TOUGHVISUAL: A USER-FRIENDLY PRE-PROCESSING AND POST-PROCESSING GRAPHICAL INTERFACE FOR TOUGHREACT

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ABSTRACT

TOUGHVISUAL is a complete Windows-based graphical user interface for the TOUGHREACT program, which is a general multiphase multicomponent reactive transport simulator, developed by introducing geochemistry into the existing multiphase fluid and heat flow code TOUGH2. The complexity of the input files (such as flow.inp, solute.inp and chemical.inp) required by TOURHREACT makes manual construction of its input files tedious and error-prone, especially for problems with a large number of elements and complex geological structures. TOUGHVISUAL streamlines the creation of the input files and helps reduce errors, so one can spend more time interpreting and analyzing the modeling results. TOUGHVISUAL builds on the experiences of previous relatively mature interface software such as PetraSim, Tougher, and Winggridder, and is presented here as an improved pre- and post-processing TOUGHREACT graphical interface. TOUGHVISUAL's advantages are as follows:

(1) It is written in the object-oriented language C++, which is convenient for management and future update.

(2) It generates regular or irregular editable and convertible MESH files, such as rectangular, triangular, quadrilateral, thiessen polygon to meet user's needs.

(3) It makes full use of existing geological data. For example, all kinds of attribute data, likes porosity, could be represented as three-dimensional scatter points, then assigned as properties to elements via three-dimensional interpolation.

(4) It translates domain properties into element properties if one builds property domains.

(5) It imports attribute data from other software and exports various common file formats to other software, so that TOUGHVISUAL shares information with other software.

(6) It displays the results of various state variables as temporal evolution curves for single or many elements, space iso-surfaces, or the contours of a cross-sectional map. This can be very helpful for users who want to display results during running time.

1. INTRODUCTION

TOUGHREACT is a general multiphase multicomponent reactive transport simulator (Xu et al., 2006) developed by introducing geochemistry into the existing multiphase fluid and heat flow code TOUGH2 (Pruess et al., 1999). Although TOUGHREACT, as initially developed, is a powerful research tool, its input files are difficult to create and error-prone, requiring using a text-based editor and assigning properties to grid elements. It is especially inconvenient if your study area is irregular or is a heterogeneous porous media. There are a few commercial programs, such as PetraSim, Wingridder, GeoCAD, and Tougher (Alcott et al., 2006; Yamamoto, 2008; Pan, 2003; Burnell et al., 2003; You Li et al., 2011), making graphical interfaces for TOUGH, but they have proved neither very flexible nor convenient.

For these reasons, our research group at Jilin University, considering the shortage of existing interfaces, attempted to develop a better interface software for TOUGHREACT, making it more user-friendly and convenient. While at present TOUGHVISUAL only supports the ECO2N module, additional modules could be easily incorporated in future versions.

2 .DESIGN OVERVIEW

This paper will briefly describe the graphical interface TOUGHVISUAL, which can be used to create input files, edit input data files, and plot TOUGHREACT simulation results. We used the Microsoft Visual Studio 2005 development tool, while utilizing OpenGL to render the model and visualize the result. This tool adapts the methods of modularization architecture. Its portion structure is shown in Figure.1.

