On The Development Of A Three-Dimensional Finite-Element Groundwater Flow Model Of The Saturated Zone, Yucca Mountain, Nevada

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ABSTRACT

Development of a preliminary three-dimensional model of the saturated zone at Yucca Mountain, Nevada, the potential location for a high-level nuclear-waste repository, is presented. The development of the model advances the technology of interfacing: (1) complex three-dimensional hydrogeologic framework modeling; (2) fully three-dimensional, unstructured, finite-element mesh generation; and (3) ground-water flow, heat, and transport simulation. The three-dimensional hydrogeologic framework model is developed using maps, cross sections, and well data that were gridded at an interval of 1500 meters by 1500 meters with variable depth over the entire model domain. A horizontal gridding interval of 500 meters by 500 meters is used to sample the northeast corner of the model domain that includes Yucca Mountain. The framework model provides different hydrogeologic units covering an irregularly shaped area of about 3,100 square kilometers. The framework-model data are used to feed an automated mesh generator, designed to discretize irregular three-dimensional solids, and to assign material properties from the hydrogeologic framework model to the tetrahedral elements. The mesh generator facilitated the addition of nodes to the finite-element mesh which correspond to the exact three-dimensional position of the potentiometric surface based on water-levels from wells, which are used for model calibration. A ground-water flow and heat simulator is run with the resulting finite-element mesh, within a parameter-estimation program. The application of the parameter-estimation program is designed to provide optimal values of permeability and specified fluxes over the model domain to minimize the residual between observed and simulated water levels.

INTRODUCTION

Yucca Mountain, Nevada is being characterized by the U.S. Department of Energy and its contractors as to its suitability as a potential site for a repository for high-level nuclear waste. Numerical models have been developed as part of this characterization of the ground-water flow system in the vicinity of Yucca Mountain. Personnel from the U.S. Geological Survey and Los Alamos National Laboratory have collaborated to develop the modeling approach presented in this paper.

The purposes for developing this model of the saturated zone of Yucca Mountain and vicinity are to: (1) estimate ground-water flow direction and magnitude from the design repository area to the accessible environment; (2) examine the complex three-dimensional behavior of flow through heterogeneous porous and fractured media; (3) account for the distribution of ground-water temperature; (4) identify the potential role of faults as barriers or conduits to ground-water flow; (5) interface high-resolution hydrogeologic-framework-model data directly into the construction of the numerical model of ground-water flow; (6) obtain optimal variable values used in the numerical model through parameter-estimation techniques; and (7) provide a means for subsequent flow, heat, and radionuclide-transport modeling using the calibrated model of the flow system.

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This paper discusses the development of a fully three-dimensional, finite-element model of the Yucca Mountain saturated-zone flow system. The following components are briefly discussed: (1) description of the numerical code of ground-water flow and heat transport; (2) construction of a three-dimensional hydrogeologic framework model and its interface with a fully three-dimensional finite-element mesh; and (3) interfacing the finite-element numerical model with a parameter estimation routine.

CONCEPTUAL MODEL

The domain selected for the model was first identified by Czarnecki and Wilson (1991). Model boundaries (fig. 1) do not coincide everywhere with ground-water divides; consequently, at certain locations lateral flow across the study-area boundary is expected. Within the model area, water in alluvium, volcanic, and carbonate rocks generally flows from north to south. Hydraulic head ranges from more than 1,100 m above sea level north of Yucca Mountain to about 600 m above sea level at the southern end of the study area at Franklin Lake playa, California (fig. 2). Hydraulic head is affected primarily by the: (1) distribution of hydrogeologic units; (2) geologic structure; (3) intensity and distribution of fracturing; and (4) proximity to recharge and discharge areas.

Recharge within the study area is assumed to be from the following sources: (1) downward and possible lateral recharge from episodic flooding of Fortymile Wash; (2) throughflow from Pahute and Rainier Mesas, which causes recharge along the northern border of the study area; (3) throughflow to the northwestern part of the Amargosa Desert; and (4) minor recharge from episodic flooding of the Amargosa River channel. Because of the present arid setting of the study area, in which precipitation ranges from about 100 to 200 mm/yr, only minor recharge is assumed to occur elsewhere in the study area.

