

FREEWAT

Free and Open Source Software Tools for Water Resource Management

EU HORIZON 2020 Project

FREE and Open Source Software Tools for WATer Resource Management

FREEWAT User Manual

Volume 2

Heat and Solute Transport in Subsurface Water Flow

by ***Iacopo Borsi***[(1)]

Version 0.3

December 5th, 2016

This version is confidential, only for FREEWAT Project Partners



This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 642224

FOREWORD

FREEWAT is an HORIZON 2020 project financed by the EU Commission under the call WATER INNOVATION: BOOSTING ITS VALUE FOR EUROPE. FREEWAT main result is an open source and public domain GIS-integrated modeling environment for the simulation of water quantity and quality in surface water and groundwater with an integrated water management and planning module. Specific objectives of the FREEWAT project are: to coordinate previous EU and national funded research to integrate existing software modules for water management in a single environment into the GIS-based FREEWAT platform and to support the FREEWAT application in an innovative participatory approach, gathering technical staff and relevant stakeholders in designing scenarios for the proper application of water policies.
The open source characteristics of the platform allow to consider this an initiative "ad includendum", as further research institutions, private developers etc. may contribute to the platform development. Capabilities integrated in FREEWAT are:

- a dedicated module for water management and planning;
- a whole module for calibration, uncertainty and sensitivity analysis;
- a module for solute transport in the unsaturated zone;
- a module for crop growth and rural water management;
- a module dedicated to time-series processing to support advanced model calibration;
- tools for dealing with groundwater quality issues;
- tools for the analysis, interpretation and visualization of hydrogeological data.

FREEWAT Development has received funding from the following projects:

1. Hydrological part has been developed starting from a former project, named SID&GRID, funded by Regione Toscana through EU POR-FSE 2007-2013 (sidgrid.isti.cnr.it).
2. Porting of SID&GRID under QGIS has been performed through funds provided by Regione Toscana to Scuola Superiore S.Anna - Project Evoluzione del sistema open source SID&GRID di elaborazione dei dati geografici vettoriali e raster per il porting negli ambienti QGIS e Spatialite in uso presso la Regione Toscana (CIG: ZA50E4058A)
3. Saturated zone solute transport simulation capability has been developed within the EU FP7-ENV-2013-WATER-INNO-DEMO MARSOL. MARSOL project receives funding from the European Union's Seventh Framework Programme for Research, Technological Development and Demonstration under grant agreement n. 619120 (www.marsol.eu)
4. The previous codes have been integrated into FREEWAT under development within EU H2020 project FREEWAT - Free and Open Source Software Tools for Water Resource Management. FREEWAT project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement n. 642224 (www.freewat.eu)
This User Manual provides guidelines to properly install and use the FREEWAT plugin.

***Project Coordinator**:*
Rudy Rossetto, Istituto di Scienze della Vita – Scuola Superiore Sant'Anna, Via S. Cecilia 3, 56127 Pisa.
Capabilities of the FREEWAT platform were tested either by the developers group and by Project Partners. However, future applications of the platform may reveal errors and drawbacks not detected to date. Users are kindly requested to notify any error in both platform and User Manual. Please send this info to: rudy.rossetto@sssup.it

***To cite this User Manual**:*
Borsi, I.. FREEWAT User Manual, Volume 2 - Heat and Solute Transport in Subsurface Water Flow. December 5th, 2016

***Text editing**:*
Giovanna De Filippis(2), Matteo Ghetta(2)

***Affiliation**:*
(1) TEA SISTEMI S.p.A., Pisa (IT)
(2) Istituto di Scienze della Vita – Scuola Superiore Sant'Anna, Pisa (IT)

Contents

Abstract ii

1 Introduction 1
- 1.1 Simulated processes . . . 1
- 1.2 Limitations (related to the FREEWAT Version v.1.0 - July 2016) . . . 2

2 Building the transport model 3
- 2.1 Creating a new transport model . . . 3
- 2.2 Basic properties of the transport model (ADV and DSP package) . . . 5
- 2.3 Sink and Source Mixing Package - SSM . . . 7
- 2.4 Reaction Package - RCT . . . 7
- 2.5 Unsaturated Solute Balance - USB . . . 8
- 2.6 Density and Viscosity dependence (VDF and VSC) . . . 11

3 Run the transport model 12

References 14

Abstract

In **FREEWAT** the hydrological model can be coupled with a solute transport model, to simulate multispecies advective and dispersive transport, both in unsaturated and saturated zone. The possibility to simulate viscosity- and density-dependent flows is present as well. Such capabilities are particularly relevant to approach studies on seawater intrusion processes (where density variations of water due to salinity effect are crucial), or for assessing geothermal plants at low and medium enthalpy.

