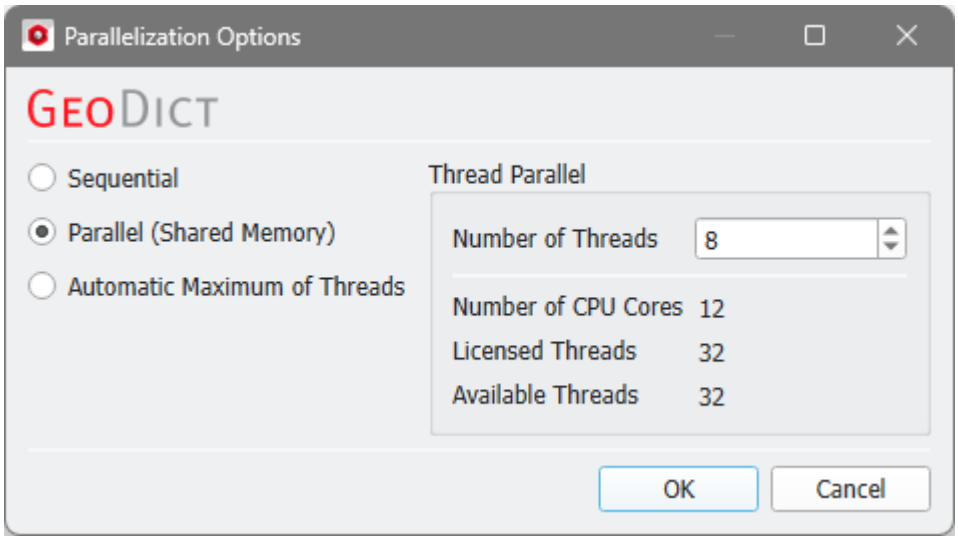


Selecting **Sequential** will not apply parallelization and only one thread is used for the computation.

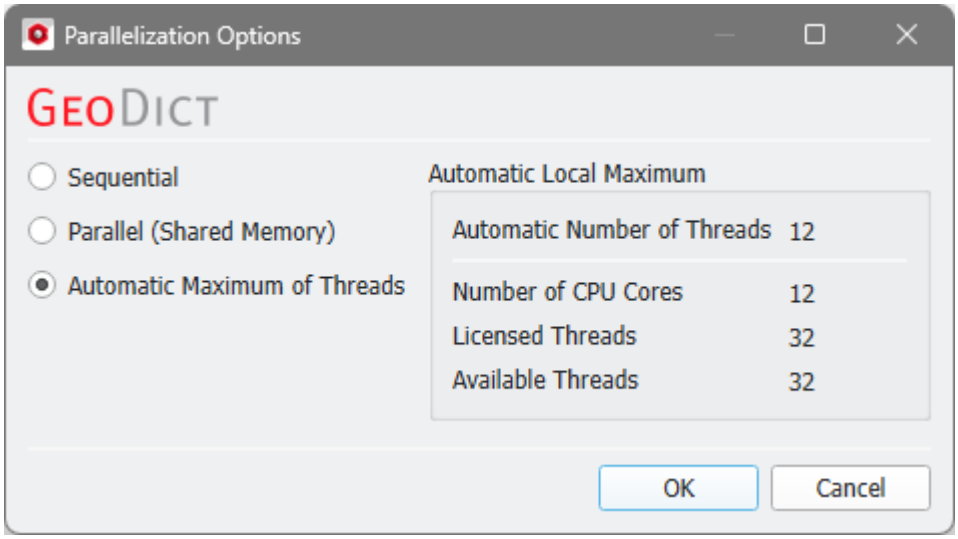


When **Parallel (Shared Memory)** is selected, the **Number of Threads** can be entered. Below, the **Number of CPU Cores** that the current machine has, the maximum number of **Licensed Threads** and the number of those licensed threads that are available (**Available Threads**) are shown in the dialog.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

parallel processes you can use, is the smallest of those three numbers.



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



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

Advanced Options

Write Compressed Volume Fields

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

If the option **Write Compressed Volume Fields** is checked, then the adaptive grid is used as compression method for writing out *.hht files. This option allows to save 80-

90% space on hard drive. The runtime for writing *.hht files is also reduced significantly. But the runtime for loading and uncompressing of compressed *.hht is increased by the amount of runtime that was saved for writing out compressed *.hht files.

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

Optimization Options

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

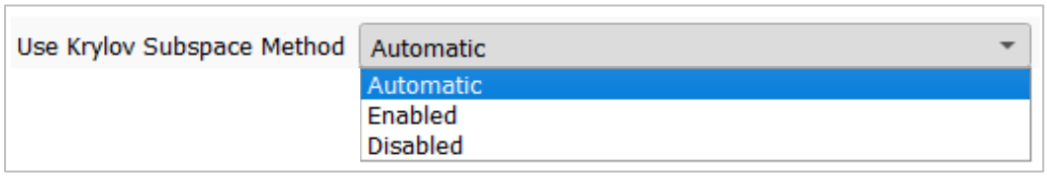
The method is available to solve the Stokes and Stokes–Brinkman equations as well as for solving mechanics, diffusion, thermal, and electrical conduction and is enabled by default.

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

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

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

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

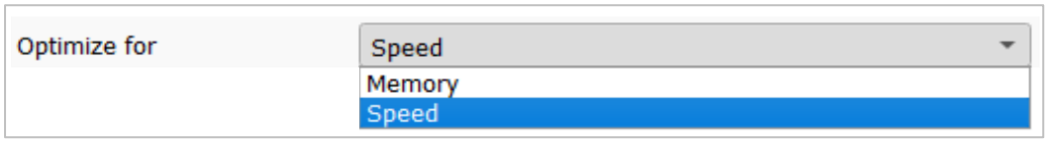


Note! In case that the Krylov subspace method (BICGStab) is used, the **Relaxation** may also be adapted automatically.

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

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

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



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

Grid Options

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

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

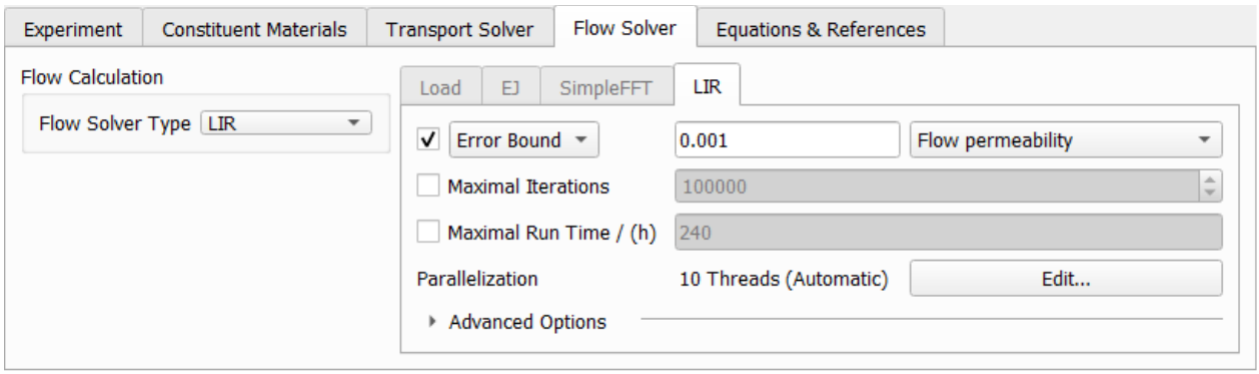
The solver can analyze the result field during the computation and improves the adaptive grid in places where more accuracy is needed. The LIR solver splits cells where a high gradient occurs.

The other **Grid Options** are fixed and shown for your reference only.

Flow Solver

Under the **Flow Solver** tab, the settings for the flow solver used in the AddiDict simulation can be chosen and its parameters can be defined. The tab is subdivided into two panels for **Flow Calculation** and **Solver Settings**.

Important! 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.

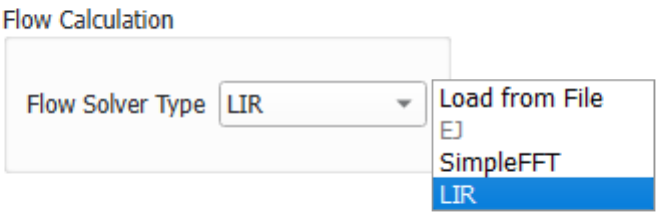


Flow Solver Panels

- Flow Calculation 91
  Choose the flow solver.
- Solver Settings 92
  Learn more about stopping criteria, parallelization, and advanced settings.

Flow Calculation

In the **Flow Calculation** panel on the top left, select the **Flow Solver Type** to be used for solving the chosen partial differential equations from the pull-down menu (EJ, SimpleFFT, or LIR). EJ cannot be selected for solving Brinkman equations.



It is also possible to choose **Load from file** to import the result file (*.gdr) 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.

Solver Settings

General Settings

Stopping Criteria

The equations are solved by an iterative approach.

Iterative Solver

The basic idea of an iterative method is to

1. Start with some initial guess for the unknown values
2. Improve the current values in each iterative step
3. Repeat the iterative process until one of the stopping criteria is reached.

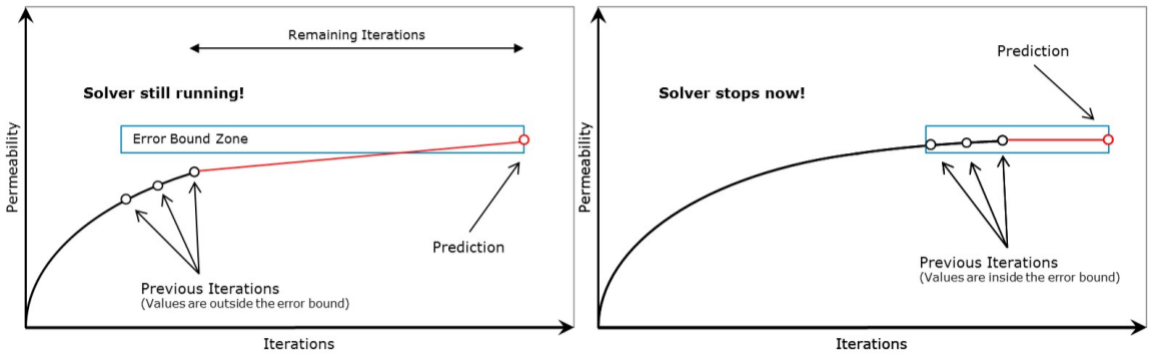
The iterative process is controlled by setting the values and activation for **Error Bound, Tolerance, Residual**, **Maximal Iterations**, and **Maximal Run Time (h**). The stopping criteria apply for each computational direction individually.

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

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

Error Bound

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



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

Tolerance

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

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

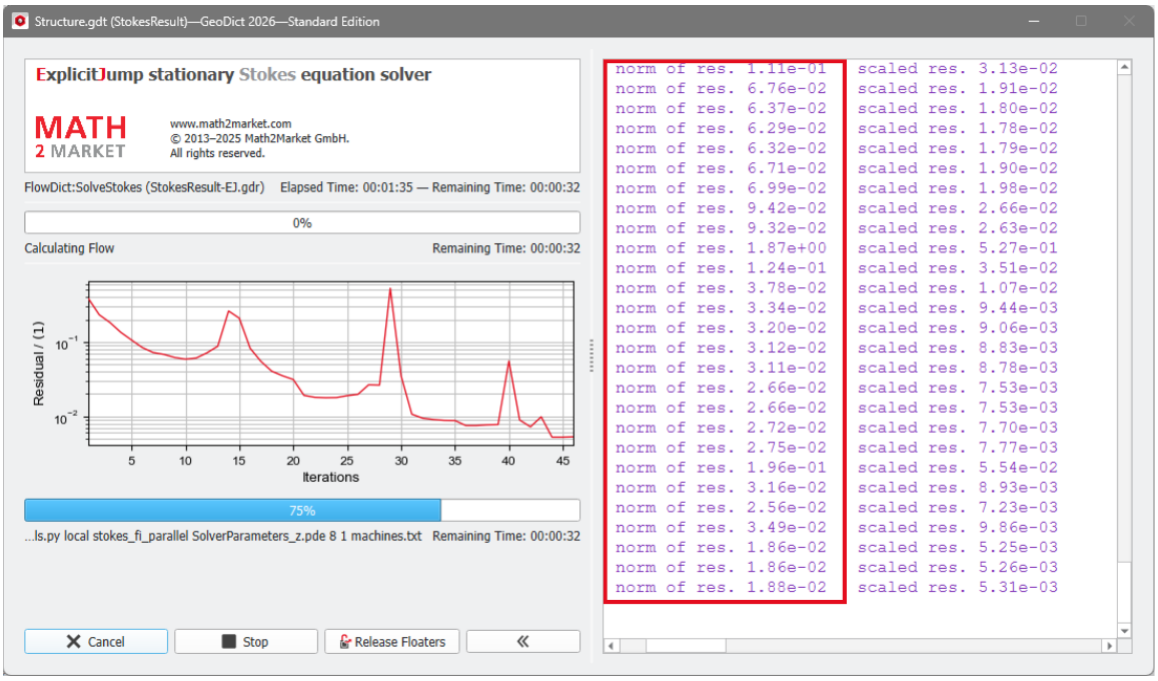
$$\max_{i\in[1,100]} \frac{x_c - x_{c-i}}{x_{c-i}} < \text{tolerance} \tag{48}$$

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

Residual

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

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



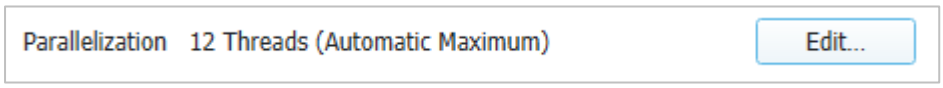
The recommendation to choose **Tolerance** or **Residual** for the **EJ** solver is based on the structure's porosity. Both give similar results for highly porous structures. For dense structures, if using the Schur Complement **Residual**, the relative norm of the residual may be small even though the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

Parallelization

Parallelization

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

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



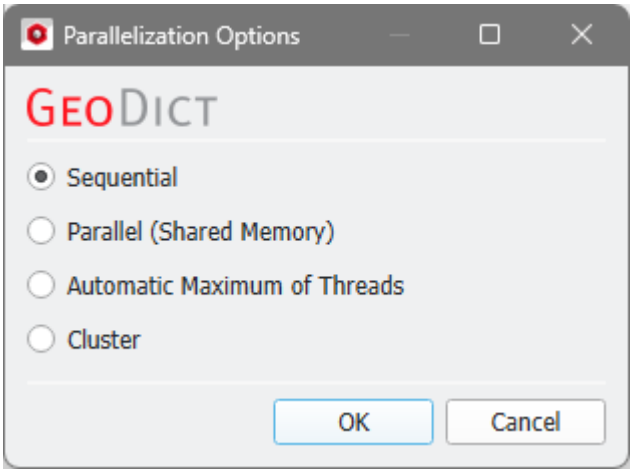
The parallelization of the solvers is done with two technical methods: **MPI Parallelization** or **Thread parallelization**. The following table shows the support of both parallelization methods:

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

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

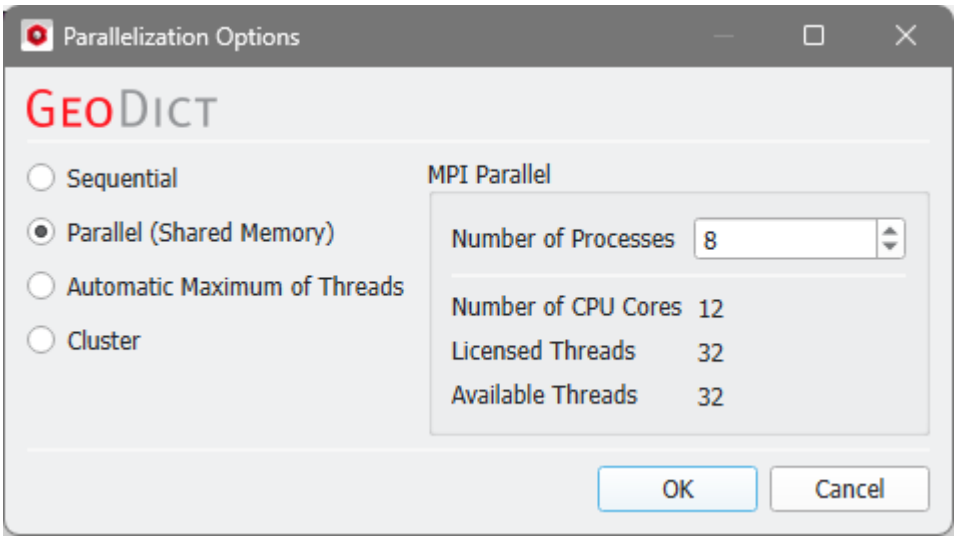
Sequential

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



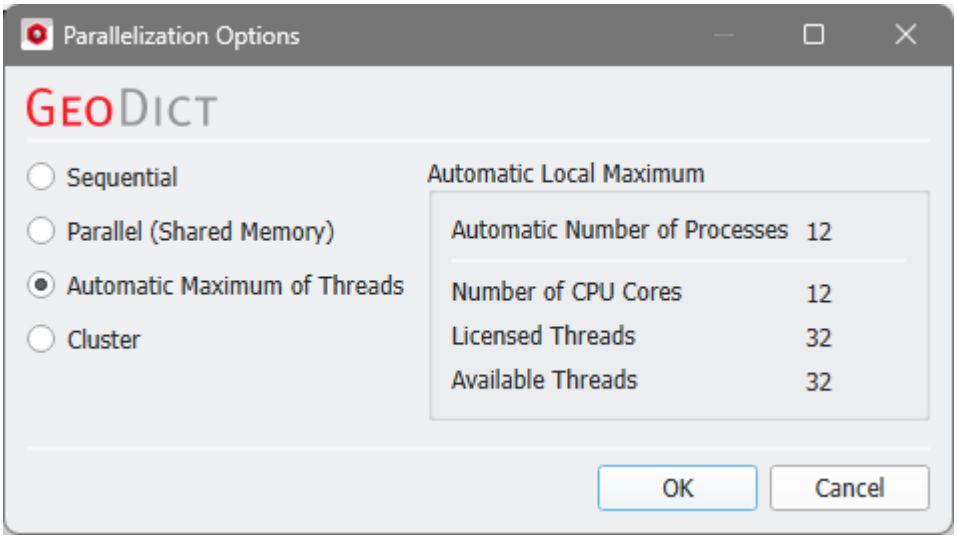
Parallel (Shared Memory)

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



Automatic Maximum of Threads

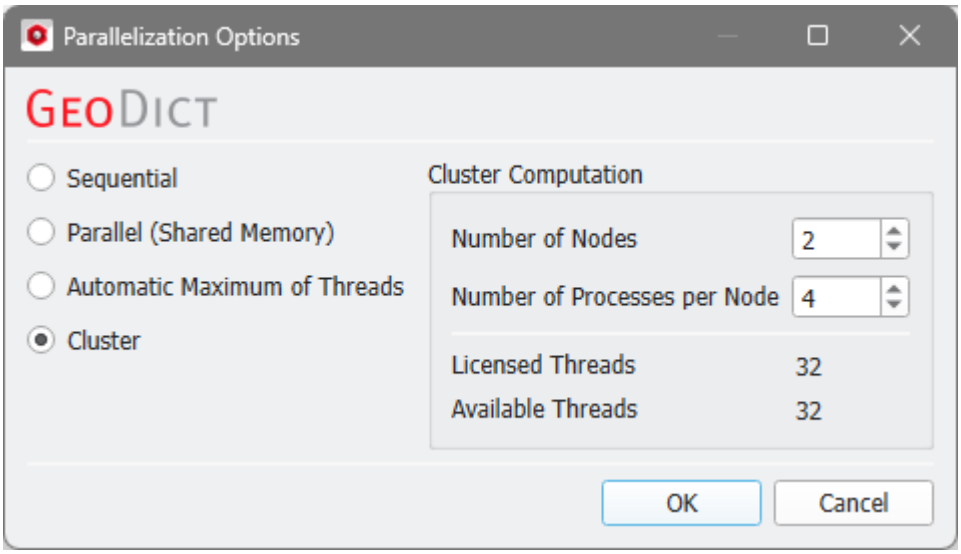
If **Automatic Maximum of Threads** is selected, the number of parallel processes is automatically selected for optimal speed, based on the CPU cores and licensed parallel processes.



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

Cluster

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

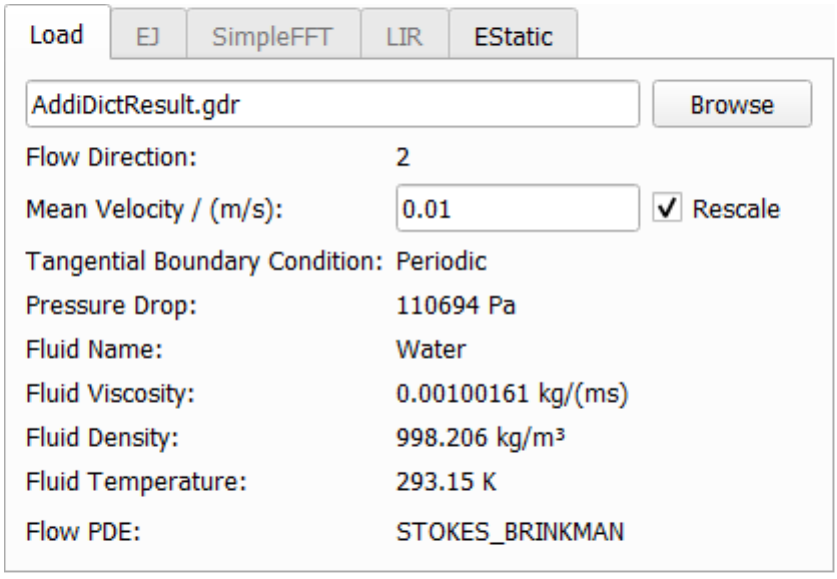


For details on how to set up and run parallel computations, consult the High Performance Computing chapter.

