



Original software publication

TOUGH2Viewer 2.0: A multiplatform tool for fully 3D Voronoi TOUGH grids

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ABSTRACT

The software TOUGH2Viewer 2.0, originally available since 2012, is an enhanced visualization software specifically designed to visualize the results of TOUGH simulations performed using structured and fully unstructured 3D Voronoi grids. 3D Voronoi grids permit a great degree of flexibility when accurate numerical simulations are required. The TOUGH family of simulators represents a set of software well-known worldwide for numerical modeling and simulation for coupled transport of water, vapor, non-condensable gas and heat in porous and fractured media. Nevertheless, TOUGH has no native enhanced pre- and post-processing tools, and several pre- and post-processing tools have been developed. Using TOUGH2Viewer the users can interactively navigate the model, a 3-dimensional virtual environment, by means of a Graphical User Interface (GUI). This new version of TOUGH2viewer allows the editing of numerical models by dedicated GUIs, adding pre-processing capabilities.

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Code metadata

Current code version	2.0
Permanent link to code/repository used of this code version	https://github.com/ElsevierSoftwareX/SOFTX_2019_384
Legal Code License	Apache License, Version 2.0
Code versioning system used	Git
Software code languages, tools, and services used	Java
Compilation requirements, operating environments & dependencies	NetBeans 8.1 IDE, Java JDK 1.8 or higher, Java3D, JFreeChart.
If available Link to developer documentation/manual	https://github.com/stebond/TOUGH2Viewer/blob/master/TutorialTOUGH2Viewer_ver.2.0.pdf
Support email for questions	stefano.bondua@unibo.it

Software metadata

Current software version	2.0
Permanent link to executables of this version	https://github.com/stebond/TOUGH2Viewer/blob/master/T2Viewer_v2.0.zip
Legal Software License	Apache License, Version 2.0
Computing platforms/Operating Systems	iOS, Linux, OS X, Microsoft Windows, Unix-like and any operative system Java and Java3D enabled.
Installation requirements & dependencies	Java and Java3D.
Link to user manual	https://github.com/stebond/TOUGH2Viewer/blob/master/TutorialTOUGH2Viewer_ver.2.0.pdf
Support email for questions	stefano.bondua@unibo.it

1. Motivation and significance

The TOUGH family of codes is one of the most widely used numerical simulators for geothermal reservoir engineering and other applications, such as underground carbon storage, nuclear waste and environmental management [1]. Developed since

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the early eighties at the Lawrence Berkeley National Laboratory (LBL, Berkeley, CA), TOUGH is written in Fortran, and the new TOUGH3 version was released recently [2]. TOUGH is a command line software and does not have a native Graphical User Interface (GUI) to generate the grid and the input files or to visualize the simulation results. TOUGH has an embedded mesh generator tool, MESHMAKER, that can generate structured grids as specified by the user [3]. For the sake of completeness, it is worth to recall that TOUGH2 is not the sole code for non-isothermal multiphase flow and transport in fractured porous media. Among the others, it is worth mentioning: Tetrad [4], FEHM [5], STARS [6], HYDROTHERM [7], MUFTE [8,9], PFLOTTRAN [10], OpenGeoSys [11], DUMU^x [12,13], FEFLOW [14], SHEMAT [15], ECLIPSE [16], Waiwera [17].

The TOUGH2Viewer [18] is a visualization and management software tool for TOUGH grids and simulation results. Initially developed for 3D structured and 2D Voronoi extruded mesh (referred in literature as 2.5D grids) [18], in 2017 it was updated to handle fully 3D Voronoi grids [19]. Now thanks to new implementations, TOUGH2Viewer, is not just a viewer, in fact it permits grid manipulation by: (i) editing the properties of the grid blocks (rock types, volume); (ii) exporting sub-grids as defined by the user; (iii) exporting simulation results for the open source visualization software Paraview [20]. Until now, no other visualization software devoted to fully unstructured 3D grids are available in the scientific literature for the TOUGH family of codes.

TOUGH2Viewer, though developed to work with TOUGH files, can be probably adapted to work with other numerical simulators by adding dedicated modules for managing different input/output file formats.

