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**FLOW123D**

version 1.6.5

**Documentation of file formats  
and brief user manual.**

**Liberec, 2011**

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## 0.1 Overview

Flow123D is a software for simulation of water flow and reactionary solute transport in a heterogeneous porous and fractured medium. In particular it is suited for simulation of underground processes in a granite rock massive. The program is able to describe explicitly processes in 3D medium, 2D fractures, and 1D channels and exchange between domains of different dimension. The computational mesh is therefore collection of 3D tetrahedrons, 2D triangles and 1D line segments.

The water flow model assumes a saturated medium described by Darcy law. For discretization, we use lumped mixed-hybrid finite element method. We support both steady and unsteady water flow.

The solute transport model can deal with several dissolved substances. It contains non-equilibrium dual porosity model, i.e. exchange between mobile and immobile pores. There is also model for several types of adsorption in both the mobile and immobile zone. The implemented adsorption models are linear adsorption, Freundlich isotherm and Langmuir isotherm. The solute transport model uses finite volume discretization with up-winding in space and explicit Euler discretization in time. The dual porosity and the adsorption are introduced into transport by operator splitting. The dual porosity model use analytic solution and the non-linear adsorption is solved numerically by the Newton method.

Reaction between transported substances can be modeled either by a SEMCHEM module, which is slow, but can describe all sorts of reactions. On the other hand, for reactions of the first order, i.e. linear reactions or decays, we provide our own solver which is much faster. Reactions are coupled with transport by the operator splitting method,

The program provides output of the pressure, the velocity and the concentration fields in two file formats. You can use file format of GMSH mesh generator and post-processor or you can use output into widely supported VTK format. In particular we recommend Paraview software for visualization and post-processing of VTK data.

The program is implemented in C/C++ using essentially PETSC library for linear algebra. The water flow as well as the transport simulation and reactions can be computed in parallel using MPI environment.

The program is distributed under GNU GPL v. 3 license and is available on the project web page: <http://dev.nti.tul.cz/trac/flow123d>

## 0.2 Basic usage

### 0.2.1 How to run the simulation.

On the Linux system the program can be started either directly or through a script `flow123d.sh`. When started directly, e.g. by the command

```
> flow123d -s example.ini
```

the program requires one argument after switch `-s` which is the name of the principal input file. Full list of possible command line arguments is as follows.

**-s** *file*

Set principal INI input file. All relative paths in the INI file are relative against current directory.

**-S** *file*

Set principal INI input file. All relative paths in the INI file are relative against directory of the INI file. This is equivalent to change directory to the directory of the INI file at the start of the program.

**-i** *path*

When there is string `${INPUT}` in the any path in the INI file, it will be replaced by given *path*.

**-o** *path*

Every relative path for any output file will be relative to this *path*.

All other parameters will be passed to the PETSC library. An advanced user can influence lot of parameters of linear solver. In order to get list of supported options use parameter **-help**. You can use script `flow123d.sh` to start parallel jobs or limit resources used by the program. This script accepts the same parameters as the program itself and further some additional parameters.

**-h**

Usage overview.

**-t** *timeout*

Upper estimate for real running time of the calculation. Kill calculation after *timeout* seconds. Can also be used by PBS to choose appropriate job queue.

**-np** *number of processes*

Specify number of parallel processes for calculation.

**-m** *memory limit*

Limits total available memory to *memory limit* bytes.

**-n** *priority*

Change (lower) priority for the calculation. See `nice` command.

**-r** *out file*

Stdout and stderr will be redirected to *out file*.

On the Windows system you have to use Cygwin libraries in order to emulate Linux API. The program with libraries can be downloaded from:

[http://dev.nti.tul.cz/~brezina/flow123d\\_packages/](http://dev.nti.tul.cz/~brezina/flow123d_packages/)

Then you can start a sequential run by command:

```
> flow123d.exe -s example.ini
```

or a parallel run by command:

```
> mpiexec.exe -np 2 flow123d.exe -s example.ini
```

The program accepts the same parameters as the Linux version, but there is no script similar to `flow123d.sh` on Windows system.

## 0.2.2 Structure of input

The principal input file of the program is an INI file which contains names of other necessary input files. Those are the file with calculation mesh (`*.msh`), the file with specification of adjacency between dimensions (`*.ngh`), the file with material description (`*.mtr`) and the file with boundary conditions for the water flow problem (`*.bcd`). For unsteady water flow you have to specify file with initial condition for the pressure (key `Input/Initial`) and optionally one can introduce file with water sources (key `Input/Sources`).

In the case of transport simulation one have to specify also the file with transport boundary conditions (`*.tbc`) and the file with transport initial condition for individual substances (`*.tic`).

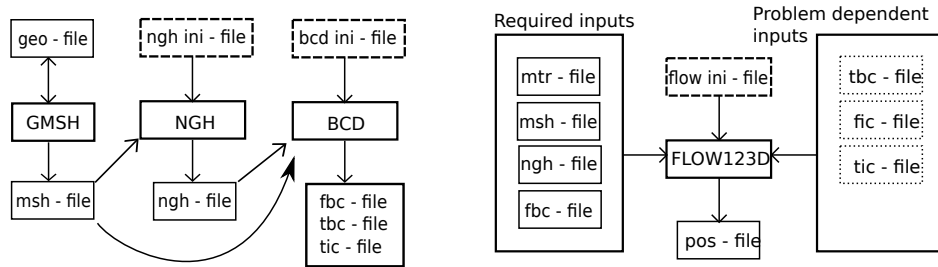


Figure 1: Preparation of input files.

For the preparation of input files we use several utilities (see Figure 1). We usually begin with a `*.geo` file as a description of the domain geometry. This come as an input for the GMSH mesh generator, which produce the mesh file. Then we run program `ngh` to produce adjacency file. Finally we can use program `bcd` for the preparation of files with boundary and initial conditions. The file with material properties has to be created manually, preferably by modifying some of the example problems. The programs `ngh` and `bcd` are distributed together with `flow123d` with their own limited documentation.

The output files can be either `*.pos` files accepted by the GMSH or one can use VTK format that can be post-processed by Paraview.

In following sections we briefly describe structure of individual input files.