Additional Settings

Load

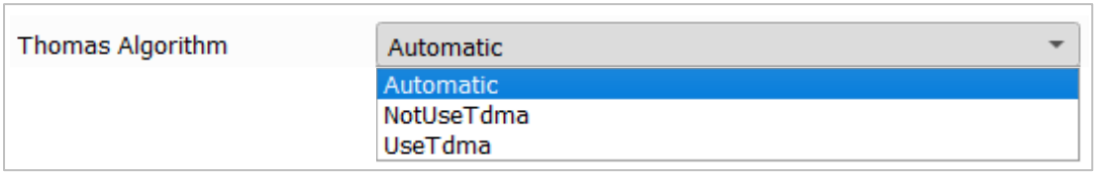
If **Load from File** has been selected from the **Flow Solver Type** menu in the **Flow Calculation** panel, choose a GeoDict result file of a previously run computation. Some information about the computation is shown. The mean velocity of the computation can be rescaled to another one by checking **Rescale** and editing the mean velocity.



SimpleFFT

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

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



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

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

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

For more information about the Thomas algorithm see here.

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

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

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

LIR

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

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

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

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

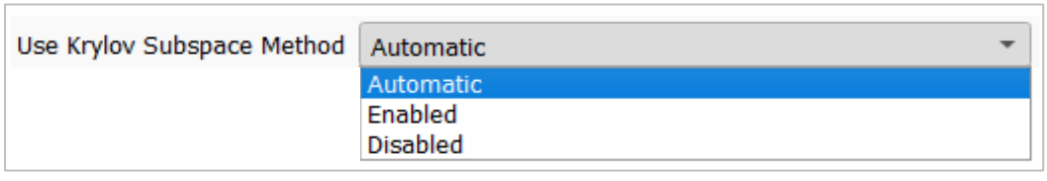
The method is available to solve the Stokes and Stokes–Brinkman equations as well as for solving mechanics, diffusion, thermal, and electrical conduction and is enabled by default.

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

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

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

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

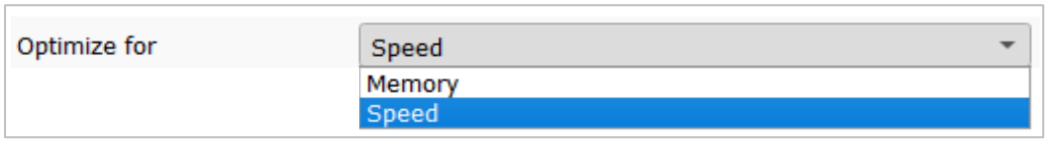


Note! In case that the Krylov subspace method (BICGStab) is used, the **Relaxation** may also be adapted automatically.

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

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

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 grid structure called LIR-tree and needs up to 10 times less runtime and memory compared to the **Regular Grid** option.

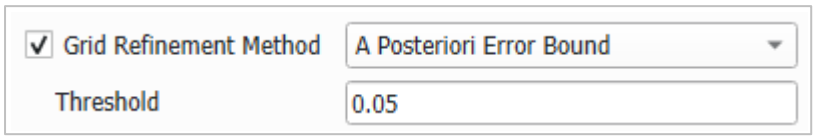
The solver can analyze the result field during the computation and improves the adaptive grid in places where more accuracy is needed. The LIR solver splits cells where a high gradient occurs.

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

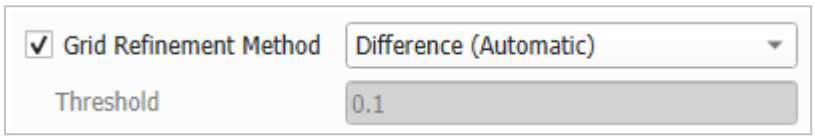
Select one of the three available refinement methods from the drop-down menu.

When **A Posteriori Error Bound** is selected, the solver targets the specified accuracy

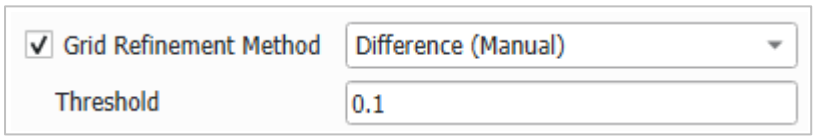
Threshold. While the **Error Bound** (set as Simulation Stopping Criterion) determines the relative error in the solution of the linear system, **A Posteriori Error Bound** refers to the relative error estimated by comparing high-order and low-order discrete solutions. The accuracy **Threshold** refers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



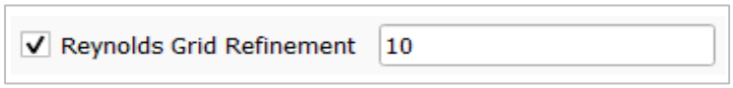
Choosing **Difference (Automatic)** leads to computational cells being split when the difference in values between neighboring cells exceeds a certain **Threshold**. The solver automatically chooses all internal parameters based on the structure and simulation settings. For this option, cells are split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



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



Activate **Reynolds Grid Refinement** to use the local Reynolds number (Re) for adaptive grid refinement.



A grid cell is split if the local Reynolds number, i.e., the ratio between inertial and viscous forces exceeds the given threshold. The Reynolds number is defined as:

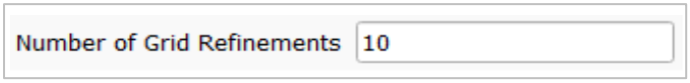
$$\mathrm{Re} = \frac{\rho \mathrm{u} \mathrm{L}}{\mu} \quad (49)$$

Reynolds Number

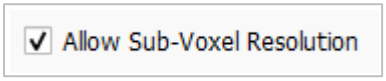
where ρ is the density of the fluid (SI units: kg/m^3), u is the velocity of the fluid (m/s), μ is the dynamic viscosity of the fluid (Pa·s or N·s/m^2 or kg/m·s), L is a characteristic length (m). For the local Reynolds number, the size of the grid cell is used for the

characteristic length.

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



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



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

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

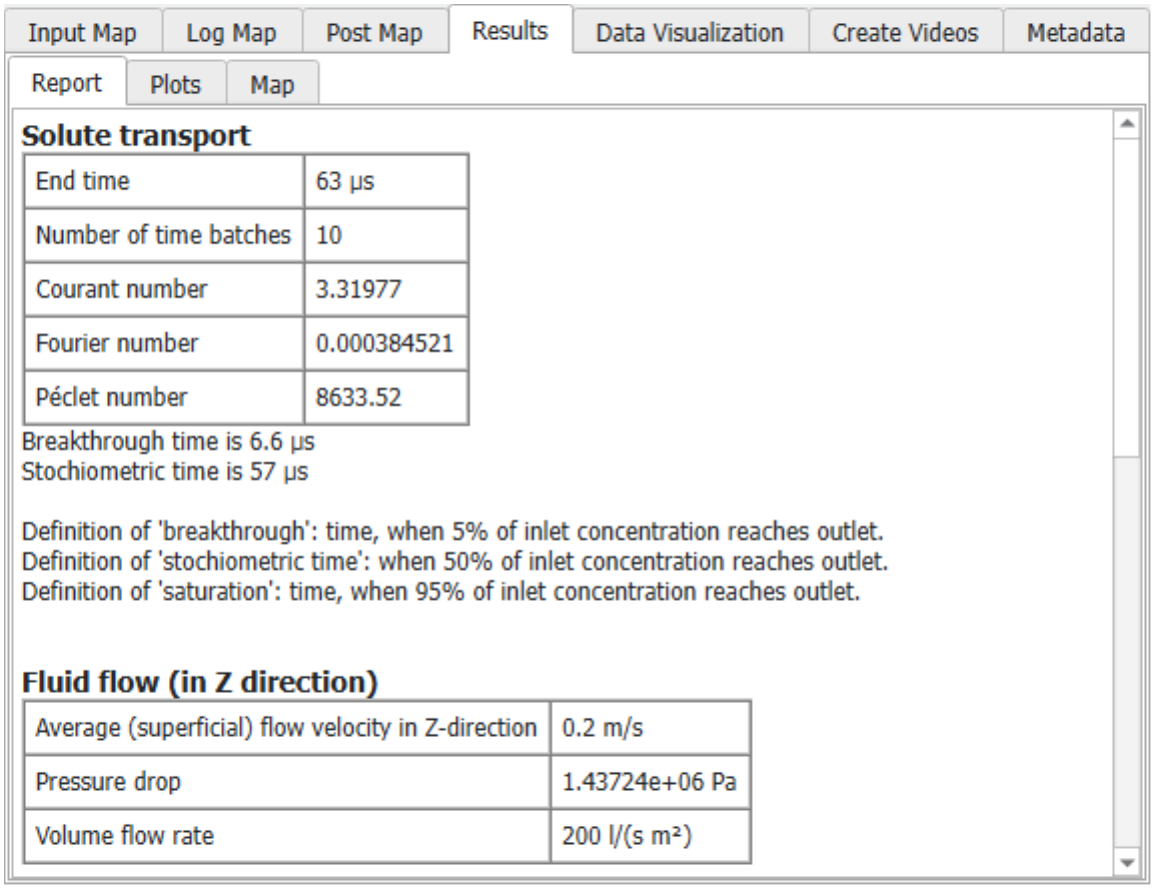
Check **Allow Grid Re-Coarsening** to allow the solver to automatically revert the grid refinement and coarsen the computational cells.

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

1.3.2 Results

After the **Transport Concentration Field** simulation is completed, the resulting files are saved in the project folder and a **Result Viewer** with the GeoDict result file opens automatically. The created GeoDict result file (*.gdr) contains seven tabs. The computational results are shown under the **Results** tab, can be loaded for visualization via the **Data Visualization** tab, and can be used to **Create Videos**. The other four tabs (**Input Map**, **Log Map**, **Post Map** and **Metadata**) display additional information about the computation.

Find more details on the general functionalities in the Result Viewer user guide.



Transport Concentration Field Results

- Report 103
  Shows the computed results.
- Plots 105
  View result plots.
- Data Visualization 107
  Load results for a graphical visualization.
- Create Videos 110
  Visualize the transport of concentration in a MP3 movie.

Report

In the **Report** subtab of the **Results** tab an overview of the simulation results is provided.

Solute Transport

At the top the **End time**, **Number of time batches**, and the more precise dimensionless numbers 79 for the **Solute Transport** are shown. All of these parameters are defined or shown in the Experiment 78 tab when setting up the transport simulation.

Solute transport	
End time	63 µs
Number of time batches	10
Courant number	3.31977
Fourier number	0.000384521
Péclet number	8633.52

Below specific characteristic times are reported:

- **Breakthrough time**: 5% of the inlet concentration reach the outlet
- **Stochiometric time**: 50% of inlet concentration reach outlet
- **Saturation time**: 95% of inlet concentration reach outlet

Breakthrough time is 6.6 µs
Stochiometric time is 57 µs

Fluid Flow

The **Average (superficial) flow velocity in Z-direction**, the **Pressure drop**, and the **Volume flow rate** are given. One of the values was set as input value in the Flow Boundary Conditions 81 when advective transport is active. The other values are then computed by the FlowDict computation.

Fluid flow (in Z direction)	
Average (superficial) flow velocity in Z-direction	0.2 m/s
Pressure drop	1.43724e+06 Pa
Volume flow rate	200 l/(s m²)

Solver Information

At the bottom of the report information on the **Transport** and **Flow solver** are shown. This includes the selected **Solver** (always LIR for the transport solver), the number of **Threads**, the **Number of cells**, **Runtime**, (**Maximum**) **Memory usage**, and the selected **Stopping criterion**. For the transport solver the runtime is separated into the **Total runtime** as sum of all time batches and an **Average runtime per batch** computed from all individual time batch runtimes.

Transport solver information

Solver	LIR
Threads	20
Number of cells	3177439
Maximum memory usage	1.033 GiB
Total runtime	15.205 min
Avg. runtime per batch	1.5205 min

Flow solver information

Solver	LIR
Threads	20
Iterations	2600
Number of cells	3105815
Runtime	1.63135 min
Memory usage	874.044 MiB
Stopping criterion	error bound

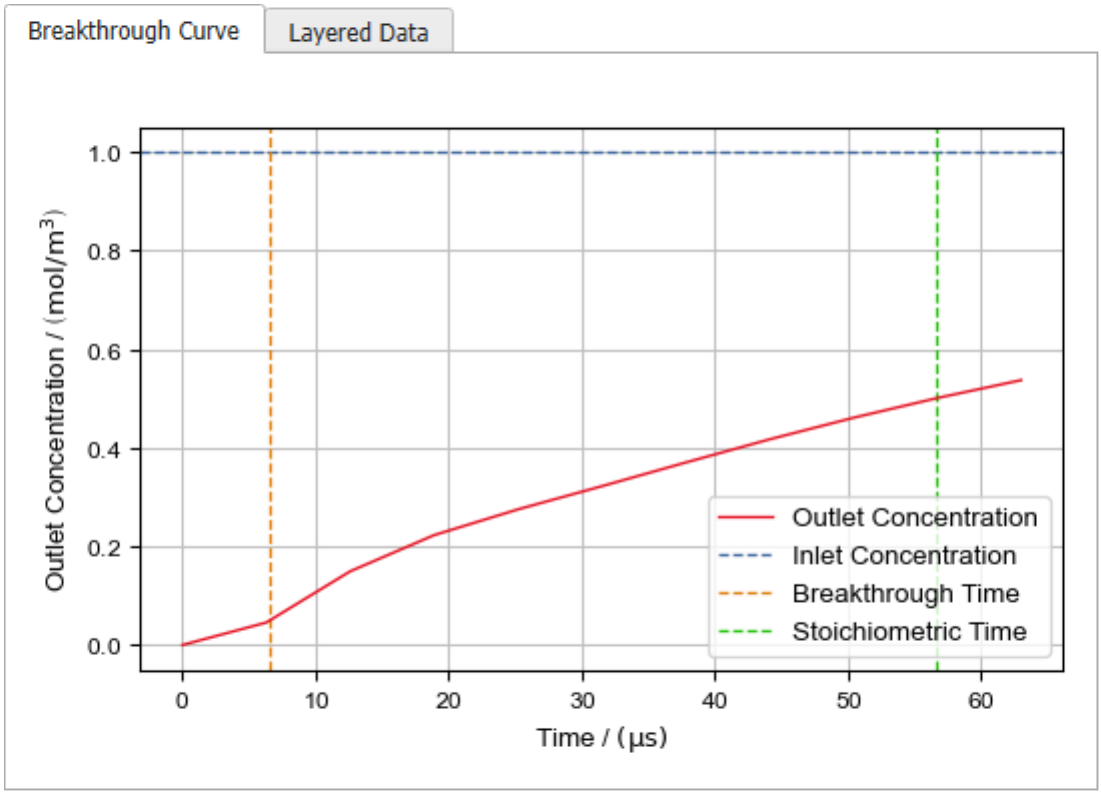
Plots

Under the **Plots** subtab twp plots are available.

Properties of the axis and graph can be modified for all plots. Right click the graph to access the settings menus. With **Edit Axis Settings**, scaling, labels and ticks of the axis as well as font sizes and legend placement can be selected. With **Edit Graph Styles**, title, style and color can be defined for each graph shown in the plot. In the menu that appears after right clicking the graph the data contained in the plot can be saved as well. More details on changing plot settings, are available in the Result Viewer user guide.

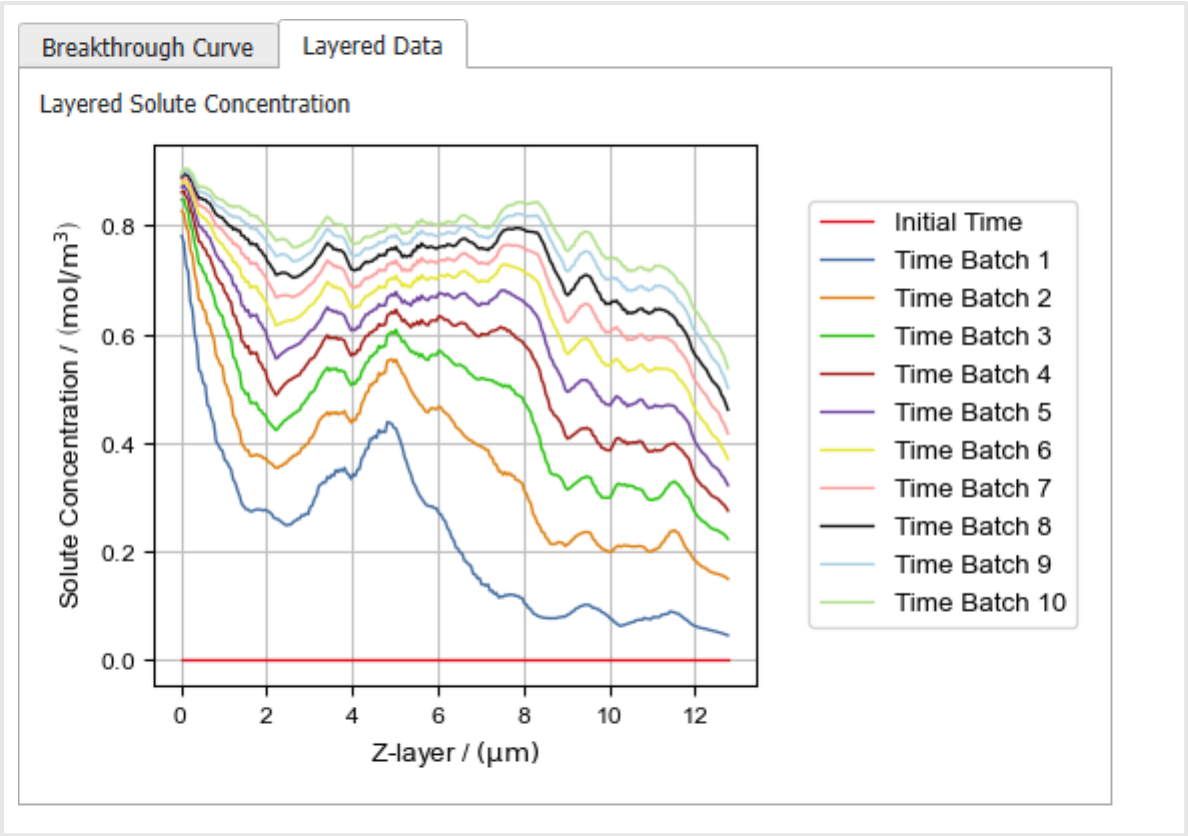
Breakthrough Curve

In the **Breakthrough Curve** plot **Outflow Concentration** in mol/m^3 is shown over the **Time**. Additionally, the inlet concentration is shown as a dashed blue line. If one the characteristic times is reached during the simulated time it is marked by a dashed vertical line. In this example the **Breakthrough** and **Stochiometric Times** were reached while **Saturation** was not achieved.



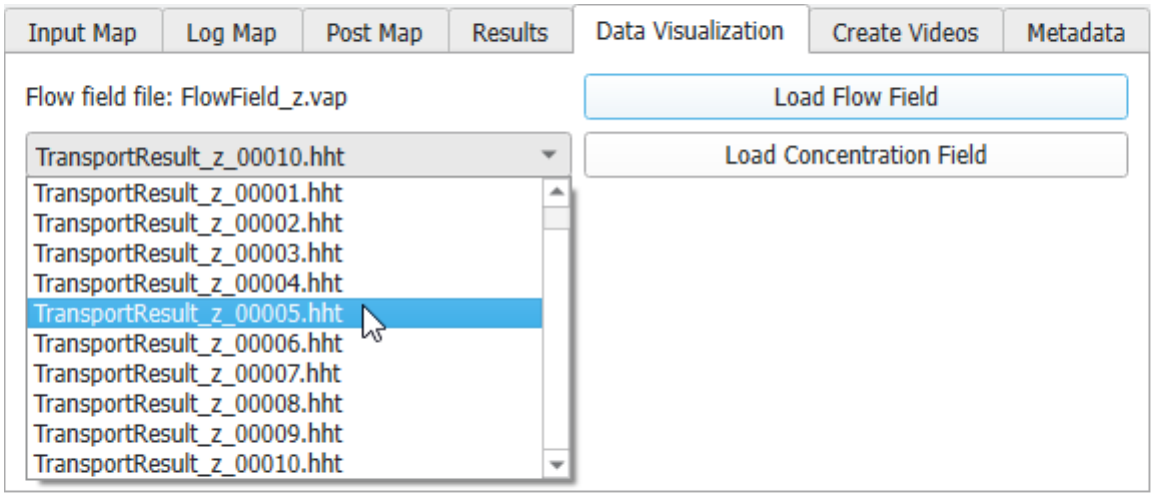
Layered Data

In this plot the **Solute Concentration** in mol/m³ is shown over the **Z-layers**. The Z-direction is always the computation direction for **Transport Concentration Field** simulation. One curve is plotted for each **Time Batch** as defined under the Experiment 78 tab.



Data Visualization

The **Data Visualization** tab enables you to load the **Concentration Fields** for each time batch defined under the Experiments 78 tab and the computed **Flow Field** for 3D visualization in the **Visualization** area of GeoDict. All files represent the field in Z-direction, which is the fixed computation direction for **Transport Concentration Field** simulations.

