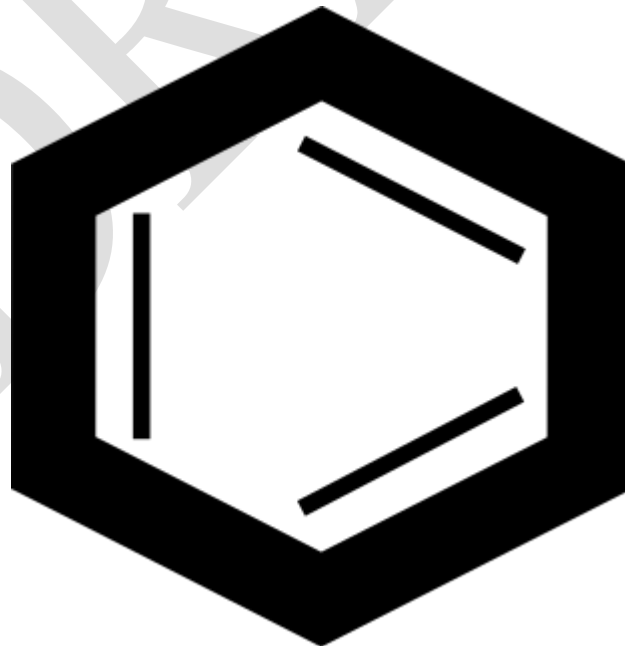


ORTi3D

OPEN REACTIVE TRANSPORT INTERFACE 3D

User's Manual of new features

For professional application in groundwater flow and reactive transport modelling



Preface

ORTI3D has recently been linked to the QGIS Geographic Information System software. The link with QGIS allows you to build large scale models, better view complex spatial information, and improve the visualization of graphical results at the end of the process. In addition, new features have been implemented in the basic interface. This document details how to use these new features.

DRAFT

Table of contents

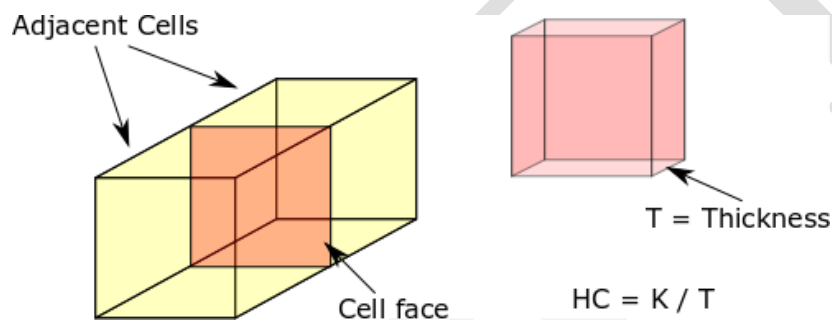
- Preface..... ii
- 1. New general features 1
 - 1.1. Horizontal Flux Barrier (HFB)..... 1
 - 1.2. Import observation data..... 2
 - 1.3. Multiplot..... 3
 - 1.3.1 Create observation zones..... 3
 - 1.3.2 Time-series graphs..... 3
 - 1.3.3 Profile graphs 4
 - 1.3.4 Calibration graph..... 5
- 2. Specific functions in QGIS..... 7
 - 2.1. Links between QGIS and ORTi3D project files..... 7
 - 2.2. Control of coordinates system 7
 - 2.3. Domain boundaries for Modflow 2000 8
 - 2.4. Grid point information..... 8
 - 2.5. Several grids to show results and contour 9

1. New general features

1.1. Horizontal Flux Barrier (HFB)

The Horizontal Flow Barrier (HFB) is used to simulate thin, vertical, low-permeability barriers that impede the horizontal flow of groundwater such as sheet pile walls, slurry trenches, or other objects which act as a barrier to flow.