Horizontal hydraulic gradients derived from the potentiometric surface range from about 0.0001 downgradient from Yucca Mountain to about 0.15 north and east of the design repository area (fig.2). Water levels used in constructing the potentiometric surface often represent a composite hydraulic head, derived from several hydrogeologic units. Depths to water range from about 3 m beneath Franklin Lake playa to about 750 m beneath Yucca Mountain. Downgradient from Yucca Mountain, in the Amargosa Desert, the potentiometric surface slopes gently toward the south (fig. 2). The potentiometric surface steepens at the Nevada-California State line (fig. 2), but flattens toward Franklin Lake playa and continues to slope slightly along the axis of the Amargosa River toward the south of Franklin Lake playa. Vertically upward hydraulic gradients are as much as 1.6, and ground-water discharge by way of evapotranspiration at Franklin Lake playa ranges from about 1 to 3 mm/d throughout the year (Czarnecki, 1990).

The cause and nature of the large hydraulic gradient (fig. 2) near Yucca Mountain are not known, although several explanations (Czarnecki and Waddell, 1984; Czarnecki and others, 1994; Fridrich and others, 1994) have been proposed: (1) faults that contain nontransmissive fault gouge or that juxtapose transmissive tuff against nontransmissive tuff; (2) the presence of a different type of lithology that is less subject to fracturing; (3) a change in the direction of the regional stress field and a resultant change in the intensity, interconnectedness, and orientation of open fractures on either side of the area with the large hydraulic gradient; (4) an apparent large gradient resulting from a disconnected, perched or semi-perched water body; or (5) a highly permeable buried fault that drains water from tuff units into a deeper regional carbonate aquifer. The gentle slope of the potentiometric surface 20 km downgradient from Yucca Mountain (fig. 2) is likely due to the presence of a transmissive aquifer of Tertiary(?) carbonate rock (Swadley and Carr, 1987).

Potentiometric and temperature data from deep holes drilled in the south-central Amargosa Desert indicate a potential upward component of ground-water flow (hydraulic gradients of 0.02) from depths as great as 600 m (Czarnecki, 1987). Upward flow is indicated by convex-upward profiles of ground-water temperature plotted as a function of depth; upward-flowing warm water causes a