## **0.3 Water flow model**

### **0.3.1 Governing equations**

### **0.3.2 Mixed-hybrid discretization**

## **0.4 Transport model**

### 0.4.1 Advection-Diffusion equation

Solute transport is governed by advection equation which can be written in the form

$$\frac{\partial c}{\partial t} + \mathbf{v} \frac{\partial c}{\partial x} = 0, \quad (1)$$

where  $c$  is concentration [ $M^3 \cdot L^{-3}$ ],  $t$  is time [ $T$ ],  $v$  is velocity [ $L \cdot T^{-1}$ ], and  $x$  is coordinate in cartesian system [ $L$ ]. Assuming solution which is constant on every element (cell centered finite volume method) and integrating equation (1) we get

$$\int_{e_i} \frac{\partial c}{\partial t} dV + \int_{e_i} \mathbf{v} \frac{\partial c}{\partial x} dV = 0.$$

After some rearrangements we obtain on  $i$ -th element ( $e_i$ )

$$\frac{\partial c_i}{\partial t} V_i + c \int_{\partial e_i} \mathbf{v} \cdot \mathbf{dS} = 0, \quad (2)$$

where  $c_i$  is average concentration in  $e_i$  and  $V_i$  its volume,  $c$  will be specified later (there are two main possibilities -  $c_i$  or concentration from neighbouring element). Term  $\frac{\partial c}{\partial t}$  we approximate by explicit Euler difference

$$\frac{\partial c}{\partial t} \approx \frac{c_i^{n+1} - c_i^n}{\Delta t}. \quad (3)$$

Where  $\Delta t$  is a time step and upper index at  $c_i$  means values in the discrete time steps  $n + 1$  and  $n$ . We assume that all elements have piecewise smooth element boundary  $\partial e$  with outwards directed normal. Inside the area  $\Omega$  we introduce internal flows. With respect to  $e_i$ , we define internal flow intake  $U_{ij}^-$  (from element  $e_j$ ) and internal flow drain  $U_{ij}^+$  (to element  $e_j$ ) as follows

$$\begin{aligned} U_{ij}^- &= \min\left(\int_{\partial e_i \cap \partial e_j, i \neq j} \mathbf{v} \cdot \mathbf{dS}, 0\right), \\ U_{ij}^+ &= \max\left(\int_{\partial e_i \cap \partial e_j, i \neq j} \mathbf{v} \cdot \mathbf{dS}, 0\right). \end{aligned} \quad (4)$$

Those flows realizes solute transport in the area  $\Omega$ . On the  $\partial\Omega$  we define external flows which will be important for transport Dirichlet boundary conditions. In the same way as for internal flows we assume (with respect to element  $e_i$ ) external flow intake  $U_{ij}^{e-}$  (from  $\partial\Omega$ ) and external flow drain  $U_{ij}^{e+}$  (to  $\partial\Omega$ ).

$$\begin{aligned} U_{ik}^{e-} &= \min\left(\int_{\partial e_i \cap \partial\Omega} \mathbf{v} \cdot \mathbf{dS}, 0\right), \\ U_{ik}^{e+} &= \max\left(\int_{\partial e_i \cap \partial\Omega} \mathbf{v} \cdot \mathbf{dS}, 0\right). \end{aligned} \quad (5)$$

Direction of the velocity  $\mathbf{v}$ , which affects sign of the  $U$ -terms is significant for the construction solution. For the solution stability it is suitable to use an upwind scheme, which can be written for finite difference on simple 1D geometry in the form

$$\begin{aligned} v > 0 : \frac{\partial c}{\partial x} &\approx \frac{c_i^n - c_{i-1}^n}{\Delta x}, \\ v < 0 : \frac{\partial c}{\partial x} &\approx \frac{c_{i+1}^n - c_i^n}{\Delta x}. \end{aligned} \quad (6)$$

This scheme can be interpreted as well as in finite volume method - in convection term one can get  $c$  value opposite the flow of the quantity  $\mathbf{v}$  direction. For every  $e_i$  we introduce itemsets  $\mathcal{N}_i, \mathcal{B}_i$  which contains indexes of neighbouring elements, local boundary conditions respectively. Assuming upwind scheme, using (4), (5), and (3) we can write solution of the equation (2) (relation between two consecutive time steps) on  $e_i$  in the form

$$c_i^{n+1} = c_i^n - \frac{\Delta t}{V_i} \left[ \sum_{j \in \mathcal{N}_i} [U_{ij}^+ c_i + U_{ij}^- c_j] + \sum_{k \in \mathcal{B}_i} [U_{ik}^{e+} c_i + U_{ik}^{e-} c_{B_{ik}}] \right]. \quad (7)$$

Where  $c_{B_{ik}}$  are values of Dirichlet boundary conditions which belong to  $e_i$ . Formula (7) can be rewritten into the matrix notation

$$\mathbf{c}^{n+1} = (\mathbf{I} + \Delta t \mathbf{A}) \cdot \mathbf{c}^n + \Delta t \mathbf{B} \cdot \mathbf{c}_B^n \quad (8)$$

Where  $\mathbf{c}$  is vector of  $c_i^{n+1}$ ,  $\mathbf{A}$  is a square matrix composed from  $\frac{U_{ij}^+}{V_i}$ ,  $\frac{U_{ij}^-}{V_i}$ , and  $\frac{U_{ij}^{e+}}{V_i}$ .  $\mathbf{B}$  is in general rectangular matrix composed from  $\frac{U_{ij}^{e-}}{V_i}$  and  $\mathbf{c}_B^n$  is vector of Dirichlet boundary conditions.matrix definition. There is one stability condition for time step which is called Courant-Friedrich-Levy condition. For the problem without sources/sinks it can be written as

$$\Delta t_{max} = \min_i \left( \frac{V_i}{\sum_j U_{ij}^+ + \sum_k U_{ik}^{e+}} \right) = \min_i \left( \frac{V_i}{\sum_j |U_{ij}^-| + \sum_k |U_{ik}^{e-}|} \right). \quad (9)$$

This condition has a physical interpretation, which can be understood as conservation law - volume that intakes/drains to/from element  $e_i$  can not be higher then element volume  $V_i$ . From algebraical point of view this condition can be seen as a condition which bounds norm of the evolution operator as follows

$$\|\mathbf{I} + \Delta t \mathbf{A} \quad \Delta t \mathbf{B}\| \leq 1. \quad (10)$$

### 0.4.2 Generalization

This approach can be used as well as for more general element connections – for compatible/non-compatible element interconnection, if we know the flow integral values ( $U_{ij}^+$  or  $U_{ij}^-$ ). The most