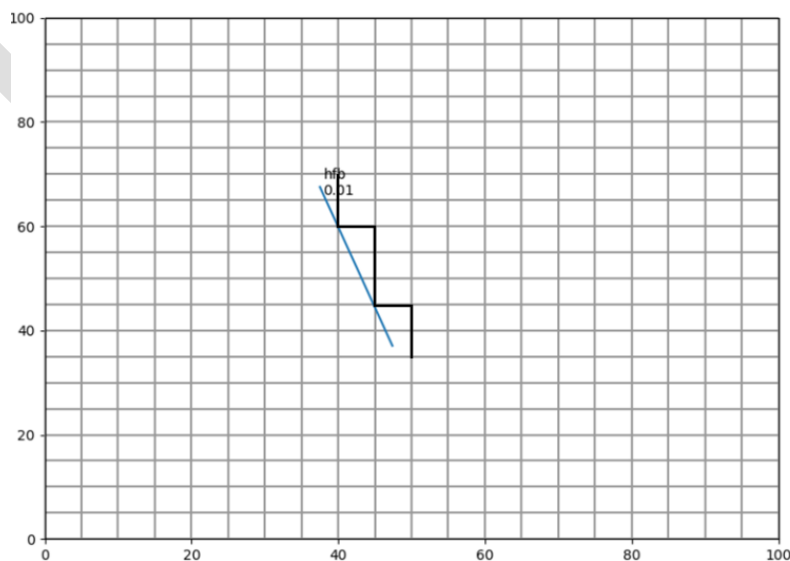
Barriers are simulated as a series of horizontal flow barrier located on the boundary between two adjacent finite-difference cells in the same layer. Barriers width is not explicitly considered, but is represented as hydraulic characteristic (HC) defined as barrier hydraulic conductivity divided by barrier thickness.



The **HFB** package is not included by default in ORTI3D. Therefore, to assign horizon barrier condition to the groundwater system, enable **HFB** package.

Horizontal Flow Barrier may be defined on distributed property values:

- Set “line” or “polyline” zones of value. ORTI3D automatically calculated the appropriate cell faces (black line) based on the intersection point of the polyline (blue line).



To assign a **Horizontal Flow Barrier** in the model:

- Choose **Modflow series - Modflow – HBF6 – hbf.3 Hydraulic Characteristic Kh/e** in the first four drop-down list under the **Spatial Attributes** section.
- Assign **Horizontal Flow Barrier** with the desired tool for assigning and editing distributed input data.
- A **Zone** window will appear.
- Set the **hydraulic characteristic (HC)** to assign at the zone in the **Zone value** box.

*Information about the **HBF** package can be found in the MODFLOW-2000 user guide on page 63, located in the **Doc** folder of your ORTI3D installation folder.*

1.2. Import observation data

ORTI3D has an import option to import observation data of three different types:

- Head observation data.
- Tracer observation data.
- Chemistry observation data.

To import observation data:

- Select **Import/Head observation data** (or Tracer observation data or Chemistry observation data) from the **Main menu** section.
- A **Head observation data** window will appear.
- Set or copy paste your **Head observation data** in the table respecting the title of each column.

The titles of the column are:

- Head observation data: Well – Layer – Time – Head
- Tracer observation data: Well – Layer – Time – Tracer
- Chemistry observation data: Well – Layer – Time – Chemical specie 1 - Chemical specie 2 ...

Well: must match the name of an **Observation zone** in the model.

Layer: For 3D model, **Layer** represents the model layer at which the **Observations** were recorded (starting from 0 increasing with depth). For 2D model, **Layer** is 0.

Time: is the time at which the **Observations** were recorded. The times indicate here must match with the **Model output times**.

Head: is the value of head in model units.

Tracer: is the value of tracer concentration in model units.

Chemical species: is the value of chemical species concentration in moles.

1.3. Multiplot

ORTi3D has a multiple graphs display option of three different types:

- Time-series graphs.
- Profile graphs.
- Calibration graphs.

1.3.1 Create observation zones

To create an observation zone see ORTi3D user's manual on page 96.

1.3.2 Time-series graphs

A time-series graph plots the change in a selected variable with time. In groundwater flow and contaminant transport modelling, time-series graphs are used to evaluate and compare temporal trends in the calculated Head, Tracer or Chemical Species Concentration at selected observation zones.

To display a **Time-Series Graph**:

- Select **Time-Series Graph** in the **Type** drop-down list under the **Results/5.Observation** section.
- Select the simulation result to display in the **Result** drop-down list under the **Results/5.Observation** section:
 - **Head** for flow simulation.
 - **Tracer** for transport simulation.
 - **Chemistry** for reactive transport simulation.
- A **Plot of result** window will appear.
- Select the desired **Observation zones** and **Layers**.
- Press the **Apply** button to display or update the **Time-Series Graph**.