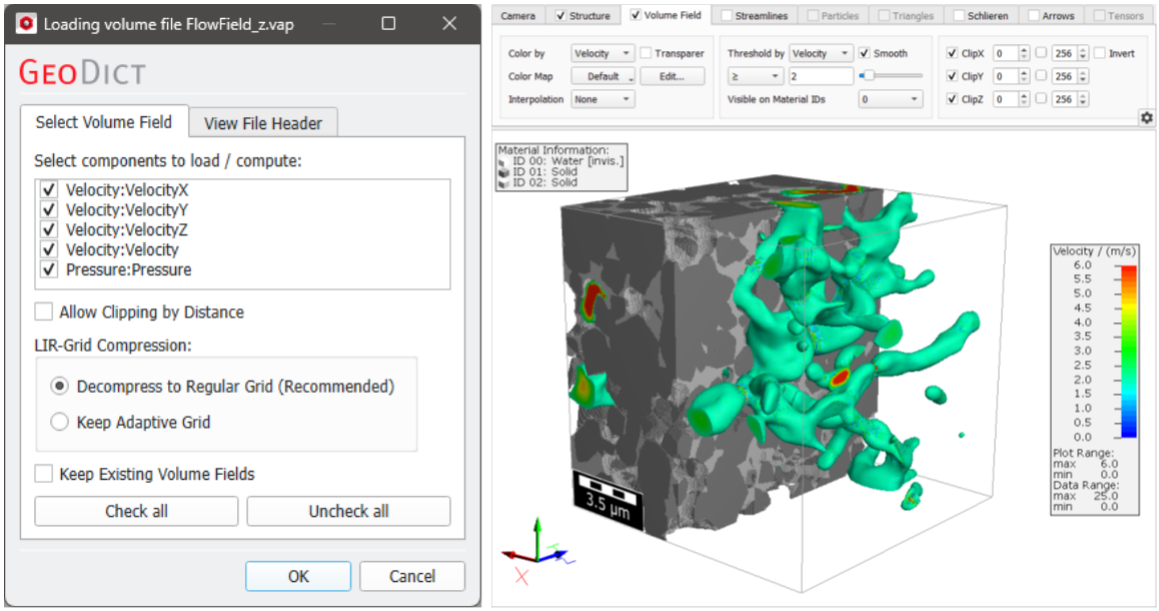


Load Flow Field

The computed results for the flow field can be loaded directly from the result file by clicking **Load Flow Field**. In the opening dialog, select the desired components of the

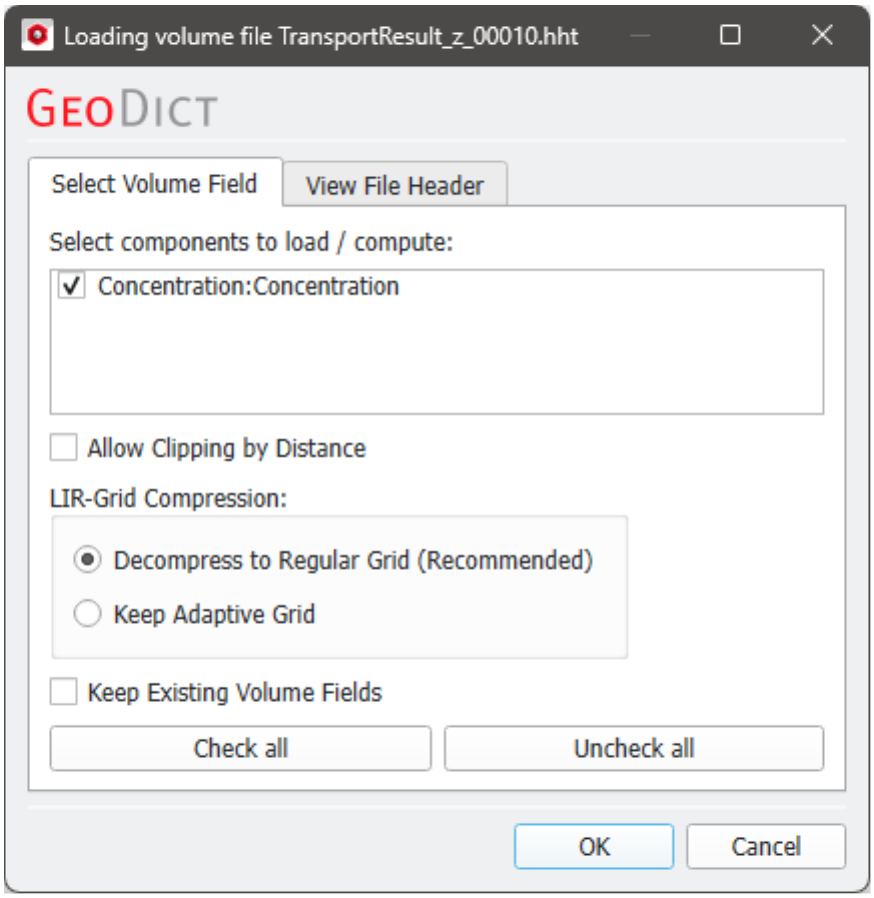
flow field to be shown. The saved fields are compressed and require decompression to enable all visualization features. When another volume field is already loaded the option **Keep Existing Volume Fields** is available.

The options available for the visualization of the flow field are the same as in FlowDict, SatuDict, or FilterDict. For more details on the available visualization options please refer to the Visualization user guide.

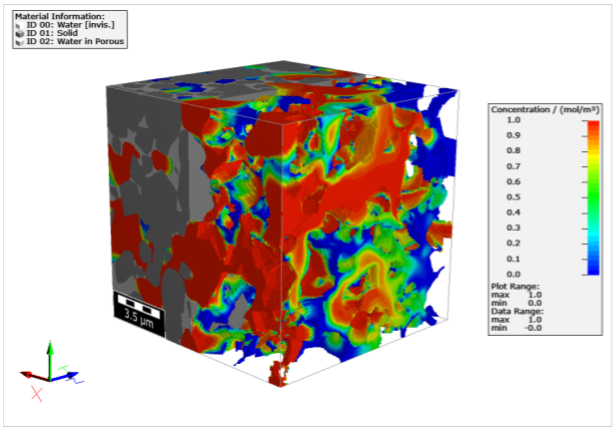


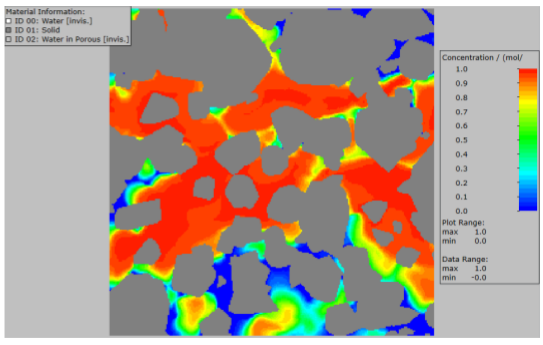
Load Concentration Field

A **Concentration Field** file (*.hht) showing the distribution of solute concentration (in mol/m^3) in the structure is created after each time batch defined in the Experiment 78 tab. After clicking **Load** for one of the concentration field files the **Loading volume file** dialog opens. In the *.hht file, only the concentration field is contained. The field may be compressed by the LIR solver and may require decompression to enable all visualization features. When another volume field is already loaded, the option **Keep Existing Volume Fields** is available. This feature allows for loading multiple time batches to visualize the transport over time.



After loading the concentration field, it is shown in the **Visualization area** of the GeoDict GUI. In the **Visualization panel**, directly above it, parameters for the visualization of the concentration field during the transport simulation are selectable under the **Volume Field** tab. The concentration field can be shown in 2D or 3D and with or without the structure.

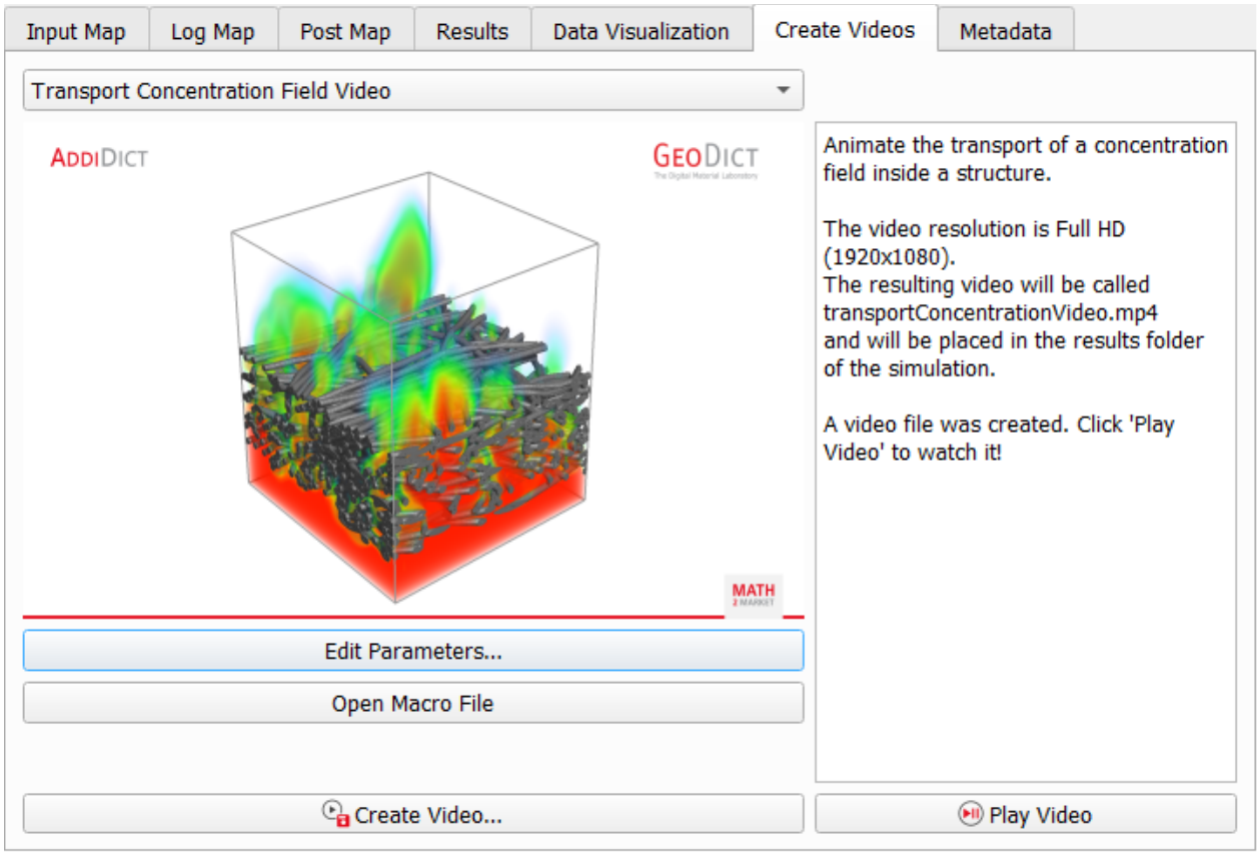




For more details on the available visualization options please refer to the Visualization user guide.

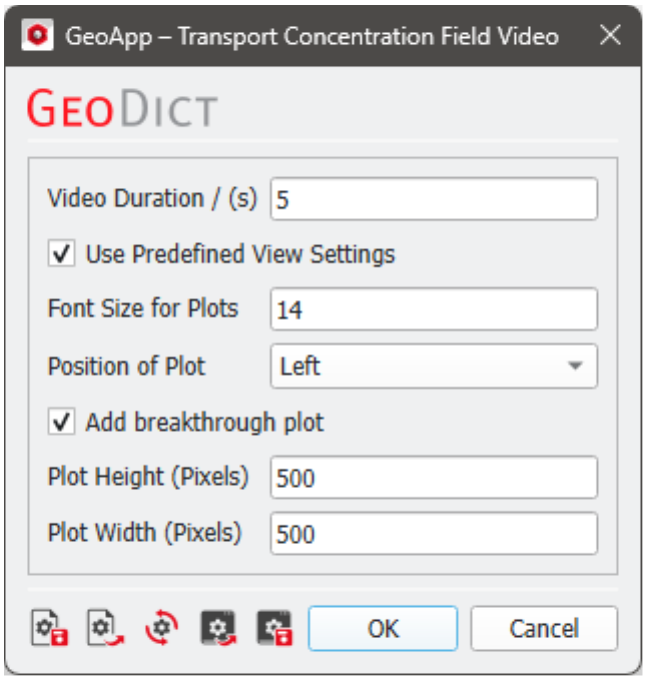
Create Videos

A predefined GeoPy macro can be used to animate the movement of the concentration field inside the structure. The created video is in Full HD and the file (**transportConcentrationVideo.mp4**) is saved to the results folder. The macro for video creation can be viewed and modified by clicking **Open Macro File**.



Under **Edit Parameters**, multiple options are available:

- **Video Duration**: Set the duration of the video in s. Time batches are distributed of the defined time.
- **Use Predefined View Settings**: When this setting is activated a predefined camera position is used to create the animation. When inactive the current view settings from the visualization area in GeoDict are used.
- **Font Size for Plots**: Define the font size for text in the breakthrough plot that can be included in the video.
- **Position of Plot**: Define the position of the breakthrough plot that can be included in the video. The plot can be positioned to the right or left of the 3D animation of the concentration field.
- **Add breakthrough plot**: When activated the breakthrough plot is shown in the video together with the animation. Each time batch the corresponding data point is added to the plot.
- **Plot Height** and **Width**: Set the size of the breakthrough plot in the video.



After setting the parameters click **Create Video** to run the macro. Once a video was created the **Play Video** button becomes active and allows for direct viewing of the video.

1.4 Adsorption

Use **Adsorption** to simulate the interaction between a solute moving through the structure and reactive porous voxels. Adsorption-based processes are widely used to remove contaminants and odors in various everyday applications. These processes often rely on materials with large internal sub-micron surfaces, such as activated carbon or zeolites.

There are two approaches available for simulating the solute movement through the structure:

1. Tracking tracer particles based on the Track Particles & Molecules 19 command, or
2. Simulating the movement of a concentration field based on the Transport Concentration Field 77 command.

The simulated solute distributions are then used to compute local adsorption reactions in reactive porous voxels. Within the porous active zone, the governing adsorption equations are solved based on the transported concentration and the equilibrium concentrations. Equilibrium concentrations are computed based on adsorption isotherms that you define. You can choose to use one of multiple isotherm models or enter measured values directly.

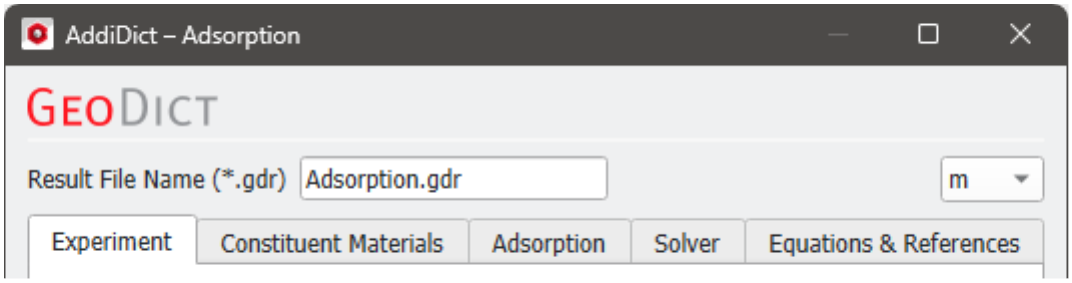
The results include the breakthrough behavior, the overall adsorption uptake, and the local adsorption distribution inside the reactive porous zones over time. These insights help determine the optimal usage durations of adsorbent materials and guide design adjustments, such as changes to the geometry, to maximize the efficiency and sustainability of valuable materials.

The Adsorption command

- Options 112
  Understand the input parameters.
- Results 144
  View the simulation results.

1.4.1 Options

Select **Adsorption** from the pull-down menu and click the **Option**'s **Edit** button to open a dialog to enter or edit the simulation options. Choose a **Result File Name** for the result file (*.gdr) fitting to your current project.



The adsorption simulation parameters are organized under the tabs: **Experiment**, **Constituent Materials**, **Adsorption**, and **Solver**. The **Equations & References** tab gives a summary of the used equations and symbols which are explained in more detail in this user guide.

Tabs of the Adsorption dialog

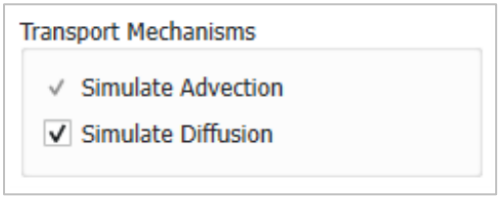
- Experiment 113
  Define flow/transport conditions and choose the used methodology.
- Constituent Materials 117
  Define the temperature and materials in your structure.
- Adsorption 120
  Specify the adsorption reaction parameters.
- Solver 127
  Set the parameters for all applied solvers.

Experiment

The **Experiment** tab is separated into five panels:

Transport Mechanisms

Select one or both of the **Transport Mechanisms** by checking the **Advection** and/or **Diffusion** boxes in the upper left part of the **Experiment** tab.



Note! For the **Tracer**-based approach, advection is always active while diffusion is optional. For the **Field**-based approach both options can be selected.

Check **Simulate Diffusion** to activate the computation of transport by diffusion. If the button is unchecked, the diffusivity is set to $D = 0$ in the particle momentum equation 6 for the **Tracer**-based approach. For the **Field**-based approach the diffusivity is set to $D_0 = 0$ in the advection-diffusion equation 12.

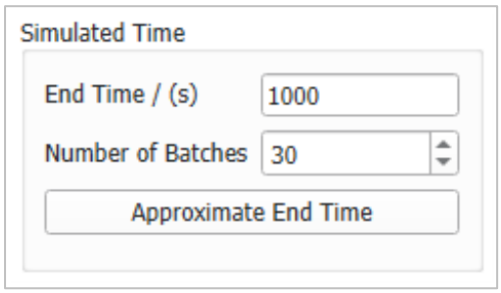
When using the **Field**-based approach, check **Simulate Advection** to activate the computation of advective transport due to the fluid flow. If unchecked, the velocity of the fluid is zero, i.e., $\vec{u} = \vec{0}$ in the advection-diffusion equation 12, and therefore, the concentration field is transported by diffusion only. In this case, the Flow Boundary Conditions 115 and the Flow Solver 91 tab set inactive.

Simulated Time

In the **Simulated Time** panel, the physical **End Time** of the simulation can be specified. The initial time is always zero. By clicking the **Approximate End Time** button, the **End**

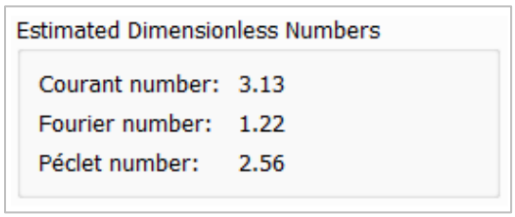
Time is automatically determined such that, for the specified average fluid velocity (defined in the Flow Boundary Conditions 115 panel by **Mean Velocity** or by **Flow Rate**), most of the solute passes through the entire structure and a complete breakthrough curve is computed. When it is unclear how to choose the **End Time**, it is highly recommended that the **Approximate End Time** used before starting the simulation. The approximation works best for high Péclet 115 numbers, i.e., when advection dominates the transport.

The simulation time can be divided into intervals (so-called "time batches"), after which the concentration field and other information is written to disk. Define the **Number of Batches**.



Estimated Dimensionless Numbers

In this panel, three **Dimensionless Numbers** are automatically estimated based on the entered parameter values, provided a structure is loaded. They give you an idea of how strongly advection and diffusion contribute to transport *before* the simulation is started. After the simulation, more precise values are listed in the report.



The **Courant number** Co quantifies the extent to which particles, molecules, or concentration fields are transported through the structure by advection during the simulation. For instance, if $\mathrm{Co} = 0.5$, then the solute (particles, molecules, or the concentration field) is advectively transported by the flowing solvent across half of the domain. The Courant number is defined as:

$$\mathrm{Co} = \frac{V\,T}{L} \tag{50}$$

where V is the characteristic velocity estimated from the flow boundary conditions, T is the simulation time (which equals the **End Time**, given that the initial time is zero), and L is the length of the structure in the through direction.

In contrast, the **Fourier number** Fo quantifies the extent to which the solute (particles, molecules, or the concentration field) is transported through the structure by diffusion during the simulation. The Fourier number is defined as:

$$\mathrm{Fo} = \frac{D\,T}{L^2} \tag{51}$$

where D is the characteristic diffusivity, taken as the maximum effective diffusivity across all existing materials.

Finally, the **Péclet number** Pe is the ratio of advective transport to diffusive transport. A Péclet number of infinity implies purely advective transport, whereas a value equal to zero corresponds to purely diffusive transport. The Péclet number is defined as:

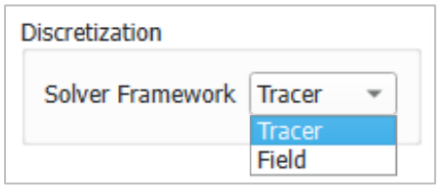
$$\mathrm{Pe} = \frac{V\,L}{D} = \frac{\mathrm{Co}}{\mathrm{Fo}} \tag{52}$$

Discretization

Select the **Solver Framework**, i.e., the approach that is used for simulating the adsorption reaction.

The **Tracer**-based approach releases clouds of molecular tracer particles for each batch. These tracer particles transport the concentration through the structure and are used to compute the adsorption reactions. This approach uses the Track Particles & Molecules 19 command in AddiDict. When you select this option the Tracer Solver 143 tab is activated.