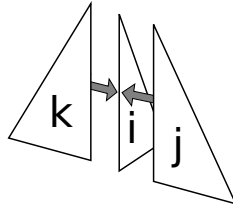


Figure 2: Edge with 3 elements

general case of connection is relation among  $n$  elements like in figure (2). For this case we define edge element indexset  $\mathcal{G}_l$  that contains all the indexes of elements which sides make  $l$ -th edge ( $g_l$ ), so that  $\mathcal{G}_l = \{i, j, k\}$ . For  $\mathcal{G}_l$  we introduce its subsets  $\mathcal{G}_{ij}$ ,  $\mathcal{G}_{ji}$ ,  $\mathcal{G}_{ik}$ ,  $\mathcal{G}_{ki}$ ,  $\mathcal{G}_{kj}$ , and  $\mathcal{G}_{jk}$ , where  $\mathcal{G}_{ij} = \mathcal{G}_{ik} = \mathcal{G}_l \setminus i = \{j, k\}$ ,  $\mathcal{G}_{ji} = \mathcal{G}_{jk} = \mathcal{G}_l \setminus j = \{i, k\}$ , and  $\mathcal{G}_{ki} = \mathcal{G}_{kj} = \mathcal{G}_l \setminus k = \{i, j\}$ .

It can be written in the same way for any edge  $g$  with more than 3 elements, it is hold  $|\mathcal{G}_g| - 1 = |\mathcal{G}_{ab}|; \forall a, b \in \mathcal{G}_g$ . For  $l$ -th edge ( $g_l$ ) we can define total edge flow  $U_{g_l}$  eg. as

$$\begin{aligned} U_{g_l} &= \sum_{m \in \mathcal{G}_{ji}} \left[ U_{mj}^+ + \frac{U_{jm}^+}{|\mathcal{G}_{ji}|} \right] = \sum_{m \in \mathcal{G}_{jk}} \left[ U_{mj}^+ + \frac{U_{jm}^+}{|\mathcal{G}_{jk}|} \right] \\ &= \sum_{m \in \mathcal{G}_{ij}} \left[ U_{mi}^+ + \frac{U_{im}^+}{|\mathcal{G}_{ij}|} \right] = \sum_{m \in \mathcal{G}_{ik}} \left[ U_{mi}^+ + \frac{U_{im}^+}{|\mathcal{G}_{ik}|} \right] \\ &= \sum_{m \in \mathcal{G}_{ki}} \left[ U_{mk}^+ + \frac{U_{km}^+}{|\mathcal{G}_{ki}|} \right] = \sum_{m \in \mathcal{G}_{kj}} \left[ U_{mk}^+ + \frac{U_{km}^+}{|\mathcal{G}_{kj}|} \right], \end{aligned} \quad (11)$$

$U_{g_l}$  with respect to any  $e_m$ ;  $m \in \mathcal{G}_l$  has to have the same value because continuity equation, for assumed incompressible flow, has to be fulfilled in every edge. Edges with more than two elements and two and more nonzero intakes to edge realize an ideal mixing (to an average concentration) with weights which will be specified later. This fact modifies equation (7) on the general mesh into the form

$$c_i^{n+1} = c_i^n - \frac{\Delta t}{V_i} \left[ \sum_{j \in \mathcal{N}_i} \left[ U_{ij}^+ c_i + \frac{U_{ij}^-}{\sum_{k \in \mathcal{G}_{ij}} \left[ U_{ki}^+ + \frac{U_{ik}^+}{|\mathcal{G}_{ij}|} \right]} \sum_{k \in \mathcal{G}_{ij}} U_{ki}^+ c_k \right] + \sum_{k \in \mathcal{B}_i} [U_{ik}^{e+} c_i + U_{ik}^{e-} c_{B_{ik}}] \right]. \quad (12)$$

The edges with total edge flow  $U_{g_l} = 0$  can occur breakdown in the equation (12) via term  $\sum_{k \in \mathcal{G}_{ij}} \left[ U_{ki}^+ + \frac{U_{ik}^+}{|\mathcal{G}_{ij}|} \right] = 0$ . This fact implies as well as numerator  $U_{ij}^- = 0$ . In order to avoid dividing by zero we have to assume computation only for nonzero flows. Concentrations  $c_k$ ,  $k \in \mathcal{G}_{ij}$  that may intakes into element  $e_i$  are weighted with weights

$$\alpha_k = \frac{U_{ki}^+}{\sum_{k \in \mathcal{G}_{ij}} \left[ U_{ki}^+ + \frac{U_{ik}^+}{|\mathcal{G}_{ij}|} \right]}, \quad (13)$$

so that the ideal mixing in this edge leads to the average concentration

$$c_{av} = \frac{\sum_{k \in \mathcal{G}_{ij}} U_{ki}^+ c_k}{\sum_{k \in \mathcal{G}_{ij}} \left[ U_{ki}^+ + \frac{U_{ik}^+}{|\mathcal{G}_{ij}|} \right]}. \quad (14)$$

Matrix notation is the same as in (8). Finally ...



## 0.5 Reaction model

## 0.6 Input files

### 0.6.1 Flow123D ini file format

In this section we briefly describe every option you can use in global INI-file. Options marked (NOT IMPLEMENTED) are not implemented in current version, but probably will be reimplemented in near future. Options marked (NOT SUPPORTED) has not been tested since they are obsolete and will be replaced by similar functionality.

#### Section: [Global]

KEY	TYPE	DEFAULT	DESCRIPTION
Problem.type	<b>int</b>	NULL	Type of solved problem. Currently supported: 1 = steady saturated flow 2 = unsteady saturated flow using MH method 4 = unsteady saturated flow using Lumped MH method
Description	<b>string</b>	<i>undefined</i>	Short description of solved problem - any text.
Stop_time	<b>double</b>	1.0	Time interval of the whole problem.[time units]
Time_step	<b>double</b>	1.0	Time step for unsteady water flow solver. [time units]
Save_step	<b>double</b>	1.0	The output with transport is written every <b>Save_step</b> . [time units]