Observation zones and Layers

The model **Observation zone** specified in the model are listed under the **Zones** tab. The Observation zone displayed on the graph can be selected under the **Zones** tab.

The Layers of the model are listed under the **Layers** tab. The model layers at which the simulation results are recorded can be selected under the **Layers** tab.

Once the desired **Observation zones** and **Layers** are selected, press the **Apply** button to display or update the **Time-Series Graph**.

Reactive transport result

For reactive transport simulations involving multiple chemical species, an additional tab labelled **Species** will appear beside the Group and Points tabs. The **Species** tab contains the list of the Chemical Species being simulated by the model. One or more of these species can be selected to plot on the Time-Series Graph.

Multiplot option can be display by:

- Observation zone: One graph for each selected Observation zone.
- Chemical species: One graph for each selected Chemical species.

To change the multiplot option:

- Select **By zone** or **By species** in the dropdown list.

Observed data

To display observed data on **Time-Series Graph**:

- Check the **Observed data** checkbox.
- Press the **Apply** button to display or update the **Time-Series Graph**.

Export Result

Simulated data at selected **Observation zone** and **Layers** can be exported by:

- Press the **Export** button.
- A **Save** window will appear. Navigate to the directory where you want save the ASCII data file.
- Indicate the file name and then click the “**Save**” button.

1.3.3 Profile graphs

A Profile graph plots the change in a selected variable in space. In groundwater flow and contaminant transport modelling, Profile graphs are used to evaluate and compare spatial trends in the calculated Head, Tracer or Chemical Species Concentration at selected observation zones.

To display a **Profile Graph**:

- Select **Profile Graph** in the **Type** drop-down list under the **Results/5.Observation** section.
- Select the simulation result to display in the **Result** drop-down list under the **Results/5.Observation** section:
 - **Head** for flow simulation.
 - **Tracer** for transport simulation.
 - **Chemistry** for reactive transport simulation.
- A **Plot of result** window will appear.
- Select the desired **Observation zones** and **Layers**.
- Press the **Apply** button to display or update the **Profile Graph**.

Observation zones and Layers

The model **Observation zone** specified in the model are listed under the **Zones** tab. The Observation zone displayed on the graph can be selected under the **Zones** tab.

The Layers of the model are listed under the **Layers** tab. The model layers at which the simulation results are recorded can be selected under the **Layers** tab.

Once the desired **Observation zones** and **Layers** are selected, press the **Apply** button to display or update the **Profile Graph**.

Reactive transport result

For reactive transport simulations involving multiple chemical species, an additional tab labelled **Species** will appear beside the **Group** and **Points** tabs. The **Species** tab contains the list of the Chemical Species being simulated by the model. One or more of these species can be selected to plot on the **Profile Graph**.

Multiplot option can be display by:

- Observation zone: One graph for each selected Observation zone.
- Chemical species: One graph for each selected Chemical species.

To change the multiplot option:

- Select **By zone** or **By species** in the dropdown list.

Observed data

To display observed data on **Profile Graph**:

- Check the **Observed data** checkbox.
- Press the **Apply** button to display or update the **Profile Graph**.

Export Result

Simulated data at selected **Observation zone** and **Layers** can be exported by:

- Press the **Export** button.
- A **Save** window will appear. Navigate to the directory where you want save the ASCII data file.
- Indicate the file name and then click the “**Save**” button.

1.3.4 Calibration graph

ORTi3D provides a Calculated vs. Observed scatter graph for evaluating the model calibration.

To display a **Calibration Graph**:

- Select **Calibration Graph** in the **Type** drop-down list under the **Results/5.Observation** section.
- Select the simulation result to display in the **Result** drop-down list under the **Results/5.Observation** section:
 - **Head** for flow simulation.
 - **Tracer** for transport simulation.
 - **Chemistry** for reactive transport simulation.
- A **Plot of result** window will appear.
- Select the desired **Observation zones**.
- Press the **Apply** button to display or update the **Profile Graph**.

Calibration Times

The Calculated vs. Observed Scatter Graph represent a snap-shot in time of the comparison between the calculated and observed values. For transient simulation, the calibration may be evaluated at different times or for all times where observed data are available.