The TOUGH input and output files are plain text ASCII files. In the TOUGH3 [2], the last release, there is the possibility to obtain simulation results in a .csv file format and in the *.tec format for the TecPlot¹ visualization software. In the simulation result files, the thermodynamic variables are given at the nodes of the grids and they refer to the volume of the discretized space. The information about the coordinates and the geometry of the block is not used in the simulation, so the results (pressure, temperature, saturation, etc.) can be visualized using the visualization software only at the nodes of the grid. It is worth mentioning that the TOUGH simulator computes the heat and mass transfer at the interface of the grid blocks by using the Integral Finite Difference method (IFDM) [21,22]. The IFDM requires that the surface area shared by two neighboring blocks be orthogonal to the segment connecting the two node blocks. This constraint is implicitly satisfied by structured orthogonal grids and Voronoi grids. In case of not compliant IFDM grids, numerical errors can arise [23]. Visualization of the simulation results obtained by TOUGH2Viewer takes into account the shape of the original geometry of each block, permitting an enhanced visualization of the simulation results on full 3D Voronoi grids.

In the scientific literature, many pre- and post-processing tools are described, including visualization software and export filters for TOUGH grids, which may be commercial, free or open source. The list of some of the most popular commercial pre- and post-processing software tools for TOUGH includes: Petrasim [24], Leapfrog [25], WinGridder [26], mView [27], GeoCad [28]. Of the free or open source software tools, the most notable are Mulgraph and MulGeom [29], G*Base [30] Simple Geothermal Modeling Environment (SGME) [31], TOUGHER [32], IGMESH [33], pyTOUGH [34,35], iMatTOUGH [36], IGMESH [37], TIM [38], AMESH [39], LaGrit [40] and MESHVORO [41].

In Table 1 it is summarized the main characteristics of the listed pre- and post-processing software. Among them, as far as we know, only TOUGH2Viewer allows the visualization and editing capabilities on 3D Voronoi grids.

2. Software description

TOUGH2Viewer is a Java application based on the Java3D library and designed for the visualization, editing and analysis of 3D structured/unstructured grids for the TOUGH family of codes. Structured grids are created, for example, by the MESHMAKER meshing tool embedded in TOUGH. Unstructured 2.5D grids are, for example, created by using TOUGH2GIS [42] that includes a modified version of AMESH [39], an open source mesh generator for 2.5D Voronoi grids. 3D fully unstructured grids (3D Voronoi grids) are those grids created by VORO2MESH [19].

2.1. Software architecture

TOUGH2Viewer contains four main modules: the input module, visualization module, edit module, export module. A detailed description of these modules will be given in the following paragraphs. Fig. 1 shows a schematic drawing of the overall architecture. The user can display the grid blocks according to a color scale of the various computed variables and/or edit the grid block properties. The edit tool allows the user to obtain overall information about the simulation trend over the time and to modify the value of parameters associate to the block of the grid. The term manipulation is intended here in the sense of being able to edit grid block properties, like material type and volume value assignment, creation/modification of the initial condition of primary variables (INCON) (for details about the INCON file, see the TOUGH2 manual), file and sub-grid exporting from the original grid.

The export module allows the user to export the numerical model and or simulation results for two purposes: (i) for visualization by means of other visualization software like Paraview; (ii) for obtain a modified, ready to use input files for TOUGH.

The grid generation task can be executed by MESHMAKER, AMESH, VORO2MESH or other grid generator software. TOUGH2Viewer is built using several types of Java 3D library data objects. The most important data object is named VoronoiPlusPlusBox() and is an extended class inherited from the Java 3D Shape3D Class and represents a single Voronoi 3D cell polytope. Other 3D data objects are the Cartesian axis, the surfaces, the polylines, the vectors, etc. which can be used in plotting the grid blocks. The object data VoronoiPlusPlusBox() stores the geometrical properties of one block; it contains the vertex coordinates, the faces and the vector normal to each face. The thermodynamic variable array is stored separately from the geometrical information relative to the blocks.

2.2. Software functionality

The following paragraphs provides an overview of the main functions made available by TOUGH2Viewer. Further details are available in the Quick Tutorial² associated with the software.

2.2.1. Input module

The input module is devoted to read all the data needed for a numerical model 3D visualization. The necessary files for the visualization of a TOUGH model are: (i) the MESH file, an ASCII file containing block names, volume and connection information for a detailed explanation of the MESH file format please refer to the TOUGH2 user's guide [3]; (ii) the geometrical file (in case of unstructured grid); (iii) the output file generated by TOUGH containing the simulation results.