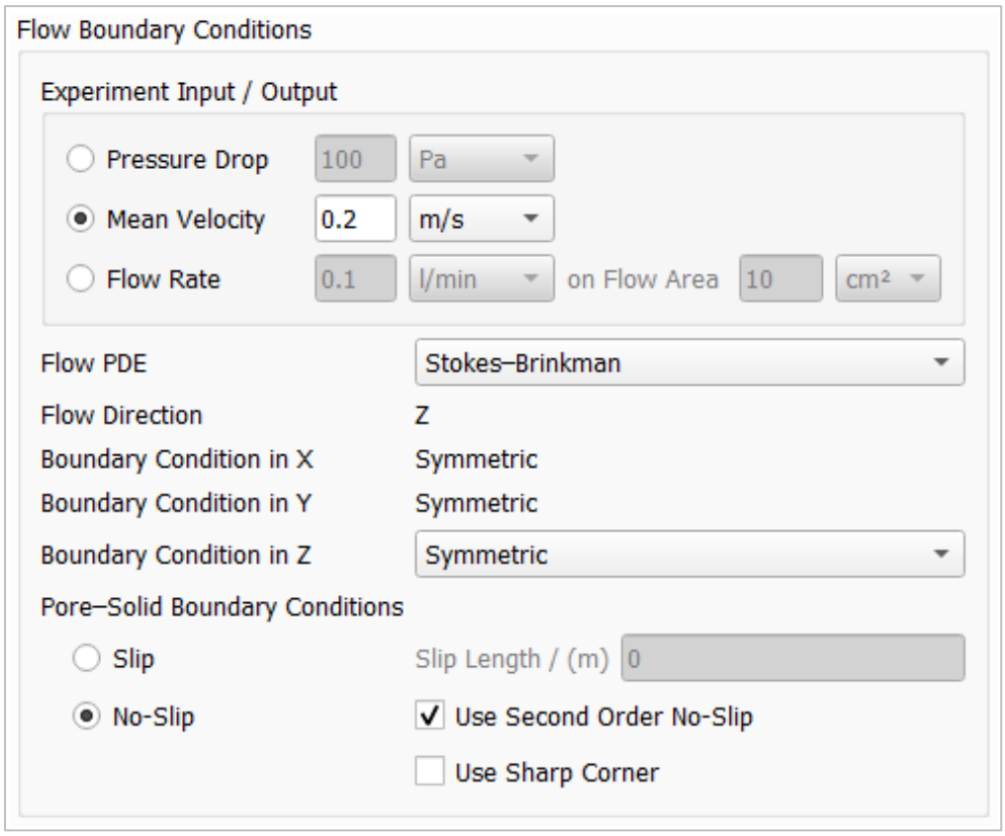
The **Field**-based approach solves the reactive transport equation and directly yields volume fields for concentration and adsorption loading. This approach is based on the Transport Concentration Field 77 command. When you select this option the Field Solver 139 tab is activated.



Flow Boundary Conditions

In the **Flow Boundary Conditions** panel, either the **Pressure Drop**, the mean flow **Velocity**, or the **Flow Rate** can be defined. Note that this part of the dialog is accessible only if Simulate Advection 113 is selected.

Important! In AddiDict, the fluid flow and transport is always computed in **Z-direction**. If another direction is required, the 3D model can be rotated with ProcessGeo prior to using AddiDict.



From the **Flow PDE** menu, you can specify the equations to be solved for computing the fluid flow field. The flow field is required to simulate the particle movements and trajectories or transport of the concentration field. (Navier-)Stokes equations describe fluid flow in structures containing only solid materials and pores. (Navier-)Stokes-Brinkman equations describe the flow through structures containing porous materials, solids, and pores. Use the Stokes equation when fluid velocities are slow or the viscosities are high, i.e., at low Reynolds numbers. The Navier–Stokes equation should be used for high fluid velocities when inertial effects cannot be neglected.

Note! The **Adsorption** command always requires (Navier-)Stokes-Brinkman equations since the Adsorbent needs to be defined as porous solid.

The used flow boundary conditions in **X** and **Y** direction are reported. For the **Track Particles & Molecules** command 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 leads to **Symmetric** flow boundary conditions.
- **Periodic** particle movement requires **Periodic** flow boundary conditions.

For the **Transport Concentration Field** and **Adsorption** commands the boundary conditions in **X** and **Y** direction are fixed to **Symmetric**.

The boundary condition in **Z** direction, can be **Periodic**, **Symmetric**, or **VinPout**. Please refer to the FlowDict user guide for more details. For the **Track Particles & Molecules** command, using the Stokes(-Brinkman) equation only allows for using **Periodic** or **Symmetric** boundary conditions, while the Navier-Stokes(-Brinkman) equation uses the **VinPout** 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. The default **Slip Length** of zero corresponds to a flow velocity of zero along the solid surface. 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, e.g., for gases when the mean free path is comparable to the pore size. The same slip length must be set for all materials in the structure. Find more details on the **Slip Length** here.

For the **No-Slip** boundary condition two additional options are available:

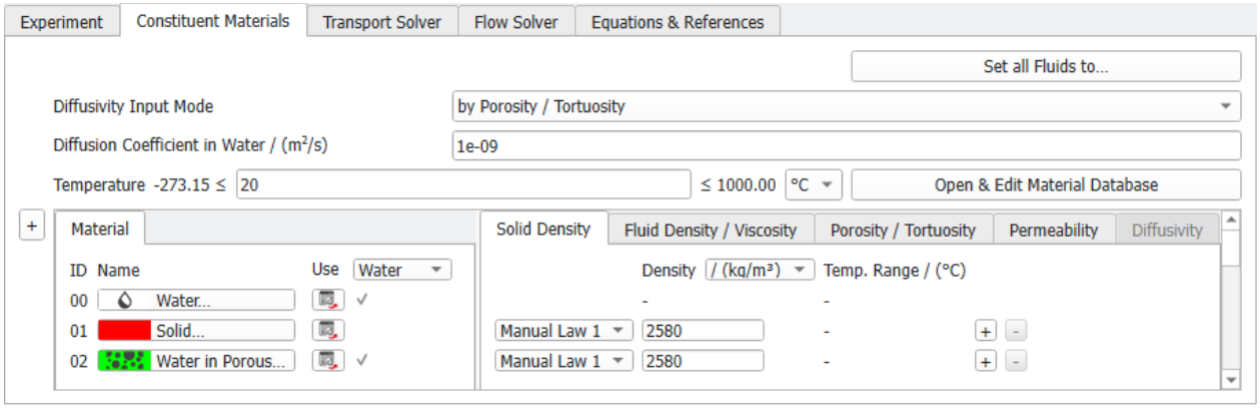
- **Use Second Order No-Slip** (default): This option sets the tangential velocity to zero at the center of the voxel surfaces and use a second order approximation of the velocity field.
- **Use Sharp Corner**: This option sets the tangential velocity to zero at the voxel corners.

Find more details on these settings in the FlowDict user guide.

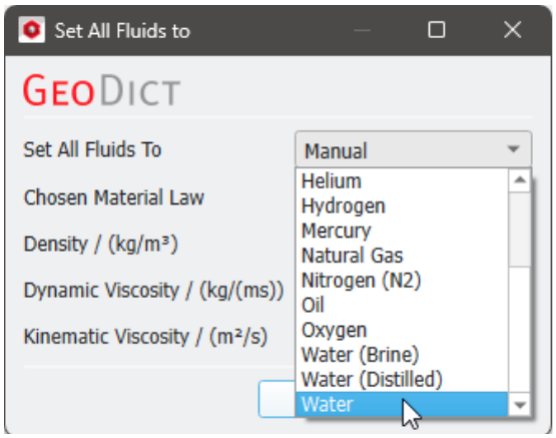
Constituent Materials

Define the materials in the structure and their properties in the **Constituent Materials** tab.

The **Temperature** 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.



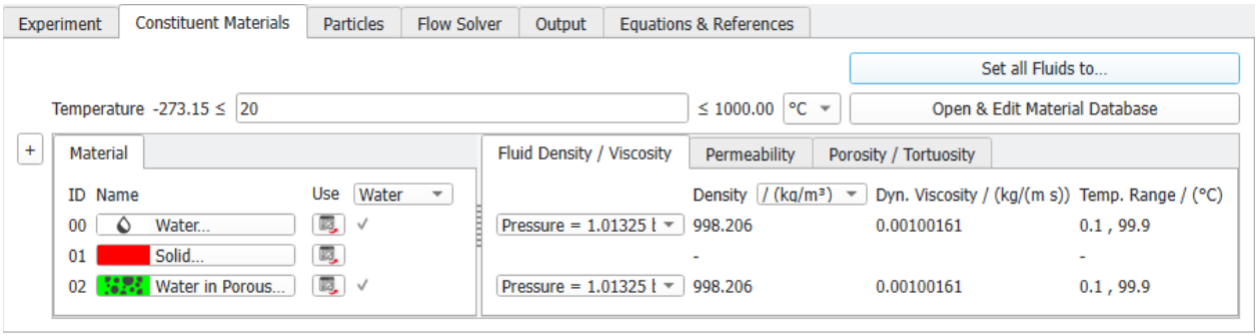
The fluid flowing through all pore and porous materials can be set by clicking **Set all Fluids to** and selecting it from the pull-down menu.



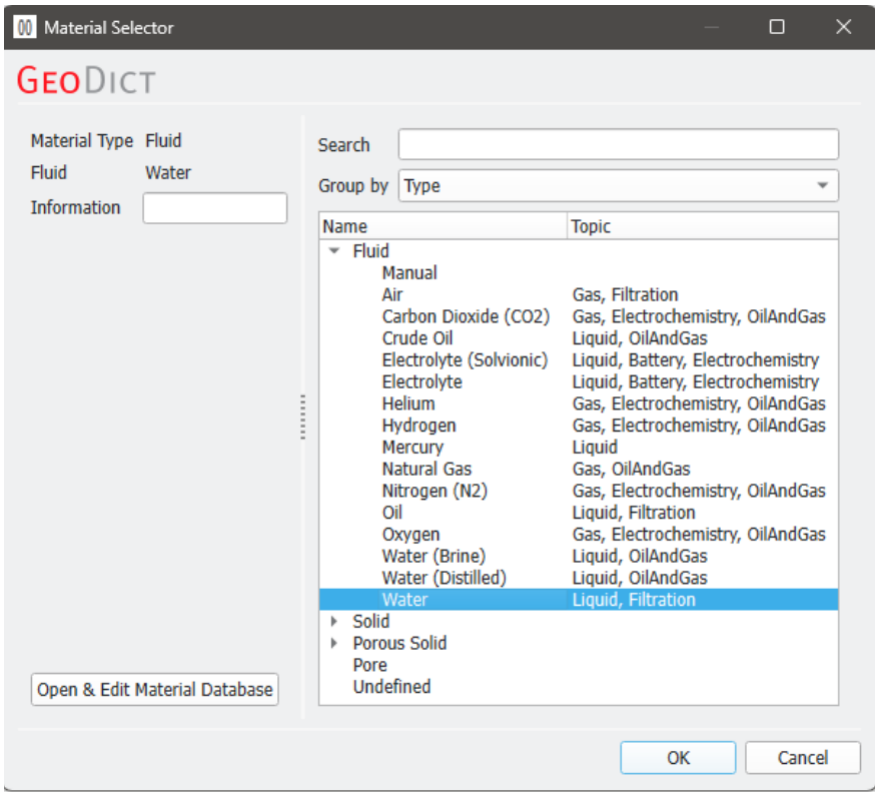
If one of the predefined fluids is used, the values for **Density**, **Dynamic Viscosity**, and **Kinematic Viscosity** are taken from the material database and are dependent on the given **Temperature** value. If **Manual** is chosen, you can enter these values manually.

Any values entered manually, e.g., those for a special type of oil, can also be added to the Material Database. Find more information on editing, expanding, and using the material database in the respective user guide.

As soon as you define 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 ID 02. The density and the dynamic viscosity of this fluid, at the selected temperature range, is shown under the **Fluid Density/Viscosity** subtab.



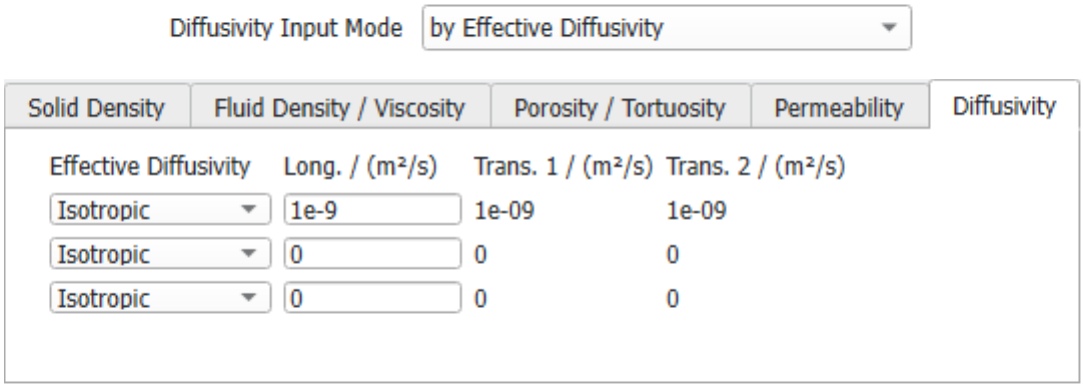
All materials assigned to the material IDs, which fall into one of the material categories (pore, porous or solid), can be selected individually through the **Material Selector** dialog, by clicking on the material's buttons. Fluid flow can occur only in pores and in porous materials.



Under the **Constituent Materials** tab the effective diffusivity of the solute in the fluid and porous materials needs to be defined. Here two options are available for the **Diffusivity Input Mode**:

by Effective Diffusivity

Select the option **by Effective Diffusivity** to activate the **Diffusivity** subtab in the bottom right of the dialog. In this subtab the **Effective Diffusivity** D_{eff} can be set for all materials manually.



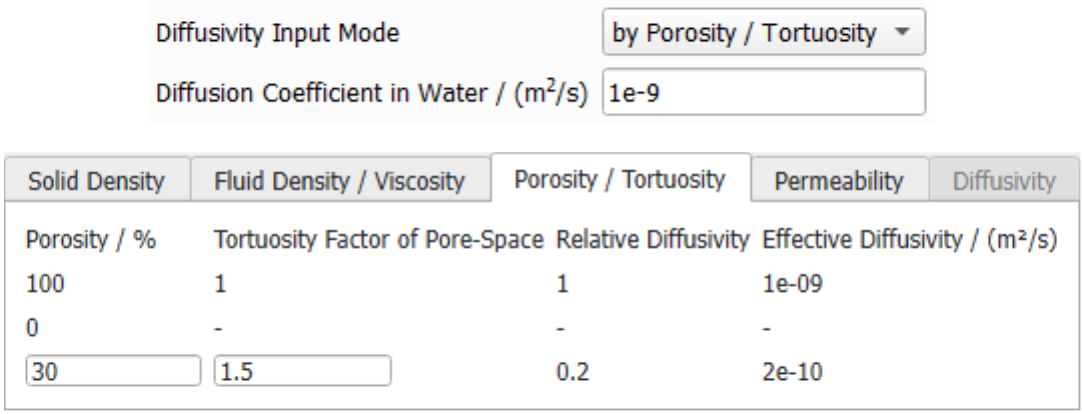
by Porosity/Tortuosity

Select **by Porosity/Tortuosity** to activate the field for the **Diffusion Coefficient in *Fluid*** and the **Porosity / Tortuosity** subtab in the bottom right of the dialog. In the

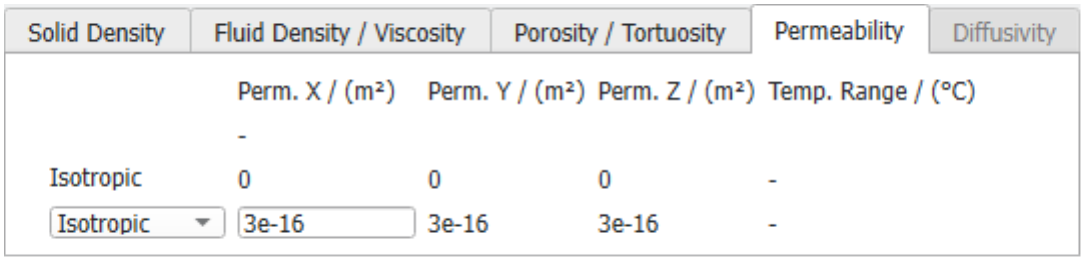
field for the **Diffusion Coefficient in *Fluid*** the diffusion coefficient D_0 for the solute in the fluid material in the structure needs to be provided, e.g., for solute in water. This value is automatically set as effective diffusivity for the fluid material. Under the **Porosity / Tortuosity** subtab the porosity ϕ and the tortuosity τ for each porous material need to be defined. These values are used to calculate the relative (D_{rel}) and effective (D_{eff}) diffusivity for each porous material:

$$D_{\mathrm{rel}} = \frac{\phi}{\tau} \tag{53}$$

$$D_{\mathrm{eff}} = D_{\mathrm{rel}} \cdot D_0 \tag{54}$$



For porous materials, their permeability needs to be defined on the **Permeability** subtab.



Adsorption

Define the adsorption reaction under the **Adsorption** tab. This tab contain three subtabs to define the individual parameters for the solute that adsorbs (**Adsorbate**), the porous material that adsorbs the solute (**Adsorbent)**, and the adsorption reaction (**Interaction**).

Define the Adsorption Reaction

- Adsorbate 121
  Define the solute that adsorbs.
- Adsorbent 123

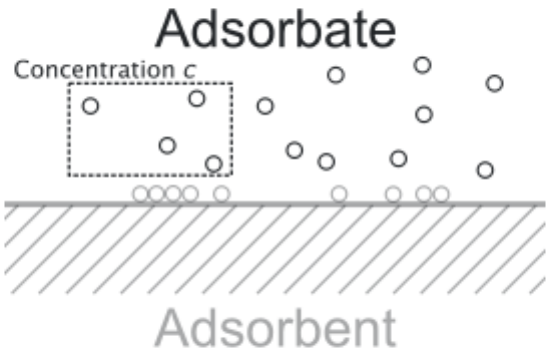
Define the Adsorption Reaction

Specify the material that adsorbs the solute.

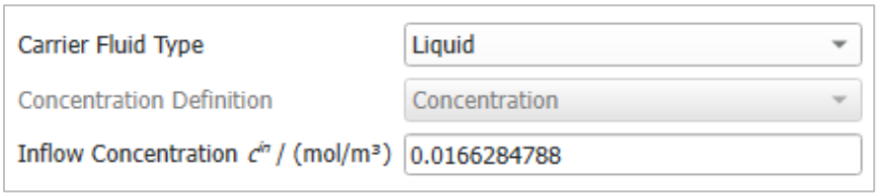
- Interaction
  Set up the adsorption reaction.

Adsorbate

Under the **Adsorbate** subtab you can define all parameters regarding the solute that adsorbs to the adsorbent solid.

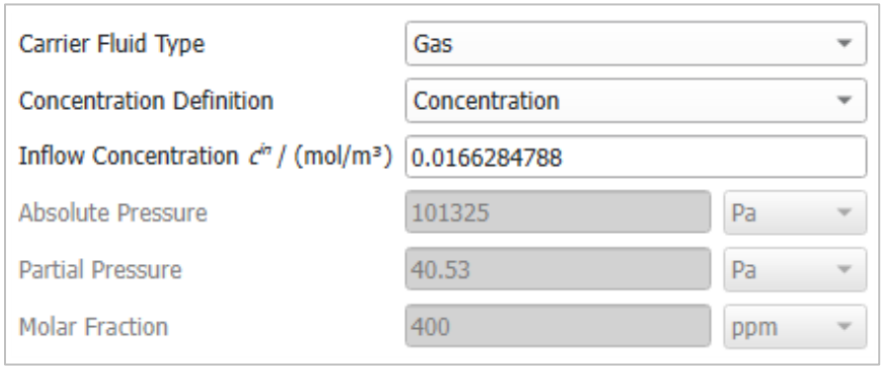


The **Carrier Fluid Type** can be a **Gas** or **Liquid** depending on what the solvent is transported by. When you select **Liquid** the **Concentration Definition** for the solute is automatically set the **Concentration** and an **Inflow Concentration** in mol/m³ must be defined.



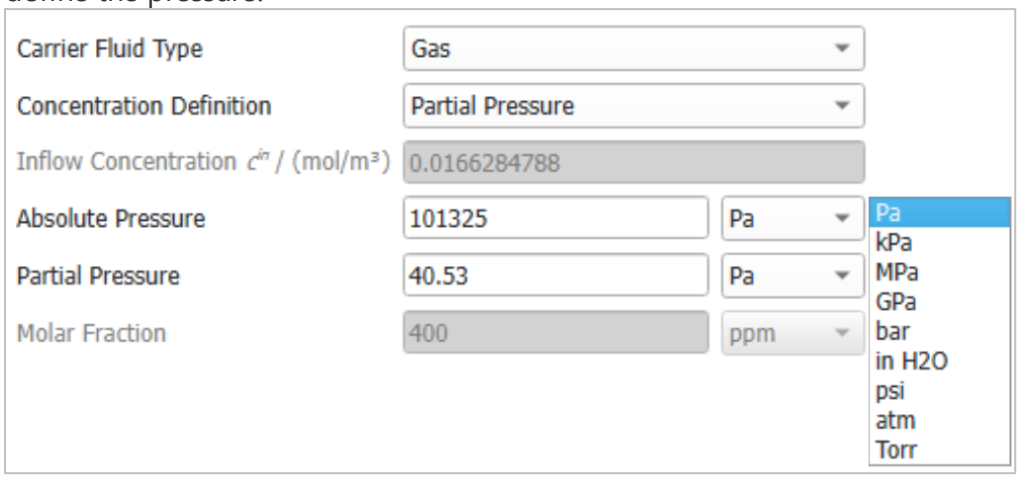
For **Gases** the **Concentration** of the solute can be **Defined** in three different ways:

- **Concentration**: Directly prescribe an **Inflow Concentration** in mol/m³ that is transported into the domain via the fluid flow.