CHAPTER 1

Introduction

In **FREEWAT** (Free and Open Source Software Tools for Water Resource Management) the hydrological model can be coupled to a solute transport model, to simulate advective and dispersive transport of several species, both in unsaturated and saturated zone. The possibility to simulate viscosity and density dependent flow is present as well. Such capabilities are particularly relevant to approach studies on seawater intrusion processes (where density variations of water due to salinity effect are crucial), or for assessing geothermal plants at low- and medium-entalpy. Simulation of heat transport (also coupled with additional chemical species) is possible just treating heat as a *species* and defining diffusive coefficient and other parameters in a coherent way.

Solute transport is solved in FREEWAT by applying the well-known MT3DMS code (A Modular Three-Dimensional Multi-species Transport Model for Simulation of Advection, Dispersion, and Chemical Reactions of Contaminants in Groundwater Systems). The User can find details on the code and documentation material at: <http://hydro.geo.ua.edu/mt3d/> Furthermore, viscosity- and density-dependendent flows are solved by applying SEAWAT (Simulation of Three-Dimensional Variable-Density Ground-Water Flow and Transport), <http://water.usgs.gov/ogw/seawat/>, which is a revised version of coupling MODFLOW with MT3DMS, taking into account variations in density and viscosity during the numerical resolution of the groundwater flow equation ([seawat]).

Finally, solute transport through vadoze zone is addressed by an estimate of the pollutant leaching from the ground surface up to the water table: here the amount of effective concentration is then used as boundary condition for the MT3DMS code in the saturated zone.

This manual is organized as follows. In Section *Simulated processes*, details on FREEWAT capabilities are presented, focusing on transport processes, while limitations and default settings are reported in Section Limitations. Description of the simulation procedure is given in Chapter *Building the transport model*.

Simulated processes

The following processes (each one corresponding to a specific package of MT3DMS or SEAWAT code) are implemented in FREEWAT.

- ADV (Advection package).
- DSP (Hydrodynamic Dispersion), taking into account mechanical dispersion and molecular diffusion phenomena.
- SSM (Sinks and Sources Terms), simulating solute mass entering the model domain through sources or leaving the model domain through sinks.
- RCT (Chemical Reactions), simulating equilibrium-controlled linear or nonlinear sorption, nonequilibrium (rate-limited) sorption, and first-order reaction that can represent radioactive decay or provide an approximate representation of biodegradation. The general formulation sorption can also be used to model kinetic mass transfer between the mobile and immobile domains in a dual-domain advection-diffusion model. No reaction among different species can be considered (namely no geochemical reaction).

- VDF (Variable Density Flow)
- VCS (Viscosity-depedent Flow)

The leaching of contaminant through the vadoze zone is solved by the module USB (Unsaturated Solute Balance), developed as original internal module of FREEWAT.

Limitations (related to the FREEWAT Version v.1.0 - July 2016)

The following packages/options can not be activated directly from FREEWAT platform (to activate them, the User needs to write or modify input files generated by FREEWAT).

- RCT (Chemical Reactions) package can be activated only in case of single species simulations (this is a temporarly limitation that will be solved in short time)
- HSS (Hydrocarbon Spill Source) package, to provide a seamless linkage to the MT3DMS transport simulator for the Hydrocarbon Spill Screening Model (HSSM) <http://www.epa.gov/water-research/hydrocarbon-spill-screening-model-hssm-windows-version>, is not implemented in FREEWAT.
- Application of SEAWAT (density- and viscosity-dependent flow) is possible only in the saturated zone.

