VORO2MESH and TOUGH2Viewer for MODFLOW

User Manual

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Summary

1 Introduction

The Finite Volume Method (FVM) allows great flexibility for the discretization of the reservoir domain. It may be used on arbitrary geometries, using structured or unstructured meshes, and it leads to robust scheme.

FVM satisfies conservation law in each finite volume of the discretization and also satisfies a global conservation, but it requires a geometrical constraint on the blocks of the grid: the connecting segment between the nodes of two adjacent blocks must be orthogonal to the shared surface between the two blocks.

The Voronoi tessellation implicitly satisfies the this FV constrain.

TOUGH family of simulators, adopts the Integral Finite Difference method (IFD), a finite volume formulation that allows the use of irregularly shaped cells. The pre and post-processor VORO2MESH and TOUGH2Viewer were specifically developed to manage full Voronoi 3D grids for the TOUGH family of simulators.

The USGS modular hydrologic model MODFLOW 6 supports a general unstructured grid based on concepts developed for MODFLOW-USG, an UnStructured Grid (USG) version of MODFLOW for simulating groundwater flow using a Control Volume Finite-Difference Formulation.

New versions of both VORO2MESH and TOUGH2Viewer with new features specifically dedicated to MODFLOW 6 have been developed.

This manual is dedicated to the new functionalities of VORO2MESH and TOUGH2Viewer for the generation and visualization of MODFLOW 6 grids and simulation results.

More detailed information about VORO2MESH and TOUGH2Viewer can be found in the User Manual of the two software downloadable from the following website: VORO2MESH at https://site.unibo.it/softwaredicam/en/software/voro2mesh; and TOUGH2Viewer at https://site.unibo.it/softwaredicam/en/software/tough2viewer.

Manuals are available after approved requests for downloading the software from the above mention links.

2 VORO2MESH grid generation

Originally tailored for the generation of 3D Voronoi grids for TOUGH, VORO2MESH capabilities have been extended to allow MODFLOW grid generation. A detailed description of VORO2MESH capabilities can be found in the VORO2EMSH user's manuals and in (Bonduà et al., 2017).

2.1 VORO2MESH installation

In order to run VORO2MESH properly, download VORO2MESH last version from https://site.unibo.it/softwaredicam/en/software/voro2mesh.

Once you have downloaded the zip package, extract it into the desired folder. The VORO2MESH executable can be located in a folder that must belong to the path of your operative systems (environment variable on operating systems specifying a set of directories where executable programs are located). Alternatively, VORO2MESH must be located into the working folder.

2.2 VORO2MESH usage

After locating the directory with voro2mesh.exe file ,VORO2MESH can be run from the DOS prompt (Windows) by typing VORO2MESH [ENTER]. For a more detailed explanation about VORO2MESH options, please refer to the VORO2MESH user manual.

VORO2MESH use a parameter file named voro.par for discretization directions. In Table 1 is shown the **voro.par** structure and keywords description. Everything that follows the comment symbol is "!"is ignored by the parser. For a complete list of the available keywords, please refer to the VORO2MESH user manual available at [https://site.unibo.it/softwaredicam/en/software/voro2mesh.](https://site.unibo.it/softwaredicam/en/software/voro2mesh)

```
!VORO2MESH parameter file
x_max=+1726500.0000 !x max
x_min=+1701500.0000 !x min
y_max=+4759500.000  !y min
y_min=+4732500.000   !y max
z_max=2000.0 !            z max
z_min=-6000.0 !           z min
toler=1.001 ! all connection with area<toler will be skipped from CONNE
toler_dist2=1.0E-06 !minimum square distance between two points. If d(p1,p2)<toler_dist2 the program
will terminate.
read_rocktype=1 !0=no,1=yes;
auto_nxnynz=1 !0=manual;1=auto. Parameter for compute the voronoi tessellation
print_vtkXML_file=1 !0=no;1=yes; The voronoi geometry will be exported to a VTK file in a vtu format
(see Paraview documentation);
n_x=10 ! number of domain subdivision for voronoi computation
n_y=10 ! number of domain subdivision for voronoi computation
n_z=1 ! number of domain subdivision for voronoi computation
r_max=2.0 !
wall_type=1 !1: regular box;2=cylinder
add_walls=0 !0:no; 1:yes. If yes, a file called "wallslist.dat" must be present. Inside, a list of ABCD have to
be present, that are parameter of the equation Ax+By+Cz+D>0 (the cutting wall)
tolerance_walls=0.1 !parameter for evaluate inside points if(ax+by+cz-d>tolerance_walls) then ok.
min_distance_from_walls=10.0 !if dist(point,walls(i))<min_distance_from_walls the node is skipped
fit_surface=3 !0:no fit; 1=execute fit ;2:fitsuface2;3:fitsurface3. if fit_surface=3, a file list called surface
list must be present.
n_layers=5 !
refine_mesh=1 !if(refine_mesh=1)norefinement;if refinemesh>1, each square is then divided in
refine_mesh^2 elements. Not implemented.
coarse_mesh=1 !if(coarse_mesh=1)no coarsening;if coarse_mesh>1, a square is then taken skipping
coarse_mesh elements. Note that refinemesh=2 and coarse_mesh=2 give the same number of elements,
but generate different meshes. Not implemented.
vertical=2 !0: the point belongs to the segment;1:the line is vertical centered;2: the line is vertical, the
node have z as multiple of 2*offset(semi regular grid).use with
variable_n_layers=1 !0=no; 1=for each xy, calculate n_layer=int(distance/offset);
offset=50.0 !if offset<0.0 then offset=min(dx,dy)
blocks_thick=70.0 !general value for blocks height;if blocks_thick <0 then blocks_thick=offset.
cut_model_top_bottom=1 !0=no; 1=yes; Node outbound from the top/bottom surface are used to
compute voronoi tessellation but are skipped from the MESH file.
assign_infinite_volume_to_boundary=0 !0=no;1=yes.
create_incon=0 !:0=no; 1=yes
read_por_perm_tables=0 ! 0=no; 1=yes
format_por_perm_tables=1 ! 1=x,y,z,por,k,[ky],[kz]; 2=gridded files(one file for each values). 2=NOT
IMPLEMENTED.
number_of_points_por_perm=1 !number of points used to calculate por and perm. Actually use 1 or 4
ONLY.
dist_mode_por_perm=0 ! 0=2D; 1=3D;
```

```
max_dist_por_perm=850.0 !
create_gener=0 !:0:no; 1=yes; 2=use mask.dat
min_2d_dist=850.0 ! when creating GENER, if we have two block with d(P1,P2)<min_2d_dist, only the lower block is taken...(feature for ENI project)
assign_roktype_to_gener=0 ! 0 no; >0 rocktype=assign_rocktype_to_gener
divide_control_inside_points=1 !0=no;1=yes;
por_perm_upscaling=1 !1=mean;2=series and parallel calculation (use 2 only with number_of_points_por_perm=4)
exclude_out_pts=1 !0=no;1=yes; points not inside the domain will not print in "in.dat.ready". During reading, outside points are skipped in any case.
two_digit=1 !0=use 3 digit exponent(example 1.403E+003);1=use two digit exponent (example: 1.4031E+03)
blocks_thick=50.0 !general value for blocks height
debug_mode=0 !0=no;1=yes
write_tough2viewer_dat=1 !0:no; 1:yes
block_names_format=0 !default=0;=0,standard A3I[len_char_eleme_name-3];=1 use I[len_char_eleme_name]
len_char_eleme_name=5 !default 5; must be 5<=len_char_eleme_name<=9
len_char_volume=10 !
len_char_eleme_surface=10 !
len_char_coordinates=10 !
len_char_d1d2=10 !
len_char_surface=10 !
len_char_cosine=10 !
CVT=0 !If CVT=1, the internal points are moved to have CVT
CVT_max_iter=50 !maximum number of iterations
k_s=0.0 !
k_cvt=0.01 !
HLBFGS_FLAG=0 !
end=end
```

Table 1– the **voro.par** file structure and keywords description

For a MODFLOW grid generation, in the voro.par file the following keyword must be set as follow:

generate_modflow2D_disu=1

Optionally, the following keywords can be set to obtain different data format in the grid file:

- IPRN_doubles=0 (default)
- IPRN_int=0 (default)

IPRN_doubles: is the Parameter for double format specification (from MODFLOW 6 – Description of Input and Output documentation[1]). The IPRN_doubles parameters values are explained in Table 2.

IPRN	Real
0	10G11.4
1	11G10.3
2	9G13.6
3	15F7.1
4	15F7.2
5	15F7.3
6	15F7.4

[1] https://water.usgs.gov/water-resources/software/MODFLOW-6/mf6io_6.2.0.pdf [Last Access 28/12/2020]

7	20F5.0
8	20F5.1
9	20F5.2
10	20F5.3
11	20F5.4

Table 2 – MODFLOW Double format specification.

IPRN_int: is the parameter for integer format specification (from MODFLOW 6 – Description of Input and Output documentation[2]. The IPRN_int parameters values are explained in Table 3.

IPRN	Integer
0	10I11
1	60I1
2	40I2
3	30I3
4	25I4
5	20I5
6	10I11
7	25I2
8	15I4
9	10I6

Table 3 – MODFLOW Integer format specification.

2.3 Generated files

A run of VORO2MESH will generate several output files, for TOUGH and MODFLOW grids. Those dedicated to MODFLOW (for a complete file description, user can refer to the MODFLOW's user manual) are:

- flow.disu: is the ASCII DISU (Unstructured discretization) file. It links to the following files, each containing the data values of the grid blocks information
    - flow.disu.area.dat: the horizontal projected block area ;
    - flow.disu.bottom.dat: the elevation of the bottom block face;
    - flow.disu.top.dat: the elevation of the top block face;
    - flow.disu.cl12.dat: is the array containing connection lengths between the center of a block and the shared face with each adjacent block;
    - flow.disu.hwva.dat: is a symmetric array of size NJA. For horizontal connections, entries in HWVA are the horizontal width perpendicular to flow. For vertical connections, entries in HWVA are the vertical area for flow;
    - flow.disu.ihc.dat: is an index array indicating the direction between a node and all its connections with adjacent nodes;
    - flow.disu.ja.dat: is a list of blocks number (n) followed by its connecting cell numbers (m) for each of the m cells connected to cell n;

where:

NJA: from the MODFLOW manual[3]: "is the sum of the number of connections and NODES. When calculating the total number of connections, the connection between cell n and cell m is considered to be different from the connection between cell m and cell n. Thus, NJA is equal to the total number of connections, including n to m and m to n, and the total number of cells".