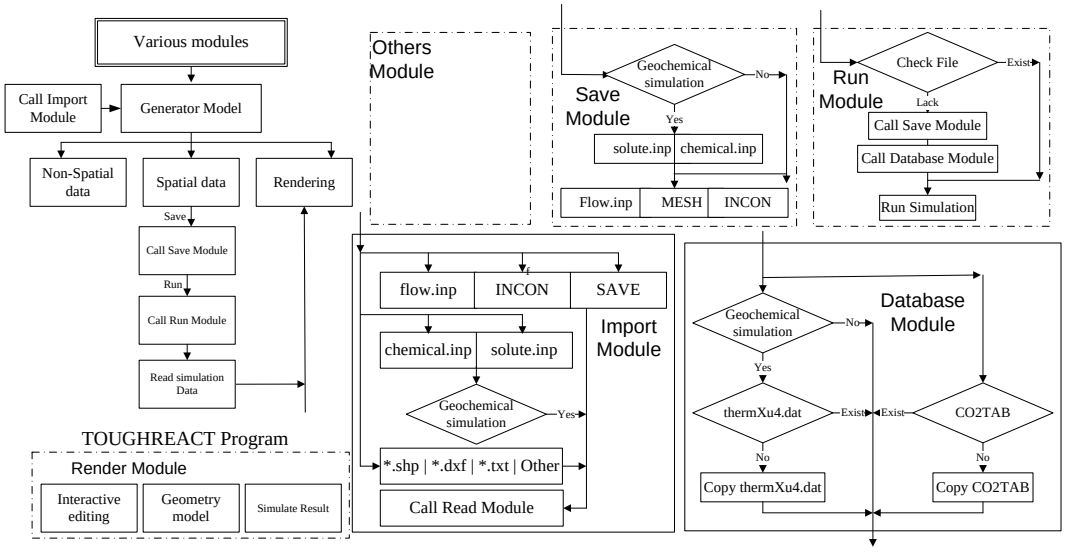


Fig. 1. Portion Structure chart in TOUGHVISUAL

3. TOUGHVISUAL INTERFACE

The TOUGHVISUAL interface software includes a pre-processor and post-processor, each consisting of different components.

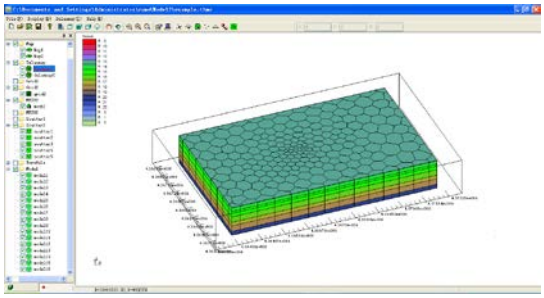


Fig. 2. Main window of TOUGHVISUAL interface

3.1. Pre-processor

TOUGH simulator's input files data are divided into many individual keyword data blocks. Different Keyword data blocks provide different information, such as ROCKS, GENER, INCON. A brief description of the processing methods is given below.

3.1.1. Geometrical Model

The geometrical model generator is one of the most important and critical steps of the interface software. One can use the mouse to draw the simulation domain boundary, and one can of course also specify the boundaries through study area coordinates. Then, the computing grid will be automatically generated by clicking the related menus. Grid shapes may be rectangular or irregular. The number of layers is unrestricted. One can use different methods for generating a geometrical model—for example, one can generate a 3-D geometrical model directly, or initially create a 2-D geometry, then carry out a simple processing step to generate a 3-D model. Three examples of geometrical models are displayed in Figures 3, 4, and 5.

Figure 3(a) shows a regular geometrical model. Note that the element size can be edited interactively in order to meet the user's needs, When the user wants to create a 3-D model, as shown in Figure 3(b), he or she needs to assign each layer's elevation. The user can of course also change the elevation within 3-D models.

Figure 4(a) displays an irregular geometrical model. The green points are the center point of the elements. The element size could be smaller in the key study or fault areas. Figure 4(b) is the corresponding 3-D model.

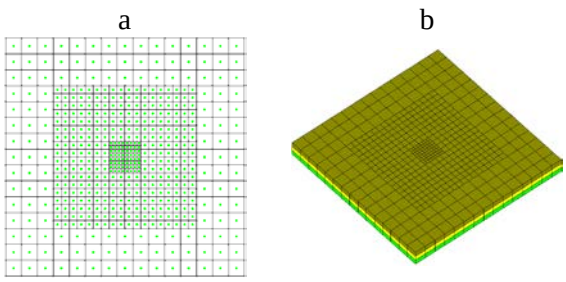


Fig. 3. Typical regular grid model. (a) Layout of a layer . (b) A 3-D model after editing.