CHAPTER 2

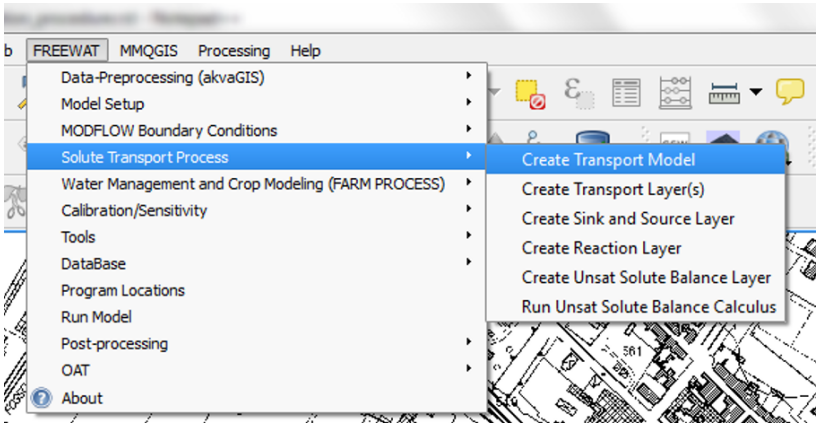
Building the transport model

Through this chapter we assume that the User has already built and run a MODFLOW model (namely the groundwater flow equation has been already solved) using FREEWAT utilities and tools described in Volume I of this manual. Concerning the code implementation, the User should be aware that the MODFLOW/MT3DMS strategy to link flow model and transport model is a binary file generated by MODFLOW (FTL file) where water flux (for each cell, and for each time step in each stress period) is saved. Then, MT3DMS will use this file as input to pass the flow regime to the transport equation solver [mt3dms]

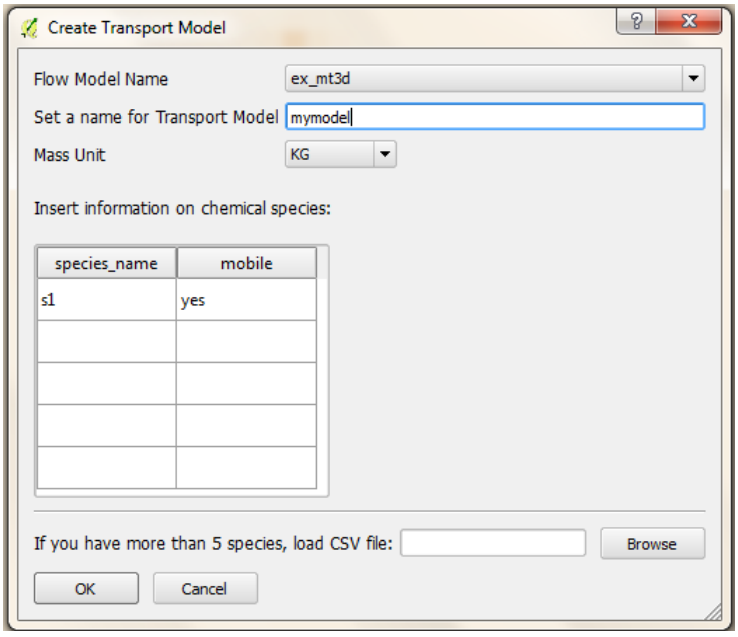
Therefore, it is assumed that the User has already created a Model (and related SpatiaLite DB), loaded in its proper QGIS project.

Creating a new transport model

The first step is the creation of a new transport model, selecting *FREEWAT -> Solute Transport Process -> Create Transport Model* menu:



The Create Transport Model GUI opens,



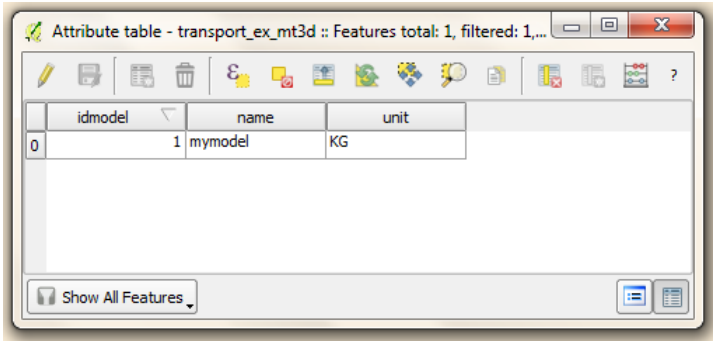
requesting the following information:

- Selection of the groundwater flow model (MODFLOW model) the User wants to couple with the transport process.
- Inserting a name for the new transport model.
- Selecting the units of measure for mass (*Kg* or *Lb*)
- Setting the **species_name** (name of the species the User wants to simulate), also specifying if it is a mobile or immobile species (setting *yes* or *no*, respectively, in the **mobile** field).