[2] https://water.usgs.gov/water-resources/software/MODFLOW-6/mf6io_6.2.0.pdf [Last Access 28/12/2020]
[3] https://water.usgs.gov/water-resources/software/MODFLOW-6/mf6io_6.2.0.pdf pag. 42[Last Access 28/12/2020]

HWVA: from the MODFLOW manual[4]: “is a symmetric array of size NJA. For horizontal connections, entries in HWVA are the horizontal width perpendicular to flow. For vertical connections, entries in HWVA are the vertical area for flow. Thus, values in the HWVA array contain dimensions of both length and area. Entries in the HWVA array have a one-to-one correspondence with the connections specified in the JA array. Likewise, there is a one-to-one correspondence between entries in the HWVA array and entries in the IHC array, which specifies the connection type (horizontal or vertical). Entries in the HWVA array must be symmetric; the program will terminate with an error if the value for HWVA for an n to m connection does not equal the value for HWVA for the corresponding n to m connection”;

m and n: two connected cells.

[4] https://water.usgs.gov/water-resources/software/MODFLOW-6/mf6io_6.2.0.pdf pag. 43[Last Access 28/12/2020]

3 TOUGH2Viewer

The TOUGH family of codes uses the IFD method, in which the segment connecting two nodes is orthogonal to the surface shared between the two grid blocks. These grids are also named perpendicular bisectors (PEBI) grids. As TOUGH has not native Graphical User Interface (GUI), TOUGH2Viwer has been created in order to visualize and manage grids for TOUGH.

TOUGH2Viewer (Bondua et al., 2012; Bonduà and Bortolotti, 2020) functionalities have been enhanced in order to visualize MODFLOW DISU grids. For an exhaustive description of the MODFLOW DISU file format, please refer to the MODFLOW input/output manual specification.

A simulation method adopting the finite volume discretization uses the block volume, surface area, and distance connection data. For this reason, the geometry of the grid blocks has not a specific file format. In order to properly visualize the grid, a specific file is created by VORO2MESH in order to be able to visualize the grid blocks with TOUGH2Viewer. The file tough2viewer.dat contains all information needed for block definition and visualization. A detailed explanation of the tough2viewer.dat file format can be found in (Bonduà et al., 2017) and in the examples folder.

Alternatively, TOUGH2Viewer can also read and visualize binary MODFLOW DISV (Vertex Discretization) grids as created by ModelMuse[5], a free and open source pre and post processing utility for MODFLOW.. ModelMuse is a graphical user interface (GUI) for the U.S. Geological Survey (USGS) models such as MODFLOW 6. models.

3.1 TOUGH2Viewer MODFLOW grid visualization and grid blocks properties editing

A detailed explanation about TOUGH2Viewer usage can be found in the TOUGH2Viewer Quick tutorial (https://site.unibo.it/softwaredicam/en/software/tough2viewer).

In this manual only dedicated MODFLOW functionalities are described.

3.1.1 TOUGH2Viewer MODFLOW GUI Input files

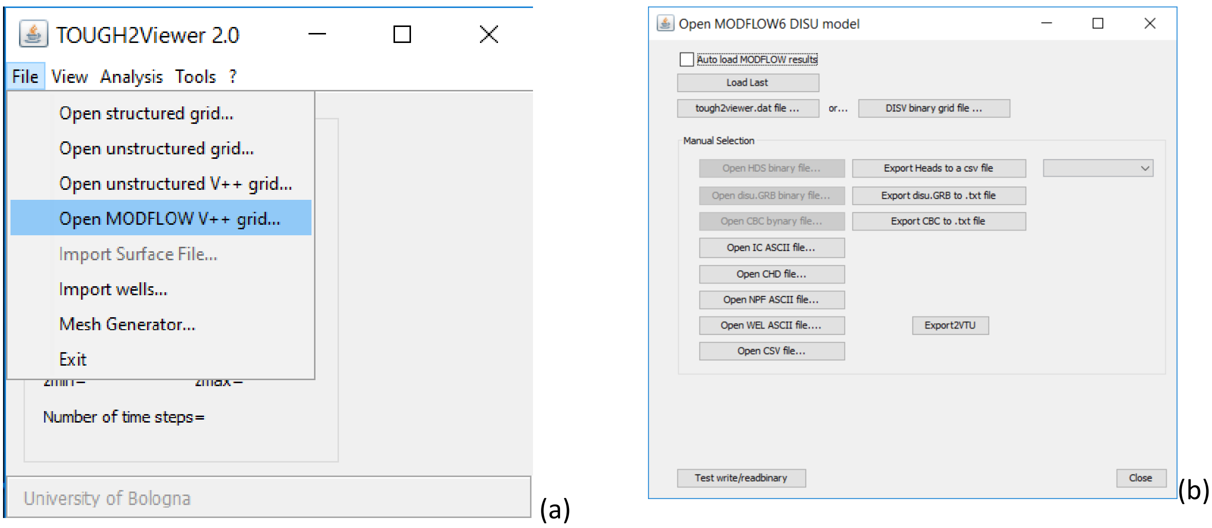

Figure 1 – (a) TOUGH2Viewer File Menu; (b) MODFLOW input file selector GUI

A dedicated GUI for MODFLOW file selection (Figure 1.b) can be activated by selecting the **MODFLOW V++ grid …** from the **File** menu item (Figure 1.a).

[5] https://www.usgs.gov/software/modelmuse-a-graphical-user-interface-groundwater-models [last access 04/02/2021]

From one of the example files, tThe first file that must be loaded is the tough2viewer.dat file by clicking the tough2viewer.dat file button.

Once the tough2viewer.dat file has been loaded, the HDS (heads) GUI button becomes active (Figure 1(b)) and the user can select the file containing the computed heads in binary format. After HDS file loading, the disu.GRB (the grid file in binary format) button becomes active and the .GRB file can be loaded. The user can iteratively load the remaining files of the simulation performed. Alternatively, is possible to check the Auto Load MODFLOW results for automated loading. Optionally, a CSV file can be loaded in order to import a set of custom variables. The custom variables can be used to create MODFLOW model input file for simulation purposes, like block permeability, initial condition, etc. …

3.1.2 TOUGH2Viewer MODFLOW results visualization

Like for TOUGH models, TOUGH2Viewer allows for a 3D visualization of the MODFLOW numerical model.

By selecting the **View->3D Block model** menu item, a dialog box will display the numerical model, as shown in the example displayed in Figure 2. The dialog box allows selecting the variable to be displayed among the loaded ones. In figure 2, visualisation of one ofthe examples from chapter 4 (02_100_CVT_Voronoi) is presented. In this Figure 2 the available variables, after file loading, are:

- Head
- Ic
- Icelltype
- K
- K22
- K33
- Angle1
- Angle2
- Angle3
- Wetdry

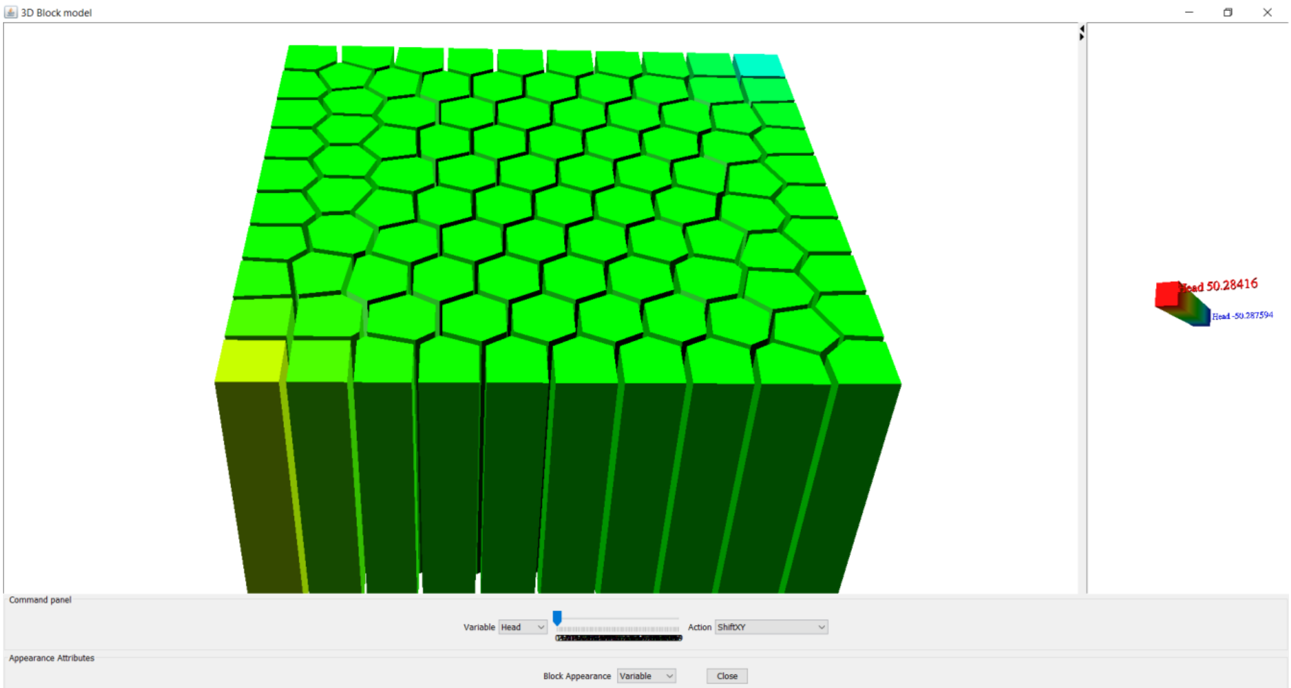

Figure 2 – 3D Block model Dialog Box.

Each of these variables can be visualised after selected from the Variable menu, as shown in Figure 2 (bottom).

3.1.3 TOUGH2Viewer input file editing/generation

MODFLOW input file includes a set of variables for numerical model specification. A dedicated GUI allows editing/modifying/generating the user defined set of variables.

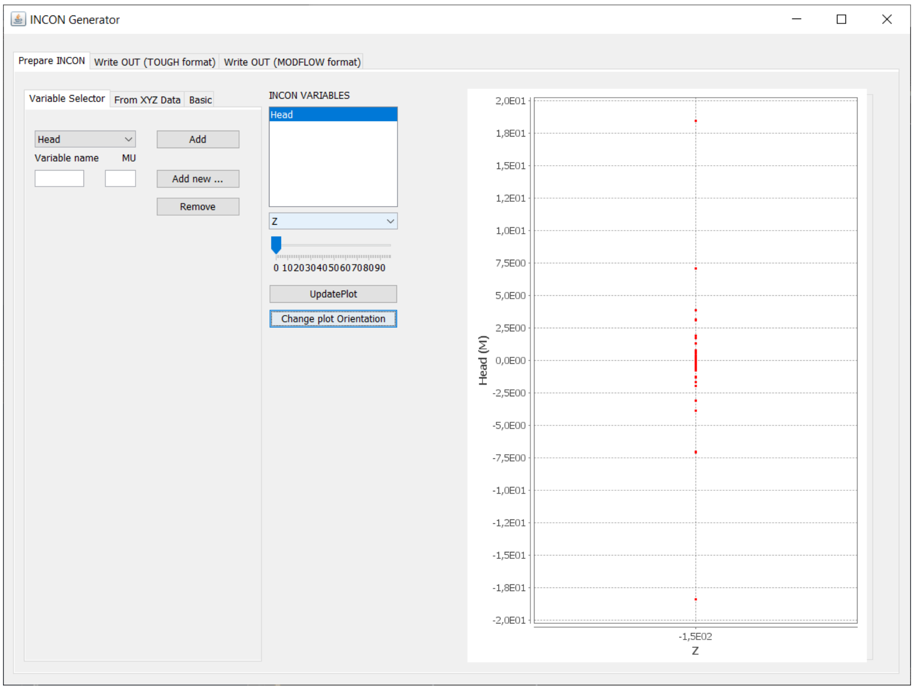

Figure 3 – INCON generator GUI for parameter editing

The Figure 3 shows the INCON generator window to set the initial conditions. The new values can be applied to all blocks, to only selected blocks or just to blocks of a certain “sub domain”, characterized by the same type of rock . From the variable dropdown list selector, the variable to be modified can be selected or new variables can be added.

