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Research paper

IGMESH: A convenient irregular-grid-based pre- and post-processing tool for TOUGH2 simulator

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ABSTRACT

As a powerful simulator with input files in fixed-format formats, the capabilities of TOUGH2 simulator urge programmers to develop the pre- and post-processing programs. A new program (IGMESH) with Graphical User Interface (GUI) is introduced. The elements for spatial discrezation are classified into domain bound, boundary for refinement, well, fault, drift and free point, which will be discreted into a series of points. The Voronoi tessellation method is employed to generate Voronoi diagrams in the plane and the relation of neighbor points in a polygon is obtained from the geometric relationship of Voronoi diagrams. Three-dimensional mesh is built based on top elevation and thickness of each model layer. IGMESH provides functions for rock type assignment, boundary conditions, interpolation method of elevation and thickness, simulation results conversion and visualization with TECPLOT software. The case studies in the Beishan area demonstrate the applicability of the approach. IGMESH software has shown to be adequate to build quasi-3D unstructured grids from the beginning of numerical model build to the results analysis, and thus will facilitate the application of TOUGH2 simulator.

1. Introduction

As a simulator for non-isothermal flows of multicomponent, multiphase fluids in porous and fractured media, TOUGH2 (Transport Of Unsaturated Groundwater and Heat) has been widely used in the studies on geothermal reservoir engineering, nuclear waste isolation and environmental assessment (Pruess et al., 2012). The most time-consuming process for TOUGH2 model users is the preparation of format-fixed input files in ASCII format, which mainly include MESH and GENER. Preparation of MESH file is the most difficult process. For example, the information of one block in MESH file consists of 80 characters, including fixed-character (default: five) code name of an element, number and increment of additional elements (ten-character), five-character material identifier, element volume (ten-character), interface area (ten-character), permeability modifier (ten-character), Cartesian coordinates of grid block centers (thirty-character) (Pruess et al., 2012). Because TOUGH2 is an integral finite difference numerical simulator, meshing tools in both finite-difference and finite-element simulation software cannot be used directly to TOUGH2 simulator. There is the missing of pre- and post-processing tools of TOUGH2, which leads to develop convenient programs. The subroutine MESHMAKER (Pruess et al., 2012) in TOUGH2 is a common regular-grid based mesh generation tool. However, in most cases, some interesting areas, such as well, fault and fracture, are needed to be refined to improve more detailed numerical simulation of fluid flow in local areas. AMESH (Haukwa, 1998) can generate irregular TOUGH meshes using Voronoi tesselation in a 2D plane and projection into the third dimension, but it is missing of Graphical User Interface (GUI) and can not show the mesh and simulated results conveniently. MeshVoro (Freeman et al., 2014) and TOUGH2GIS (Berry et al., 2014) show the powerful function in 3D mesh building with software development kits of Voro++ and GRASS GIS, respectively, but post-processor is weak in the two software. The commercial software, such as mView (Avis et al., 2012), PetraSim (Alcott et al., 2006) and WINGRIDDER (Pan, 2003), can generate such irregular grids. However, all the processes in the pre- and post-processing programs for TOUGH2 include domain discretization, rock type assignment, presentation of non-uniform thickness of model layer, boundary conditions, grid generation, visualization of simulation results along cross-sections and in

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three dimension. Up to now, there is still a lack of thorough programs which operate all the processes concerned with TOUGH2. So the TOUGH2-targeted irregular-grid-based pre-processing (Wellmann et al., 2012) and post-processing (Bonduá et al., 2012) should be further developed.

Usually, the results from TOUGH2 are visualized with commercial software TECPLOT (Tecplot Inc., 2013), a famous post-processing software. The objectives of the paper are to present a new Irregular Grid-based pre- and post-processing tool (IGMESH) with graphical user interfaces for TOUGH2 simulator and demonstrate its applications. IGMESH software is developed in C++. First, the workflow of IGMESH will be described. Second, how two-dimensional unstructured grids are built will be presented. Third, the quasi-three-dimensional (denoted as quasi-3D in short) model build, including top elevation of model, and thickness of each model layer, will be discussed. Also, a series of data, such as rock type assignment, boundary conditions, sources and sinks, grid generation and cross-section set, can be inputted by the model users. Finally, a case study in the Beishan area will be used to demonstrate the applicability of the software.