If the User has more than 5 species to be inserted, there is the possibility to upload a CSV file, having exactly the same structure as the table here presented: in particular, the three fields in firs row have to be declared with same name as in the GUI.

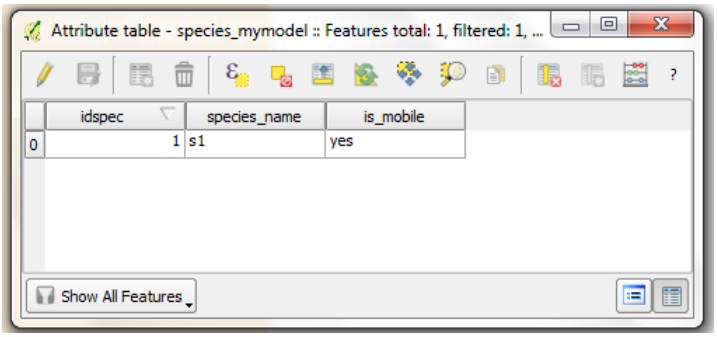
After running this tool, two new tables are created in the model DB:

1. The **transport_modelname** table (where *modelname* is the name of the groundwater flow model). In this table the list of transport models linked to the groundwater flow model *modelname* are listed. Therefore, if the User decides to create another one (or more than one) transport models, this table will be updated, and having as many records as the number of transport model associated to the selected groundwater flow model.



2. The **species_transportname** table (where *transportname* is the name of the transport model set before, *mymodel+*

*in the example). This table reports the species selected for the model: their name and the property mobile *yes* or *not*.* The User can modify this table (add or remove or modify) by setting the layer in editing mode and then saving the changes before closing the editing session.

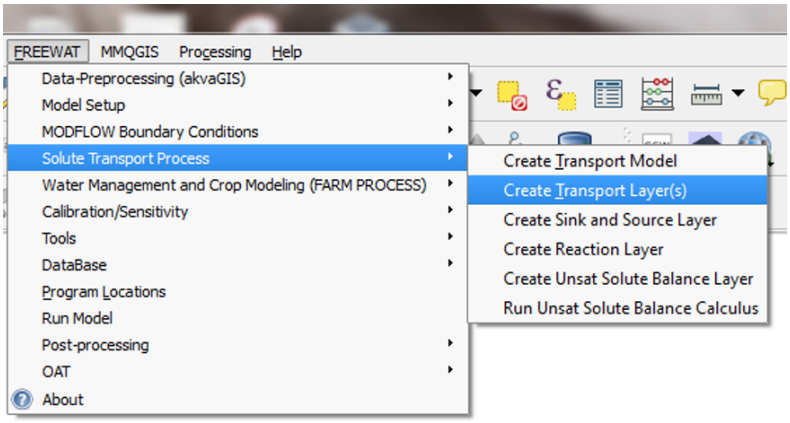


Next step is to assign basic properties to the model.

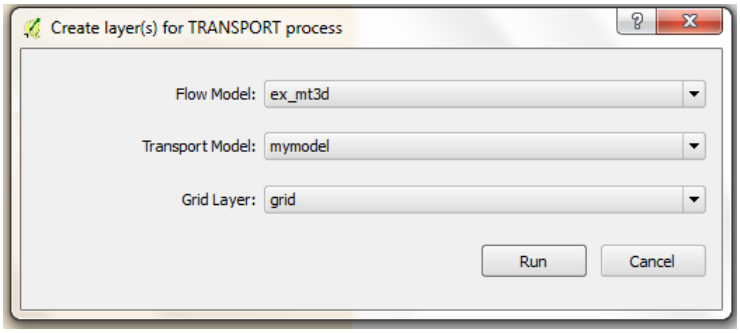
Basic properties of the transport model (ADV and DSP package)

Once the model is defined, the User has to set the basic properties, such as initial condition, active/non-active cells, effective porosity. Such pieces f information are passed to the model by defining new Model Data Objects (MDOs), the **transport layer(s)**: they are a replication of the **model layer(s)** defined for the corresponding groundwater flow model, and they are used to set basic properties (for each hydrological layer presents in the model), as described below.