² https://github.com/stebond/TOUGH2Viewer/blob/master/TutorialTOUGH2Viewer_ver.2.0.pdf

¹ <https://www.tecplot.com/>

Table 1
List of some pre- and post-processing tools for TOUGH grid generation and visualization.

Software name	2D/3D Structured grids visualization	2.5D Voronoi grids visualization	Fully 3D Voronoi grids visualization	3D Voronoi grids editing	Filter export for external viewer	Commercial	Source Code Availability
AMESH	NO	NO	NO	NO	NO	NO	YES
G*Base	YES	YES	NO	NO	NO	NO	NO
IGMESH	YES	YES	NO	NO	NO	NO	NO
iMatTOUGH	YES	NO	NO	NO	NO	NO	YES
LaGrit	YES	YES	YES	NO	YES	NO	YES
Leapfrog	YES	YES	NO	NO	YES	YES	NO
MESHVORO	NO	NO	NO	NO	YES	NO	NO
MulGeom	YES	NO	NO	NO	NO	NO	NO
MulGraph	YES	NO	NO	NO	NO	NO	NO
TIM	YES	YES	NO	NO	NP	NO	YES
mView	YES	YES	NO	NO	NO	YES	NO
Petrasim	YES	YES	NO	NO	NO	YES	NO
pyTOUGH	YES	YES	NO	NO	YES	NO	YES
TOUGH2GIS	YES	YES	NO	NO	NO	NO	YES
TOUGH2Viewer	YES	YES	YES	YES	YES	NO	YES
TOUGHER	YES	NO	NO	NO	NO	NO	NO
VORO2MESH	NO	NO	NO	NO	YES	NO	NO
WinGridder	YES	YES	NO	NO	NO	YES	NO
SGME	YES	NO	NO	NO	NO	NO	NO

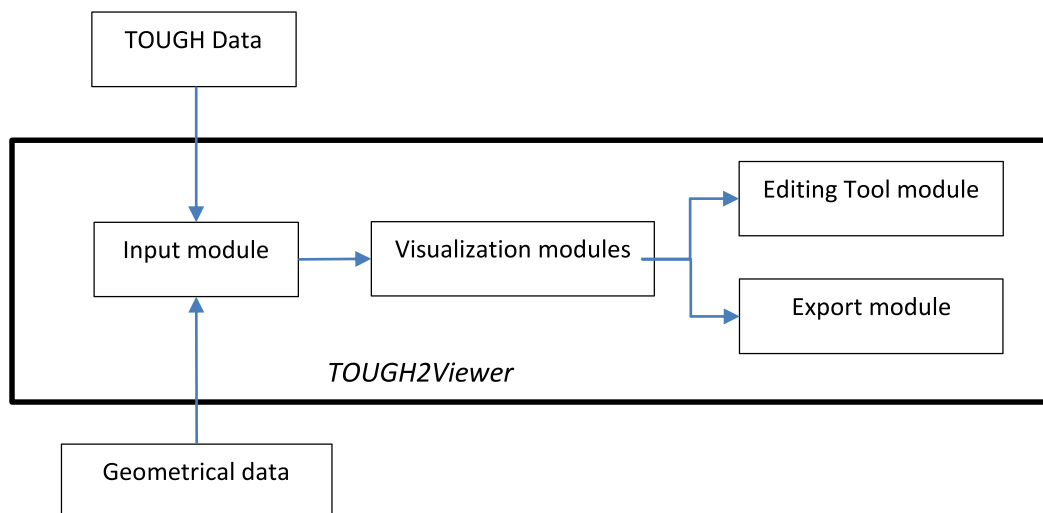


Fig. 1. Schematic drawing of the TOUGH2Viewer architecture.. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

In the followings the main subroutines of the module:

ReadMESHfile(meshFileName)

The MESH file of TOUGH contains the parameters of the discretized space using the IFDM. The function `ReadMESHfile()` reads and stores in memory the information contained in the file that contains the grid properties (MESH file, in the terminology of TOUGH). Example of block's data (defined under the keyword `ELEME` of TOUGH) are rock type, node coordinates, volume, etc. The file contains also information about the connections between neighboring grid blocks, like distance between nodes, surface area, etc. (organized under the keyword `CONNE` of TOUGH). For detailed information about the TOUGH input file format, see the TOUGH user guide [3].