To select the option time at which the calibration graph is displayed:

- Select the desired time in the **Time** dropdown list.
- Select **All** to display the calibration graph at all times where observed data are available.

Export Result

Calculated vs. Observed data at selected **Observation zone** can be exported by:

- Press the **Export** button.
- A **Save** window will appear. Navigate to the directory where you want save the ASCII data file.
- Indicate the file name and then click the “**Save**” button.

2. Specific functions in QGIS

2.1. Links between QGIS and ORTi3D project files

The Open and Save function of QGIS project file are linked with the ORTi3D plugin when an ORTi3D model is opened. In QGIS, to Open and Save project file:

- Select **Project/Open** or **Project/Save** from the **Main menu** section.

Links between the open and save function of QGIS project file and ORTi3D plugin are the following:

- When the ORTi3D plugin is loaded but no ORTi3D model is open, no changes are made to the **Open** and **Save** functions of the QGIS project file.
- When QGIS specific layers and model layers (ORTi3D specific layers) are opened in QGIS, the **Save** function allows to:
 - Save the QGIS specific layers in a project file.
 - Ask if the user want to save the ORTi3D project file (.orti file).
- When the user **Opens** a QGIS project file located in a folder with an ORTi3D project file:
 - QGIS specific layers are loaded from the QGIS project file.
 - ORTi3D specific layers are created from the ORTi3D project file.

For these features to be available:

- QGIS and ORTi3D project files must be in the save project folder.
- QGIS project file must be open from the **Main menu** section and NOT from the **Recent Projects** section available when QGIS is opened.

NB: in QGIS the ORTi3D specific layers are created as memory layers and the existing information is not stored (only the name of the layers is kept). So when opening a QGIS project file located in a folder with an ORTi3D project file, the ORTi3D specific layers which are in the project (the empty ones) are deleted and new layers are created.

2.2. Control of coordinates system

Usually with QGIS, data are projected in a given **Coordinate Reference System (CRS)**. When ORTi3D plugin is activated, the CRS of ORTi3D specific layers have to be defined. The easier way is to use the same **CRS** for ORTi3D specific layers and QGIS project.

To define QGIS project **CRS**:

- Select **Project/Properties...** from the **Main menu** section.
- A **Project Properties** window will appear.
- Click on **CRS** in the left-hand corner of the status bar.
- Choose the QGIS project **CRS** in the box **Recently used coordinate reference systems** or **Coordinate reference system of the world**.

Then, all new QGIS and ORTi3D specific layers will get the QGIS project **CRS** automatically.

To define manually (or modify) the **CRS** of a QGIS or ORTi3D specific layer:

- **Right click** to the name of the layer in the **Layers panel**.
- Select **Set CRS/Set Layer CRS...**
- Choose the **CRS** for the layer in the box **Recently used coordinate reference systems** or **Coordinate reference system of the world**.

Note that QGIS 3 automatically includes the On-The-Fly Projection which means that when a QGIS project **CRS** is defined, all layers that are then loaded, no matter what coordinate reference system they have, will be automatically displayed in the QGIS project **CRS** defined. This behavior must be used only by experienced users.

2.3. Domain boundaries for Modflow 2000

In QGIS, the size of the domain can be specified by defining a zone directly on a map. Note that in MODFLOW the domain have to be rectangular.

To define spatially the domain boundary in QGIS:

- Select **Modflow series - Modflow – DIS – dis.1 Domain** in the first four drop-down list under the **Spatial Variables** section.
- Select **Zone** in the Type drop-down list.
- Edit the ORTi3D specific layer **Ldis.1 Domain**.
- Draw a **rectangular** area with the **Add Line Feature** tool of QGIS.
- A **Zone** window will appear.
- Set a name of the zone in the **Zone Name** box, and click on **OK**.
- Select **1.Model – Grid** button under the **Model parameters** section.
- A popup window will appear. Click on **OK** to use the zone drawn in the dis.1 Domain as limit for the domain.


Then, the dialog for the grid will contain the coordinates of the corners of the rectangle drawn. The coordinates may be modified or adjusted manually with **1.Model – Grid** button under the **Model parameters** section.

2.4. Grid point information


The value of the spatialized parameters or the result of the simulations, in each cell of the model grid, can be displayed using the QGIS **Identify Feature** tool.