#### Section: [Input]

KEY	TYPE	DEFAULT	DESCRIPTION
Mesh	<b>string</b>	NULL	Name of file containing definition of the mesh for the problem.
Material	<b>string</b>	NULL	Name of file with hydraulic properties of the elements.
Boundary	<b>string</b>	NULL	Name of file with boundary condition data.
Neighbouring	<b>string</b>	NULL	Name of file describing topology of the mesh.
Initial	<b>string</b>	NULL	Name of file with initial condition for pressure head [length].
Sources	<b>string</b>	NULL	Name of file with definition of fluid sources. This is optional file, if this key is not defined, calculation goes on without sources.
sources_formula	<b>string</b>	NULL	Expression for sources as function of space coordinates $x, y, z$ . See documentation of FParser library: <a href="http://warp.povusers.org/FunctionParser/fparser.html#literals">http://warp.povusers.org/FunctionParser/fparser.html#literals</a>

## Section: [Transport]

KEY	TYPE	DEFAULT	DESCRIPTION
Transport_on	<b>YES/NO</b>	NO	If set "YES" program compute transport too.
Sorption	<b>YES/NO</b>	NO	If set "YES" program include sorption too.
Dual_porosity	<b>YES/NO</b>	NO	If set "YES" program include dual porosity too.
Reactions	<b>YES/NO</b>	NO	If set "YES" program include reactions too.
Concentration	<b>string</b>	NULL	Name of file with initial condition for concentrations of individual substances.
Transport_BCD	<b>string</b>	NULL	Name of file with boundary condition for transport.
Sources	<b>string</b>	<i>undefined</i>	Name of file with sources of species for transport.
Transport_out	<b>string</b>	NULL	Name of transport output file.
Transport_out_im	<b>string</b>	NULL	(NOT IMPLEMENTED IN 1.6.5) Name of transport immobile output file.
Transport_out_sorp	<b>string</b>	NULL	(NOT IMPLEMENTED IN 1.6.5) Name of transport sorbed output file.
Transport_out_im_sorp	<b>string</b>	NULL	(NOT IMPLEMENTED IN 1.6.5) Name of transport sorbed immobile output file.
N_substances	<b>int</b>	-1	Number of substances.
Substances	<b>string</b>	<i>undefined</i>	Names of the substances separated by commas.
bc_times	<b>list of doubles</b>	NULL	Times for changing boundary conditions. If you set this variable, you have to prepare a separate file with boundary conditions for every time in the list. Filenames for individual time level are formed from BC filename by appending underscore and three digits of time level number, e.g. <b>transport_bcd_000,</b> <b>transport_bcd_001, etc.</b>

Section: **[Run]**

KEY	TYPE	DEFAULT	DESCRIPTION
Screen_verbosity	<b>int</b>	0	Nonzero value turn on a more verbose mode (more messages on screen), however everything is in the log file.
Pause_after_run	<b>YES/NO</b>	NO	Wait for Enter after end of program in order to keep output screen open.

## Section: [Solver]

KEY	TYPE	DEFAULT	DESCRIPTION
Use_last_solution	<b>YES/NO</b>	NO	If set to "YES", uses last known solution for chosen solver.
Solver_name	<b>string</b>	petsc	Type of linear solver. Supported solvers are: <b>petsc</b> , <b>petsc.matis</b> (experimental)
Solver_params	<b>string</b>	NULL	PETSc options to override default choice of iterative solver and preconditioner (use with care). In particular to use UMFPACK sequential direct solver set: <b>Solve_params = "-ksp preonly -pc_type lu -pc_factor_mat_solver_package umfpack"</b> To use parallel direct solver MUMPS use: <b>Solve_params = "-ksp preonly -pc_type lu -pc_factor_mat_solver_package mumps -mat_mumps_icntl_14 5"</b>
Keep_solver_files	<b>YES/NO</b>	NO	(NOT SUPPROTED IN 1.6.5) If set to "YES", files for solver are not deleted after the run of the solver.
Manual_solver_run	<b>YES/NO</b>	NO	(NOT SUPPROTED IN 1.6.5) If set to "YES", programm stops after writing input files for solver and lets user to run it.
Use_control_file	<b>YES/NO</b>	NO	(NOT SUPPROTED IN 1.6.5) If set to "YES", programm do not create control file for solver, it uses given file.
Control_file	<b>string</b>	NULL	(NOT SUPPROTED IN 1.6.5) Name of control file for situation, when <b>Use_control_file</b> YES.
NSchurs	<b>int</b>	2	Number of Schur complements to use. Valid values are 0,1,2. The last one should be the fastest.
Solver_accuracy	<b>double</b>	1e-6	When to stop solver run - value of residum of matrix. Useful values from 1e-4 to 1e-10. Bigger number = faster run, less accuracy.
max_it	<b>int</b>	200	Maximum number of iteration of linear solver.

Section: **[Output]**

KEY	TYPE	DEFAULT	DESCRIPTION
Write_output_file	<b>YES/NO</b>	NO	If set to "YES", writes output file.
Output_file	<b>string</b>	NULL	Name of the output file for water flow output.
Output_file_2	<b>string</b>	NULL	(NOT IMPLEMENTED IN 1.6.5) Name of the output file (type 2).
Output_digits	<b>int</b>	6	(NOT IMPLEMENTED IN 1.6.5) Number of digits used for floating point numbers in output file.
Output_file_type	<b>int</b>	1	(NOT IMPLEMENTED IN 1.6.5) Type of output file 1 - GMSH like format 2 - Flow data file 3 - both files (two separate names)
Pos_format	<b>string</b>	ASCII	Output file format. One can use: ASCII, BIN, or VTK_SERIAL_ASCII
balance_output	<b>string</b>	NULL	Name of file for output of water boundary fluxes and balance of sources over material subdomains.

Description: Options controlling output file of the program

## Section: [Semchem\_module]

KEY	TYPE	DEFAULT	DESCRIPTION
Compute_reactions	Yes/No	"No"	NO = transport without chemical reactions YES = transport influenced by chemical reactions
Output_precision	int	1	Number of decimal places written to output file created by Semchem_module.
Number_of_further_species	int	0	Concentrations of these species are not computed, because they are ment to be unexghaustible.
Temperature	double	0.0	Temperature, one of state variables of the system.
Temperature_Gf	double	0.0	Temperature at which Free Gibbs Energy is specified.
Param_Afi	double	0.0	Parameter of the Debuy-Hückel equation for activity coefficients computation.
Param_b	double	0.0	Parameter of the Debuy-Hückel equation for activity coefficients computation.
Epsilon	double	0.0	Epsilon specifies relative norm of residuum estimate to stop numerical algorithms used by Semchem_module.
Time_steps	int	1	Number of transport step subdivisions for Semchem_module.
Slow_kinetics_substeps	int	0	Number of substeps performed by Runge-Kutta method used for slow kinetics simulation.
Error_norm_type	string	"Absolute"	Through wich kind of norm the error is measured.
Scalling	boolean	"No"	Type of the problem preconditioning for better convergence of numerical method.