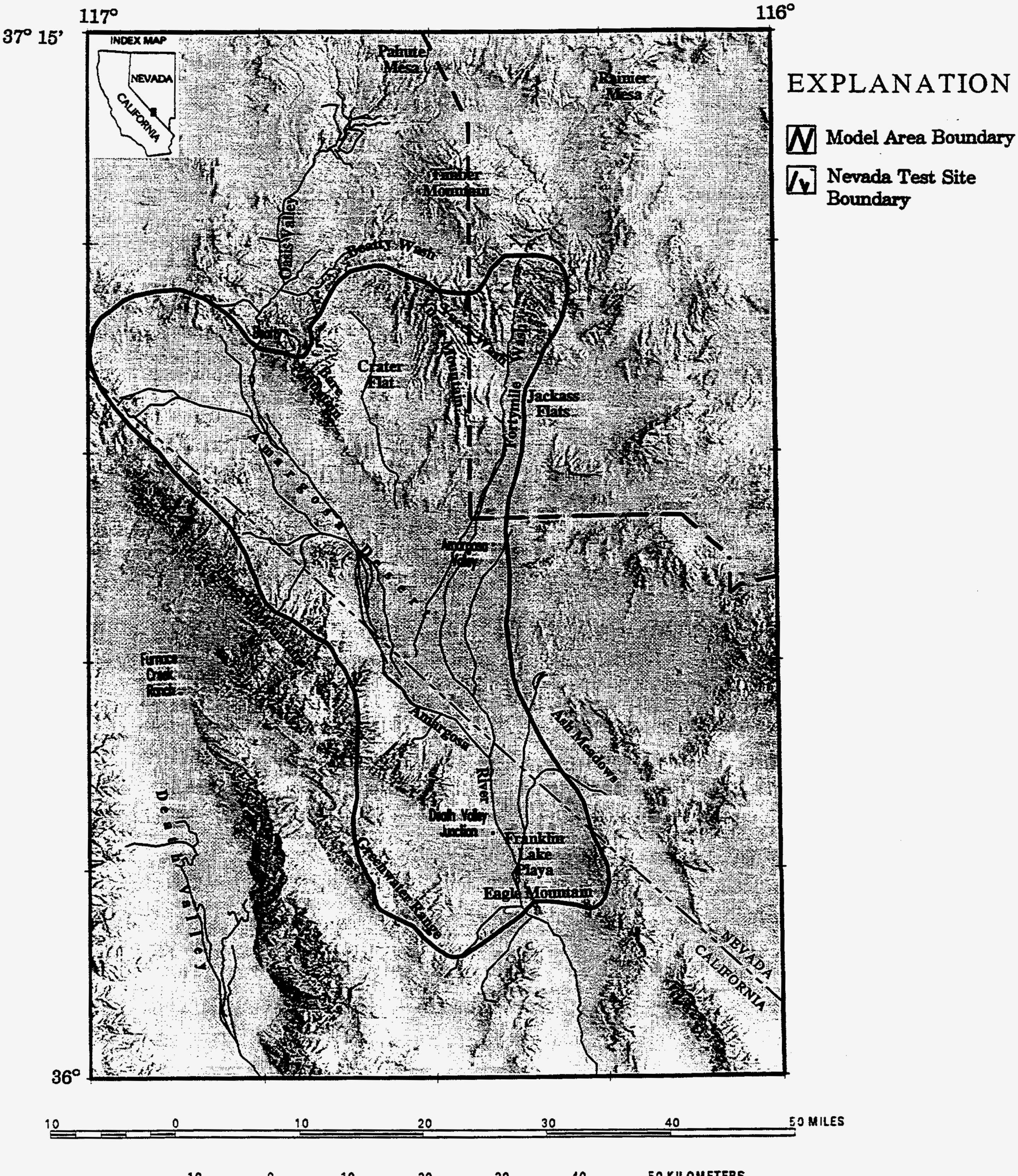

Figure 1. —Model area.