ReadTOUGHViewer_dat(tough2viewer_dat_FileName)

In case of 3D Voronoi grids created by `VORO2MESH`, the geometrical information about the block (vertex, faces and face normal) are stored in the file named `tough2viewer.dat`. The information stored in the file permits geometrical definition of the

block, needed for the 3D visualization. More details about file format can be found in [19].

ReadT2_data(T2outputFileName)

The TOUGH simulation output is a plain text file containing information about the thermo-physical properties of the block, but it also contains information about the details of the evolution of the simulation itself (convergence, numerical problems, computation time, etc.). The structure of this file depends on the Equation of State (EOS) used for the simulation and on the level of message detail activated by the user. For further details about the output files, please refer to [3].

2.2.2. Visualization module

It is essentially composed by a set of windows for the graphic representation of the grid and for the simulation results visualization.

Model3D()Visualization

The `Model3D()` window is the most important functionality of TOUGH2Viewer (see for example [Figs. 2](#) and [4](#)). It creates a 3D

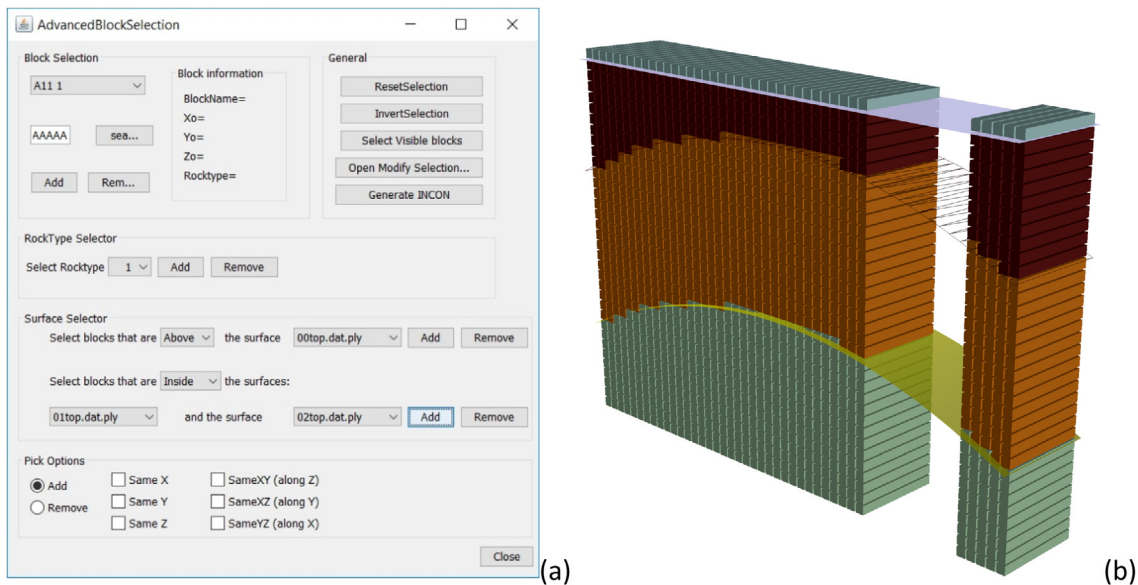


Fig. 2. (a) AdvanceBlockSelection dialog window: user can select blocks by block name, rocktype, surfaces, coordinate, visibility. (b) 3D structured grid example. Rock type assignment was performed using TOUGH2Viewer. A region of the model is hidden from view using the SetVOI->hideVOI function. The separation interfaces between domains are shown.