On the right side of the window, a plot of the variable versus x, y, or z can be visualized by clicking the **UpdatePlot** button. In the example of Figure 3, the “ic” variable is plotted.

The values of a variable can be assigned basically in two different ways listed below.

The first one uses the Inverse Distance Weighted (IDW) method on the data inputted from a CSV file, which contains information about, see Figure 4.

The CSV file must contain at least 4 columns. 3 variables are reserved to the node coordinates for each block, see Figure 4 (buttons on(x, y, z). The others are the top).variables to be used for the variables assignation/creation. The IDW (Inverse Distance Weighted method) options allow the user to use all the coordinates or just use the selected ones, the maximum number of points to be used in the interpolation. The dropdown menu allow to select the column containing the different coordinate (one the file has been loaded, the “Item 1” dropdown list will contain the column name of the loaded CSV file.

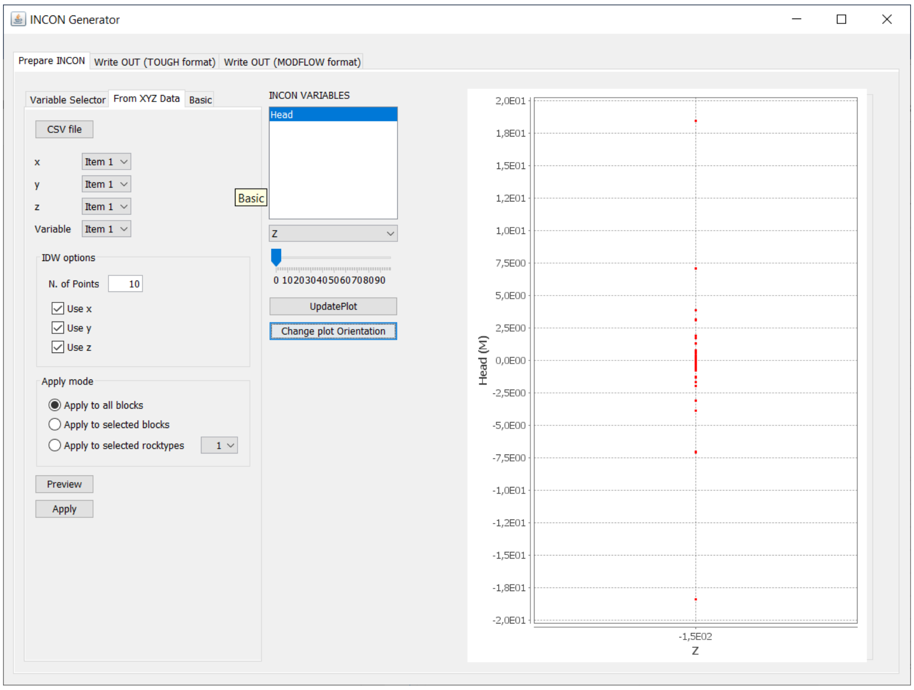

Figure 4 – XYZ data interpolator.

The second method of variable editing (**basis tab**) uses a linear combination defined as:

variable=a*x+b*y+c*z+Costconstant

where Cost is a constant (increment).

The user must specify the coefficient of the linear equation a, b, c, and the constant (see Figure 5).

The button **ChangePlot Orientation** allow changing the layout of the preview plot.

The **C and Const** panel allow to compute the C and the CONST value of the ax+by+cz+CONST=0 equation passing from 2 points, z1 and z2.

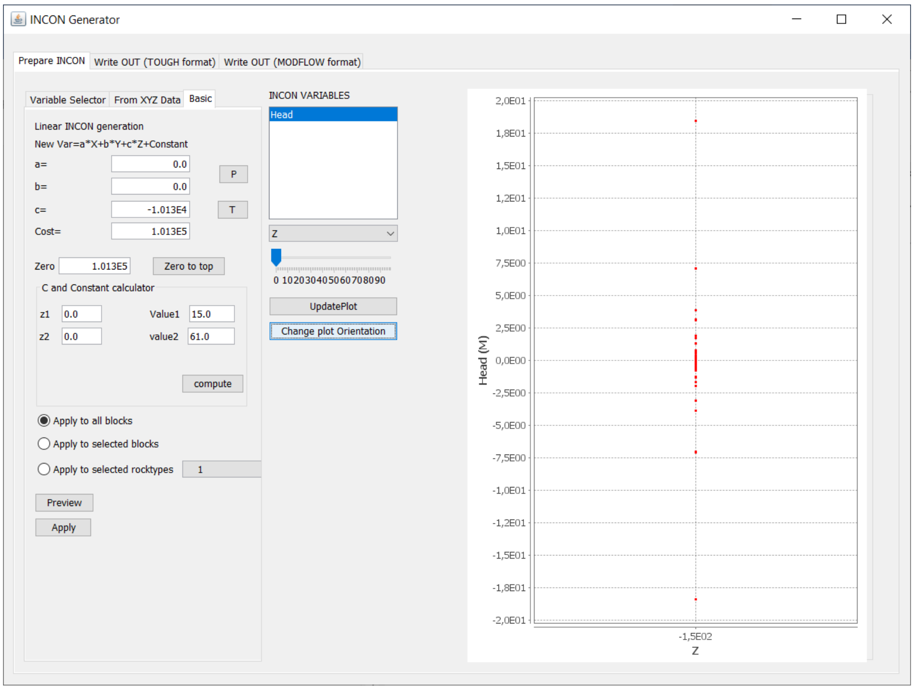

Figure 5 – INCON generator windows for using the linear xyz function.

The **write OUT MODFLOW** tab (Figure 6 and Figure 7) allows exporting the values of the variables in the two classical file format of MODFLOW: table data or <node> <variable> data format.

In Figure 6 , the exporting preview of the ic edited variable is shown, using the table format, while in Figure 7 is shown a preview of *by node* exporting capabilities.

The user can specify if type of the variable to be exported is INTEGER or DOUBLE. Depending on the variable type, the user can specify also the IPRN variable format (refer to the MODFLOW 6 – Description of Input and Output[6] for further details).

The preview content of the variable can be exported by saving it as a text file or just by the classical copy and paste native command of the operative system.

Note that the header, containing the directives of simulation print out, can be modified manually by the user.

It is worth to mention that in some cases, the variable value should not benot be assigned to all blocks. For example, the *.well files usually contain just the blocks nodes in which the well flow rate is specified, while the remaining blocks implicitly are assumed by MODFLOW for ato have the flow rate equal to zero. To undefined blocks, TOUGH2viewer assigns a default value of -1.0E10.

To avoid the printing of these meaningless values, the user can specify a threshold value to avoid the presence of non- valid values in the output file (for example by setting the default threshold value =-1000).

[6] https://water.usgs.gov/ogw/modflow/mf6io.pdf

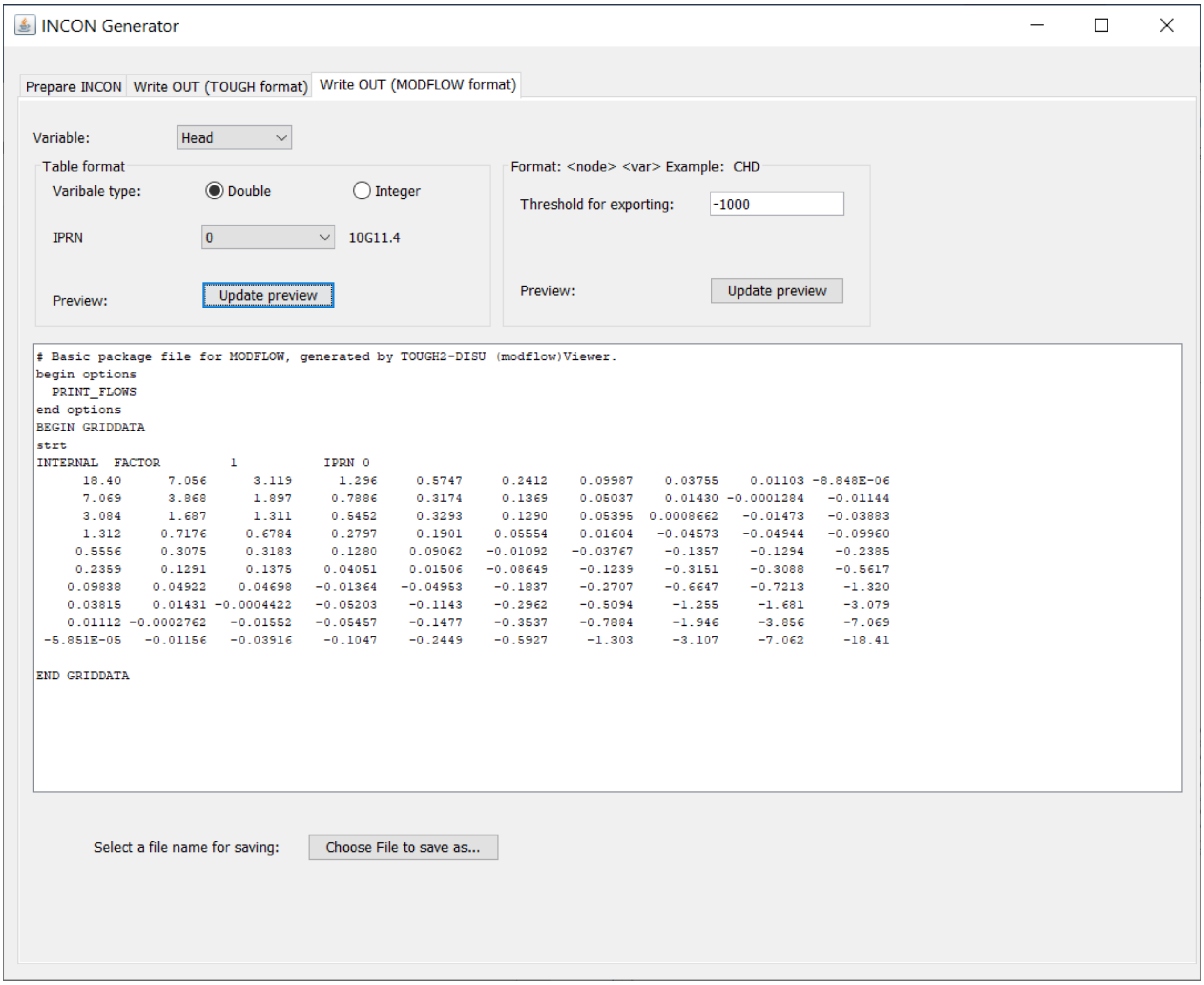

Figure 6 – "Table format" exporting preview.