From the main menu, *FREEWAT -> Solute Transport Process -> Create Transport Layer(s)*

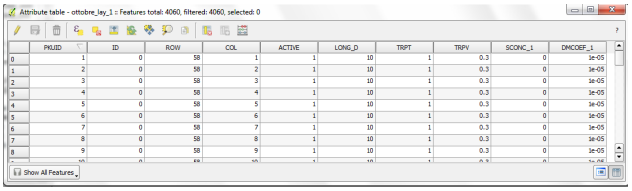


The following GUI appears



where the name for both groundwater and transport model are requested, along with the reference **grid layer**. Once the bottom *Run* has been pushed, the algorithm creates as many MDOs as the number of model layers of the flow model, assigning the standard name **transportname_lay_1**, **transportname_lay_2**, ..., **transportname_lay_N** according to the number (N) of model layers defined. Each transport layer reports (for each cell of the model grid), the following fields (see also the screen shot below, as example):

- *ACTIVE*: set -1, 0 or 1, to set the cell as constant-concentration cell, inactive, or active, respectively (as for the model layer)
- *LONG_D*: value of longitudinal dispersivity (a_L).
- *TRPT*: ratio of the horizontal transverse dispersivity, a_{TH}, to the longitudinal dispersivity.
- *TRPV*: ratio of the vertical transverse dispersivity, a_{TV}, to the longitudinal dispersivity.
- **For each species:**
    1. *SCONC*: initial concentration.
    2. *DMCOEFF*: coefficient of molecular diffusion.



Note: the other crucial parameter to solve the transport equation is the **effective porosity**. Such a value, to be set for each layer, is defined in the flow model layer, and identified as **NE**. Therefore, once the above properties for each transport layer have been set, the User has to go to the flow model layers and set the **NE** value there.

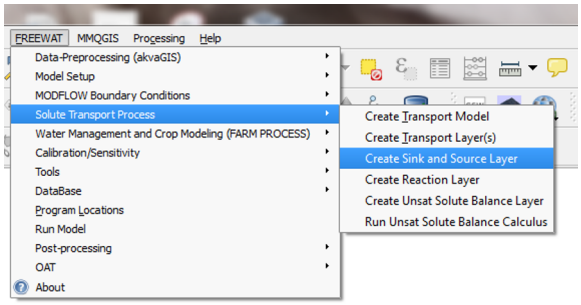
Note: the coefficients above described (namley: **LONG_D**, **TRPT**, **TRPV** and **DMCOEFF**) must be specified only if the User wants to activate the dispersion package (DSP). Otherwise, the User can leace the default values, due to the fact that the code will not consider such values. The possibility to activate/inactivate DSP is given in the GUI *Run Model* (see below 3_runmodel).

Sink and Source Mixing Package - SSM

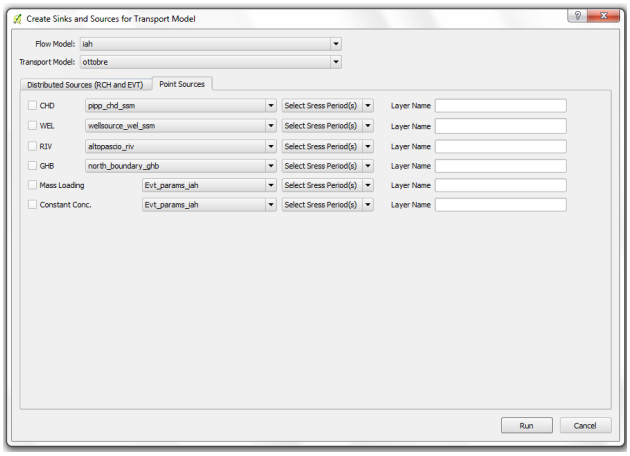
Whenever in the flow model is present (at least) a sink-source pacckage (like WEL, CHD, RIV, etc.), the User has to specify the behaviour of the solutes with respect to these stresses, since they rapresent a potential sink/source term of the transport equation [mt3dms]

In this case, the User has to create an MDO for each point-wise or linear source (like WEL, CHD or RIV, for instance) and for distributed sources (like RCH or EVT).