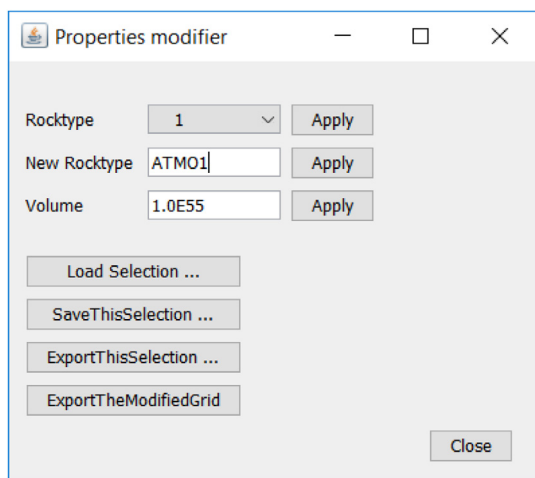


Fig. 3. Properties modifier dialog. Properties of the selected block can be changed: a different rocktype can be assigned, a new volume can be set. The new properties of the selected blocks can be saved, a new grid can be created or the modified grid with the new parameters can be exported.

virtual scene where the grid of the numerical model can be visualized. Each block is built using the vertex coordinates as read by the ReadTOUGH2Viewer_dat() function. Blocks are pickable and by choosing the appropriate Model3D option, information about the block properties can be visualized or the fluid-petro-thermo properties associated to the block can be modified. Among several selection methods, it is worth noting the selection utility function, SelectNeighbors(), that allows selection of all connected blocks starting from an initial selected block.

For model inspection, a set of splitting mode commands enables the user to view internal portions of the model. Volumes of Interest (VOI) can be defined to hide/visualize parts of the grid model.

Other functions include: preset views (top, bottom, right, left front, back), 2D Plots (thermodynamic variables), snapshot, block

find, single or multiple selections, sub grid exports, rock type modifications, auto snapshot and auto rotate functions.

3D_Flow() Visualization

The TOUGH computes the heat and mass transfer between block faces. This kind of variable is a vector, as it has a 3D orientation. The Flow3D visualization function allows the user to visualize the vector sum of the flow vectors at the nodes, allowing a quick overview of the evolution behavior of the numerical model. Fig. 5 shows an example.

Visualization options

The visualization option dialog box allows the user to set and edit visualization parameters. Main visualization options include:

- Visualization filter: blocks can be visualized/hidden by setting a min and max threshold for the variables shown;
- 3D Block model Object: blocks can be hidden/visualized based on rock type values. A stretch factor can be applied to better understand block geometry. Axis and background color can be modified by the user;
- 3D flow vector properties, like normalized vector length and color scale settings.

2.2.3. Editing tool module

Properties_modifier()

The properties modifier dialog window (Fig. 3) allows the modification of the rocktype and/or the volume value of the selected blocks. The blocks selection can be performed by the Advanced Block Selection function, allowing selection by simple clicking or by using surfaces files for the definition of regions in the 3D space.

INCON_Generator()

The initial conditions file generator allows the user to set initial condition values (under the keyword INCON of TOUGH) in various ways: by block, by rock type or by user selected blocks. The definition of the initial condition of the primary variables depends on the EOS being used in the simulation. The INCON_Generator() dialog allows the assignment to the selected

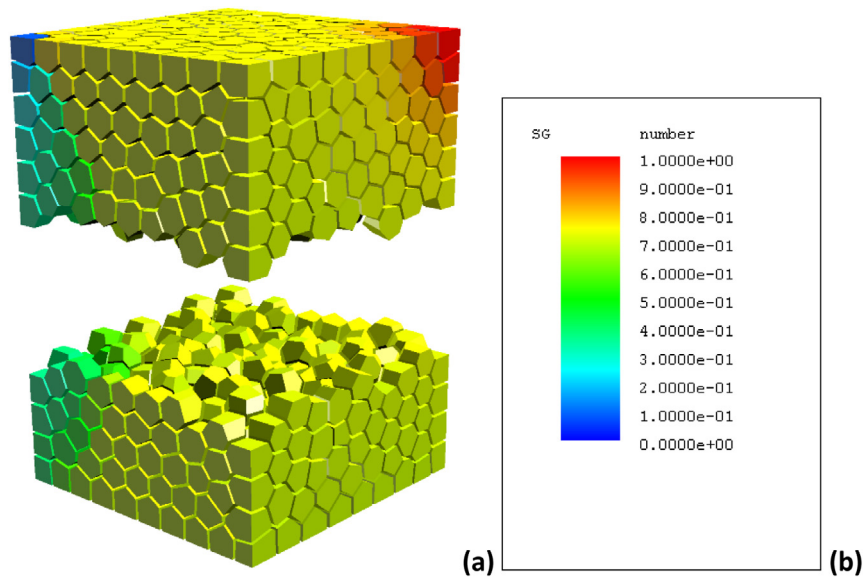


Fig. 4. 3D unstructured grid example visualization using TOUGH2Viewer. The model is $1000 \times 1000 \times 1000 \text{ m}^3$ and the color scale refers to gas saturation variable (SG in the terminology of TOUGH). Rock type assignment has been done with VORO2MESH. The grid is visualized using the ShiftXY() function to allow internal inspection. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

blocks the INCON values using (i) linear correlation; (ii) interpolation of table data imported as CSV file or interpolation of xyz raw data using the inverse distance weighted method.