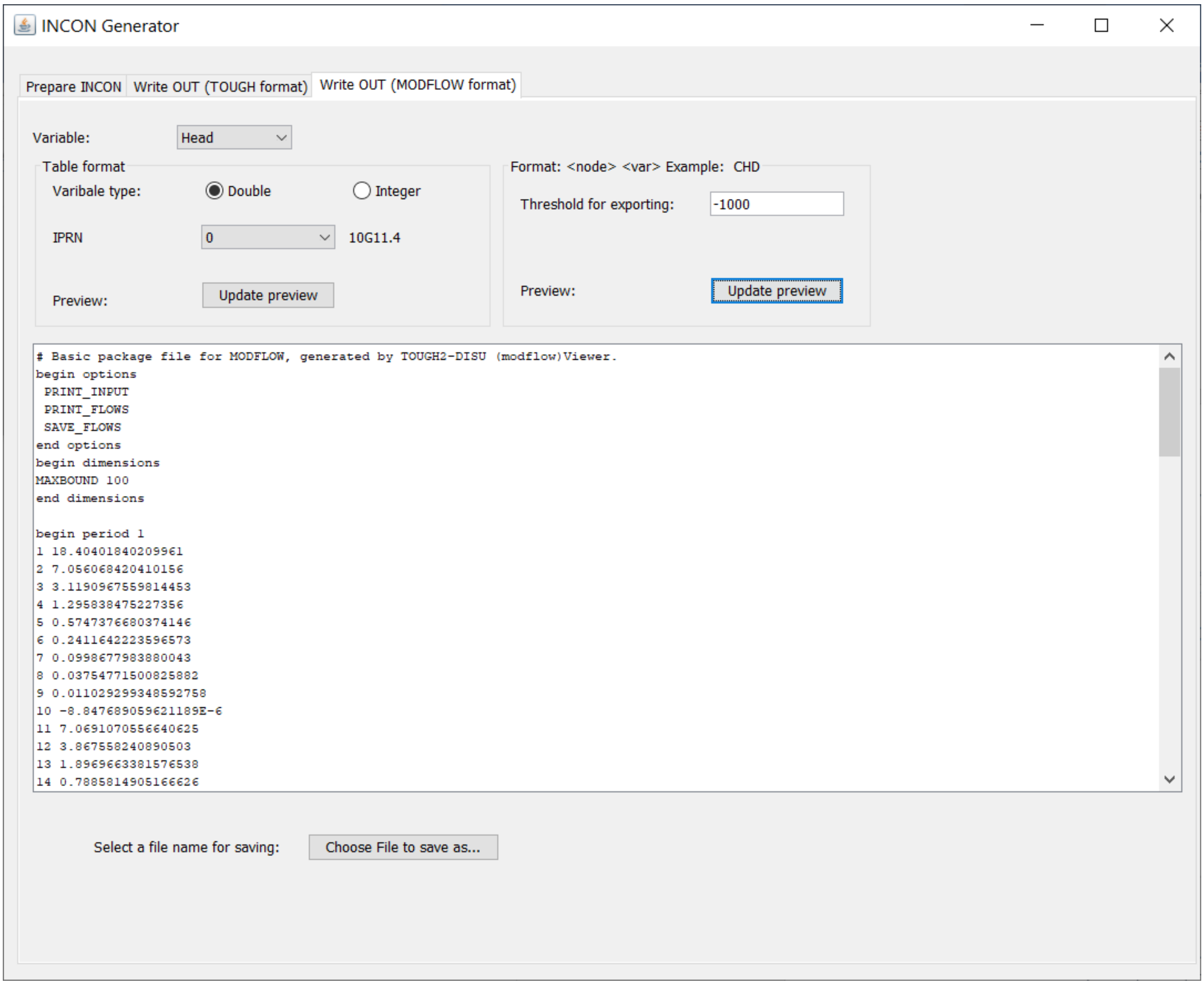

Figure 7 – "by node" exporting preview.

3.2 TOUGH2Viewer Results exporting

3.2.1 Paraview file exporting

Among the several functionalities of TOUGH2Viewer, it is worth mentioning the Export to Paraview capability. After the model has been loaded in TOUGH2Viewer (and/or csv file reading, variable editing, etc.), the model can be exported into a convenient format, like a vtu PARAVIEW file format (Figure 8).

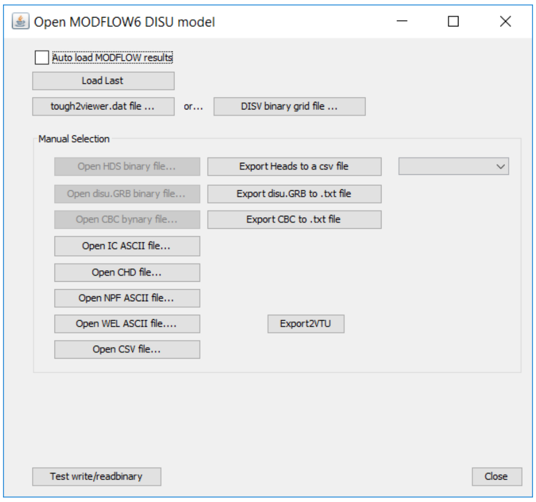

Figure 8 – Export2VTU button to export the MODFLOW model in a vtu format.

The exporting function allows generating a VTU file for each time step. Optionally, by the dropdown menu, it is possible to select and export only one of the listed time steps. Exported file contains all the variable data loaded and, if loaded, the csv data imported. Figure 9 shows an example of a MODFLOW model exported by TOUGH2Viewer and displayed with Paraview.

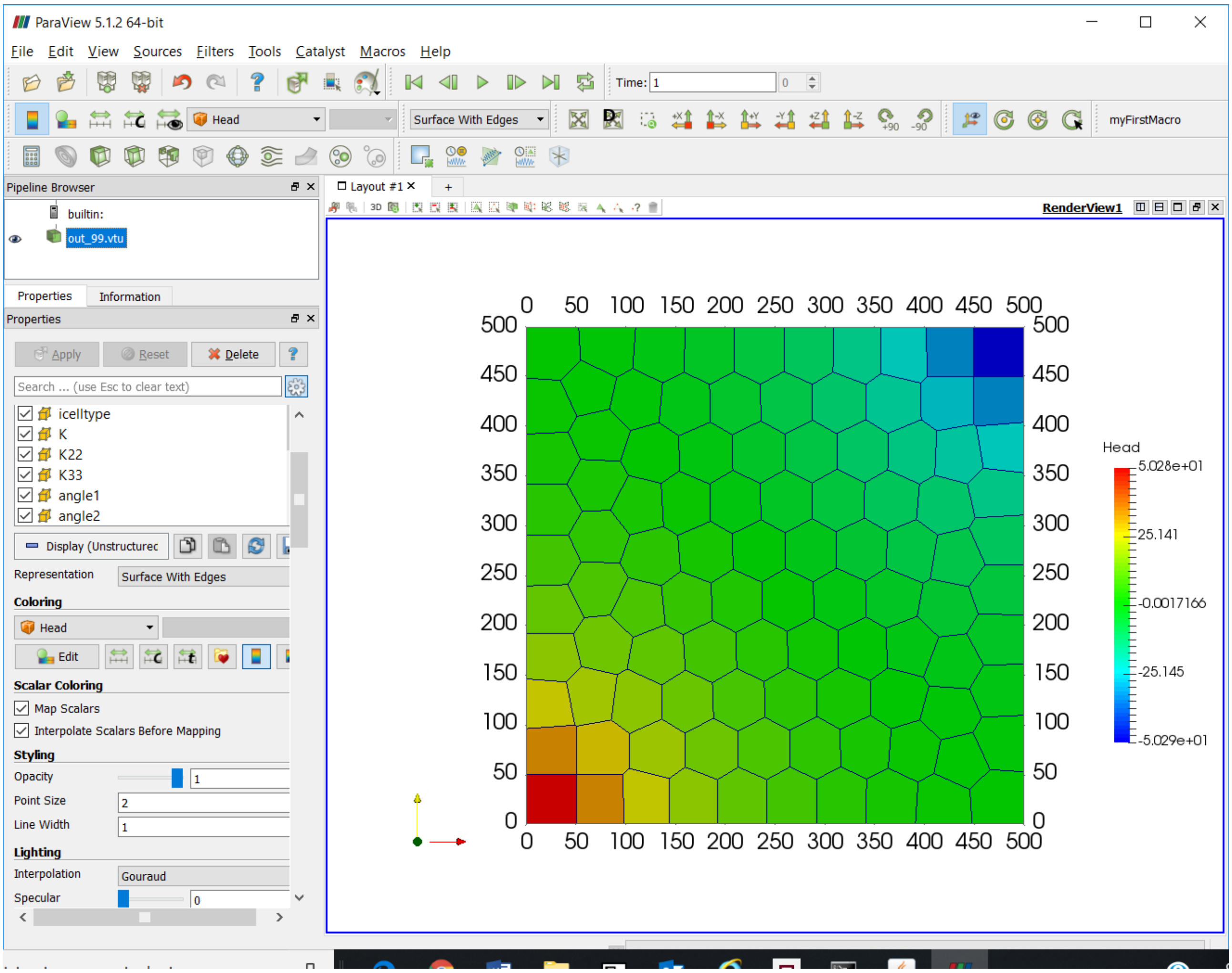

Figure 9 – A Modflow model exported by TOUGH2Viewer and displayed with Paraview.

3.2.2 CSV file exporting

Some of the MODFLOW 6 output files are available only in binary format. TOUGH2Viewer allows ASCII file exporting (txt and csv) of the loaded files in a convenient format that can be used for data analysis and interpretation of the results by using other software.

MODFLOW 6 files that can be converted from binary to ASCII format are: HDS, GRB, and CBC files.