Section: **[Aqueous\_species]**

KEY	TYPE	DEFAULT	DESCRIPTION
El_charge	<b>int</b>	0	Electric charge of an Aqueous_specie particle under consideration.
dGf	<b>double</b>	0.0	Free Gibbs Energy valid for TemperatureGf.
dHf	<b>double</b>	0.0	Enthalpy
Molar_mass	<b>double</b>	0.0	Molar mass of Aqueous_species.

Section: **[Further\_species]**

KEY	TYPE	DEFAULT	DESCRIPTION
Specie_name	<b>string</b>	""	Name belonging to Further_specie under consideration.
dGf	<b>double</b>	0.0	Free Gibbs Energy valid for TemperatureGf.
dHf	<b>double</b>	0.0	Enthalpy
Molar_mass	<b>double</b>	0.0	Molar mass of Further_species.
Activity	<b>double</b>	0.0	Activity of Further_species.

Section: **[Reaction\_i]**

KEY	TYPE	DEFAULT	DESCRIPTION
Reaction_type	<b>string</b>	"unknown"	Type of considered reaction (Equilibrium, Kinetics, Slow_kinetics).
Stoichiometry	<b>int</b>	0	Stoichiometric coefficients of species taking part in <i>i</i> -th reaction.
Kinetic_constant	<b>double</b>	0.0	Kinetic constant for determination of reaction rate.
Order_of_reaction	<b>int</b>	0	Order of kinetic reaction for participating species.
Equilibrium_constant	<b>double</b>	0.0	Equilibrium constant defining <i>i</i> -th reaction.



Section: **[Reaction\_module]**

KEY	TYPE	DEFAULT	DESCRIPTION
Compute_decay	Yes/No	"No"	It enables to switch on simulation of radioactive decay or first order reactions.
Nr_of_decay_chains	int	0	How many decay chains are considered.
Nr_of_FoR	int	0	How many first order reactions are defined.

Section: **[Decay\_i]**

KEY	TYPE	DEFAULT	DESCRIPTION
Nr_of_isotopes	int	0	It defines the number of isotopes which does the current section [Decay_i] work with.
Substance_ids	array of int	NULL	Sequence of ids describing the order of isotopes in decay chain.
Half_lives	array of double	NULL	Contain half-lives belonging to isotopes defined by ids.
Bifurcation_on	Yes/No	"No"	It makes it possible to define branches in current [Decay_i].
Bifurcation	array of double	NULL	It defines a percentage, which is the first isotope in current [Decay_i] decaying to products.

Section: **[FoReact\_i]**

KEY	TYPE	DEFAULT	DESCRIPTION
Kinetic_constant	double	0.0	It defines kinetic constant which is the corresponding half-life computed from.
Substance_ids	array of int	NULL	It contains a couple of indices of substances which are taking part in first order reactions described in current section FoReact.i.

## 0.6.2 Mesh file format version 2.0

The only supported format for the computational mesh is MSH ASCII format produced by the GMSH software. You can find its documentation on:

<http://geuz.org/gmsh/doc/texinfo/gmsh.html#MSH-ASCII-file-format>

Comments concerning Flow123d:

- Every inconsistency of the file stops the calculation. These are:
  - Existence of nodes with the same *node-number*.
  - Existence of elements with the same *elm-number*.
  - Reference to non-existing node.
  - Reference to non-existing material (see below).
  - Difference between *number-of-nodes* and actual number of lines in nodes' section.
  - Difference between *number-of-elements* and actual number of lines in elements' section.

- By default Flow123d assumes meshes with *number-of-tags* = 3.

*tag1* is number of material (reference to .MTR file) in the element.

*tag2* is number of geometry region in which the element lies.

*tag3* is partition number (CURRENTLY NOT USED).

In accordance with specification of GMSH mesh format.

- Currently, line (*type* = 1), triangle (*type* = 2) and tetrahedron (*type* = 4) are the only supported types of elements. Existence of an element of different type stops the calculation.
- Wherever possible, we use the file extension .MSH. It is not required, but highly recommended.

### 0.6.3 Material properties file format, version 1.0

The file is divided in two sections, header and data. The extension `.MTR` is highly recommended for files of this type.

```
$MaterialFormat
1.0 file-type data-size
$EndMaterialFormat
$Materials
number-of-materials
material-number material-type <material-type-specific-data> [text]
...
$EndMaterials
$Storativity
material-number <storativity-coefficient> [text]
...
$EndStorativity
$Geometry
material-number geometry-type <geometry-type-specific-coefficient> [text]
...
$EndGeometry
$Sorption
material-number substance-id sorption-type <sorption-type-specific-data> [text]
...
$EndSorption
$SorptionFraction
material-number <sorption-fraction-coefficient> [text]
...
$EndSorptionFraction
$DualPorosity
material-number <mobile-porosity-coefficient> <immobile-porosity-coefficient>
<nonequilibrium-coefficient-substance(0)> ...<nonequilibrium-coefficient-substance(n-1)>
[text]
...
$EndDualPorosity
$Reactions
reaction-type <reaction-type-specific-coefficient> [text]
...
$EndReactions
```

where:

*file-type* `int` — is equal 0 for the ASCII file format.

*data-size* `int` — the size of the floating point numbers used in the file. Usually *data-size* = `sizeof(double)`.

*number-of-materials* `int` — Number of materials defined in the file.

*material-number* **int** — is the number (index) of the n-th material. These numbers do not have to be given in a consecutive (or even an ordered) way. Each number has to be given only once, multiple definition are treated as inconsistency of the file and cause stopping the calculation (exception \$Sorption section).

*material-type* **int** — is type of the material, see table.

<*material-type-specific-data*> — format of this list depends on the *material - type*.

<*storativity-coefficient*> **double** — coefficient of storativity

*geometry-type* **int** — type of complement dimension parameter (only for 1D and 2D material), for 1D element is supported type 1 - cross-section area, for 2D element is supported type 2 - thickness.

<*geometry-type-specific-coefficient*> **double** — cross-section for 1D element or thickness for 2D element.