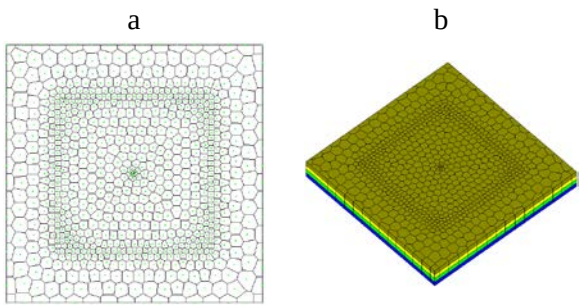


Fig. 4. Typical irregular grid model. (a) Layout of one layer. (b) Irregular geometry model displays in 3-D

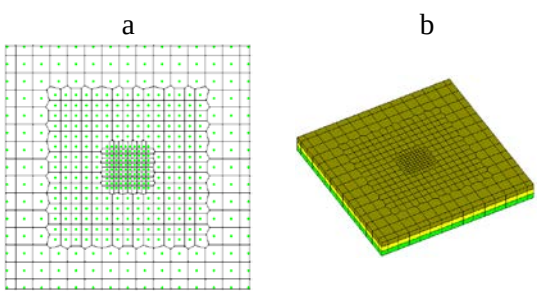


Fig. 5. Regular/irregular grid model. (a) Layout of a layer. (b) 3-D view of the model

In this process, calculating the interface area between two connected elements and element's volume is very important. TOUGHVISUAL mostly uses two methods for achieving this. One can use Equation (1) (Gelder, 1995) to compute the area of an interface of any polygon with N vertices P_i (i=1..N). This formula for computing area is very effective for any polygon in 2-D or 3-D. Moreover, the volume of a polyhedron R, with N vertices and m faces (F1,F2,…Fm), is given in Equation (2). The user can change a complex polygon into a simple polygon first, then compute its area and volume. Finally, using ELEME and CONNE data, the MESH file can be generated. Element properties will inherit the default value, which one can change if needed.

$$A = \frac{1}{2}\sum_{i=1}^{N} P_i \times P_{i+1} \qquad (1)$$

$$V = \frac{1}{3}\sum_{j=1}^{m} F_j \bullet A_j \qquad (2)$$

3.1.2. ROCKS

This keyword data block mainly introduces material (rock) properties, which can be set by the material tab. In default, all blocks will be assigned to the first rock type. The user can then modify the block's material according to the study area's geological conditions. There are three methods to finish this data block: Figures 6 and 7 show two methods; the third method is reserved for use with other modules. When you save this model, these values will be written into the flow.inp file according to the original TOUGH fixed format. When changing a block's material zone, one must select the blocks—see Figures 6 and 7.

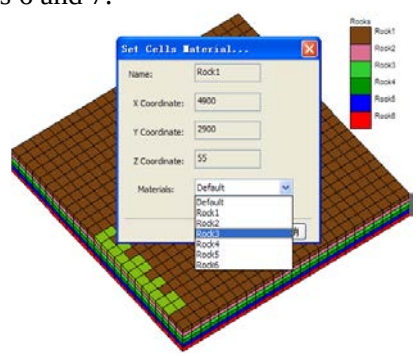


Fig. 6. Modification of gridblocks's material zone.

Fig. 7. The second method for modifying the grid-block's material zone.

3.1.3. GENER

Similar to assigning gridblocks to ROCKS data, the user can select a sink or source block to inject/product mass or heat. The associated parameter values to be set are shown in Figure 8.

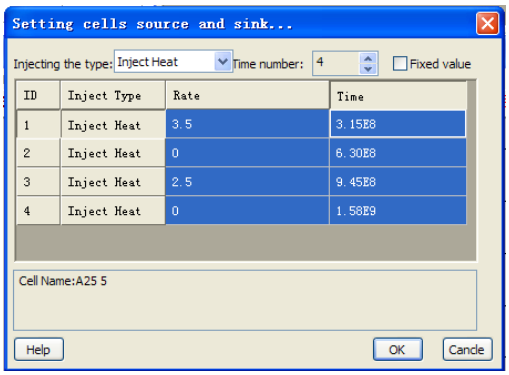


Fig. 8. Defining sinks or sources for a block

3.1.4. Boundary condition

Two basic boundary types can be specified. For the Dirichlet condition, the user can assign large volumes, so that their thermodynamic conditions or state variables, such as pressure and temperature, do not change during the simulation time—see Figure 7 (the fourth column of the cell attribute's tab). Boundary conditions can also be handled by introducing sinks or sources of appropriate rates into the elements, specified in the GENER data block.