4 Example Tutorials

In this chapter, a number of example tutorials aretutorials are explained to allow new users of VORO2MESH and TOUGH2Viewer to learn how to generate the input files for a MODFLOW simulation and how to visualize the simulation results. Before starting with the tutorial examples, make sure you have downloaded TOUGHT2Viewer version for MODFLOW visualisation with examples and VORO2MESH from DICAM SOFTWARE site (links for download are in Introduction Chapter), MODFLOW 6. and ModelMuse (links for download are in the chapter below)

For MODFLOW input/output file format, the user can refer to the MODFLOW user guide.

Finally, a basic set of instructions will be given to visualize these files in PARAVIEW.

4.1 MODFLOW installation

Download and install MODFLOW 6 from https://www.usgs.gov/software/modflow-6-usgs-modular-hydrologic-model, and Model Muse https://www.usgs.gov/software/modelmuse-a-graphical-user-interface-groundwater-models [last accessed 15th of December, 2020] Dowloaded MODFLOW 6 should contain several folders:

- bin
- doc
- examples
- make
- msvs
- src
- srcbmi
- utils.

Move downloaded zip file to a desired folder like “D:\” and extract the zipped files.

After zip extraction, navigate the folder tree and located the example folder.

4.2 Examples installation

The zip file containing the example folder can be downloaded from the following link:

VORO2MESH and TOUGH2Viewer tool set for MODFLOW link: [https://site.unibo.it/softwaredicam/en/voro2mesh-and-tough2viewer-for-unstructured-voronoi-modflow-grids/darcy.zip/@@download/file/ VORO_T2V_MODFLOW_Examples.zip]

Download and extract the VORO_T2V_Examples.zip file. The uncompressed folder “VORO_T2V_Examples”.

We suggest of copying/move the VORO_T2V_MODFLOW_Examples folder from the TOUGH2Version for MODFLOW in to the example folder of downloaded MODFLOW 6 sofware. Otherwise, it is necessary to properly set the executable folder path of the OS environmental variables.

The examples refer to a numerical simulationsnumerical simulation of two problems: (i) Darcy flow; (ii) Five Spot flow.

4.3 Darcy problem conceptual model

The Darcy problem is a simple simulation of a Darcy flow in a square domain of 700 x 700 x 100 m^3, with homogeneous permeability and steady state flow.

The Darcy flow is obtained by setting a constant head at the left and right borders of the domain:

The most left grid block head=1 m;

The most right grid block head=0;

The initial head conditions of the remaining grid blocks are set to zero meters.

The model is simulated by using two grids:

- 01_DARCY_DISV

- 02_DARCY_VORONOI

4.3.1 01_DARCY_DISV

The numerical model is the same of the **ex06-mfusg1disv** MODFLOW example folder. To start the MODFLOW simulation, user must use the "run.bat" file that is present in the same folder. (please check if the directory which batch file opens is mf6.exe file, otherwise it can be easily changed by right click on the run.bat file – select 'edit' and manually insert the location of mf6.exe file – for example: E:\mf6.2.0\bin\mf6.exe)

4.3.1.1 TOUGH2Viewer visualization

After simulation run is terminated, results can be visualized in TOUGH2Viewer by loading the file as shown in Table 4.

Run TOUGH2Viewer by double clicking on the run4186.bat command file from, located in to the "dist" folder of TOUGH2Viewer folder.(refer to the TOUGH2Viewer[7] user manual for details).

Command button	File to select
DISV binary grid file …	flow.disv.grb
Open HDS binary file …	flow.hds
Open CBC binary file …	Flow.cbc
Open IC ASCII file …	flow.ic
Open CHD file …	flow.chd
Open NPF file …	flow.npf

Table 4 – Command button and the list of files to be selected for the visualization of the 01_DARCY_DISV simulation results with TOUGH2Viewer..

After files loading, the results visualization is generated by selecting the **View->3D Block Model** menu item command as shown in Figure 10.

[7] https://site.unibo.it/softwaredicam/en/software/tough2viewer

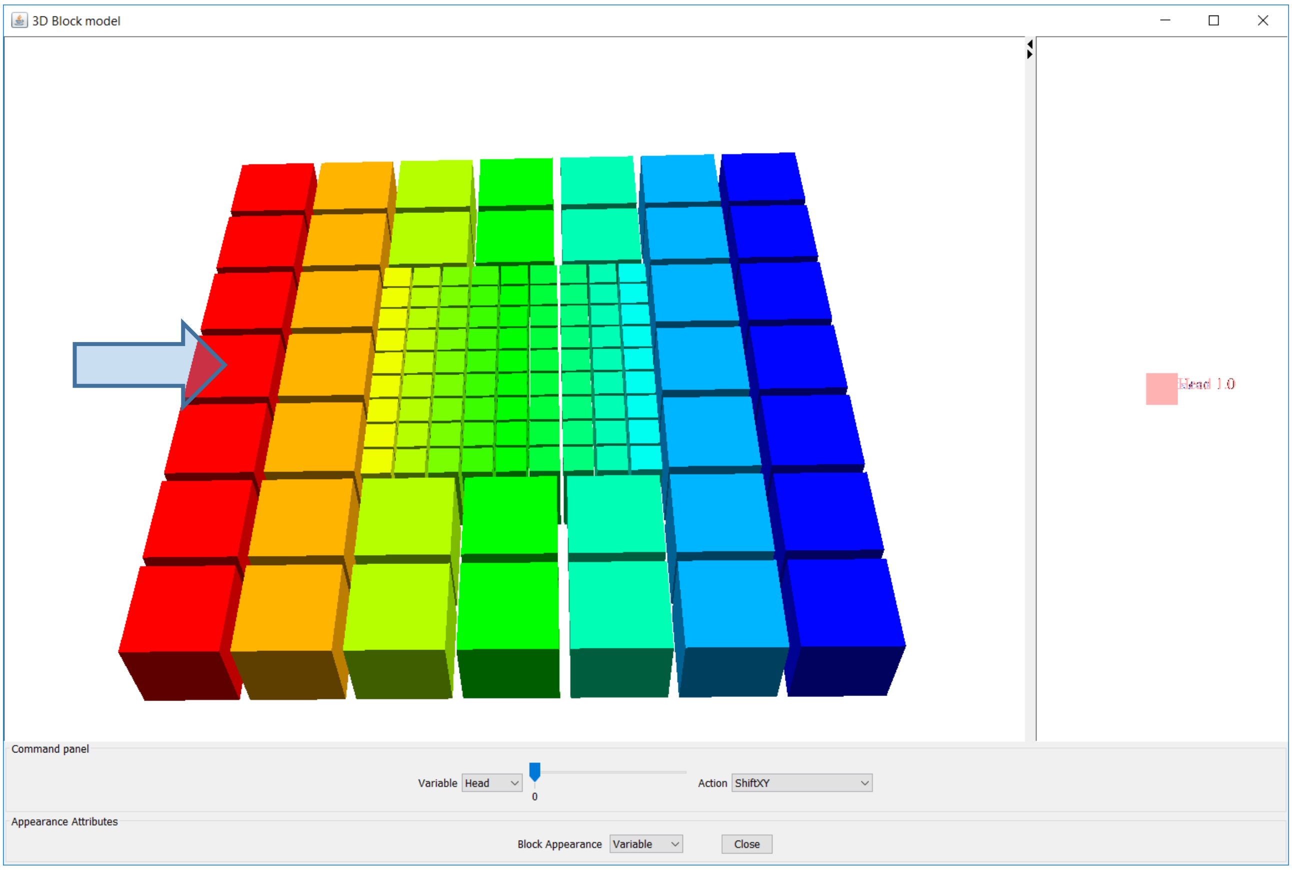

Figure 10 – 3D model visualization of the Darcy DISV simulation. The arrow indicates the block to be selected using the Get2Plot function to obtain the plot of Figure 11

From the Action menu, the user can select the Get2DPlot to obtain a horizontal profile of the desired variable (the Head along the x direction in this example). By selecting the middle block of the most left columns of the model, as shown in Figure 10, a 2D plot is generated, as shown in Figure 11. The plot shows the Head computed variable versus the x direction. As expected, the head varies linearly from head=1 m (x=50 m) to head=0 m (x=650 m).

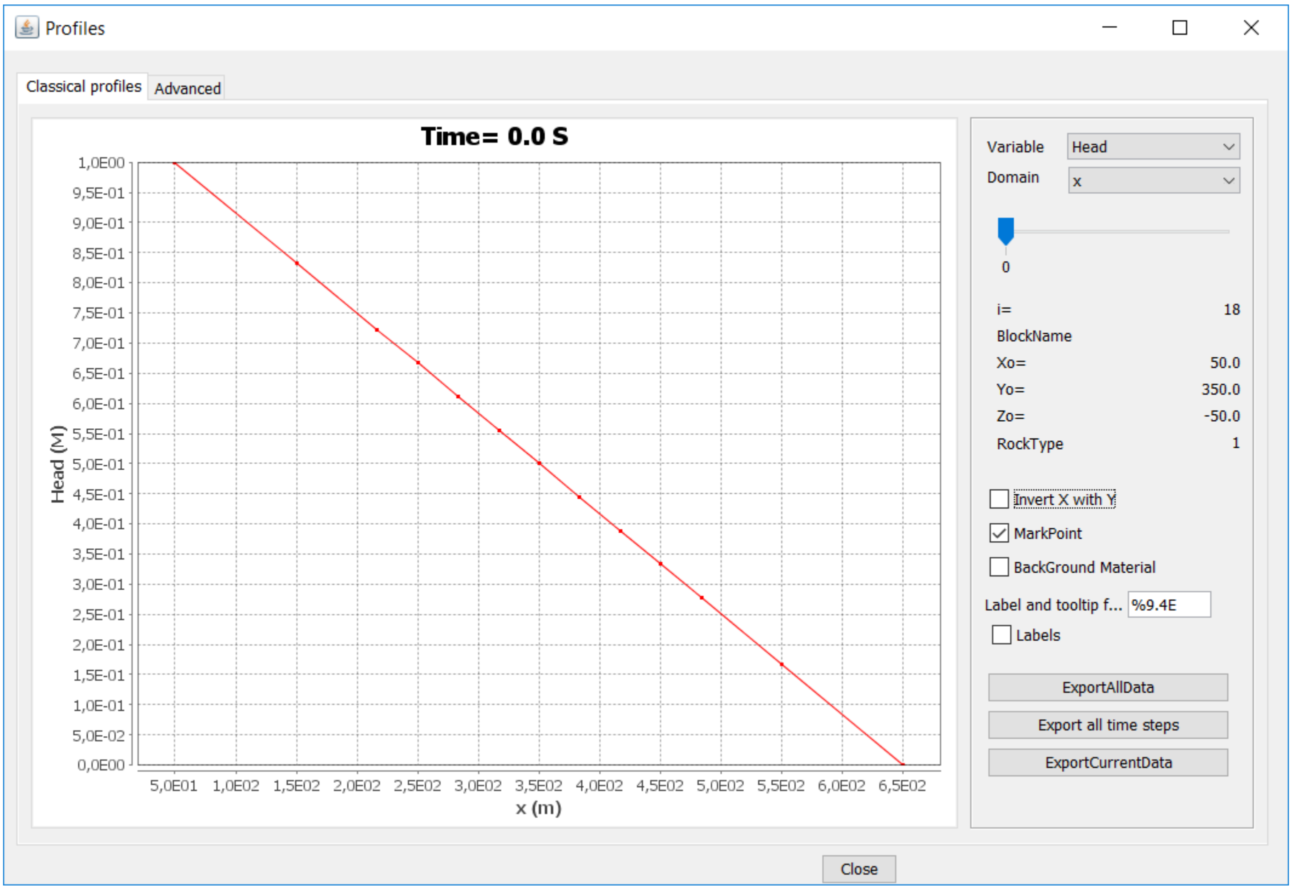

Figure 11 – Head profile in the x direction.