*substance-id* **int** — refers to number of transported substance, numbering starts on 0.

*sorption-type* **int** — type 1 - linear sorption isotherm, type 2 - Freundlich sorption isotherm, type 3 - Langmuir sorption isotherm.

<*sorption-type-specific-data*> — format of this list depends on the *sorption - type*, see table.

Note: Section \$Sorption is needed for calculation only if *Sorption* is turned on in the *ini* file.

<*sorption-fraction-coefficient*> **double** — ratio of the "mobile" solid surface in the contact with "mobile" water to the total solid surface (this parameter (section) is needed for calculation only if *Dual\_porosity* and *Sorption* is together turned on in the ini file).

<*mobile-porosity-coefficient*> **double** — ratio of the mobile pore volume to the total volume (this parameter is needed only if *Transport\_on* is turned on in the ini file).

<*immobile-porosity-coefficient*> **double** — ratio of the immobile pore volume to the total pore volume (this parameter is needed only if *Dual\_porosity* is turned on in the ini file).

<*nonequilibrium-coefficient-substance(i)*> **double** — nonequilibrium coefficient for substance  $i$ ,  $\forall i \in \langle 0, n - 1 \rangle$  where  $n$  is number of transported substances (this parameter is needed only if *Dual\_porosity* is turned on in the ini file).

*reaction-type* **int** — type 0 - zero order reaction

<*reaction-type-specific-data*> — format of this list depends on the *reaction - type*, see table.

<i>material-type</i>	<i>material-type-specific-data</i>	Description
11	$k$	$\mathbf{K} = (k)$
-11	$a$	$\mathbf{A} = \mathbf{K}^{-1} = (a)$
21	$k$	$\mathbf{K} = \begin{pmatrix} k & 0 \\ 0 & k \end{pmatrix}$
22	$k_x \quad k_y$	$\mathbf{K} = \begin{pmatrix} k_x & 0 \\ 0 & k_y \end{pmatrix}$
23	$k_x \quad k_y \quad k_{xy}$	$\mathbf{K} = \begin{pmatrix} k_x & k_{xy} \\ k_{xy} & k_y \end{pmatrix}$
-21	$a$	$\mathbf{A} = \mathbf{K}^{-1} = \begin{pmatrix} a & 0 \\ 0 & a \end{pmatrix}$
-22	$a_x \quad a_y$	$\mathbf{A} = \mathbf{K}^{-1} = \begin{pmatrix} a_x & 0 \\ 0 & a_y \end{pmatrix}$
-23	$a_x \quad a_y \quad a_{xy}$	$\mathbf{A} = \mathbf{K}^{-1} = \begin{pmatrix} a_x & a_{xy} \\ a_{xy} & a_y \end{pmatrix}$
31	$k$	$\mathbf{K} = \begin{pmatrix} k & 0 & 0 \\ 0 & k & 0 \\ 0 & 0 & k \end{pmatrix}$
33	$k_x \quad k_y \quad k_z$	$\mathbf{K} = \begin{pmatrix} k_x & 0 & 0 \\ 0 & k_y & 0 \\ 0 & 0 & k_z \end{pmatrix}$
36	$k_x \quad k_y \quad k_z \quad k_{xy} \quad k_{xz} \quad k_{yz}$	$\mathbf{K} = \begin{pmatrix} k_x & k_{xy} & k_{xz} \\ k_{xy} & k_y & k_{yz} \\ k_{xz} & k_{yz} & k_z \end{pmatrix}$
-31	$a$	$\mathbf{A} = \mathbf{K}^{-1} = \begin{pmatrix} a & 0 & 0 \\ 0 & a & 0 \\ 0 & 0 & a \end{pmatrix}$
-33	$a_x \quad a_y \quad a_z$	$\mathbf{A} = \mathbf{K}^{-1} = \begin{pmatrix} a_x & 0 & 0 \\ 0 & a_y & 0 \\ 0 & 0 & a_z \end{pmatrix}$
-36	$a_x \quad a_y \quad a_z \quad a_{xy} \quad a_{xz} \quad a_{yz}$	$\mathbf{A} = \mathbf{K}^{-1} = \begin{pmatrix} a_x & a_{xy} & a_{xz} \\ a_{xy} & a_y & a_{yz} \\ a_{xz} & a_{yz} & a_z \end{pmatrix}$

Note: all variables (  $k, k_x, k_y, k_z, k_{xy}, k_{xz}, k_{yz}, a, a_x, a_y, a_z, a_{xy}, a_{xz}, a_{yz}$  ) are of the double type.

<i>sorption-type</i>	<i>sorption-type-specific-data</i>	Description
1	$k_D[1]$	$s = k_D c$
2	$k_F[(L^{-3} \cdot M^1)^{(1-\alpha)}] \quad \alpha[1]$	$s = k_F c^\alpha$
3	$K_L[L^3 \cdot M^{-1}] \quad s^{max}[L^{-3} \cdot M^1]$	$s = \frac{K_L s^{max} c}{1 + K_L c}$

Note: all variables (  $k_D, k_F, \alpha, K_L, s^{max}$  ) are of the double type.

<i>reaction-type</i>	<i>reaction-type-specific-data</i>	Description
0	$substance-id[1] \quad k[M \cdot L^{-3} \cdot T^{-1}]$	$\frac{\partial c_m^{[substance-id]}}{\partial t} = k$

Where  $c_m^{[substance-id]}$  is mobile concentration of substance with id *substance-id* and  $\Delta t$  is the internal transport time step defined by CFL condition.

*text* **char**[] — is a text description of the material, up to 256 chars. This parameter is

optional.

### Comments concerning 1-2-3-FLOW:

- If *number-of-materials* differs from actual number of material lines in the file, it stops the calculation.

## 0.6.4 Boundary conditions file format, version 1.0

The file is divided in two sections, header and data.

```
$BoundaryFormat
1.0 file-type data-size
$EndBoundaryFormat
$BoundaryConditions
number-of-conditions
condition-number type <type-specific-data> where <where-data> number-of-tags <tags>
[text]
...
$EndBoundaryConditions
```

where

*file-type* **int** — is equal 0 for the ASCII file format.

*data-size* **int** — the size of the floating point numbers used in the file. Usually *data-size* = sizeof(double).

*number-of-conditions* **int** — Number of boundary conditions defined in the file.