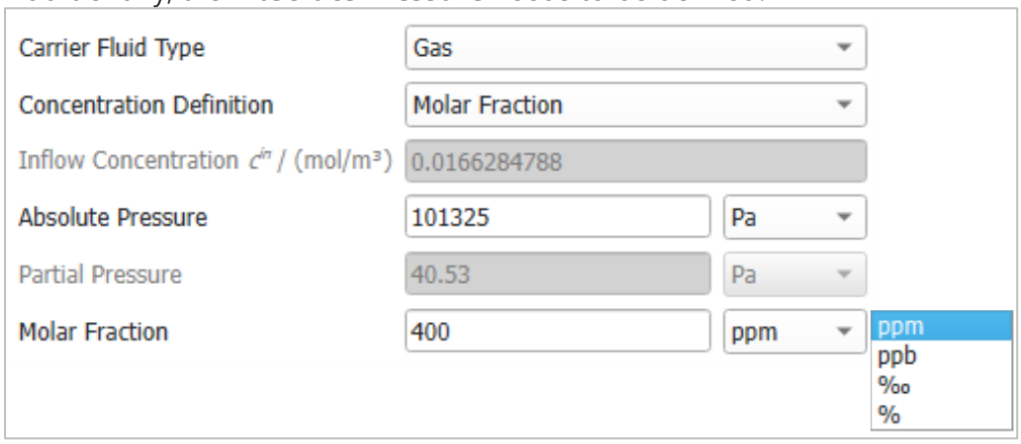


- **Partial Pressure**: Define the **Partial Pressure** of the gas that adsorbs to the adsorbent. The **Partial Pressure** is the pressure of that gas as if it alone occupied the entire volume of the original gas mixture at the same temperature. The **Absolute Pressure** is the sum of the partial pressures of the gases in the mixture. You can select from a wide range of units to

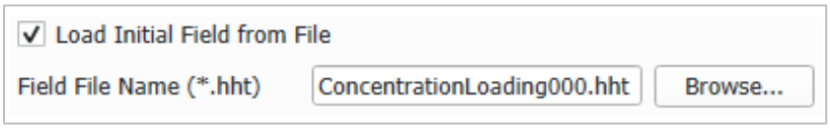
define the pressure.



- **Molar Fraction**: Define the **Molar Fraction** which is the ration between the amount of the solute substance and the total amount of all substances in a mixture. The fraction can be expressed in parts per million (**ppm**), parts per billion (**ppb**), per mil (**‰**), or percent (**%**). Additionally, the **Absolute Pressure** needs to be defined.



An **Initial Concentration** c^0 in mol/m³ can be defined in one of two ways. An **Initial Field** can be loaded by selecting the checkbox and clicking **Browse**. Through this option, an initial distribution of the solute in solution in the structure can be defined. For each time batch, AddiDict automatically generates a *ConcentrationLoadingXXX.hht* file. This file contains two volume fields: the **Concentration** and the **Loading**. Here the **Concentration**, i.e., the distribution of the solute in the structure is used as input. Therefore, the output of a previous adsorption simulation can easily serve as the input for subsequent runs. Alternatively, *.hht files can be manipulated with Python scripting.

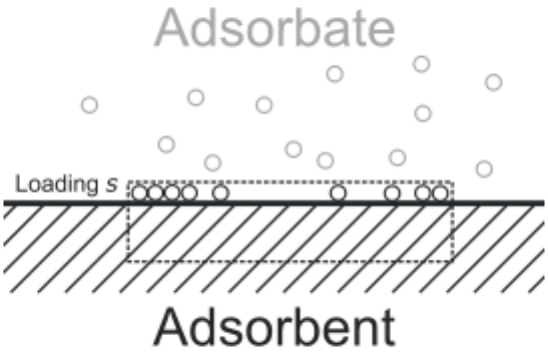


Alternatively a **Constant Value** for the **Initial Concentration** of the solute in the structure can be defined.

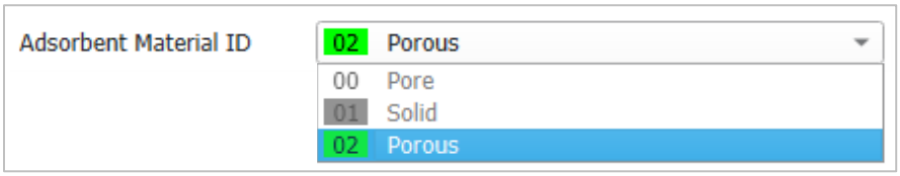
If none of these options is selected the **Initial Concentration** is c^0 = 0 mol/m³.

Adsorbent

Under the **Adsorbent** subtab you can define all settings regarding the material that adsorbs the solute species.



Select the **Material ID** of your **Adsorbent**. You can only select porous solids as adsorbent and only one adsorbent material can be selected.



An **Initial Sorbent Loading** s^0 in mol/kg can be defined in one of two ways. An **Initial Field** can be loaded by selecting the checkbox and clicking **Browse**. Through this option, an initial distribution of the solute adsorbed to the adsorbent can be defined. For each time batch[113], AddiDict automatically generates a *ConcentrationLoadingXXX.hht* file. This file contains two volume fields: the **Concentration** and the **Loading**. Here the **Loading**, i.e., the distribution of the solute adsorbed to the adsorbent, in the structure is used as input. Therefore, the output of a previous adsorption simulation can easily serve as the input for subsequent runs. Alternatively, *.hht files can be manipulated with Python scripting.

Alternatively a **Constant Value** for the **Initial Sorbent Loading** of the solute in the structure can be defined.

If none of these options is selected the **Initial Sorbent Loading** is $s^0 = 0$ mol/m^3.

Interaction

Under the **Interaction** subtab you can define all parameters regarding the adsorption reaction.

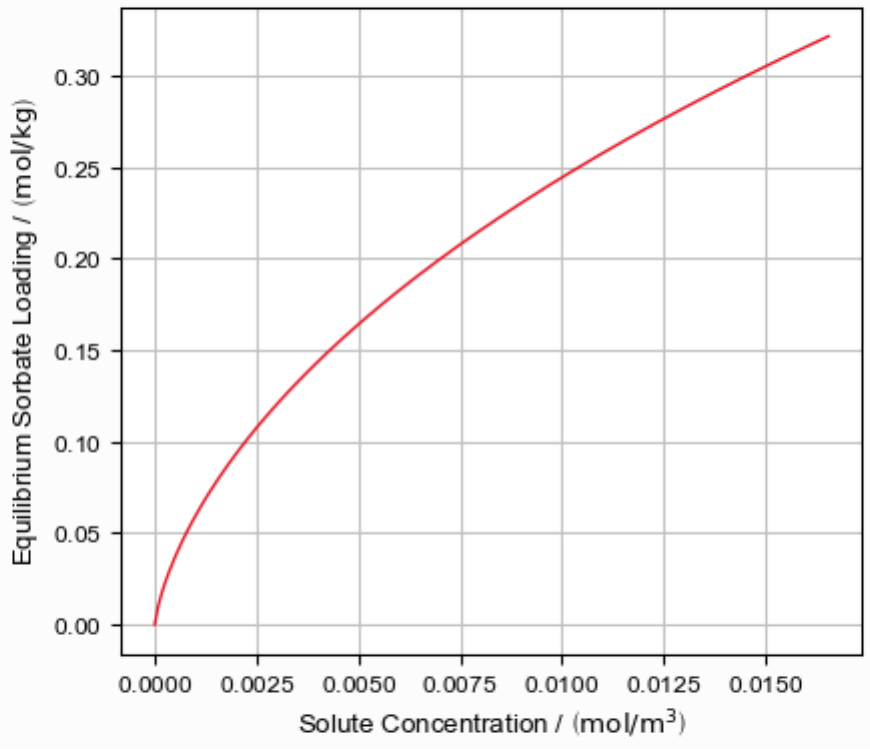
Rate

At the top the rate of the adsorption reaction needs to be defined. Currently, only the **Linear Driving Force** rate type is available. Find a description and the equation of this rate type here. The **Linear Driving Force** rate requires a **Rate Constant k_{ldf}** that is applied in the Rate Equation. Define this parameter below in kg/(m³ s). This parameter controls the speed of the sorption reaction.

Rate Type	Linear Driving Force
Rate Constant k_{ldf} / (kg/(m³ s))	3
Rate Equation:	$R(c,s) = k_{ldf}\,(\varphi(c) - s)$

Isotherm $\varphi(c)$

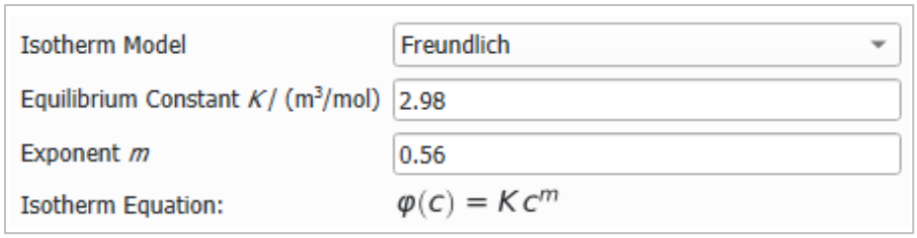
Select one of five **Isotherm Models** to describes how the solute distributes between the liquid or gas phase and the surface of the adsorbent at constant temperature. These models mathematically relate the amount of adsorbed solute to the equilibrium concentration of the solute in the surrounding phase. To the right of the parameter fields, the isotherm is shown in a plot. The plot is automatically updated when selecting a different model or changing one of the parameters.



Freundlich

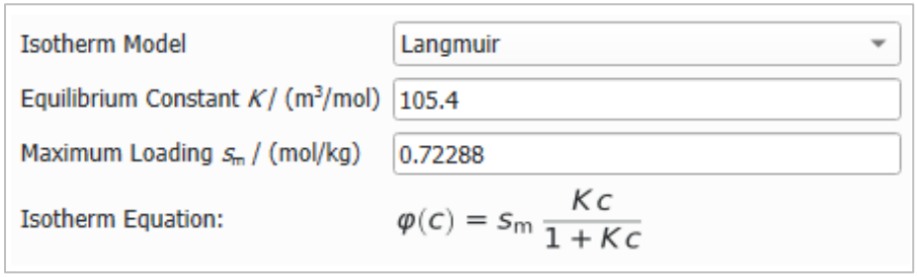
Choose the Freundlich isotherm model when you want to model adsorption on heterogeneous surfaces with sites of varying adsorption energies and without monolayer coverage or a finite number of adsorption sites. The Freundlich isotherm

model requires the definition of two parameters: the equilibrium constant K (m^3/mol) and the empirical exponent m.



Langmuir

Choose the Langmuir isotherm model[15] when you want to model monolayer adsorption on a surface with a finite number of identical sites, where each site can hold only one solute molecule. The Langmuir isotherm model requires the definition of two parameters: the equilibrium constant K (m^3/mol) and the maximum loading s_m (mol/kg). The default values are for the adsorption of CO_2 on a zeolite surface (see Coker and Knox, 2014[158]).



Table

If you have laboratory measurements with pairs of solute **Concentration** and adsorbent **Loading** you can select the **Table** option to directly use your data to prescribe the isotherm curve. The data can be copied from other sources such as *.txt or excel files and pasted to the table.

Isotherm Model: Table

	Concentration c / mol/m³	Loading s / mol/kg
1	0	0
2	0.0017296	0.131191
3	0.00345921	0.199755
4	0.00518881	0.252565
5	0.00691842	0.296762
6	0.00864802	0.335303
7	0.0103776	0.369763
8	0.0121072	0.401098
9	0.0138368	0.429943
10	0.0155664	0.456747
11		

Tóth

Use the Tóth isotherm model[16] for systems that deviate from the ideal monolayer adsorption behavior described by the Langmuir isotherm model[15]. This can happen especially at low and intermediate pressures. The Tóth isotherm model requires the definition of three parameters: the equilibrium constant K (m³/mol), the Tóth heterogeneity parameter[16] t, and the maximum loading s_m (mol/kg).

Isotherm Model: Toth

Equilibrium Constant K / (m³/mol): 32.12

Exponent t: 0.204

Maximum Loading s_m / (mol/kg): 13.32

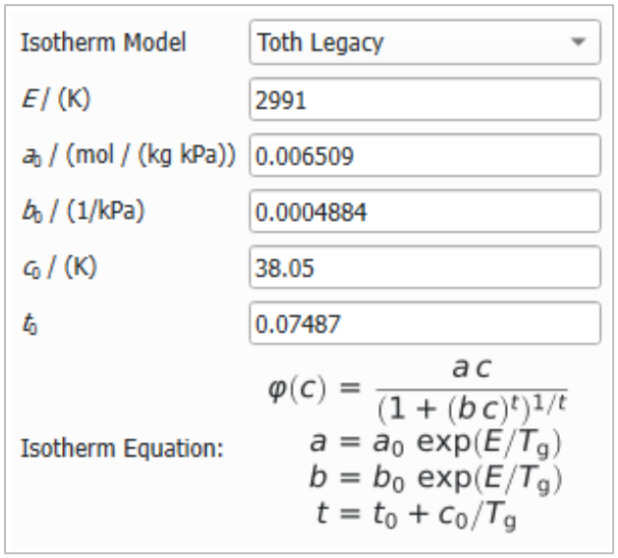
Isotherm Equation:

$$\varphi(c) = s_m \frac{Kc}{(1 + (Kc)^t)^{1/t}}$$

Tóth Legacy

The Tóth Legacy isotherm model[16] uses a different definition of the Tóth isotherm and was previously available in the Adsorption GeoApp in GeoDict 2025.

For the **Tóth Legacy** model the Tóth parameters E, a_0, b_0, c_0, and t_0 need to be provided. The default values are based on the adsorption of CO_2 on a zeolite surface (see CO_2/13X in table 1 of Coker and Knox, 2014 [158]).

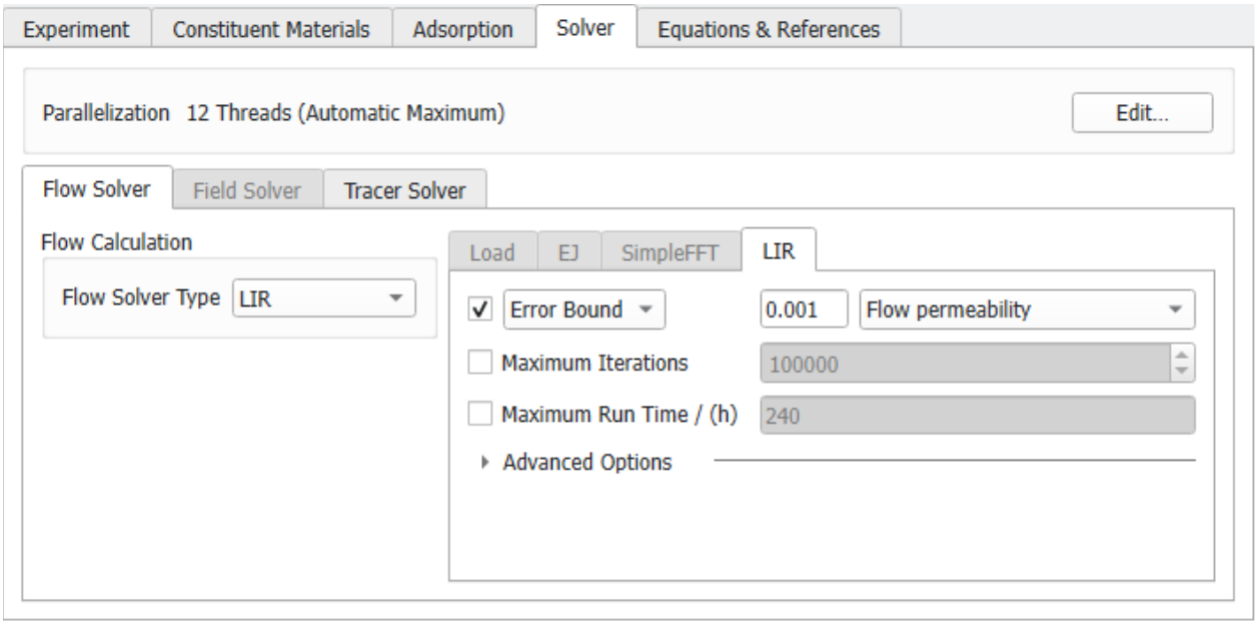


Solver

Under the **Solver** tab all parameters for the used solvers can be defined. Which subtabs are active depends on the settings defined under the Experiment [113] tab.

The **Flow Solver** subtab is active when Simulate Advection [113] is selected in the **Experiment** tab. For the Tracer-based approach this setting is always active but for the Field-based approach it can be deactivated.

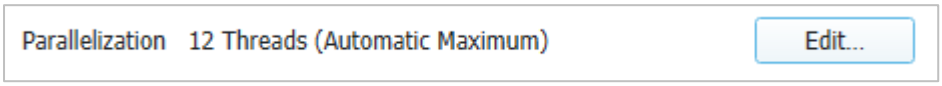
Only one of the **Field Solver** and **Tracer Solver** subtabs can be active at a time. Which subtab is active depends on the selected Solver Framework [115] in the **Experiment** tab.



Parallelization

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

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



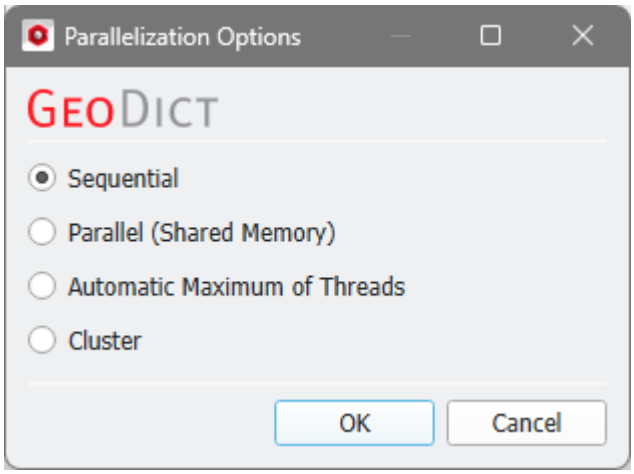
The parallelization of the solvers is done with two technical methods: **MPI Parallelization** or **Thread parallelization**. The following table shows the support of both parallelization methods:

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

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

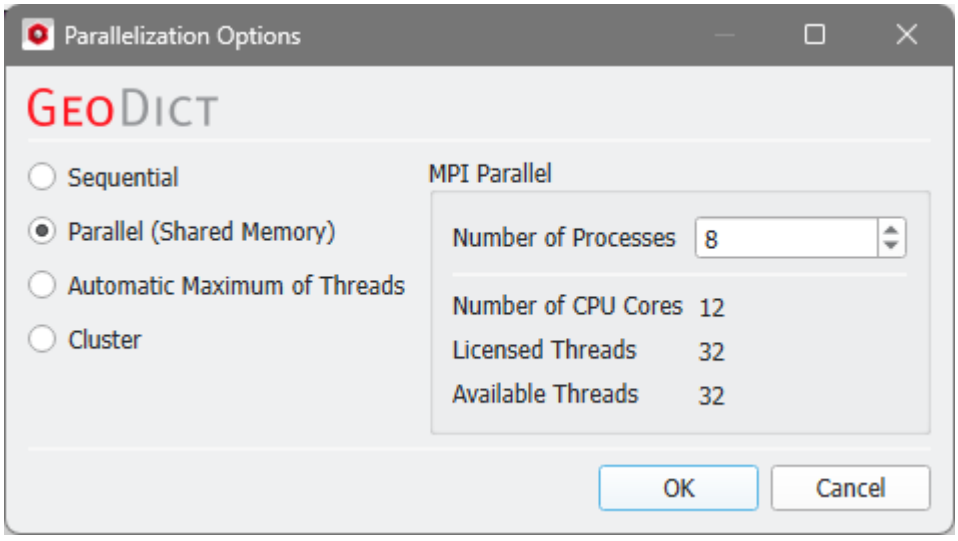
Sequential

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



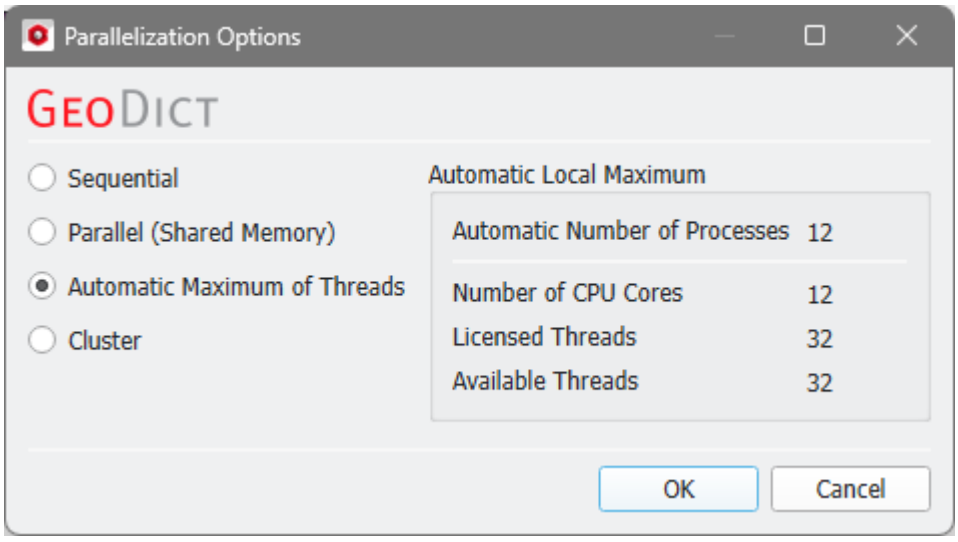
Parallel (Shared Memory)

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



Automatic Maximum of Threads

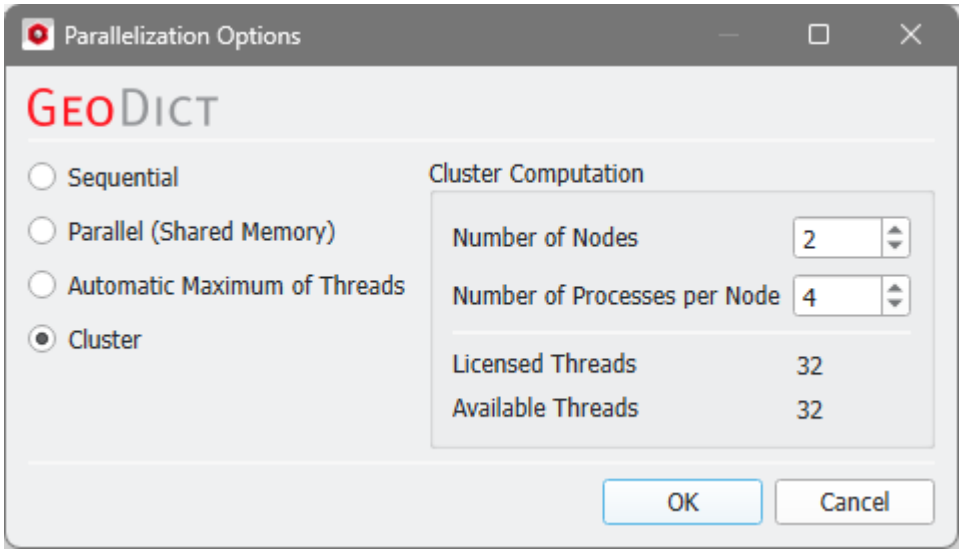
If **Automatic Maximum of Threads** is selected, the number of parallel processes is automatically selected for optimal speed, based on the CPU cores and licensed parallel processes.