3.1.5. Initial condition

All gridblocks are assigned the default initial conditions. The temperature is calculated according to geothermal gradient, and the pressure is calculated according to hydrostatic pressure. The defaults can be overwritten using a simple mouse operation. In addition, the user can import or connect to the existing initial condition, such as the SAVE file.

Figure 9 shows how a user can modify the block's initial condition after selecting the target blocks. The selected blocks will then have the same initial conditions. If one wants to define different initial values for different blocks, one should adopt another method (Figure 10).

Figure 11 show how a user can restart a model by connecting the save/savechem file, generated in a previous run. Then the program will take the corresponding processing for the initialization.

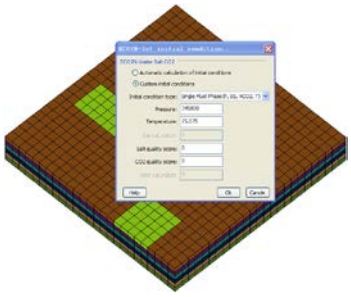


Fig. 9. One method to modify the block's initial conditions

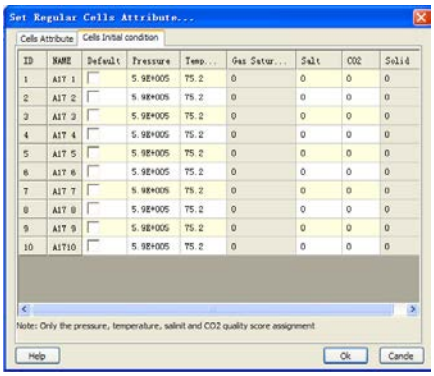


Fig. 10. Another method to modify the block's initial conditions.

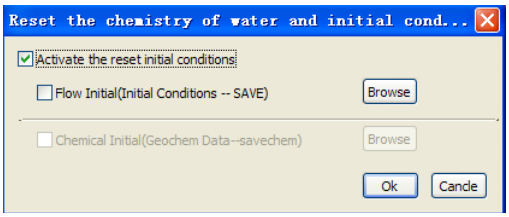


Fig. 11. Connection to a existing initial condition file.

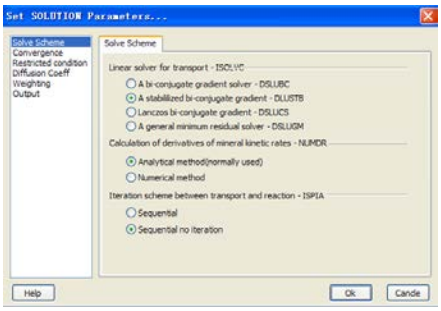
3.1.5. PARA, MULTI, TIMES and SOLVR Keywords

According to the menu operation, the user can also finish the parameters assigned for PARA, MULTI, TIMES, and SOLVER data blocks.

3.1.6. Solute.inp file

This solute.inp file in the original TOUGH-REACT program contains various flags and input parameters for calculations of reactive transport (Xu et al., 2006), such as diffusion coefficients, tolerance limits, and output control. Parameters in this file are organized in various displayed menus, as shown on Figure 12**.**

a



b

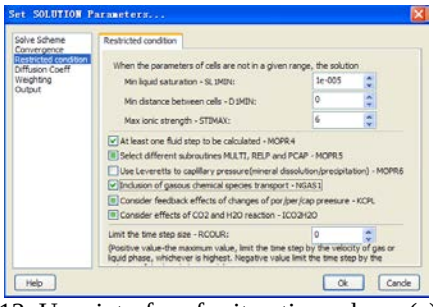
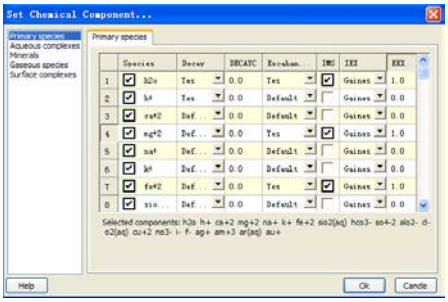