To get grid point information of a spatialized parameter:

- Select the parameter to display with the first four drop-down list under the **Spatial Variables** section.
- Check the **view** checkbox. The spatialized values of the parameter will be displayed in the **Parameters** ORTi3D specific layer.
- Click on the **Parameters** ORTi3D specific layer in the **Layer** panel.

- Select the **Identify Feature** tool  of QGIS:
- Left click on a cell to get the value of the parameter in the **Identify Results** panel. Set the **Current Layer** mode in the **Identify Results** panel to only display information about the **Parameters ORTi3D** specific layer.

To get grid point information of a simulation result:

- Select the simulation result to display (Head, Tracer or Chemical species) under the **Results** section.
- The spatialized values of the simulation result will be displayed in the **Simulation result (Head, Tracer or Chemistry)** ORTi3D specific layer.
- Click on the **Simulation result (Head, Tracer or Chemistry)** ORTi3D specific layer in the **Layer** panel.
- Select the **Identify Feature** tool  of QGIS:
- Left click on a cell to get the simulation result in the **Identify Results** panel. Set the **Current Layer** mode in the **Identify Results** panel to only display information about the **Parameters ORTi3D** specific layer.

2.5. Several grids to show results and contour

In QGIS, simulation results will be display in three different ORTi3D specific layers:

- Head layer for flow simulation.
- Tracer layer for transport simulation.
- Chemistry layer for reactive transport simulation.

To display the simulation result:

- Select the simulation result to display (Head, Tracer or Chemical species) under the **Results** section.
- The spatialized values of the simulation result will be displayed in the **Simulation results (Head, Tracer or Chemistry)** ORTi3D specific layer.

To get the contour of the simulation result:

- First rasterize the **Simulation results (Head, Tracer or Chemistry)** ORTi3D specific layer:
 - Select **Raster – Conversion - Rasterize (Vector to Raster)** tool under the main menu of QGIS.
 - To get more information of this tool: https://docs.qgis.org/2.8/en/docs/user_manual/processing_algs/gdalogr/gdal_conversion/rasterize.html
- Secondly create contour from the rasterized QGIS specific layer:
 - Select **Raster – Extraction – Contour ...** tool under the main menu of QGIS.

3. Parameter optimization: PEST

ORTI3D allow writing the main PEST files and running PEST. One file **MUST** be provided in the model project directory:

- The observation file which **MUST** be called « **pest_obs.txt** ».

3.1. PEST input data

3.1.1 Pest parameters

In ORTI3D, parameters to optimize may be selected from the interface. There are two different types of parameters:

- Background parameters: distributed model parameters for which the value is applied in all cells of your model (cf. section 4.2.1 of the manual).
- Zone parameters: distributed model parameters for which the value is applied in zones (cf. section 4.2.2 of the manual).

To select PEST background parameters:

- \bar{p}_b
- Click on the “Pest background parameters” button under the Parameter/5.Pest section.
 - Select the type of parameters that you want to optimize. Note that there is different tab for flow, transport and reactive model parameters.
 - Click the “Ok” button.
 - Check the “Use” box of the parameters to optimize and choose:
 - The min and max value of the parameters values during the optimization (cf. Pest manual).
 - The transformation of parameter during the optimization (cf. Pest manual).
 - The name of the group to assign each parameter to (cf. Pest manual).Note that there is different tab for flow, transport and reactive model parameters.
 - Click the “Ok” button.

To select PEST zone parameters:

- \bar{p}_z
- Click on the “Pest zone parameters” button under the Parameter/5.Pest section.
 - Select the type of parameters that you want to optimize. Note that there is different tab for flow, transport and reactive model parameters.
 - Click the “Ok” button.
 - Check the “Use” box of the parameters to optimize and choose:
 - The min and max value of the parameters values during the optimization (cf. Pest manual).
 - The transformation of parameter during the optimization (cf. Pest manual).
 - The name of the parameter group to assign each parameter to (cf. Pest manual).Note that there is different tab for flow, transport and reactive model parameters.
 - Click the “Ok” button.