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

Cluster

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



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

Individual Solver Settings

- Flow Solver 131
  Choose and set up the applied flow solver.
- Field Solver 139
  Set the parameters for the concentration field transport solver.

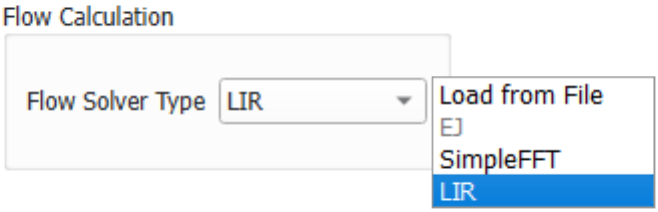
Individual Solver Settings

- Tracer Solver 143
  Define the tracer particles.

Flow Solver

Flow Calculation

In the **Flow Calculation** panel on the top left, select the **Flow Solver Type** to be used for solving the chosen partial differential equations from the pull-down menu (EJ, SimpleFFT, or LIR). EJ cannot be selected for solving Brinkman equations.



It is also possible to choose **Load from file** to import the result file (*.gdr) 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.

Important! The EJ solver cannot be selected to solve Brinkman equations applied to porous materials. Therefore, the EJ solver cannot be selected to simulate adsorption, since the adsorbent must always be porous.

Solver Settings

Stopping Criteria

The equations are solved by an iterative approach.

Iterative Solver

The basic idea of an iterative method is to

1. Start with some initial guess for the unknown values
2. Improve the current values in each iterative step
3. Repeat the iterative process until one of the stopping criteria is reached.

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

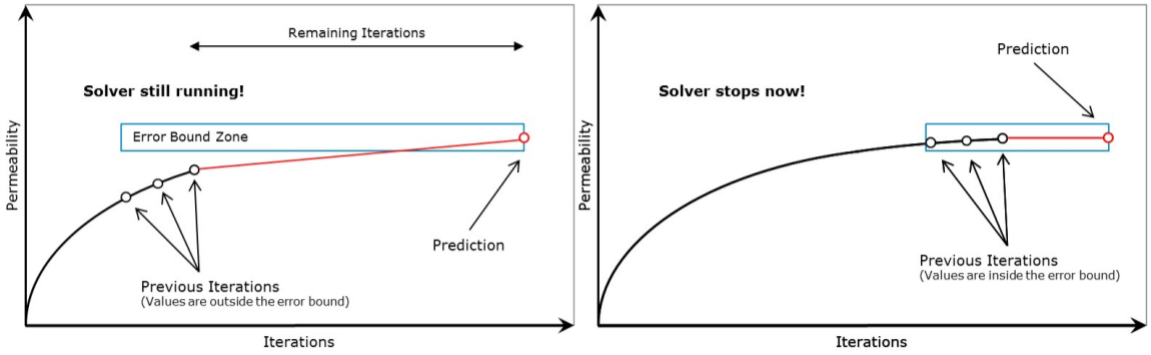
apply for each computational direction individually.

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

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

Error Bound

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



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

Tolerance

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

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

$$\max_{i\in[1,100]} \frac{x_c - x_{c-i}}{x_{c-i}} < \text{tolerance} \tag{55}$$

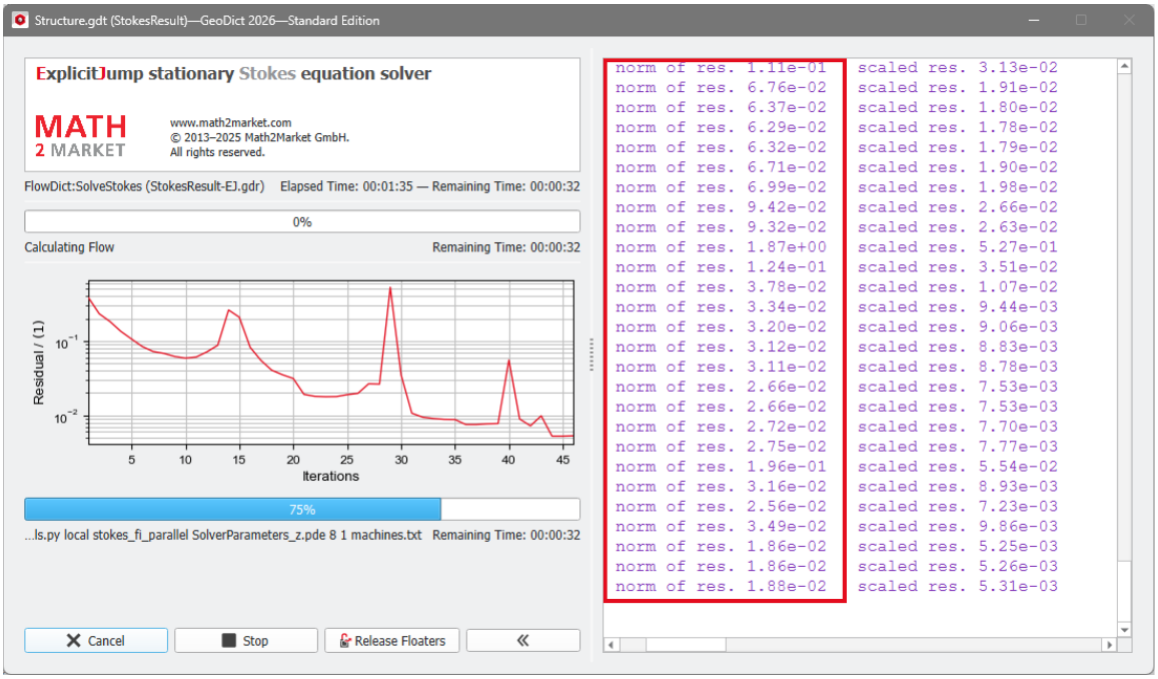
The computation is stopped if the maximal relative change is smaller than the value

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

Residual

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

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



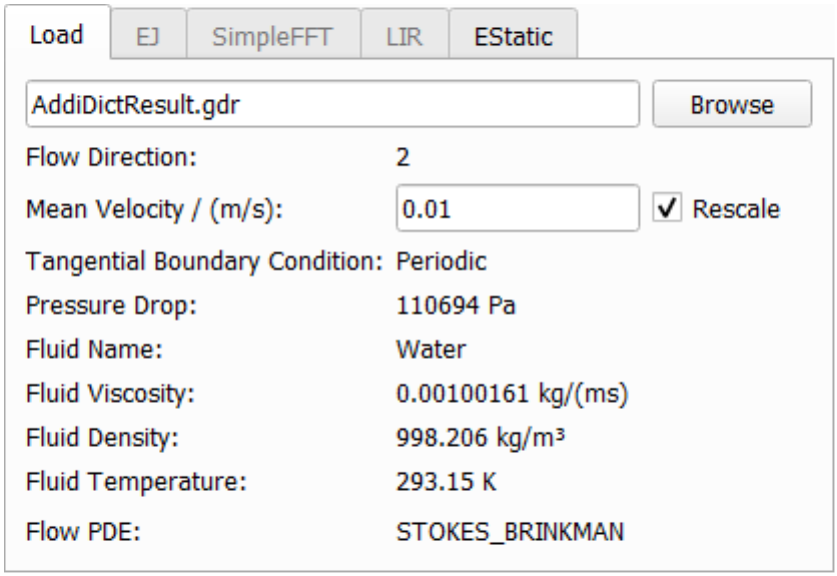
The recommendation to choose **Tolerance** or **Residual** for the **EJ** solver is based on the structure's porosity. Both give similar results for highly porous structures. For dense structures, if using the Schur Complement **Residual**, the relative norm of the residual may be small even though the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

Additional Settings

Load

If **Load from File** has been selected from the **Flow Solver Type** menu in the **Flow**

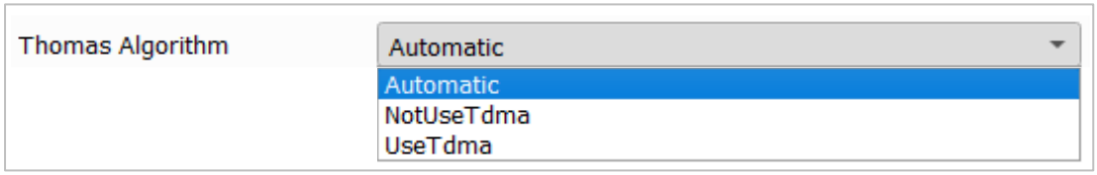
Calculation panel, choose a GeoDict result file of a previously run computation. Some information about the computation is shown. The mean velocity of the computation can be rescaled to another one by checking **Rescale** and editing the mean velocity.



SimpleFFT

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

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



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

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

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

For more information about the Thomas algorithm see here.

Depending on the material parameters and geometrical structure of the structure, the underlying mathematical problem can vary in complexity, thus influencing the behavior

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

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

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

LIR

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

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

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

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

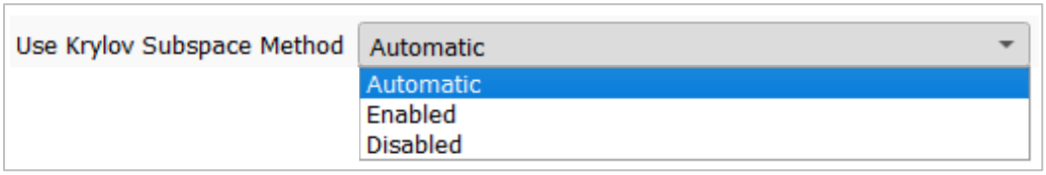
The method is available to solve the Stokes and Stokes–Brinkman equations as well as for solving mechanics, diffusion, thermal, and electrical conduction and is enabled by default.

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

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

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

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

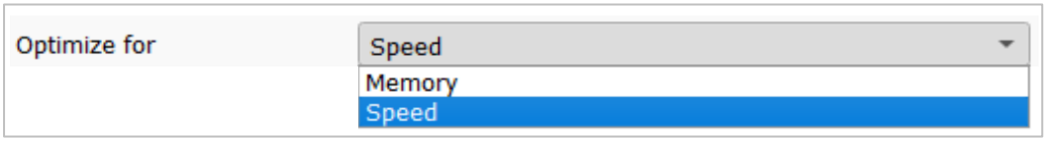


Note! In case that the Krylov subspace method (BICGStab) is used, the **Relaxation** may also be adapted automatically.

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

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

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.

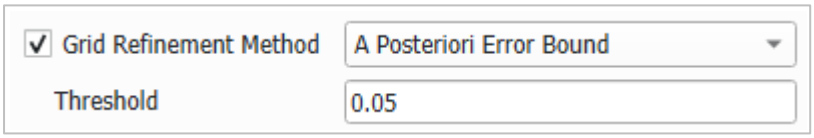
The default option is **LIR-Tree** and should always be used. The solver uses an adaptive grid structure called LIR-tree and needs up to 10 times less runtime and memory compared to the **Regular Grid** option.

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

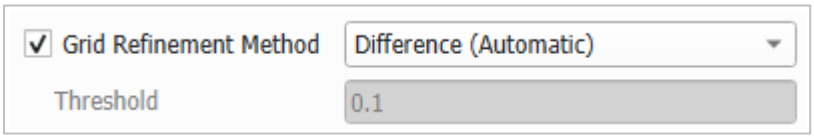
The solver can analyze the computed field and refines the adaptive grid during the computation at locations where more accuracy is needed. The LIR solver splits cells where a high gradients occur when the **Grid Refinement Method** is enabled. In this case, the additional parameters **Number of Grid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

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

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

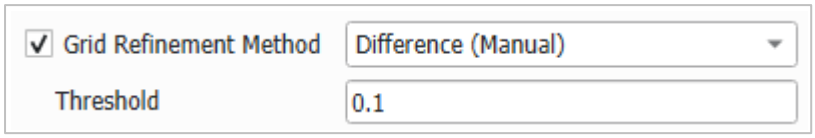


Choosing **Difference (Automatic)** leads to computational cells being split when the difference in values between neighboring cells exceeds a certain **Threshold**. The solver automatically chooses all internal parameters based on the structure and simulation settings. For this option, cells are split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

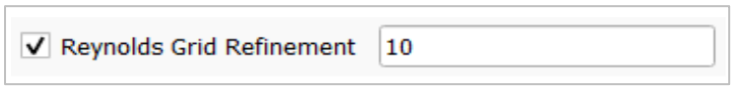


Selecting **Difference (Manual)** also causes the computational cells to be split when the difference in values between neighboring cells exceeds the specified **Threshold**. You can specify all parameters (Threshold and Number of Grid Refinements) for the grid refinement manually. For this option, cells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

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



Activate **Reynolds Grid Refinement** to use the local Reynolds number (Re) for adaptive grid refinement.



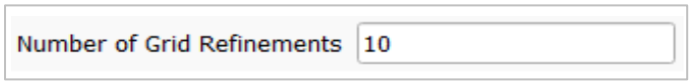
A grid cell is split if the local Reynolds number, i.e., the ratio between inertial and viscous forces exceeds the given threshold. The Reynolds number is defined as:

$$\mathrm{Re} = \frac{\rho \mathrm{u} \mathrm{L}}{\mu} \quad (56)$$

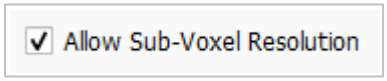
Reynolds Number

where ρ is the density of the fluid (SI units: kg/m^3), u is the velocity of the fluid (m/s), μ is the dynamic viscosity of the fluid (Pa·s or N·s/m^2 or kg/m·s), L is a characteristic length (m). For the local Reynolds number, the size of the grid cell is used for the characteristic length.

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



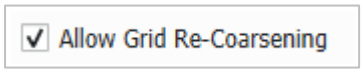
When **Allow Sub-Voxel Resolution** is enabled, the solver is allowed to split computational cells to sizes smaller than the voxel length.



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

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

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

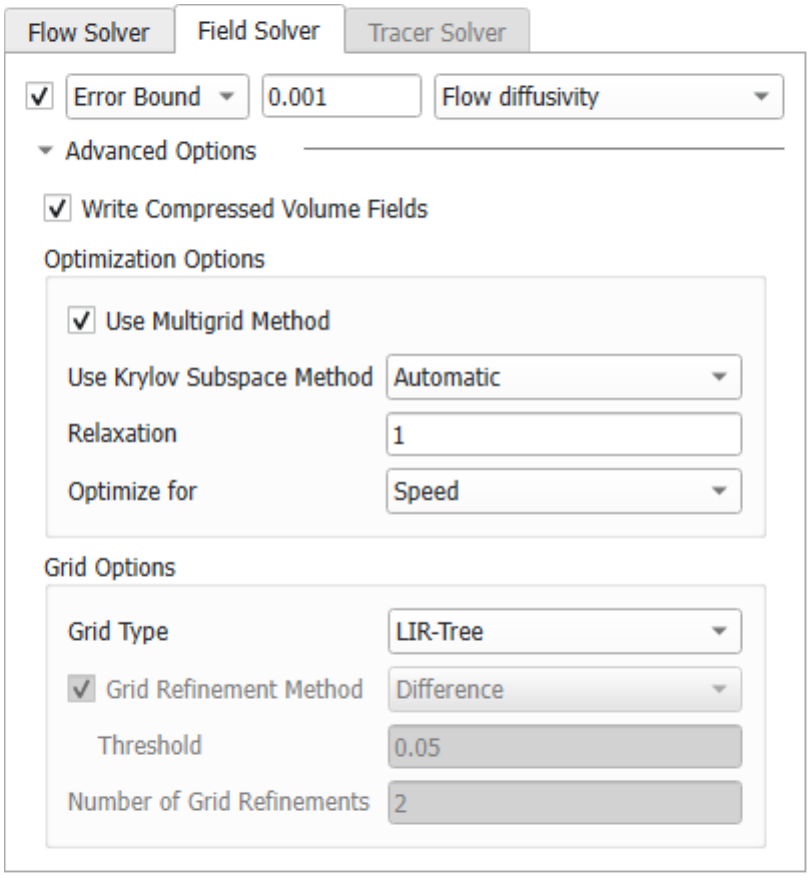


This means, grid refinement is done temporarily. Afterwards, the cells are merged as

soon as accuracy is not needed anymore. This reduces the memory and runtime requirements.

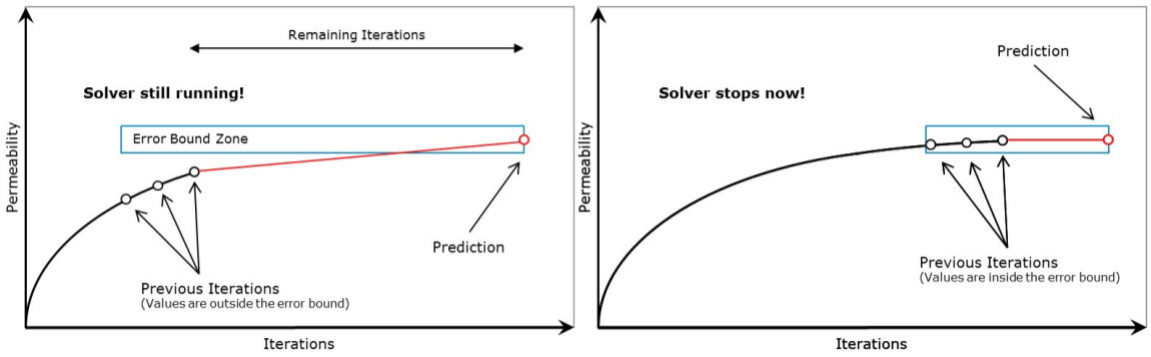
Field Solver

Under the **Field Solver** tab, several options regarding the solver for the transport of the concentration field are available. The solution algorithm for concentration field transport is integrated into the LIR solver only.



Stopping Criterion

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



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

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

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

$$\max_{i\in[1,100]} \frac{x_c - x_{c-i}}{x_{c-i}} < \text{tolerance} \tag{57}$$

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

Advanced Options

Write Compressed Volume Fields

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

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

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

Optimization Options

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

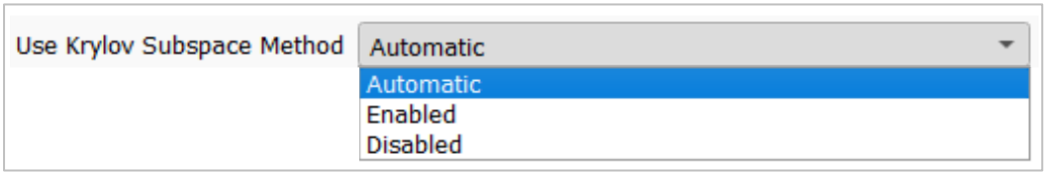
The method is available to solve the Stokes and Stokes–Brinkman equations as well as for solving mechanics, diffusion, thermal, and electrical conduction and is enabled by default.

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

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

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

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

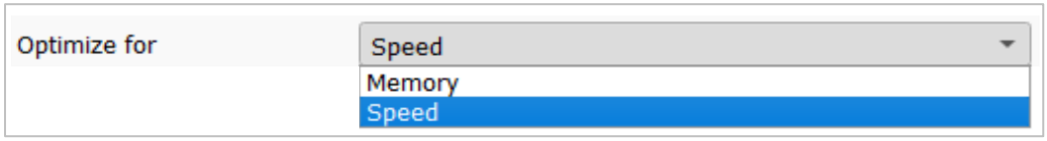


Note! In case that the Krylov subspace method (BICGStab) is used, the **Relaxation** may also be adapted automatically.

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

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

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



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

Grid Options

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

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

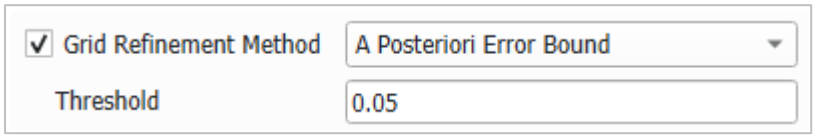
The solver can analyze the result field during the computation and improves the adaptive grid in places where more accuracy is needed. The LIR solver splits cells where a high gradient occurs.

For the following options the settings cannot be changed from the default values. The default values are shown for you information:

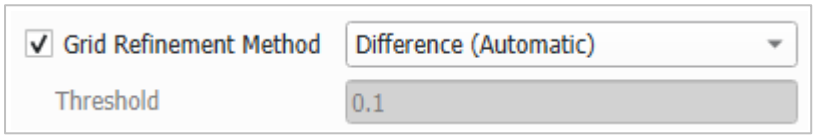
The solver can analyze the computed field and refines the adaptive grid during the computation at locations where more accuracy is needed. The LIR solver splits cells where a high gradients occur when the **Grid Refinement Method** is enabled. In this case, the additional parameters **Number of Grid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

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

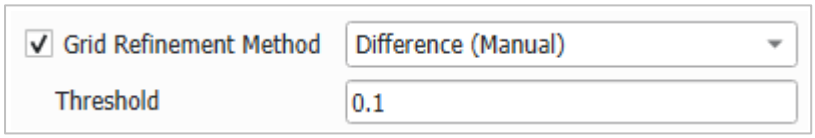
When **A Posteriori Error Bound** is selected, the solver targets the specified accuracy **Threshold**. While the **Error Bound** (set as Simulation Stopping Criterion) determines the relative error in the solution of the linear system, **A Posteriori Error Bound** refers to the relative error estimated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



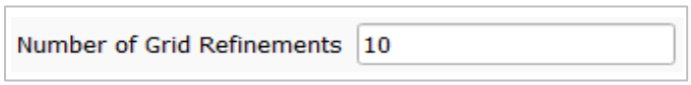
Choosing **Difference (Automatic)** leads to computational cells being split when the difference in values between neighboring cells exceeds a certain **Threshold**. The solver automatically chooses all internal parameters based on the structure and simulation settings. For this option, cells are split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



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



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



Tracer Solver

Under the **Tracer Solver** tab, options regarding the tracers used for tracking the solute concentration are available.