Fig. 12. User interface for iteration scheme(a) and run constraints(b)

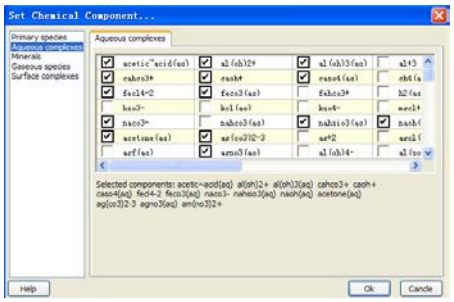
3.1.7. Chemical.inp file

This file is used to define the geochemical system (number of aqueous component species, minerals, gases, and sorbed species considered in the simulation). The file also includes the initial composition of water, minerals, and gases for different zones that are assigned to gridblocks. With this interface, the user can readily define the geochemical parameters and properties to be associated to gridblocks.

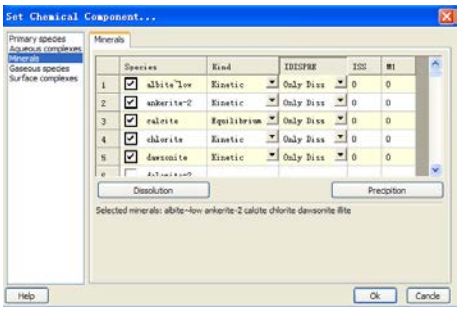
a



b



c



d

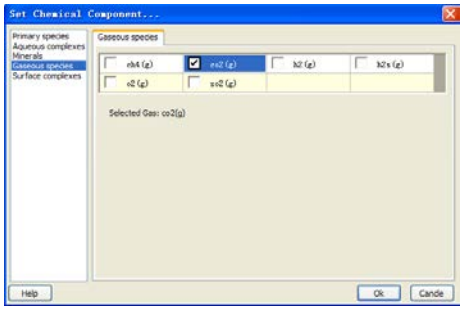
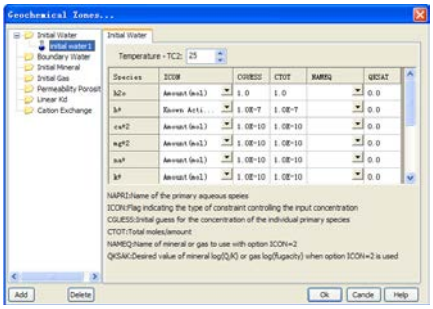


Fig. 13. Interface for primary species (a), aqueous component species (b), mineral phases (c), and gaseous species (d).

a



b

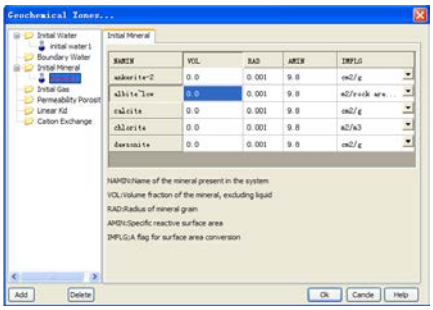


Fig. 14. Initial composition of water (a) and mineral phases (b)

3.2. Running the model

Before running the model, one should make sure that all data are saved. Then, the user selects "Run" on the menu, and the Run model dialog box will appear. Use the combox to select the graph type within which progress data will be displayed, as shown in Figure 15.

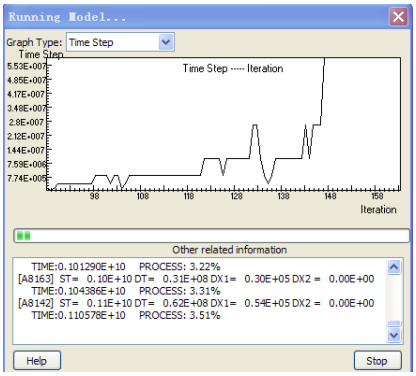


Fig. 15. Simulation progress and time step size.

There are three graph types: Time step versus number of iterations, Error versus number of iterations, and simulation-time progress versus number of iterations. For different graph types, the user will receive different information.