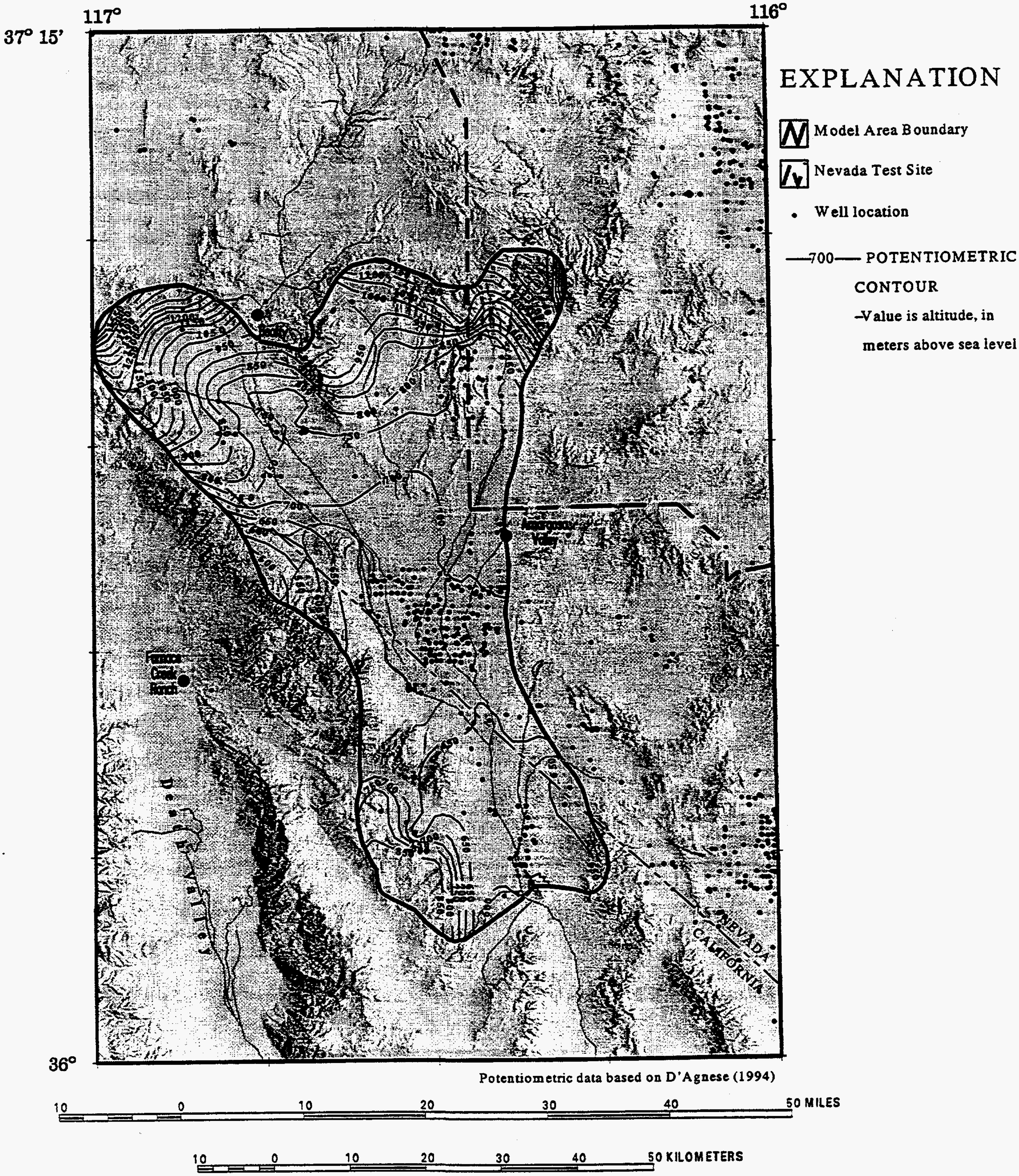

Figure 2. —Potentiometric surface.

temperature at a specific depth that is higher than that expected for a linear geothermal gradient.

Potentiometric data also indicate that a ground-water divide probably exists in the Greenwater Range, between the Amargosa Desert and Death Valley, California. Hydraulic head beneath the Greenwater Range is as much as 875 m above sea level; whereas, hydraulic head in the Amargosa Desert is about 620 m above sea level, and is below sea level in Death Valley.

DESCRIPTION OF NUMERICAL CODE

The FEHMN (Finite Element Heat Mass and Nuclide) computer code is used to simulate flow and transport through both the unsaturated and saturated zones. FEHMN is a nonisothermal, multiphase flow and transport code. It simulates the flow of water and air, and the transport of heat and contaminants, in 2- and 3-D saturated or partially saturated, heterogeneous porous media. The code includes comprehensive reactive geochemistry and transport modules and a particle tracking capability. Fractured media can be simulated using an equivalent continuum, discrete fracture, dual porosity or dual permeability approach. The basic conservation equations, constitutive relations and numerical methods are described in Zyvoloski and Dash (1990), Zyvoloski and others (1991), Reeves (1994), and Zyvoloski and others (1995a,b).

Conservation Equations

FEHMN solves three conservation equations: conservation of total fluid mass (air and water), conservation of air, and conservation of solute (contaminant). The mass of the solute is assumed to be small enough not to affect the total fluid mass balance. When energy transport mechanisms are considered, such as evaporative processes, a fourth conservation equation is necessary: conservation of energy.

Constitutive Relations

FEHMN requires information about air and water properties (and their derivatives) as functions of temperature (T) and pressure (P). Rational function approximations are used to estimate these variables in FEHMN, where the rational functions are a ratio of polynomials. For water, polynomial coefficients were obtained by fitting data from the National Bureau of Standards/Nuclear Regulatory Commission Steam Tables (Harr and others, 1984). The density of air is assumed to obey the ideal gas law.

FEHMN also requires information about the relation between relative permeabilities, capillary pressures and air-water saturations. Several well known functions (for example, Brooks-Corey; van Genuchten) are available to the user. This capability is important because the current domain for this application of FEHMN extends from land surface down to the saturated zone.

Numerical Methods

FEHMN uses a finite-element/finite-volume method to discretize the conservation equations to be solved. Newton-Raphson iteration is applied to the fully coupled system of equations. This system of equations is solved with multi-degree of freedom preconditioned conjugate gradient methods, using generalized minimum residual (GMRES) acceleration techniques.

INTEGRATION OF 3-D HYDROGEOLOGIC FRAMEWORK MODEL

To examine the complex 3-D behavior of flow through heterogeneous porous and fractured media, a detailed model of the hydrogeologic framework was developed. Development of a 3-D hydrogeologic framework model begins with the assembly of primary data: digital elevation models (DEM), geologic maps and sections, and lithologic logs. Each of these primary data can be manipulated by standard Geographic Information Systems (GIS); however the merging of these diverse data types to form a single coherent 3-D digital model requires more specialized Geoscientific Information System (GSIS) software.