To input such an information, go to *FREEWAT -> Solute Transport Process -> Create Sink and Source Layer*



and the following GUI appears:

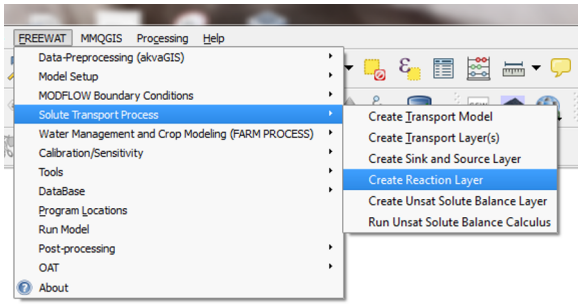


For any source/sink type (namely for each stress package of the flow model), the User has to select in the menus the corresponding MDO created for the flow model. Furthermore, for each package the stress periods where this source/sink is active has to be selected in the *Select Stress Period(s)* menu, checking the stress period(s) to be included.

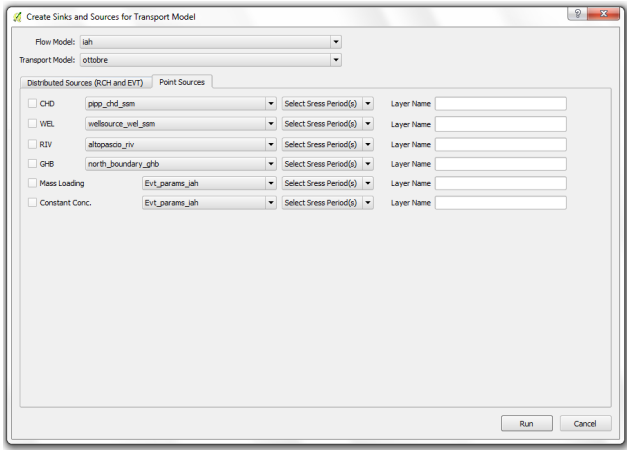
The algorithm will produce a number of new MDOs as the number of packages selected. These MDOs will be used to input data relative to the corresponding SSM stress.

Reaction Package - RCT

The reaction package can be activated from *FREEWAT -> Solute Transport Process -> Create Sink and Source Layer*



The GUI to create this MDO requires as input the model name, the grid layer and the name the User wants to assign to the new MDO.



In this MDOs the User has to set the parameters needed for the sorption and reaction terms, namely:

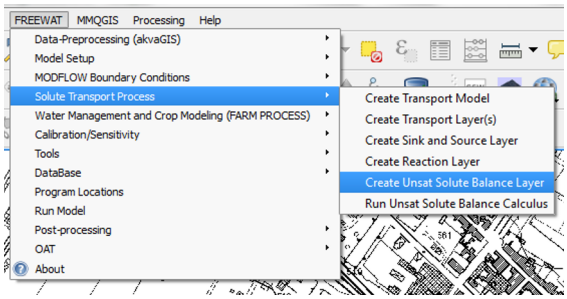
- *RHOB*: bulk density of the soil (for each layer)
- *PRSITY2*: porosity of the immobile domain (for each layer), i.e., the ratio of pore spaces filled with immobile fluids over the bulk volume of the aquifer medium, when the simulation is intended to represent a dual-domain system.
- Sorption and reaction parameters (for each layer and for each species), according to the sorption and reaction models considered for the model [mt3dms]

Unsaturated Solute Balance - USB

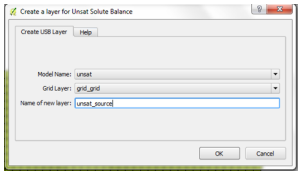
To take into account the leaching process of a contaminant present at the ground surface, the User can apply the USB module, which solves the following problem: if one (or more) area(s) on the ground surface are affected by the presence of a pollutant species, it is necessary to estimate (for each stress period in the model) how much concentration of this pollutant reaches the water table, and eventually spread out following the ground water flow. USB will compute this estimate.