3.3. Post-Processor

The fast visualization of modeling results is very important, so that dynamic analysis can be conducted with minimum delay. For this purpose, post-processing has been developed for modeling results, 3-D iso-surfaces, contour maps, cross sections, piper plots, and temporal evolution plots. In addition, modeling results can be animated.

Using the presented modules, one can create all sorts of figures, such as color-filled contour figures, which may be saved in several formats, including *.shp, *.dxf, *grd, *csv and *.bmp. The data from different modules can be converted to one another. One can import all kinds of popular file formats, likes *.shp, *.dxf, *.grd , *.csv, and so on. These modules also provide some suitable interpolation algorithms. Making full use of these functions, the user will find that they are very useful and convenient.

4. EXAMPLES

Here we present two examples to illustrate the advantages and usefulness of TOUGHVISUAL. Through simple mouse clicking, one can complete the pre-processing of input files for TOUGH2/TOUGHREACT. Analyses of numerical simulations are readily accessible to rapidly evaluate model results.

4.1. Regular Grid Model

The geometry of a model for a CO_2 injection problem is shown in Figure 16(a). This model contains 3750 elements, with 10,325 connections among them. Each layer is color-coded, and the properties of each layer can be varied, especially the mineralogical and hydraulic properties. CO_2 is injected into the center of the sixth layer at a constant pressure.

a b

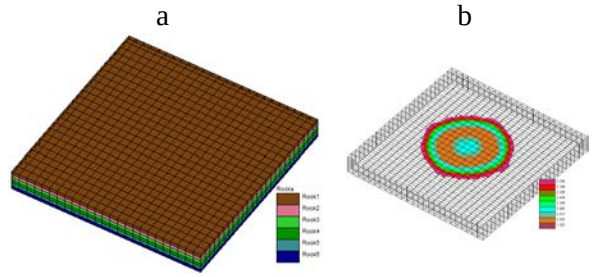


Fig. 16. Regular grid model (a). Result of the model displayed after 30 years (b).

By setting the iso-surface options, the iso-surface maps of P, T, and other state variables will be produced. Figure 16(b) shows the simulated results after 30 years. Image details can be controlled—for instance, the number of iso-surfaces and the data range. If only one time step is selected, the contour map will overlay the finite-difference grid. If more than one time step is selected, then the selected contour maps will be dynamically shown.

a b

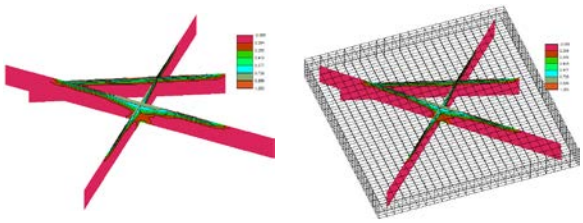
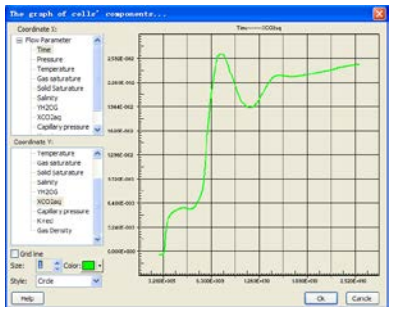


Fig. 17. Cross-sectional contour

To get a cross-sectional contour, the user should first draw the cross-hatching with the help of a mouse, then select the available state variables and plot time. The user can rotate, pan, and zoom the image interactively. By selecting the animation display, one could view the change in the simulated result over time. Finally, the user can export the image. In a similar manner, for one or more elements, the user can plot resulting variables in terms of temporal evolution—see Figures 18.

a



b

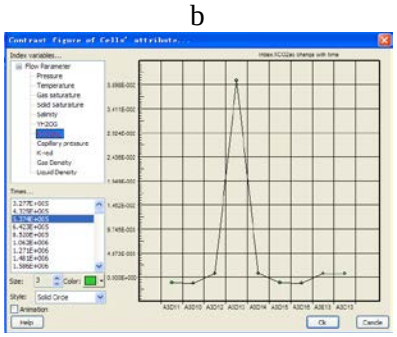


Fig. 18. Temporal evolution for one element (a). Attributed plot for multiple elements (b)

In many cases, it is very useful to display the distribution of each component in the system. Different times would have different distribution—see Figure 19.