*condition-number* **int** — is the number (index) of the n-th boundary condition. These numbers do not have to be given in a consecutive (or even an ordered) way. Each number has to be given only once, multiple definition are treated as inconsistency of the file and cause stopping the calculation.

*type* **int** — is type of the boundary condition. See below for definitions of the types.

<*type-specific-data*> — format of this list depends on the *type*. See below for specification of the *type-specific-data* for particular types of the boundary conditions.

*where* **int** — defines the way, how the place for the condition is prescribed. See below for details.

<*where-data*> — format of this list depends on *where* and actually defines the place for the condition. See below for details.

*number-of-tags* **int** — number of integer tags of the boundary condition. It can be zero.

< *tags* > *number-of-tags*\***int** — list of tags of the boundary condition. Values are separated by spaces or tabs. By default we set *number-of-tags*=1, where *tag1* defines group of boundary conditions, "type of water" in our jargon. This can be used to calculate total fluxes through the boundary group.

[*text*] **char**[] — arbitrary text, description of the fracture, notes, etc., up to 256 chars. This is an optional parameter.

## Types of boundary conditions and their data

*type* = 1 — Boundary condition of the Dirichlet's type

*type* = 2 — Boundary condition of the Neumann's type

*type* = 3 — Boundary condition of the Newton's type

<i>type</i>	<i>type-specific-data</i>	Description
1	<i>scalar</i>	Prescribed value of pressure (in meters [m])
2	<i>flux</i>	Prescribed value of flux through the boundary
3	<i>scalar sigma</i>	Scalar value and the $\sigma$ coefficient

*scalar*, *flux* and *sigma* are of the `double` type.

## Ways of defining the place for the boundary condition

*where* = 1 — Condition on a node

*where* = 2 — Condition on a (generalized) side

*where* = 3 — Condition on side for element with only one external side.

<i>where</i>	<i>&lt;where-data&gt;</i>	Description
1	<i>node-id</i>	Node id number, according to .MSH file
2	<i>elm-id sid-id</i>	Elm. id number, local number of side
3	<i>elm-id</i>	Elm. id number

The variables *node-id*, *elm-id*, *sid-id* are of the `int` type.

## Comments concerning 1-2-3-FLOW:

- We assume homegeous Neumman's condition as the default one. Therefore we do not need to prescribe conditions on the whole boundary.
- If the condition is given on the inner edge, it is treated as an error and stops calculation.
- Any inconsistence in the file stops calculation. (Bad number of conditions, multiple definition of condition, reference to non-existing node, etc.)
- At least one of the conditions has to be of the Dirichlet's or Newton's type. This is well-known fact from the theory of the PDE's.
- Local numbers of sides for *where* = 2 must be lower than the number of sides of the particular element and greater then or equal to zero.
- The element specified for *where* = 3 must have only one external side, otherwise the program stops.



## 0.6.5 Neighbouring file format, version 1.0

The file is divided in two sections, header and data. The extension `.NGH` is highly recommended for files of this type.

```
$NeighbourFormat
1.0 file-type data-size
$EndNeighbourFormat
$Neighbours
number-of-neighbours
neighbour-number type <type-specific-data>
...
$EndNeighbours
```

where

*file-type* **int** — is equal 0 for the ASCII file format.

*data-size* **int** — the size of the floating point numbers used in the file. Usually *data-size* = `sizeof(double)`.

*number-of-neighbours* **int** — Number of neighbouring defined in the file.

*neighbour-number* **int** — is the number (index) of the n-th neighbouring. These numbers do not have to be given in a consecutive (or even an ordered) way. Each number has to be given only once, multiple definition are treated as inconsistency of the file and cause stopping the calculation.

*type* **int** — is type of the neighbouring.

*<type-specific-data>* — format of this list depends on the *type*.

### Types of neighbouring and their specific data

*type* = 10 — “Edge with common nodes”, i.e. sides of elements with common nodes. (Possible many elements)

*type* = 11 — “Edge with specified sides”, i.e. sides of the edge are explicitly defined. (Possible many elements)

*type* = 20 — “Compatible”, i.e. volume of an element with a side of another element. (Only two elements)

*type* = 30 — “Non-compatible” i.e. volume of an element with volume of another element. (Only two elements)

<i>type</i>	<i>type-specific-data</i>	Description
10	<i>n_elm eid1 eid2 ...</i>	number of elements and their ids
11	<i>n_sid eid1 sid1 eid2 sid2 ...</i>	number of sides, their elements and local ids
20	<i>eid1 eid2 sid2 coef</i>	Elm 1 has to have lower dimension
30	<i>eid1 eid2 coef</i>	Elm 1 has to have lower dimension

*coef* is of the **double** type, other variables are **ints**.

## Comments concerning 1-2-3-FLOW:

- Every inconsistency or error in the .NGH file causes stopping the calculation. These are especially:
  - Multiple usage of the same *neighbour-number*.
  - Difference between *number-of-neighbours* and actual number of data lines.
  - Reference to nonexistent element.
  - Nonsense number of side.
- The variables *sid?* must be nonnegative and lower than the number of sides of the particular element.

### 0.6.6 Sources file format, version 1.0

The file is divided in two sections, header and data. The extension `.SRC` is highly recommended for files of this type.

```
$SourceFormat
1.0 file-type data-size
$EndSourceFormat
$Sources
number-of-sources
eid density
...
$EndSources
```

where

*file-type* `int` — is equal 0 for the ASCII file format.

*data-size* `int` — the size of the floating point numbers used in the file. Usually *data-size* = `sizeof(double)`.

*number-of-sources* `int` — Number of sources defined in the file.

*eid* `int` — is id-number of the element, where the source lies.

*density* `double` — is the density of the source, in volume of fluid per time unit. Positive values are sources, negative are sinks.

#### Comments concerning 1-2-3-FLOW:

- Every inconsistency or error in the `.SRC` file causes stopping the calculation. These are especially:
  - Multiple usage of the same *source-number*.
  - Difference between *number-of-sources* and actual number of data lines.
  - Reference to nonexisting element.

# ASCII post-processing file format version 1.2

File format of this file comes from the GMSH system. Following text is copied from the GMSH documentation.