Note: In case the simulation involves more than one component (contaminant), the following steps must be repeated for each component.

First, the User has to define the zone(s) on which the contaminant is present. To do that, go to the grid MDO and select the cells that form the zone(s) of interest. With this selection active, activate the USB source definition from *FREEWAT -> Solute Transport Process -> Create Unsat Solute Balance Layer*

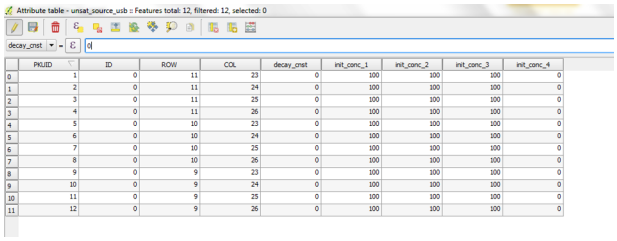


The GUI to create this MDO requires as input the model name, the grid layer and the name the User wants to assign to the new MDO.

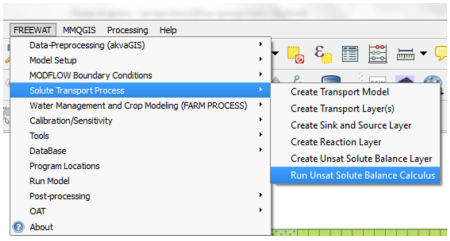


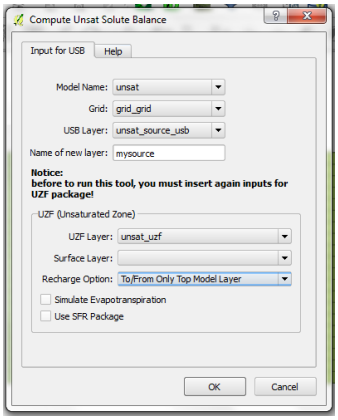
In this MDOs the User has to set the initial condition for each stress period, namely the value of solute concentration at the ground surface, in terms of Mass per volume of water (e.g. Kg/m^3) , and the decay constant, i.e. :

- *init_conc_1*: solute concentration (for each stress period)
- *decay_cnst*: decay constant, as a rate term (T^-1).



Using such a datum, it is possible to estimate how much of this source (at the ground level) can reach the water table, and eventually acting as source for the saturated flow transport problem. This is done by the USB algorithm included in FREEWAT. To to do that, open *FREEWAT -> Solute Transport Process -> Run Unsat Solute Balance Calculus*



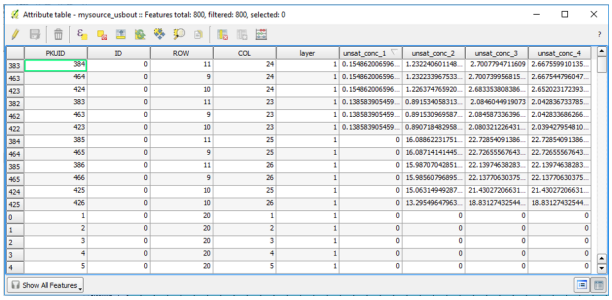


In this GUI the following info are needed:

- *Model name*: the name of the flow model
- *Grid*: the name reference grid layer
- *USB Layer*: the MDO created before where initial concentration at the ground surface have been set
- *Name of the new layer*: the name to assign to the new MDO

Furthermore, through this GUI, the model including the UZF package must be run again, since the aim is to print out the UZF budget for all the cells intersecting the source zone.

Therefore, after running again the model (this is done automatically by the code), USB algorithms ends with a creation of a new MDO, in which for each stress period the amount of concentration that reached the water table is reported, as **unsat_conc_n** field, where **n** is the n-th stress period.