Sub-grid export function

The sub grid export function allows the selection and exportation of a part of the grid (a sub grid), allowing therefore the creation of a new grid. User can select the blocks using the advance block selection dialog or using the Select Neighbors function. The Select Neighbors function searches iteratively for all the blocks connected to a selected block up to a selected number of connections.

Statistical and plot functions

The overall behavior of the numerical model is synthetized in a statistical report of the simulation results and the global mass and heat balance can be displayed in tables or plotted for all simulated time steps.

2.2.4. Export module

Among the many export functions of TOUGH2Viewer, the following are worthy of note: (i) numerical model export, (ii) raw data export, (iii) manipulated model export.

The numerical models created with MESHMAKER or with VORO2MESH and read by TOUGH2Viewer can be exported in a format that can be read by Paraview as .vtu files (unstructured grid file format).

Other file formats used for the simulated output files include PLY and csv.

A modified grid is easily exported by generating a new TOUGH MESH file with the modified grid properties, the INCON file and the geometrical tough2viewer.dat file, which in case of sub-grid generation contains only the geometrical information of the sub-grid.

3. Illustrative examples

We show the main features of the TOUGH2Viewer software on two examples of data-sets, a simplified 2D structured grid model, and a 3D Voronoi unstructured model.

3.1. Structured model

In this example, a set of 3 surfaces defines 4 geological horizons used for the rock type assignment. Fig. 2, created by means of TOUGH2Viewer, shows the 3D structured numerical model jointly with the surfaces. The “empty” model (that is the model without the rock type assigned) was generated by VORO2MESH. Alternatively, it can be built with MESHMAKER. Using the TOUGH2Viewer Advanced Block Selection Function, it was possible to select blocks with greater or lower elevation or select blocks identified by one surface or between two surfaces respectively by the AdvancedBlockSelection dialog of Fig. 2.a. Using the Properties modifier dialog window, rock type and volume assignment were then automatically assigned to the selected blocks. After rock type and INCON assignment, the numerical model was exported by generating the modified MESH and the INCON files in a format that can be directly used as TOUGH input files. In Fig. 2.b a region of blocks was hidden from the visualization by using the option hide VOI (Volume of Interest) of the function setVOI A step by step guide for this model can be found in the TOUGH2Viewer Quick tutorial.

3.2. 3D unstructured grid visualization

In case of fully unstructured 3D Voronoi grids (see Fig. 4), visualization of the grid requires a complete geometrical description of the discretized space. This information is read by TOUGH2Viewer from the file named tough2viewer.dat.

The grid was generated by VORO2MESH [19] using Centroidal Voronoi Tessellation. After MESH generation, blocks with particular properties, like the generation block (GENER keyword of TOUGH, for a detailed explanation about GENER block, please refer to the TOUGH2 User's guide [3]) or boundary conditions blocks, can be defined by simply clicking on it using the AdvanceBlockSelection dialog. In the example showed, the INCON for obtaining the steady state before fluid injection/production simulation has been generated by TOUGH2Viewer considering hydrostatic pressure, bi-phase conditions, constant non-condensable gas saturation (CO_2) and salt (NaCl) content. For further details about the model generation procedure, please refer to the TOUGH2Viewer Quick tutorial.