===== BEGIN OF INSERTED TEXT =====

The ASCII post-processing file is divided in several sections: one format section, enclosed between `$PostFormat-$EndPostFormat` tags, and one or more post-processing views, enclosed between `$View-$EndView` tags:

`$PostFormat`

`1.2 file-type data-size`

`$EndPostFormat`

`$View`

`view-name nb-time-steps`

`nb-scalar-points nb-vector-points nb-tensor-points`

`nb-scalar-lines nb-vector-lines nb-tensor-lines`

`nb-scalar-triangles nb-vector-triangles nb-tensor-triangles`

`nb-scalar-quadrangles nb-vector-quadrangles nb-tensor-quadrangles`

`nb-scalar-tetrahedra nb-vector-tetrahedra nb-tensor-tetrahedra`

`nb-scalar-hexahedra nb-vector-hexahedra nb-tensor-hexahedra`

`nb-scalar-prisms nb-vector-prisms nb-tensor-prisms`

`nb-scalar-pyramids nb-vector-pyramids nb-tensor-pyramids`

`nb-text2d nb-text2d-chars nb-text3d nb-text3d-chars`

`<time-step-values>`

`<scalar-point-values>`

`<vector-point-values>`

`<tensor-point-values>`

`<scalar-line-values>`

`<vector-line-values>`

`<tensor-line-values>`

`<scalar-triangle-values>`

`<vector-triangle-values>`

`<tensor-triangle-values>`

`<scalar-quadrangle-values>`

`<vector-quadrangle-values>`

`<tensor-quadrangle-values>`

`<scalar-tetrahedron-values>`

`<vector-tetrahedron-values>`

`<tensor-tetrahedron-values>`

`<scalar-hexahedron-values>`

`<vector-hexahedron-values>`

`<tensor-hexahedron-values>`

`<scalar-prism-values>`

`<vector-prism-values>`

`<tensor-prism-values>`

```

<scalar-pyramid-values>
<vector-pyramid-values>
<tensor-pyramid-values>
<text2d> <text2d-chars>
<text3d> <text3d-chars>
$EndView

```

where:

*file-type* is an integer equal to 0 in the ASCII file format.

*data-size* is an integer equal to the size of the floating point numbers used in the file (usually, *data-size* = sizeof(double)).

*view-name* is a string containing the name of the view (max. 256 characters).

*nb-time-steps* is an integer giving the number of time steps in the view.

*nb-scalar-points*, *nb-vector-points*, ... are integers giving the number of scalar points, vector points, ... in the view.

*nb-text2d*, *nb-text3d* are integers giving the number of 2D and 3D text strings in the view.

*nb-text2d-chars*, *nb-text3d-chars* are integers giving the total number of characters in the 2D and 3D strings.

*time-step-values* is a list of *nb-time-steps* double precision numbers giving the value of the time (or any other variable) for which an evolution was saved.

*scalar-point-value*, *vector-point-value*, ... are lists of double precision numbers giving the node coordinates and the values associated with the nodes of the *nb-scalar-points* scalar points, *nb-vector-points* vector points, ..., for each of the *time-step-values*.

For example, *vector-triangle-value* is defined as:

```

coord1-node1 coord1-node2 coord1-node3
coord2-node1 coord2-node2 coord2-node3
coord3-node1 coord3-node2 coord3-node3
comp1-node1-time1 comp2-node1-time1 comp3-node1-time1
comp1-node2-time1 comp2-node2-time1 comp3-node2-time1
comp1-node3-time1 comp2-node3-time1 comp3-node3-time1
comp1-node1-time2 comp2-node1-time2 comp3-node1-time2
comp1-node2-time2 comp2-node2-time2 comp3-node2-time2
comp1-node3-time2 comp2-node3-time2 comp3-node3-time2
...

```

*text2d* is a list of 4 double precision numbers:

```
coord1 coord2 style index
```

where *coord1* and *coord2* give the coordinates of the leftmost element of the 2D string in screen coordinates, *index* gives the starting index of the string in *text2d-chars* and *style* is currently unused.

*text2d-chars* is a list of *nb-text2d-chars* characters. Substrings are separated with the ‘^’ character (which is a forbidden character in regular strings).

*text3d* is a list of 5 double precision numbers

*coord1 coord2 coord3 style index*

where *coord1*, *coord2* and *coord3* give the coordinates of the leftmost element of the 3D string in model (real world) coordinates, *index* gives the starting index of the string in *text3d-chars* and *style* is currently unused.

*text3d-chars* is a list of *nb-text3d-chars* chars. Substrings are separated with the ‘^’ character.

===== END OF INSERTED TEXT =====

More information about GMSH can be found at its homepage:  
<http://www.geuz.org/gmsh/>

## Comments concerning FFL0W20:

- FFL0W20 generates .POS file with four views: Elements’ pressure, edges’ pressure, interelement fluxes and complex view. First three views shows ”raw data”, results obtained by the solver without any interpolations, smoothing etc. The fourth view contains data processed in this way.

**Elements’ pressure:** Contains only *scalar-triangle-values*. Triangles are the same as the elements of the original mesh. We prescribe constant value of the pressure on the element, as it was calculated by the solver as the unknown  $p$ . Therefore, the three values on every triangle are the same.

**Edge pressure:** Contains only *scalar-line-values*. The lines are the same as the edges of the elements of the original mesh. We prescribe constant value of the pressure on the edge, as it was calculated by the solver as the unknown  $\lambda$ . Therefore, the two values on every edge are the same.

**Interelement flux:** Contains *vector-point-values* and *scalar-triangle-values*. The *scalar-triangle-values* carry no information, all values are set to 0, these are in the file only to define a shape of the elements. The points for the *vector-point-values* are midpoints of the sides of the elements. The vectors are calculated as  $u\mathbf{n}$ , where  $u$  is value of the flux calculated by the solver and  $\mathbf{n}$  is normalized vector of outer normal of the element’s side.

**Complex view:** Contains *scalar-triangle-values* and *vector-point-values*. The *scalar-triangle-values* shows the shape of the pressure field. The triangles are the the same as the elements of the original mesh. Values of pressure in nodes are interpolated from  $p_s$  and  $\lambda_s$ . The *vector-point-values* shows the velocity of the flow in the centres of the elements.

## 0.7 Output files

## Output data

On every run we collect some basic profiling informations. After all computations these data are written into the file `profiler%y%m%d_%H.%M.%S.out` where %y, %m, %d, %H, %M, %S are two digit numbers representing year, month, day, hour, minute, and second of the program start time.

### 0.7.1 Output data fields of water flow modul

### 0.7.2 Output data fields of transport

### 0.7.3 GMSH viewer remarks

### 0.7.4 Paraview viewer remarks