4.3.2 02_DARCY_VORONOI

In this example, Darcy problem is solved by using a Voronoi grid. Using the same node coordinates of the previous problem, a new grid has been generated by using VORO2MESH.

4.3.2.1 VORONOI Grid generation

In the VORO2EMSH subfolder of the 02_DARCY_VORONOI folder, the following files are present:

- voro.par
- in.dat

open a terminal and at the command prompt type VORO2MESH [enter].

A set of files will be generated by VORO2MESH, as specified in the chapter 2.3.

Copy the following files into the one level up folder (do not rename these files):

1. flow.disu;
2. flow.disu.area.dat;
3. flow.disu.bottom.dat;
4. flow.disu.top.dat;
5. flow.disu.cl12.dat;
6. flow.disu.hwva.dat;

- flow.disu.ihc.dat;
- flow.disu.ja.dat;

- tough2viewer.dat

Run the MODFLOW simulation by using the "run.bat" file. After the MODFLOW simulation run is terminated, TOUGH2Viewer is used to visualize simulation results.

4.3.2.2 TOUGH2Viewer visualization

The files to be load in TOUGH2Viewer are summarized in Table 5.

Command button	File to select
tough2viewer.dat file …	tough2viewer.dat
Open HDS binary file …	flow.hds
Open disu.GRB binary file …	flow.disv.grb
Open CBC binary file …	Flow.cbc
Open IC ASCII file …	flow.ic
Open CHD file …	flow.chd
Open NPF file …	flow.npf

Table 5 - Command button and the list of files for the 02_DARCY_VORONOI model visualization.

By selecting the **View->3D Block Model**, the visualization of the MODFLOW simulation results is displayed (see Figure 12).

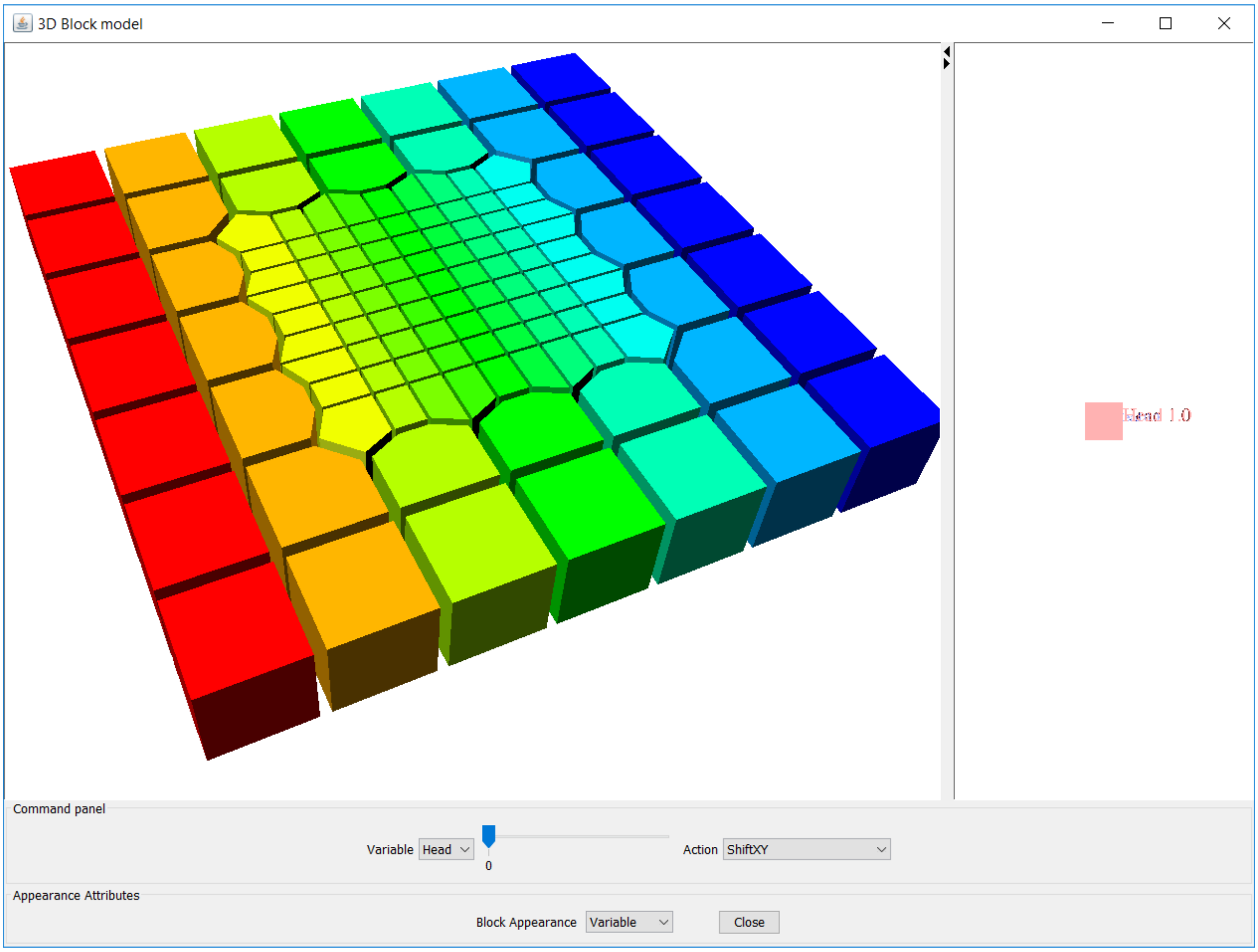

Figure 12 – 3D block model visualization of the 02_Darcy Voronoi grid simulation results.

As in the previous example, from the dropdown variable dropdown menu it is possible to visualize the other variables and obtain 2D plots of the variables versus the x and y direction.

4.4 5 spot problem examples

4.4.1 Conceptual model

All the following examples refer to the same conceptual model. The model reproduces the classical five spot problem. The five spot problem is a production/injection scheme in a confined aquifer. The production/injector wells are located at the nodes of a staggered infinite grid, as shown in Figure 13.

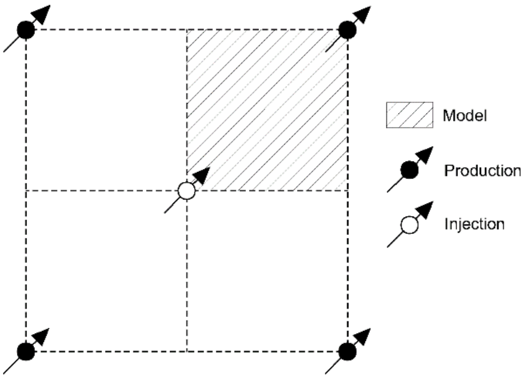

Figure 13 – Conceptual model of the 5 spot problem.

The dimension of the numerical model areis 500x500 m^2, aquifer thickness 300 m, hydraulic conductivityk=1.0E-004 m/s, storage SS=1. 0E-005 (m^{-1}), specific yield SY=2. 0E-002 m^2).

4.4.2 General instructions for grid generation

For each Voronoi example in the 03_MODFLOW_EXAMPLES\FIVE_SPOT folder, there is a VORO2MESH subfolder, except for the quadtree grid generated by ModelMuse. In the VORO2EMSH subfolder are present the following files:

- voro.par
- in.dat

open a terminal and at the command prompt, type VORO2MESH [enter].

A set of files will be generated by VORO2MESH, as specified in the chapter 2.3.

Copy the following files into the one level up folder (do not rename these files):

7. flow.disu;
8. flow.disu.area.dat;
9. flow.disu.bottom.dat;
10. flow.disu.top.dat;
11. flow.disu.cl12.dat;
12. flow.disu.hwva.dat;

- flow.disu.ihc.dat;
- flow.disu.ja.dat;
- tough2viewer.dat

The example folder containcontains now all files needed for a MODFLOW simulation run.

4.4.3 MODFLOW simulation run

The simulation run can be obtained by launching the batch file "run.bat" or by typing run.bat from the command prompt.

After MODFLOW simulation run is terminated, the MODFLOW output files will be present in the same folder.

4.4.4 TOUGH2Viewer results visualization

Run TOUGH2Viewer by double clicking on the run4186.bat command file from, located in to the “dist” folder of TOUGH2Viewer folder(refer to the TOUGH2Viewer[8] user manual for detail).

By the **File** menu item navigate and select **MODFLOW6 V++ grid …** (Figure 1.a). Click the **TOUGH2Viewer.dat file …** button and select the tough2viewer.dat file where you have located the example folder.

Continue loading files by clicking the buttons that are progressively activated (HDS or BHD, disu.GRB, CBC, IC etc. …).

After files loading, you can also export the file to Paraview by clicking the **Export2VTU** command button. As the simulations contain 100 times steps, we suggest to just the export the last time step using the dropdown menu.

You can now explore the simulation results by selecting the **View->3D block model** command.

For a more detailed explanation about the TOUGH2Viewer functionalities, users are demanded/recommended to refer to the TOUGH2Viewer quick guide downloadable from http://softare.dicam.unibo.it/tough2viewer.