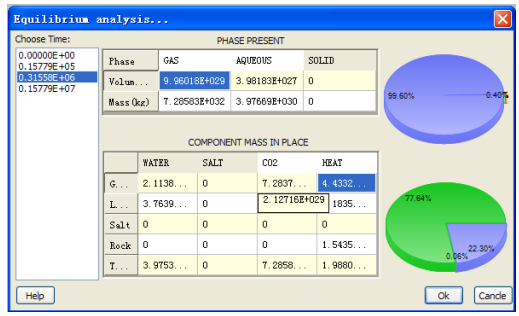


Fig. 19. Component distribution plot

4.2 Building Grid Model from a Geological Model

The second case involves geologic complexity; therefore, we need first to create an adequate geologic model. Once that is done, we can determine the modeling domain area, because in this case the geologic model is very large, about 18 km^2. The geologic model was directly built from 494 available boreholes with minimal user intervention (Figure 20). We must identify the scope of the study, covering an area of 800×500 m^2. Figure 21 displays the numerical grid. This model contains 1912 elements with 7049 connections. Finally, we transfer the properties of the geologic model into the modeling grid (Figure 22a).

a b

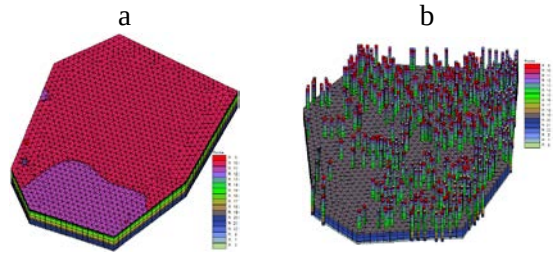


Fig. 20. Generation of a geologic model from borehole data. (a) 3D view of the geologic model. (b) Geologic model with boreholes

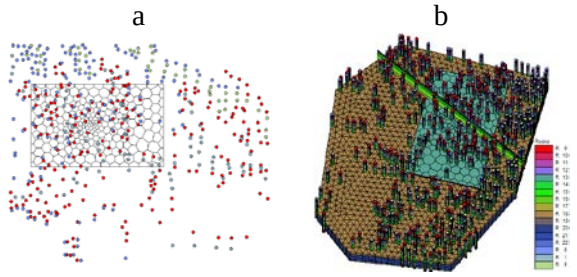


Fig. 21. Determination of the study area. (a) Plan view. (b) 3D view

Figure 21(a) shows the study area using either the black line diagram (a), or the sea-green area in (b).

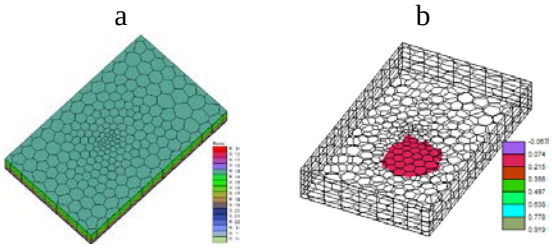


Fig. 22. Grid model (a), Result of the model (b).

Figure 22(a) shows the grid model in 3-D view. As illustrated in Figure 22(b), the user can select any time and available variables (Sl, Sg., etc.) for plotting.

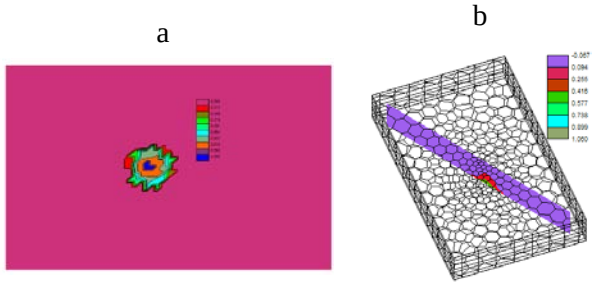


Fig. 23. Sg contours (a) and cross-sectional contour (b)

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