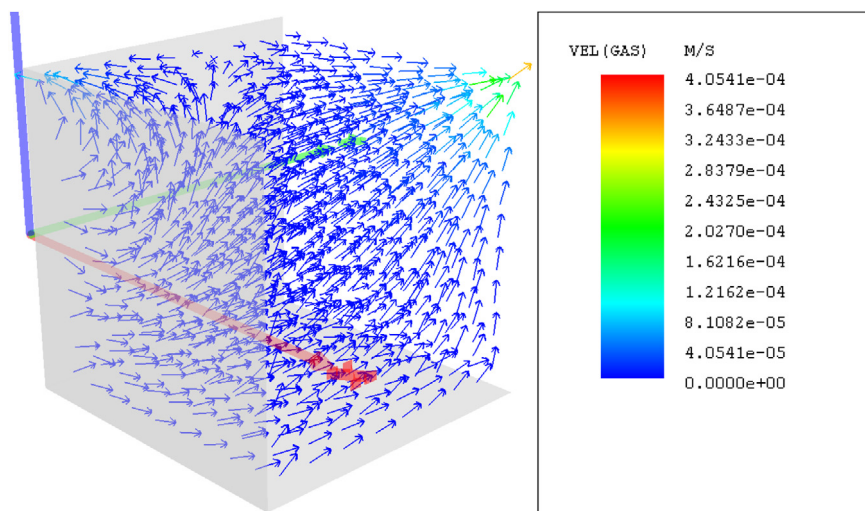


Fig. 5. TOUGH2Viewer vector flow visualization module. The vector variable visualized is VEL(GAS) (m/s) (gas velocity). The colored line segments are: red the x, green the y, and blue the z axes. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

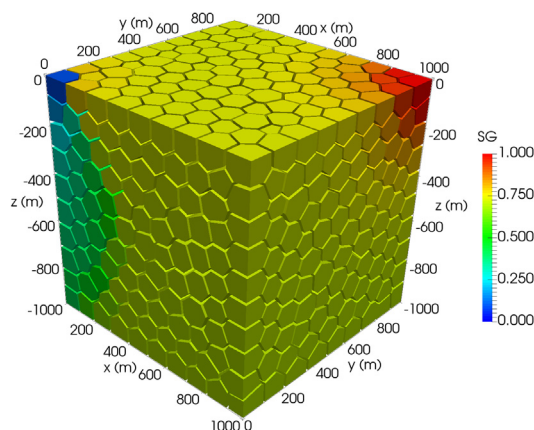


Fig. 6. 3D unstructured grid visualization using Paraview. Saturation of Gas (SG) color scale. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

Using the export function Export2VTU, the simulated results were exported into a set of vtu files and Fig. 6 shows the same model visualized with Paraview. Paraview is a powerful 3D visualization software that can enhance data visualization by a set of filters and primitives for scientific visualization (among the other, it is worth to mention grid blocks, vector field, isosurfaces, transparency, slicing, threshold, etc...). On the other hand, it has no dedicated editing or input filters functions for TOUGH2 grids.

4. Impact

The use of 3D Voronoi grids in the field of numerical simulations is growing and consequently also the dedicated tools developed for model visualization.

TOUGH2Viewer gives efficient insight into the implementation of structured and unstructured 3D Voronoi grid visualization and management for TOUGH numerical models. Grid editing, as well as the creation of the necessary file for the TOUGH simulation within a GUI environment, make it possible to generate numerical models in an efficient way. It follows the concept of “what you see is what you get”, as the user can easily observe differences on simulation results or grid changes between different models by means of visual inspection of the model.

The TOUGH2Viewer is intended for new users approaching the TOUGH world for the first time, as well as for experienced users who intend to deploy the power of fully unstructured grids without the limitations due to the 3D Voronoi grid and results visualization.

TOUGH2Viewer, though developed to work with TOUGH files, can be adapted to other numerical simulators by adding new dedicated input modules for different file formats.

5. Conclusions

TOUGH2Viewer enables visualization and grid editing of TOUGH numerical models. The new functionality of grid editing makes it possible to generate numerical models in quick steps and with visual assistance. The export function improves visualization by means of access to open source visualization software like Paraview, and can help the user to improve visualization of the numerical model results. TOUGH2Viewer is now freely available to the scientific community as a binary Java jar file and/or source code. The software is currently not used in commercial settings, but the Apache License, Version 2.0 of TOUGH2Viewer allows for its integration into commercial tools.

CRediT authorship contribution statement

S. Bonduà: Conceptualization, Methodology, Software, Validation, Formal analysis, Investigation, Data curation, Writing - original draft, Visualization, Supervision. **V. Bortolotti:** Conceptualization, Writing - review & editing, Supervision.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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