4.4.5 01_10x10_STRUCTURED

After loading the files needed for visualization (see the 3.1.1 Paragraph), by selecting the **View->3D Block Model** menu item command button, the model will be visualized as shown in Figure 14

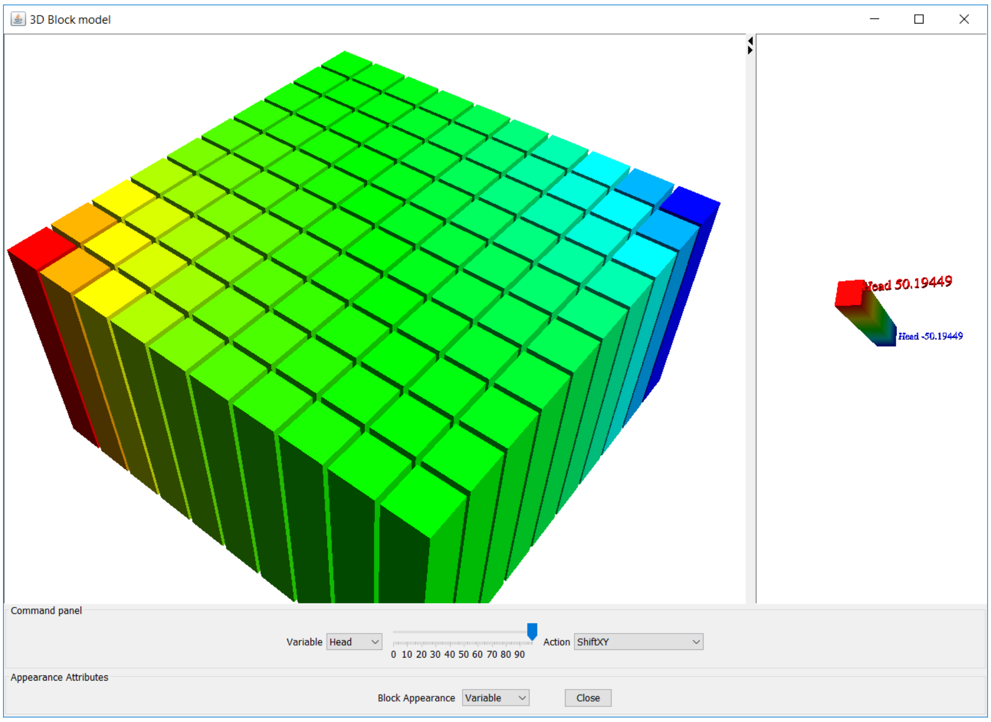

Figure 14 – 01_10x10_Structured model visualization 3D Block Model visualization.

[8] https://site.unibo.it/softwaredicam/en/software/tough2viewer

Information of a block can be obtained by selecting the **QuickInfo** item from the dropdown Action and pick a block by double clicking on it.

In figure 15 a profile of the Head of the block named “11” vs time is shown. As previously described, the profile is obtained using the “Get2DPlot” functionality.

The user can also obtain a 3D Flow visualization by using the **View->3D Flow Vector visualization** as shown in the Figure 16**.**

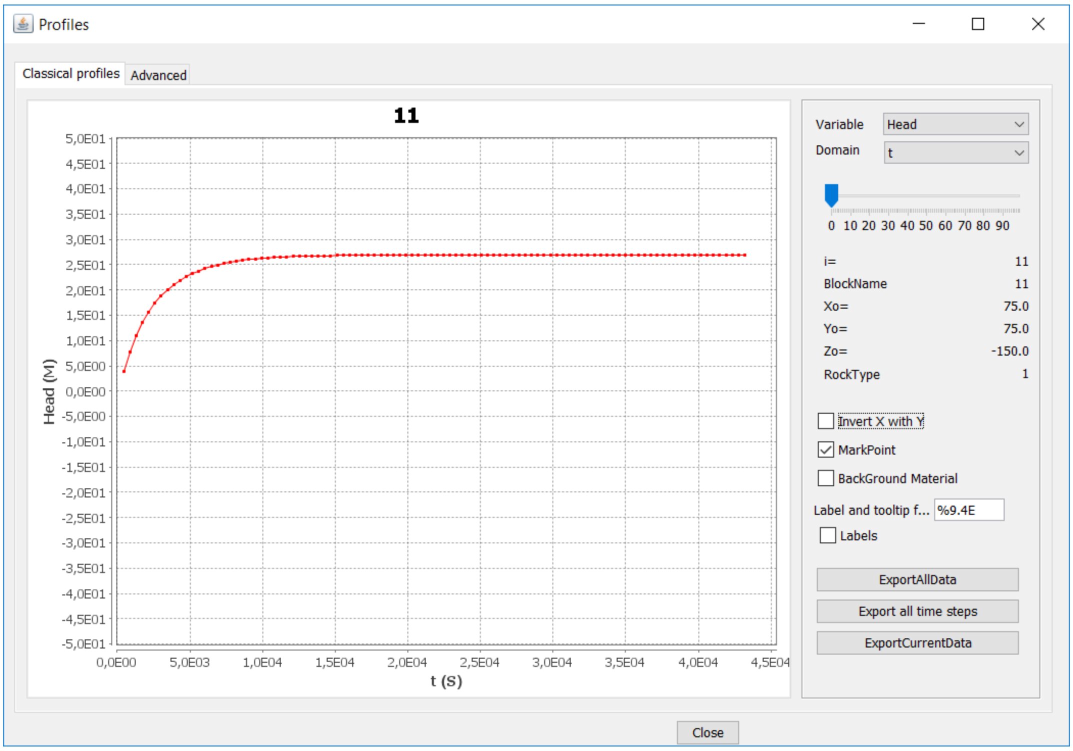

Figure 15 –Head vs time plot. The plot is obtained by using the Get2DPlot item of the dropdown Action menu and by double clicking the “11” block.

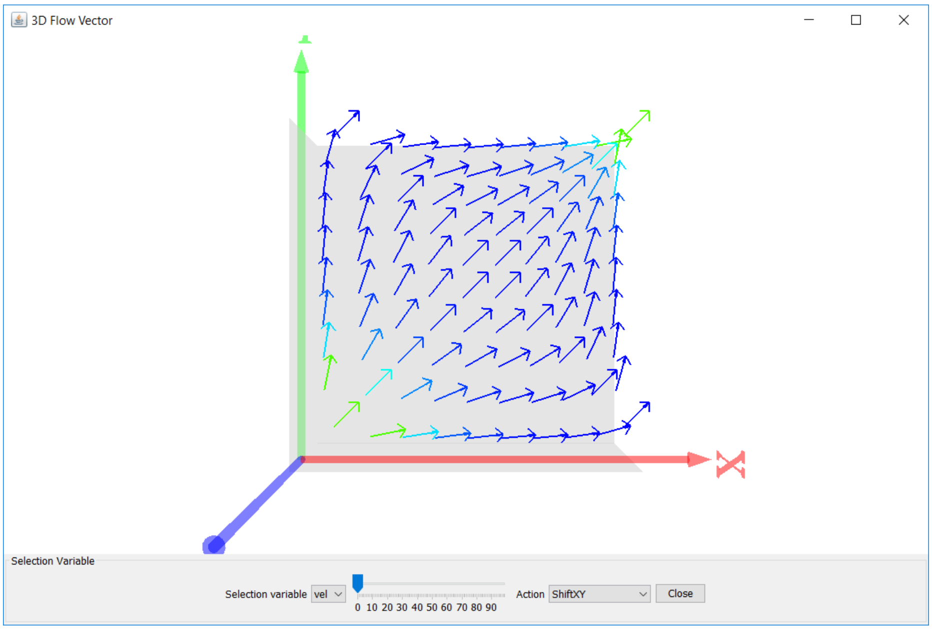

Figure 16 – 3D Flow vector visualization.

4.4.6 02_100_CVT_VORONOI

In this example, a CVT VORONOI grid has been built by VORO2MESH.

As in the previous example, after files loading the model will be show as in Figure 17

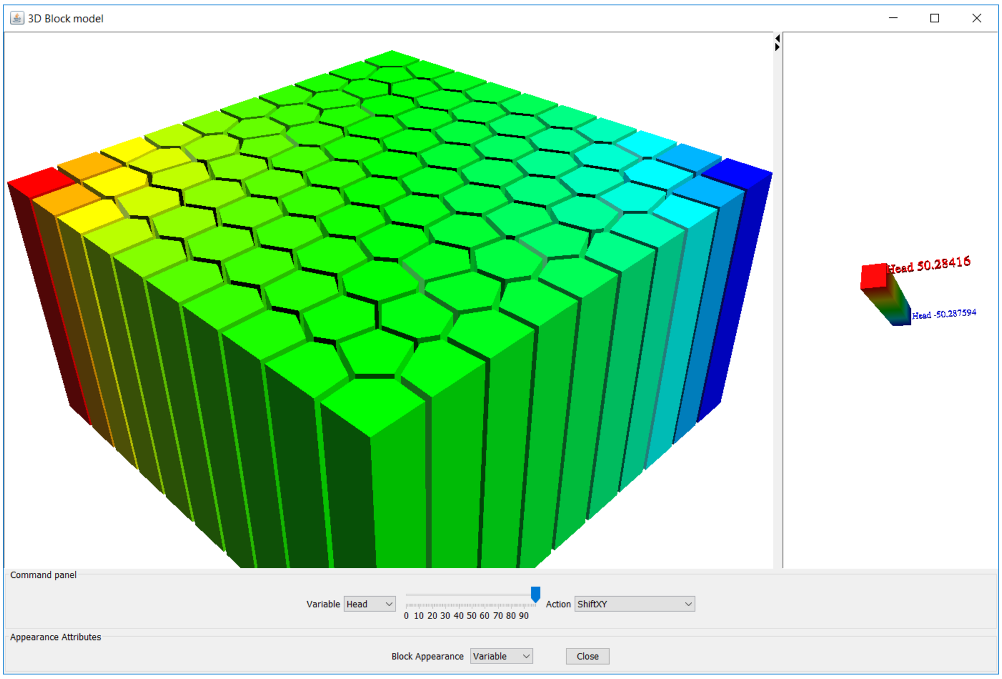

Figure 17 - 02_100_CVT_VORONOI 3D Model visualization

As in the previous example, the 3D Flow Vector and 2D plots can be visualized.

4.4.7 03_QUADTREE_14902_WELLS_REFINED

This example has been created by using the ModelMuse GUI for MODFLOW.

Open the project file 03_QUADTREE_14902_WELLS_REFINED.gpt with ModelMuse, it is enough to double click on it if you have downloaded the ModelMuse. After the model is loaded in ModelMuse, run the simulation by selecting the gree 'run' bottun from the toolbar. After the simulation is terminated, results can be visualized with TOUGH2Viewer and can be exported in vtu files for a Paraview visualization.

In this caseTo visualize the results in TOUGH2Viewer, open TOUGH2 viewer by running run4186.bat file from TOUGH2Viewer folder, the files to be load in to thechoose **Input MODFLOW6 V++ grid** and files to be loded are… dialog box are:

- 03_QUADTREE_14902_WELLS_REFINED.disv.grb
- 03_QUADTREE_14902_WELLS_REFINED.bhd
- 03_QUADTREE_14902_WELLS_REFINED.cbc
- 03_QUADTREE_14902_WELLS_REFINED.ic
- 03_QUADTREE_14902_WELLS_REFINED.npf
- 03_QUADTREE_14902_WELLS_REFINED.wel

By using the **DISV binary grid file…** command button, select the file:

03_QUADTREE_14902_WELLS_REFINED.disv.grb.

Load the remaining file by using the other file command buttons.

Using the dropdown list time step selector, select the last time step (in order to avoid generating 100 files), and then press **Export2VTU** button for a Paraview file exportation. Load the vtu file model to Paraview. Select the “head” variable and the apply button. The model will be shown as in Figure 18.