Finally, to set these quantity as constant concentration at layer 1 of the model, as boundary condition for MT3DMS simulation, the User performs the following steps:

1. Create a MDO for the SSM package, corresponding to Constant Concentration type (if not already defined), as described in *Sink and Source Mixing Package - SSM*: this should be done only considering the cells corresponding to the source zone. To do that, the User can also use the USB source MDO, which reports only the grid cells of the source; alternatively, the User can use the reference grid layer, but selecting the interested cells before.
2. Use the tool *FREEWAT -> Tools -> Copy from Vector Layer* to copy the field **unsat_conc_n** to **CSSMS_sp_n_m**, where **n** is the n-th stress period and **m** is the m-th component.

Remark 4: In case of a multi-component simulation, as stated in Remark 3, the User has to recall that a single MDO containing the USB output has to be created for each component. Therefore, step 2 above has to be repeated for each component, passing on a case-by-case basis only the concentrations relative to the component addressed.

Finally, the User can run the transport model using this SSM MDO, proceeding as described in Section 3.

Density and Viscosity dependence (VDF and VSC)

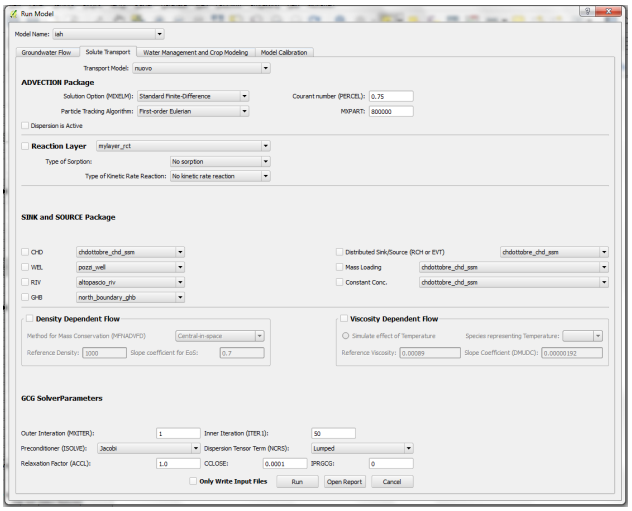
For these packages no gridded or tabled data are needed, but only the specification of some coefficient and option is required.

Therefore, no MDO creation is required, and the User will set the desired option directly in the Run Model GUI (see *Run the transport model*)

CHAPTER 3

Run the transport model

Once tables and MDOs for the transport model have been created (see *Building the transport model*), the Run Model GUI can be accessed, selecting the tag named *Solute Transport*



This GUI allows to input all the additional information needed to run a MT3DMS (or SEAWAT) simulation, namely:

- The name of flow model associated to the transport model.
- Options for the numerical solution of the advection term.
- Possibility to activate the dispersion term (by checking the flag **Dispersion is Active**)
- MDO and option for the reaction process
- MDOs for the Sink and Source Mixing package
- Possibility to activate the Density Dependent Flow (VDF), and corresponding options and parameters
- Possibility to activate the Viscosity Dependent Flow (VCS), and corresponding options and parameters
- Options and parameters for the numericla solver (GCG)

Remark: notice that, if VDF and/or VCS are selected, before to click on Run button, the User has to include under Program Locations the executable of SEAWAT code.

From this step on, the User can follow the same instruction valid for the flow model (i.e. writing only input file, running the model, opening the text report).

Finally, simulation results can be converted in raster output using the **view Model Output** sub-menu, opening the **Post-processing** menu, and performing the same procedure followed for the flow model simulation.

References

Langevin C.D., Thorne D.T. Jr., Dausman A.M., Sukop M.C. and Guo Weixing (2007). SEAWAT Version 4: A Computer Program for Simulation of Multi-Species Solute and Heat Transport: U.S. Geological Survey Techniques and Methods Book 6, Chapter A22, 39 p.

Morway Eric D., Niswonger Richard G., Langevin Christian D., Bailey Ryan T., Healy Richard W. (2013). Modeling Variably Saturated Subsurface Solute Transport with MODFLOW-UZF and MT3DMS, GROUNDWATER, Vol. 51, no. 2.

Zheng Chunmiao, and P. Patrick Wang (1999). MT3DMS, A modular three-dimensional multi-species transport model for simulation of advection, dispersion and chemical reactions of contaminants in groundwater systems; documentation and user's guide, U.S. Army Engineer Research and Development Center Contract Report SERDP-99-1, Vicksburg, MS, 202 p.