Tracer Particles

The **Tracer per inflow voxel** parameter defines how many particles are used to track the solution concentration. The number given is multiplied with the number of pore and porous voxels at the inflow boundary. This parameter controls the precision of the adsorption simulation. A higher number of tracers increases precision. However, runtime also increases. The concentration of the adsorbing solute is not changed by this parameter, it is only distributed more finely/coarsely in the fluid.

Note! We recommended to use at least the default value of **5** tracers per inflow voxel.

Random Seed

Define the **Random Seed** that is used for defining the initial particle positions. The same random seed produces identical results, whereas results with different random seeds are similar but not identical.

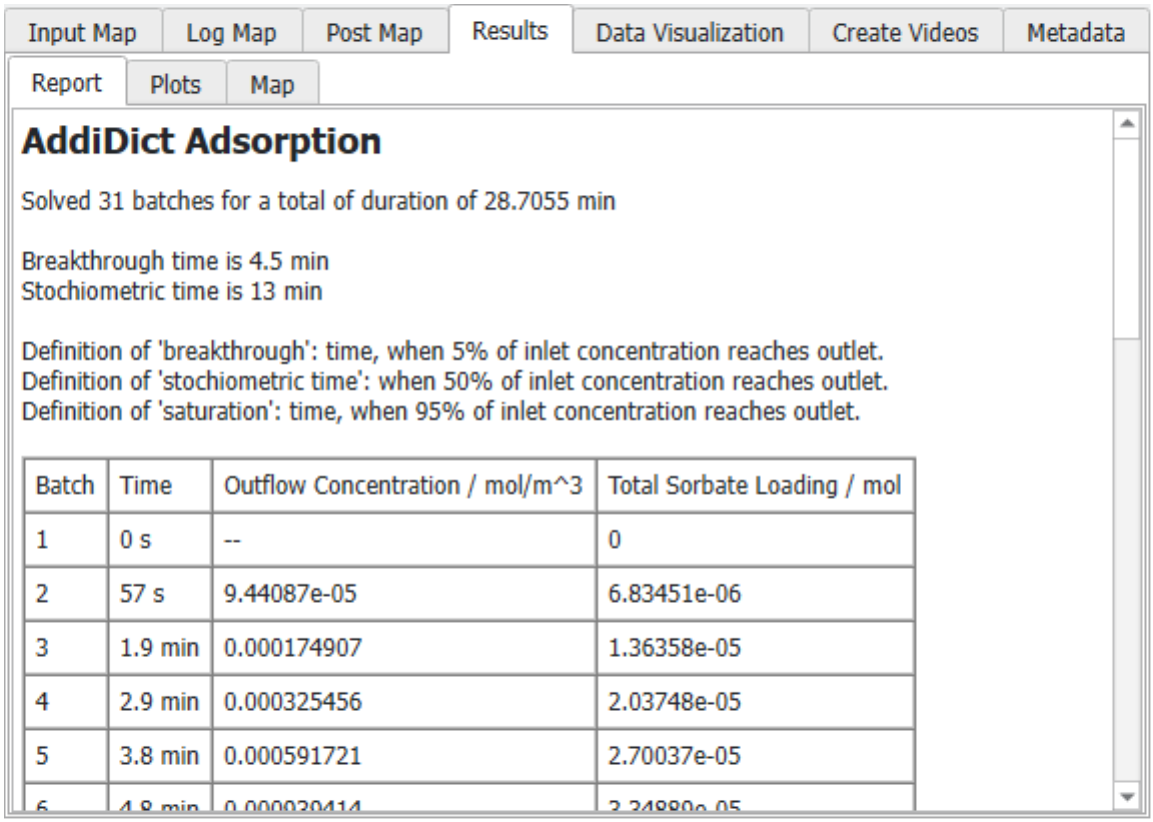
Calculate Concentration Field

Check **Calculate Concentration Field** to compute a concentration field based on the tracer particle cloud. This concentration field is only created during the post-processing and is not used during the simulation. It is similar to the resulting concentration field from the field solver and can be used as input to prescribed an initial concentration.

1.4.2 Results

After the **Adsorption** simulation is completed, the resulting files are saved in the project folder and a **Result Viewer** with the GeoDict result file opens automatically. The created GeoDict result file (*.gdr) contains seven tabs. The computational results are shown under the **Results** tab, can be loaded for visualization via the **Data Visualization** tab, and can be used to **Create Videos**. The other four tabs (**Input Map**, **Log Map**, **Post Map** and **Metadata**) display additional information about the computation.

Find more details on the general functionalities in the Result Viewer user guide.



Adsorption Results

- Report 145
  Shows the computed results.
- Plots 146
  View result plots.
- Data Visualization 149
  Load results for a graphical visualization.
- Create Videos 150
  Visualize the adsorption process in a MP3 movie.

Report

In the **Report** subtab of the **Results** tab an overview of the simulation results is provided.

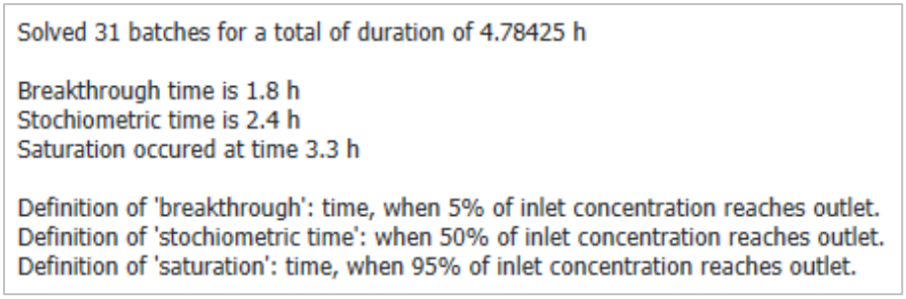
Characteristic Times

At the top of the report the **Number of Batches** with one additional initial batch and the total simulated time is provided. Both of these parameters need to be defined under the Experiment 113 tab when setting up the simulation.

Below the **Breakthrough**, **Stochiometric**, and **Saturation** times are provided. The values provide the times at which a certain amount of the inlet concentration has reached the outlet:

- For the **Breakthrough** time **5%** of the inlet concentration has reached the outlet.
- for the **Stochiometric** time **50%** of the inlet concentration has reached the outlet.
- for the **Saturation** time **95%** of the inlet concentration has reached the outlet.

When one of these conditions has not yet been reached, the corresponding characteristic time is not displayed here.



Table

Below the characteristic times a table containing the **Batch**, **Time**, **Outflow Concentration** in **mol/m³**, and the **Total Sorbate loading** in **mol** is provided. The data shown in this table is the basis for the plots shown in the respective subtab 146.

Batch	Time	Outflow Concentration / mol/m^3	Total Sorbate Loading / mol
1	0 s	--	0
2	57 s	9.44087e-05	6.83451e-06
3	1.9 min	0.000174907	1.36358e-05
4	2.9 min	0.000325456	2.03748e-05
5	3.8 min	0.000591721	2.70037e-05
6	4.8 min	0.000939414	3.34889e-05
7	5.7 min	0.00149661	3.97438e-05
8	6.7 min	0.0021505	4.57284e-05
9	7.7 min	0.00287185	5.14149e-05
10	8.6 min	0.00376958	5.67302e-05

Plots

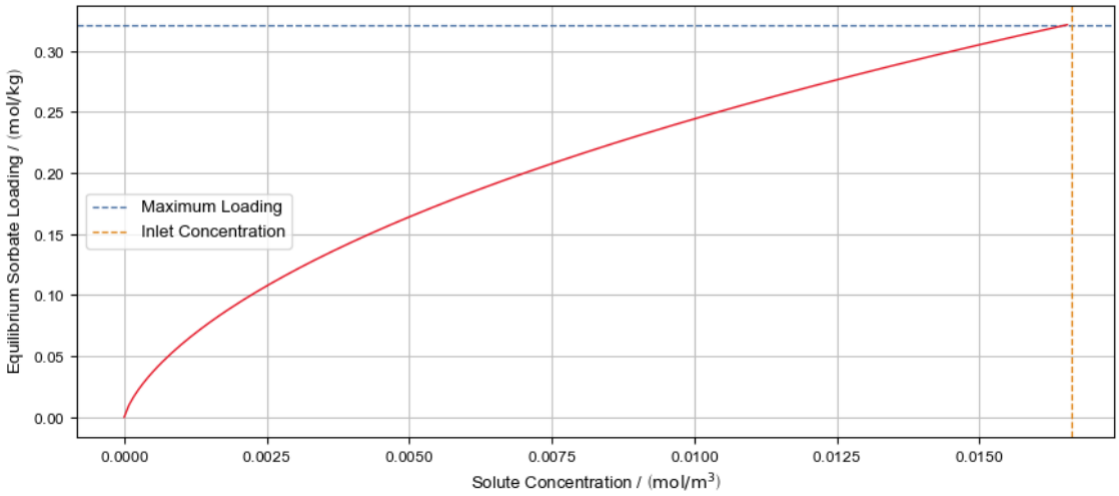
Under the **Plots** subtab, several plots are available.

Properties of the axis and graph can be modified for all plots. Right click the graph to access the settings menus. With **Edit Axis Settings**, scaling, labels and ticks of the axis as well as font sizes and legend placement can be selected. With **Edit Graph Styles**, title, style and color can be defined for each graph shown in the plot. In the menu that appears after right clicking the

graph the data contained in the plot can be saved as well. More details on changing plot settings are available in the Result Viewer user guide.

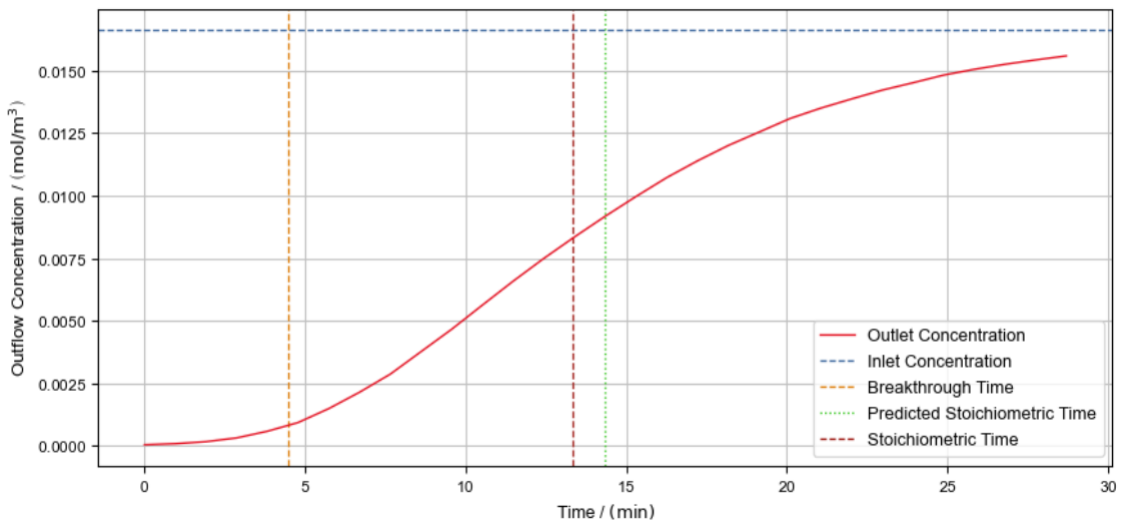
Isotherm

The **Isotherm** plot shows the applied **Isotherm**, i.e., **Equilibrium Sorbate Loading** over the **Solute Concentration**. This plot is identical to the one shown when setting up the adsorption reaction in the Adsorption - Interaction 124 tab. Additionally, the **Maximum Loading** possible with this structure and the interaction settings as well as the defined Inlet Concentration 121 are shown.



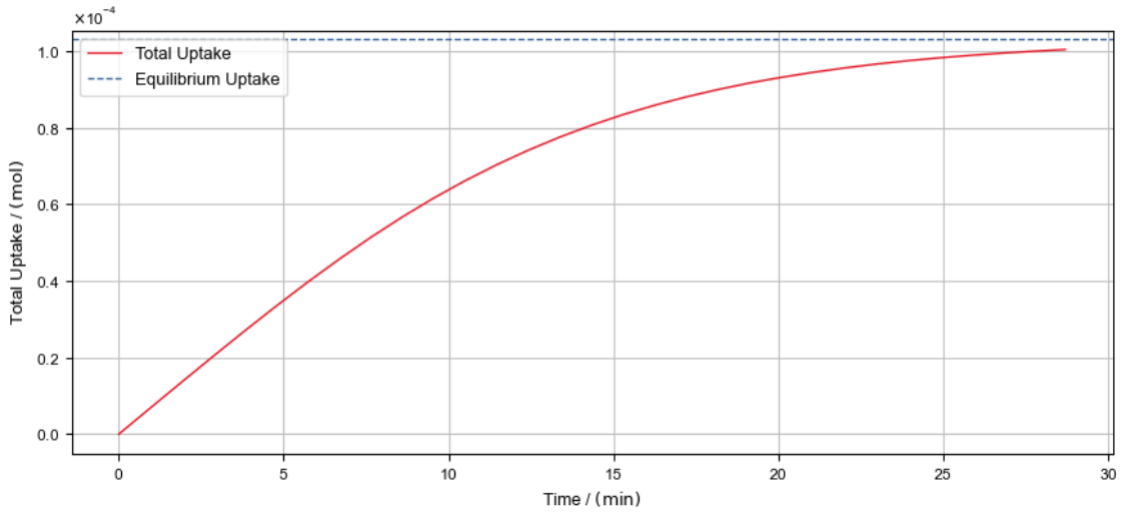
Breakthrough Curve

The **Breakthrough Curve** plot shows the **Outlet Concentration** of the solute over time. The **Inlet Concentration** shown as a dashed blue line is the maximum value that this plot can reach and was defined under the Adsorbate 121 subtab. When available the characteristic times 145 (**Breakthrough**, **Stochiometric**, and **Saturation**) are displayed as vertical dashed lines. Additionally, a **Predicted Stochiometric Time** is shown as a dotted green line. This value is based on the same computation as the Approximate End Time 113 button that is available when setting up the adsorption simulation.



Total Uptake

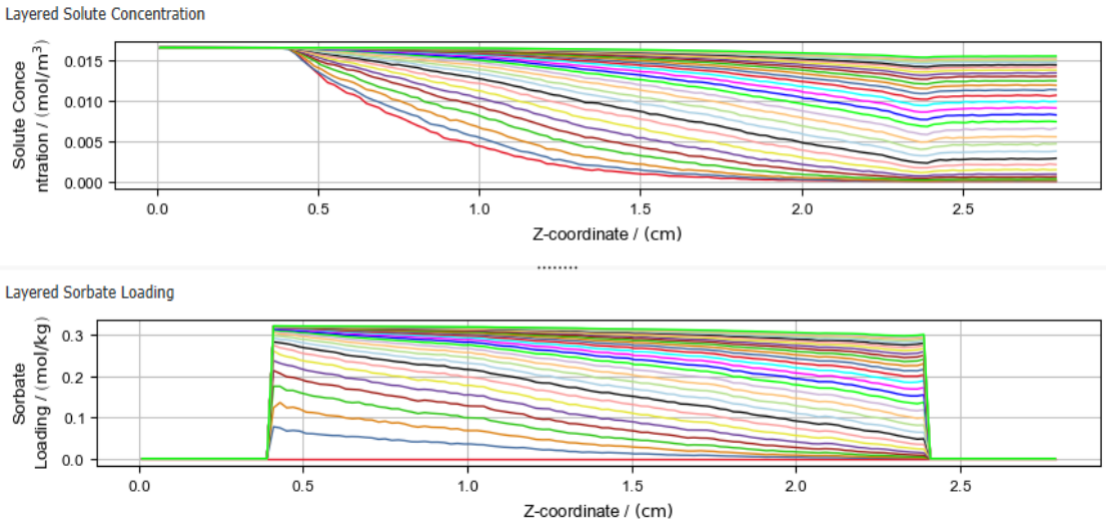
The **Total Uptake** plot shows the total amount of adsorbed species in mol over time and in addition to the breakthrough curve provides a good indication of the full saturation time. The maximum of this plot is the **Equilibrium Uptake** that depends on the structure and parameters set under the Adsorption - Interaction tab



Layered Data

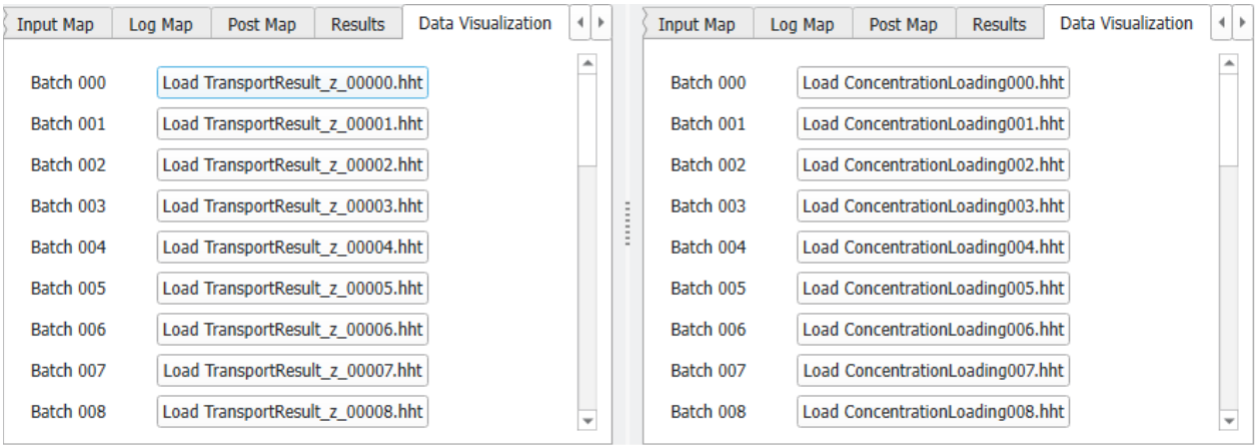
The **Layered Data** plot consists of two separate plots showing the **Solute Concentration** in **mol/m³** and the **Sorbate Loading** in **mol/kg** for each layer in the **Z** direction, which is the fixed computation direction. For each batch one graph is added to the plot allowing you to see the progress of adsorption occurring throughout the

structure. For a clearer plot, right-click the plot area to access the **Graph Styles** to select only some of batches to be shown.



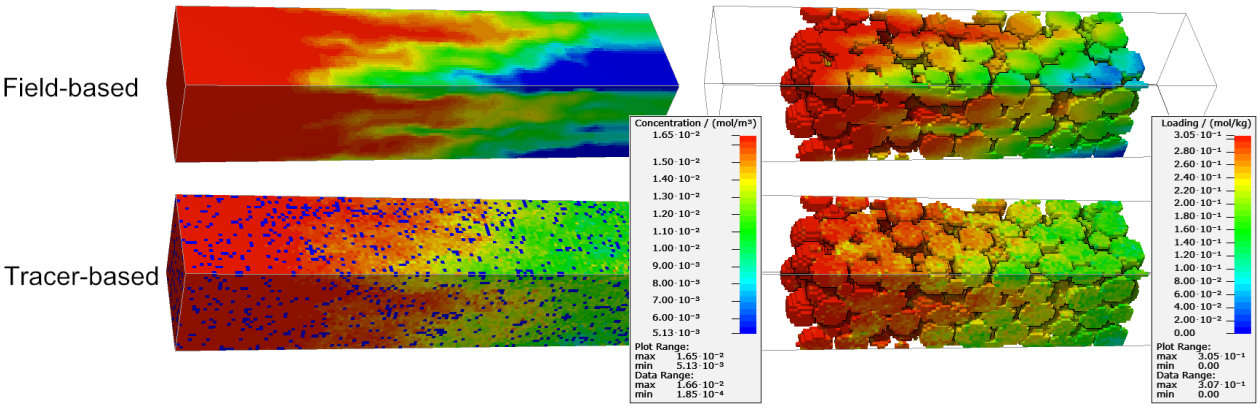
Data Visualization

The **Data Visualization** tab enables you to load for each batch the **Concentration Loading *.hht** when using the Tracer-based[115] approach or the **Transport Result *.hht** when using the Field-based[115] approach for 3D visualization in the **Visualization** area of GeoDict. Additionally, when using the Tracer-based[115] approach the **Trajectory File** of the particles can be loaded as described here[68]. For both approaches the computed **Flow Field** is available as well. All files represent the field in Z-direction, which is the fixed computation direction for **Adsorption** simulations.