3.1.2 Pest observations

The data file formats currently supported by ORTI3D for the observation file (**pest_obs.txt**) is ASCII text files (.TXT). The file must contain on the first line the keywords **Type**, **Well**, **Time**, **Value**, **Weight** and **Group** and on the following lines your PEST observations information. This information has to be provided on one line for each point, as follows (in bold the key words that must contain the file and between hook the information provided by the modeler):

Type	Well	Time	Value	Weight	Group
'Type'	'Name'	'Time'	'Value'	'Weight'	'Group'
...
...
'Type'	'Name'	'Time'	'Value'	'Weight'	'Group'

'**Type**' is the keyword used to specify the type of observation or the name of species for chemical observations:

- For flow model 'type' = Head.
- For transport model: 'type' = Tracer.
- For reactive transport model: 'type' = the name of the chemical specie.

'**Name**' is the name of the observation zone.

'**Time**' is the time at which the simulated values at the observation zone are read.

'**Value**' is the value of the observed data.

'**Weight**' is the weight of the value of the observed data (cf. PEST manual).

'**Group**' is the name of the observation group to assign each observation to (cf. Pest manual).

For example:

Type	Well	Time	Value	Weight	Group
Head	obs1	50	10.5	1	GPH
Tracer	obs1	50	500	1	GPT

3.2. PEST run settings

To set PEST run settings:

- P** • Click on the "**Parameter**" button under the **Parameter/5.Pest** section.
- Choose the category of settings in the first drop-down list.
- Choose the sub-category of settings in the second drop-down list.
- Modify or select your variable.
- Click the "**Apply**" button.

The category of PEST run settings are:

SYS: To select the operating system used for run the model and specify the path of model project directory. On **sys.1:** If you use ORTI3D on windows and run PEST on windows then select windows. In this case, the pest file will be written in your model project directory. If you use ORTI3D on windows and run PEST on linux then select linux. In this last case you can specify the model project directory path used on linux on **sys.2.**

CTD: To specify the variables in “control data” section of PEST control file (cf. PEST manual).

SVD: To specify the variables in “singular value decomposition” section of PEST control file (cf. PEST manual).

PGR: To specify the variables required for each parameter group in “parameter groups” section of PEST control file (cf. PEST manual).

OBS: To specify observation transformation for the computation of objective function (for advance users).

REG: To specify the variables in optional “regularisation” section of PEST control file (cf. PEST manual). To use this option PESTMODE have to be selected on regularization: Select regularization under **Parameter/5.Pest** section **CTD/ctd.1-Control Data 11/PESTMODE.**

PPP: To specify the variables in optional “PEST++” section of PEST control file (cf. PEST++ manual).

3.3. Running PEST

3.3.1 Write Pest files

To write PEST files:



- Click on the “**Write**” button under the **Parameter/5.Pest** section.
- A **files written** window will appear.
- Click the “**Ok**” button.

The following files have been created:

- **runmod.bat:** This is the batch file that PEST will run as “the model”. First the pre-processing code **scriptPest1.py** is running following by the model (MODFLOW or/and MT3DMS and PHT3D). To finish the post-processing code **scriptPest2.py** is executed.
- **pest_tpl.txt:** is the template file used by PEST to write the optimized parameters in the file **pest_run.txt.**
- **scriptPest1.py:** script used to write the new optimized parameter into the model project files (.orti files) and rewrite the input model files.
- **scriptPest2.py:** allow to read the simulated observation values from the model output and write them in the file **pest_out.txt.**
- **pest.ins:** an instruction file allowing PEST to read the file **pest_out.txt.**

3.3.2 Check Pest files

ORTI3D use the **pestchk** application of the PEST suite to check if the pest files are correctly written. To check if there is no error in PEST files:

- ☑ • Click on the “**Pestchk**” button under the **Parameter/5.Pest** section.
- A message will appear in the **window command prompt**. Read the message in the **cmd** to check if there is error.
- Press a key to continue in the **cmd**.
- A **file checked** window will appear.
- Click the “**Ok**” button.

3.3.3 Running Pest

When all files needed by PEST are written in the model project directory, PEST can be run.

To run PEST:

- ▶ • Click on the “**Run**” button under the **Parameter/5.Pest** section.
- A **window command prompt** will appear during the PEST execution and will disappear automatically at the end of the simulation.
- At the end of the simulation, a window with the message **Normal termination of Pest** will appear.
- Click the “**Ok**” button.