2. Workflow of IGMESH

The workflow of IGMESH is shown in Fig. 1. In each project, 2D grid is required to be formulated from discrete points, which are obtained from basic elements including domain bound, boundary for refinement, well, fault, drift and free points. When well data are collected, the elevation of top layer and the thicknesses of each model layer at each well are known. The elevation of each model layer for all discrete points can be obtained by the method of data interpolation, such as kriging and inverse distance weighting method. Input data, such as zonation of rock types, sources and sinks, boundary condition and grid generation, can be assigned to blocks of the grid by GUI. The cross-sections have to be assigned from two or more neighboring discrete points. Grid generation will separate the regional mesh by active and inactive gridblock assignment into two sub-mesh, which can be used to establish local numerical model from regional numerical model. After the simulation of TOUGH2 is finished, the output data can be directly converted to TECPLOT data for all grids and the prescribed cross-sections. Compared with other pre- and pro-processing software, IGMESH has main features: (i) user-friendly 2D mesh and quasi-three-dimensional mesh construction for regular and irregular grids; (ii) convenient operation in zonation of rock types or data interpolation for highly heterogeneous media; (iii) simulation results visualization with TECPLOT software for 3D and cross-section at different times from the model build to results analysis; (iv) implement of mesh generation by active/inactive grids assignment as well as grid name search by GUI.

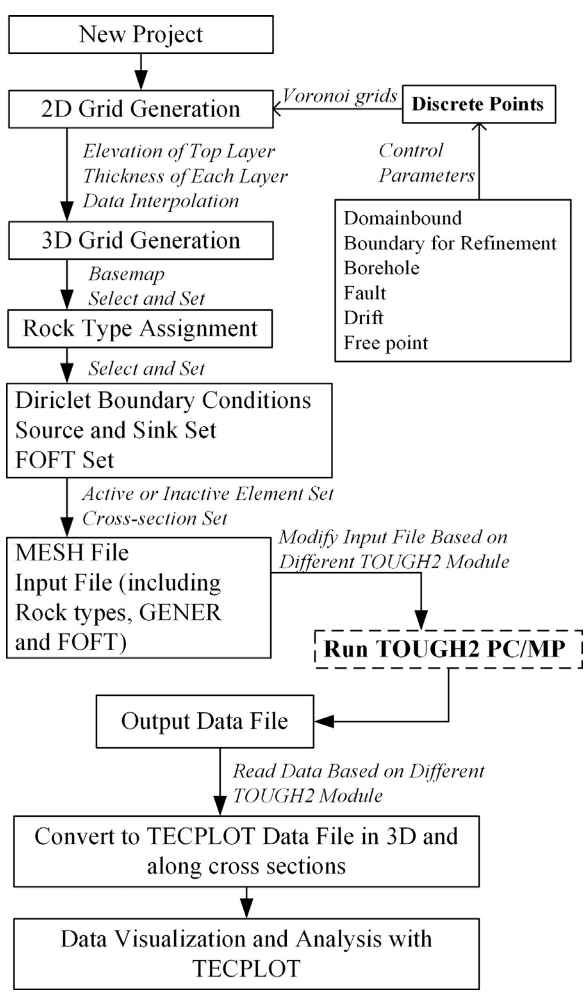

Fig. 1. Workflow of IGMESH.

For better presenting fluid flow and heat transport in local areas, mesh is required to be refined in area of interest. The information for mesh generation includes domain bound, boundary and parameters for refinement, well, fault, drift and free point. Elements are divided into discrete points according to different control method (Fig. 2). For example, the basic parameters of domain bound and refined area discretation is the interval along x (dx) and y axis (dy), and the rotation angle of x axis (θ), respectively. Well is divided by factors including the inner well radius, the farthest distance and interval factor. Free point is user-defined point.

The basic elements for 2D mesh generation consist of unique domain bound, a series of refined areas, wells, faults and drifts. For example, there are one domain bound, two refined areas, and seven wells in Fig. 3a. Domain bound, refined area, well element are discreted into red points, green and blue points, respectively. The Voronoi tessellation method is used to generate Voronoi diagrams in the plane and the relation of neighbor points in a polygon is obtained from the geometric relationship of Voronoi diagrams (Voronoi, 1908; Ahuja, 1982). The Voronoi diagrams are shown in Fig. 3b. The mesh data with different rock types, can be converted to gridblock-centered data and displayed in the TECPLOT software. The rock type at the top layer is shown in Fig. 3b. The cross-sections can be given by GUI, such as AA′ and BB′ in Fig. 3b. The cross sections along AA′ and BB′ can be seen in Fig. 3c and d, respectively. Pinch-out of lithology cannot be described with the mesh system because the mesh remain the same for each layer. However, different lithology can be assigned with different rock types, which can be used to represent pinch-out of lithology (Fig. 3c and d).

When Voronoi polygons are built, the variables, such as distance of two adjacent gridblocks and the area of a gridblock, can be calculated from the relation of Voronoi polygons. n is set as the number of nodes for a polygon. As shown in Fig. 4, assume S_p be the area of the Voronoi polygon ABCD (n=4). I and J are the center of two adjacent polygons. d_{i1} and d_{i2} are the distance of two adjacent polygons in the plane (Fig. 4a). d_u and d_d are the vertical distance of two adjacent polygons (Fig. 4b). M_u and M_d are the thickness of the upper and lower model layers. L_i is the length of each side of the polygon. V_{Iu} is the volume of a gridblock. The key parameters, S_p and V_{Iu}, can be calculated from the following formulae.