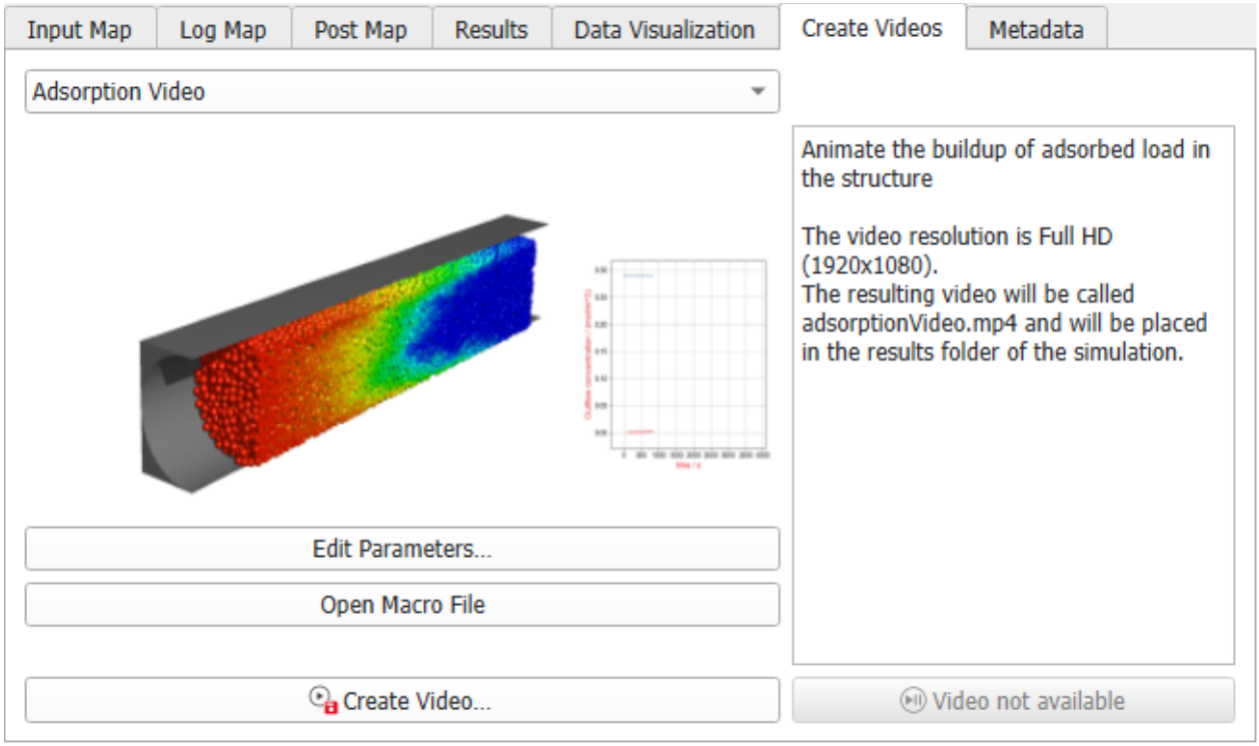
The ***.hht** volume files contain volume fields for the **Concentration** of the solute and the **Loading** of adsorbate in the porous adsorbent. When using the Tracer-based[115] approach the **Concentration** field is only available if the corresponding option[144] under the **Tracer Solver** subtab was selected.

Note! The Tracer-based 115 concentration field can have voxels that are not passed by any particle trajectory. These voxels are shown with a concentration of zero because no concentration reached them. This is an artifact of this approach. To reduce the number of voxels with zero concentration you can increase the number of tracers per inflow voxel 143.



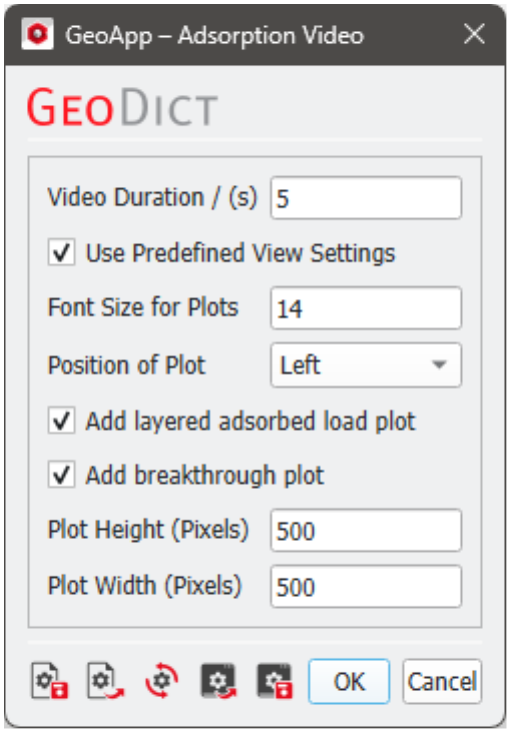
Create Videos

A predefined GeoPy macro can be used to animate the buildup of adsorbed load in the structure. The created video is in Full HD and the file (**adsorptionVideo.mp4**) is saved to the results folder. The macro for video creation can be viewed and modified by clicking **Open Macro File**.



Under **Edit Parameters**, multiple options are available:

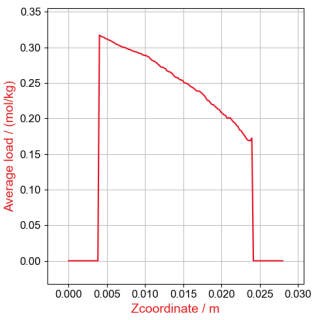
- **Video Duration**: Set the duration of the video in s. Time batches are distributed of the defined time.
- **Use Predefined View Settings**: When this setting is activated a predefined camera position is used to create the animation. When inactive the current view settings from the visualization area in GeoDict are used.
- **Font Size for Plots**: Define the font size for text in the breakthrough plot that can be included in the video.
- **Position of Plot**: Define the position of the plot that can be included in the video. The plot can be positioned to the right or left of the 3D animation of the adsorbed load. If both plots are added this is the position of the layered adsorbed load plot
- **Add layered adsorbed load plot**: When activated the layered adsorbed load plot is shown in the video together with the animation. Each time batch the adsorbed load per layer is updated.
- **Add breakthrough plot**: When activated the breakthrough plot is shown in the video together with the animation. Each time batch the corresponding data point is added to the plot.
- **Plot Height** and **Width**: Set the size of the breakthrough plot in the video.

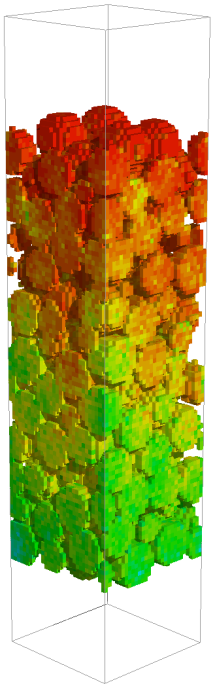


After setting the parameters click **Create Video** to run the macro. Once a video was created the **Play Video** button becomes active and allows for direct viewing of the video.

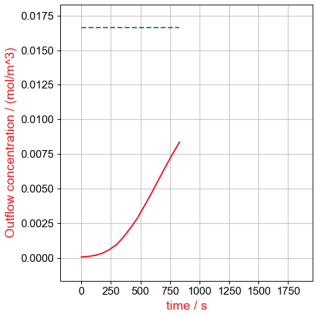
An exemplary video that was generated using **Create Video** is shown below. Please click on the play button to start the video.

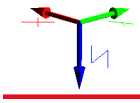
ADDIDICT





GEODICT
The Digital Material Laboratory



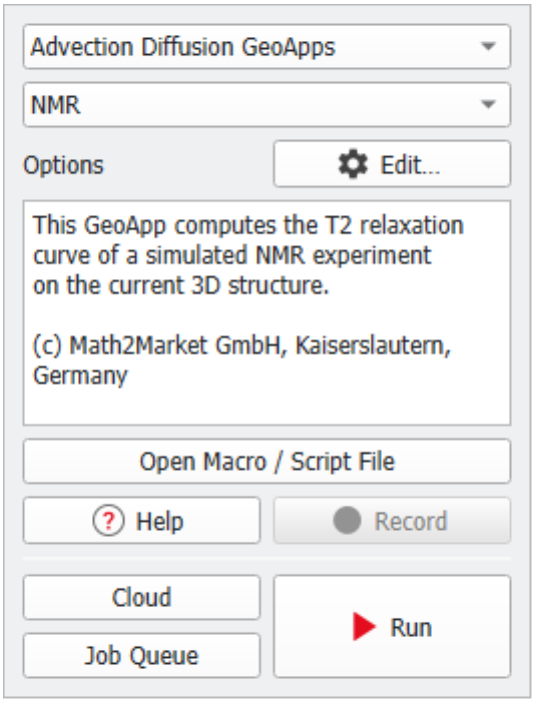


MATH 2 MARKET

1.5 Advection Diffusion GeoApps

Under the **Advection Diffusion GeoApps** the GeoApps for the AddiDict module can be accessed.

Currently, only the **NMR** GeoApp is selectable here. Click the **Edit** button to open the parameter dialog for the GeoApp where you can define the settings. Click the **Open Macro / Script File** button to open the underlying macro file your default text editor.



AddiDict GeoApps

- NMR 153
  Compute the T2 relaxation curve of a NMR experiment.

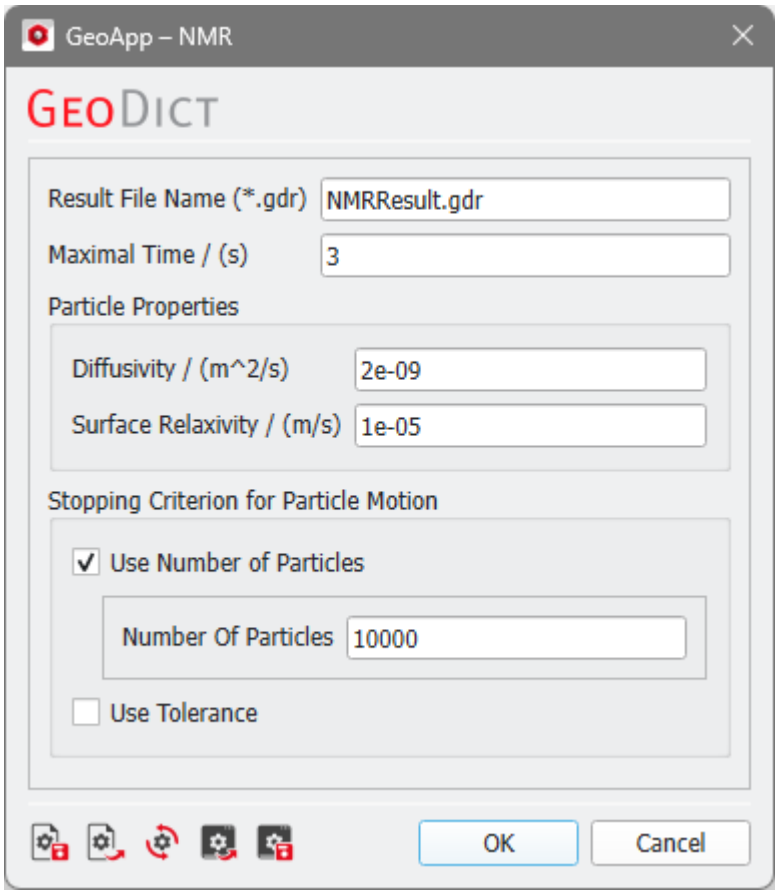
1.5.1 NMR

The **NMR** app computes the T2 relaxation curve of a simulated NMR experiment on the current 3D structure.

Modules needed to run this GeoApp:

AddiDict

After loading a structure, click **Edit** to open the **NMR** parameters dialog.



First, define the **Result File Name**.

The **Maximal Time** is the time duration of the particle tracking.

Under **Particle Properties** define the **Diffusivity** of particles in the fluid (the default 2e-9 m^2/s refers to the self-diffusion coefficient of water) and the **Surface Relaxivity** of the pore wall material.

As **Stopping Criterion for Particle Motion** either choose **Use Number of Particles** (the number of walkers to be simulated) or **Use Tolerance** (give the result deviation tolerance, then particles are added until the tolerance is reached).

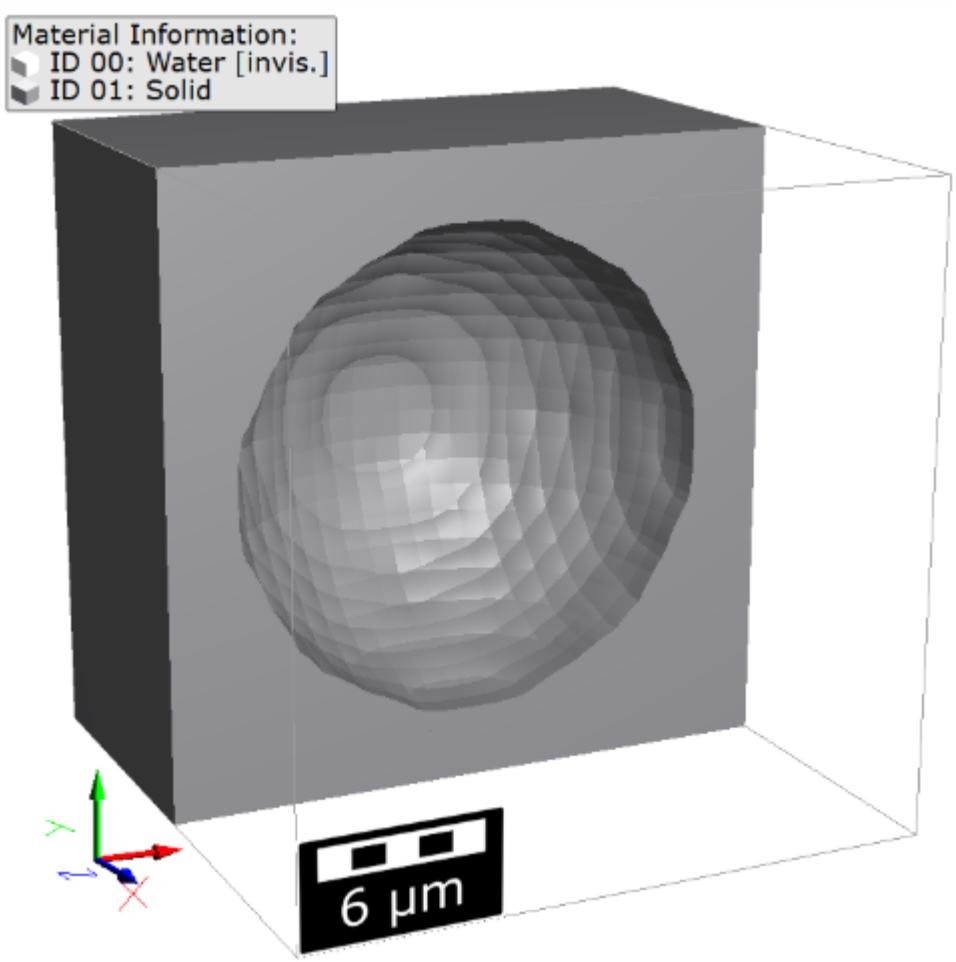
Two NMR simulation examples, one for a Bentheim sandstone and the other for an Obernkirchen sandstone are found in the tutorial Random-walk method to simulate T2 of NMR.

Click **OK** to close the dialog, go back to the GeoApp section, and click **Run**.

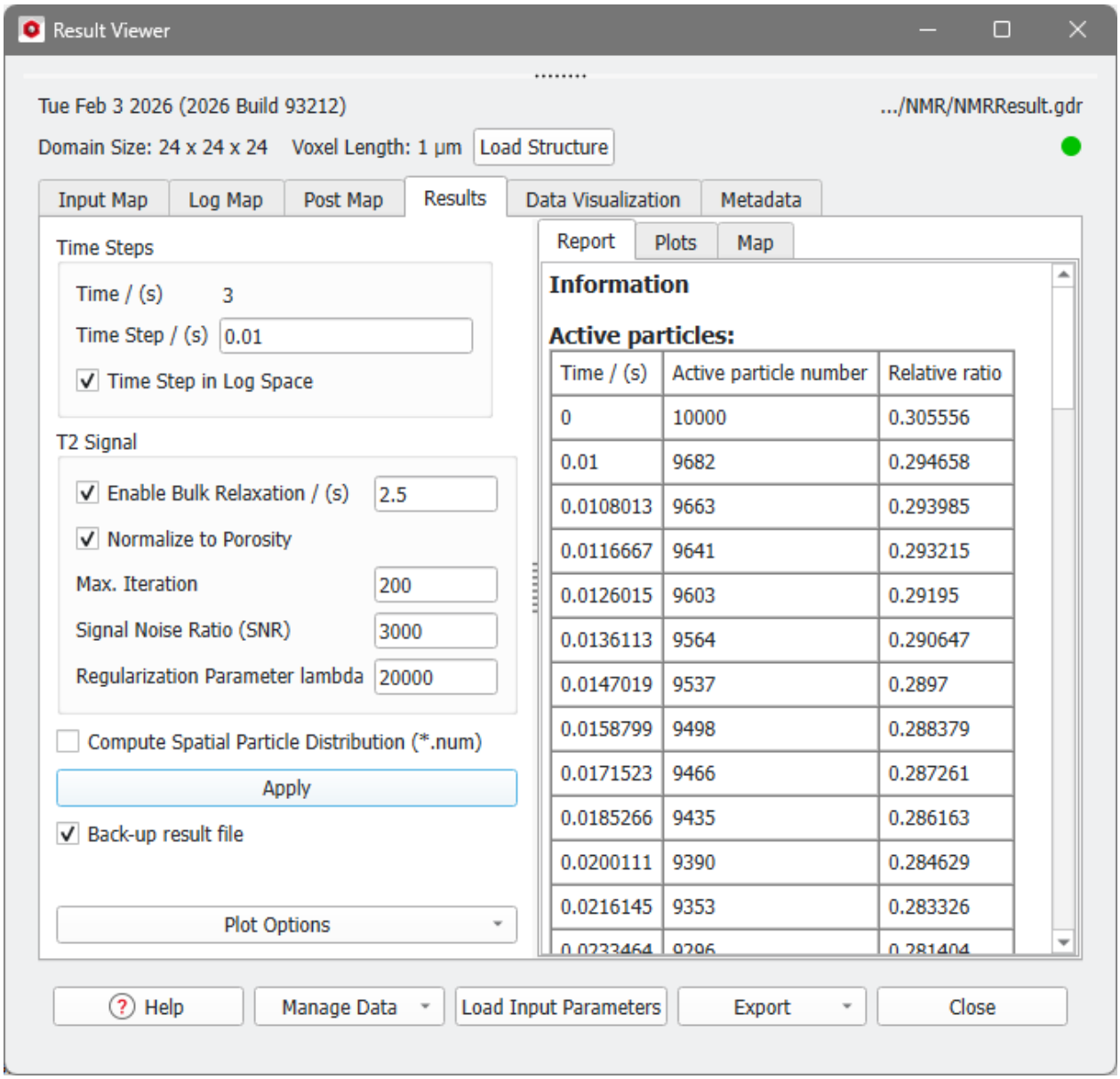
Results

When the simulation finishes, the **Result Viewer** of the result file (*.gdr) opens automatically.

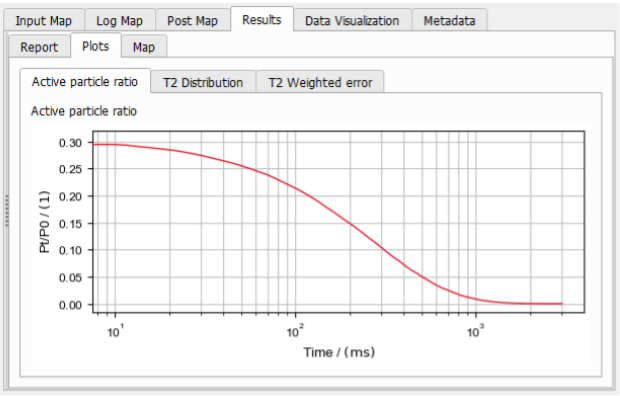
In the example, an NMR experiment was run on a cube with one spherical pore; here clipped in Z-direction.

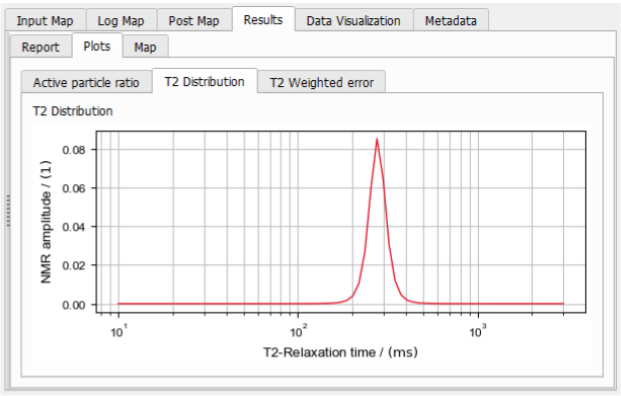


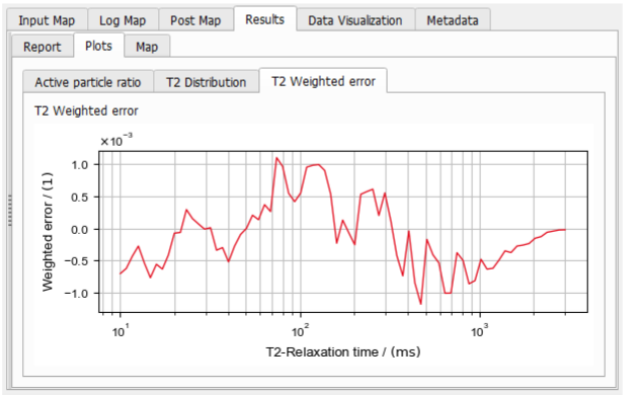
The **Results - Report** subtab of the **Result Viewer** shows the table for the number of **Active particles** and the resulting relative ratio vs. the simulation time.



In the **Results - Plots** subtab, the plot of **Active particle ratio**, corresponding to the values of the **Active particles** table, the plot of **T2 Distribution**, and **T2 Weighted error** are shown. For more details on the results, refer to the NMR tutorial linked above.


Input Map
Log Map
Post Map
Results
Data Visualization
Metadata
Report
Plots
Map
Active particle ratio
T2 Distribution
T2 Weighted error
Active particle ratio
Pt/P0 / (1)
Time / (ms)


Input Map
Log Map
Post Map
Results
Data Visualization
Metadata
Report
Plots
Map
Active particle ratio
T2 Distribution
T2 Weighted error
T2 Distribution
NMR amplitude / (1)
T2-Relaxation time / (ms)


Input Map
Log Map
Post Map
Results
Data Visualization
Metadata
Report
Plots
Map
Active particle ratio
T2 Distribution
T2 Weighted error
T2 Weighted error
Weighted error / (1)
T2-Relaxation time / (ms)

1.6 References

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