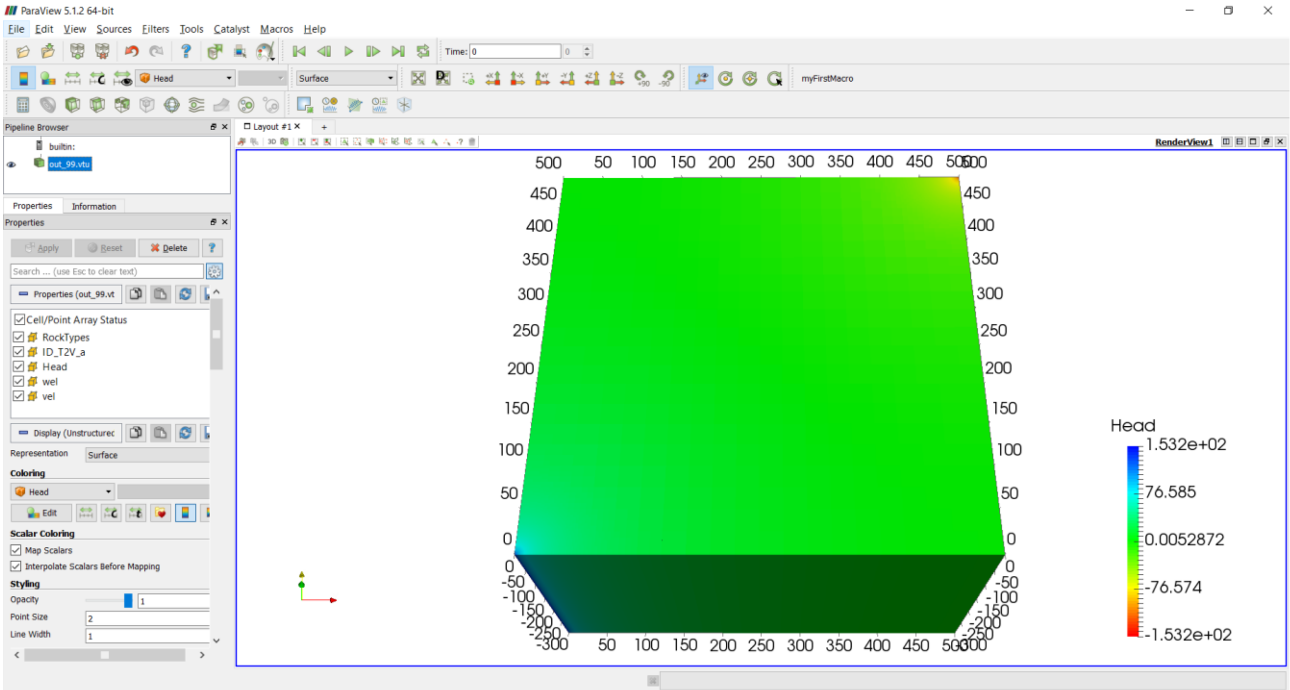

Figure 18 - 03_QUADTREE_14902_WELLS_REFINED 3D “Head” visualization.

4.4.8 04_VORONOI_WELLS_REFINED

The grid of this example has been generated by VORO2MESH. The grid node has been obtained using a Weighted CVT approach implemented in VORO2MESH.

The folder contains all the files needed for a MODFLOW simulation run. Double click on the “run.bat” batch file to run the MODFLOW simulation.

After the MODFLOW simulation RUN is completed, the user can load the simulation results files in TOUGH2Viewer. Model visualisation MODFLOW results will be displayed as showed in Figure 19 (Head).

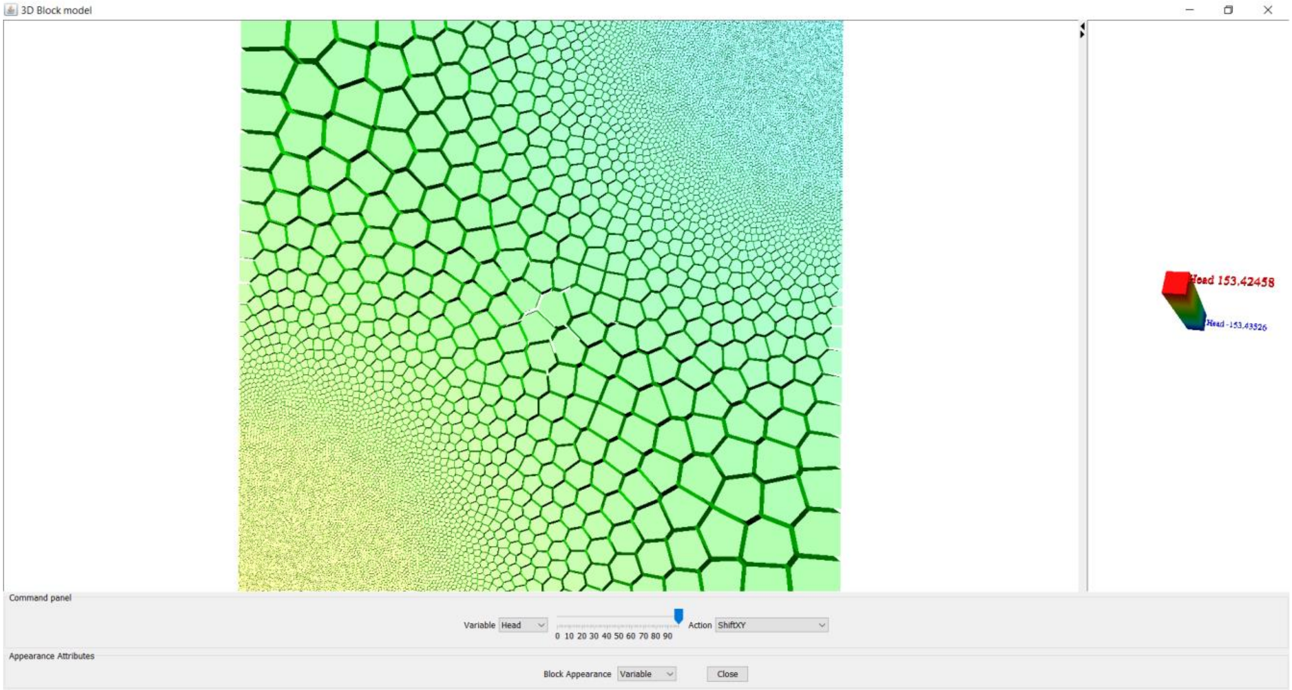

Figure 19 - 04_VORONOI_WELLS_REFINED 3D Block Model visualization.

4.4.9 05_QUADTREE_41422_WELLS_A

The 05_QUADTREE_41422_WELLS_A is a quadtree grid obtained using ModelMuse. The project file is named 05_QUADTREE_41422_WELLS_AND_LINE_REFINED.gpt. Like in the previous case case (4.4.7 03_QUADTREE_14902_WELLS_REFINED), user can visualize simulation results by using TOUGH2Viewer and loading the DISV GRB grid and the other file as explained in the 4.3.2.2. In Figure 20, the model 05_QUADTREE_41422_WELLS_AND_LINE_REFINED is visualized by Paraview.

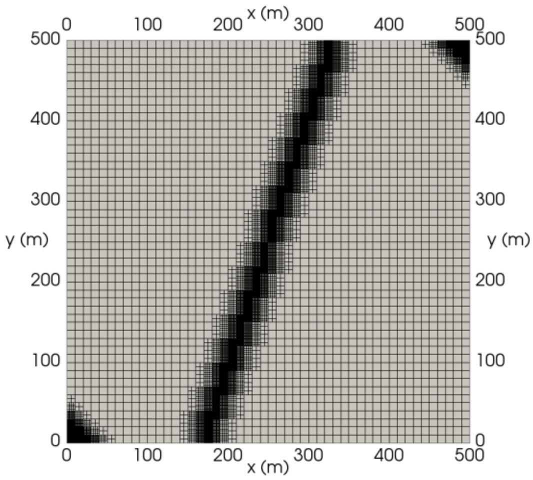

Figure 20 – 05_QUADTREE_41422_WELLS_A Paraview visualization

4.4.10 06_VORONOI_WELLS_AND_LINE_REFINED

The 06_VORONOI_WELLS_AND_LINE_REFINED grid is CVT grid obtained with VORO2MESH. The coordinates of the nodes have been generated using a weighted Lloyd algorithm (Lloyd, 1982) implemented in VORO2MESH. The voro2mesh folder contains coordinates of the nodes (in.dat file) seed points needed for the grid generation. Results can be visualized by using TOUGH2Viewer and/or Paraview.

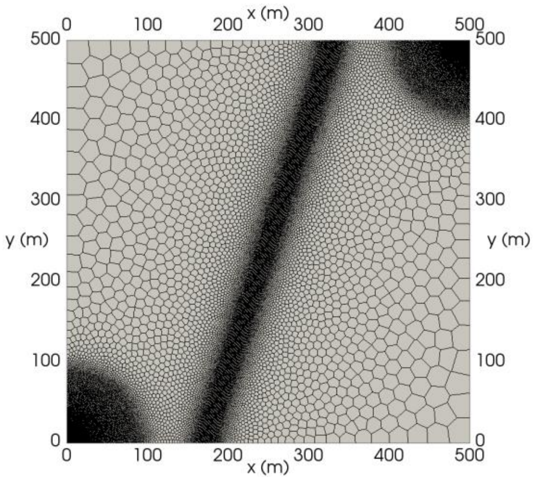

Figure 21 - 06_VORONOI_WELLS_AND_LINE_REFINED grid, Paraview visualization

5 References

Bonduà, S., Battistelli, A., Berry, P., Bortolotti, V., Consonni, A., Cormio, C., Geloni, C., Vasini, E.M., 2017. 3D Voronoi grid dedicated software for modeling gas migration in deep layered sedimentary formations with TOUGH2-TMGAS. Comput. Geosci. 108, 50–55. https://doi.org/https://doi.org/10.1016/j.cageo.2017.03.008

Bondua, S., Berry, P., Bortolotti, V., Cormio, C., 2012. TOUGH2Viewer: A post-processing tool for interactive 3D visualization of locally refined unstructured grids for TOUGH2. Comput. Geosci. 46, 107–118. https://doi.org/10.1016/j.cageo.2012.04.008

Bonduà, S., Bortolotti, V., 2020. TOUGH2Viewer 2.0: A multiplatform tool for fully 3D Voronoi TOUGH grids. SoftwareX 12, 100596. https://doi.org/https://doi.org/10.1016/j.softx.2020.100596

Lloyd, S.P., 1982. Least Squares Quantization in PCM. IEEE Trans. Inf. Theory 28, 129–137. https://doi.org/10.1109/TIT.1982.1056489

Tough2Viewer user manual

MODFLOW 6 manual

VORO2MESH manual.