Construction of a 3-D framework model involves four steps: (1) DEM data are combined with geologic maps to provide a series of points locating surfaces of individual geologic units; (2) geologic sections and lithologic logs are used to provide locations of geologic units in the subsurface; (3) interpolation of both surface and subsurface positions for each geologic unit is done with sophisticated gridding and contouring software which incorporate unit offsets across faults; (4) a geologic framework model is developed when individual surfaces are combined, utilizing appropriate stratigraphic principles to control their sequence and lateral extent.

The hydrogeologic framework model initially was developed for the area bounded by latitude 35°N and 38°N and longitude 115°W and 118°W, that encompasses the Death Valley regional ground-water flow system. The regional model represents approximately 100,000 km^2 and extends to depths of 10 km. The area has a semiarid to arid climate and is located within the southern Great Basin, a subprovince of the Basin and Range physiographic province. Elevations range from about -90 m to +3600 m; thus the region includes a diversity of climate regimes and associated ground-water recharge and discharge conditions. Additional subdivision of hydrogeologic units was done on an area bounded by latitude 36°N and 37°15'N and longitude 116°W and 117°W resulting in the identification of 16 hydrogeologic units. This refined framework will be used in the flow model that only covers 3,100 km^2.

The geology used in the framework model is typical of the Basin and Range; that is, a variety of intrusive and extrusive igneous, sedimentary, and metamorphic rocks that were subjected to several episodes of compressional and extensional deformation. The present-day topographic relief resulted in large part from Late-Cenozoic tectonism.

For the purposes of ground-water flow modeling, the hydrogeologic framework model (HFM) can be used to develop appropriate permeability values derived from hydraulic conductivity. Bedinger and others (1984) developed a series of curves defining the distribution of hydraulic conductivity for some of the hydrogeologic units contained in the HFM. These hydraulic-conductivity values likely are affected by depth and by the degree and type of faulting. The 3-D HFM contains attributes defining the hydrogeologic unit, depth, and faulting conditions for each cell. A set of rules were developed to reclassify the HFM to include hydraulic conductivity based on these attributes (Faunt, 1994, pp. 142-143). Thus, by assessing the effect of each of these attributes, appropriate hydraulic-conductivity values can be derived for each cell.

3-D FINITE-ELEMENT MESH CONSTRUCTION

After constructing a 3-D HFM, an automated finite-element mesh-generation computer program, GEOMESH (Gable and others, 1995), is used to construct a computational grid of tetrahedral elements in three dimensions. There are three basic criteria to ensure grid integrity and quality in translating from an HFM to a finite-element grid. First, the final grid must preserve the geometry of the HFM input. All material interfaces, layer truncations, external boundaries and model geometry must be preserved. Although this is a straight-forward process, it does not ensure grid quality. Second, grid quality is ensured by always producing a Delaunay grid (Gable and others, 1995), which has desirable qualities when implementing finite-element equation solvers. In two dimensions, a Delaunay triangulation of a point set produces a grid where the circumscribed circle of every triangle will not have any points in its interior. The third criteria is that the geometric coupling coefficients of the finite-element mesh are all positive and form a semi-positive coefficient matrix (Trease and Dean, 1990).

The data structure of an HFM has a number of features that must be dealt with to produce a computational grid. The HFM is an ordered array of hexahedral (8 node, 6 face) elements, whose array of IxJxK elements has (I+1)x(J+1)x(K+1) nodes. However, a large number of these elements may have to be eliminated. The reason for this is that if a hydrogeologic layer pinches out to zero thickness, the HFM does not eliminate the layer from the data structure, it simply continues the layer with zero thickness. This can produce zero-volume elements that must be removed. Also, because the HFM representation must have a rectangular shape in map view, irregular areas are modeled by assigning null values to cells outside the area of interest. These null elements must also be eliminated. When this process is finished the model is an unstructured, hexahedral, finite-element representation of the hydrogeologic model.

Hexahedral elements are then converted to tetrahedral elements. Each hexahedra can be broken into five, six or twenty-four tetrahedra, the later being used for this model. Delaunay criteria are enforced without allowing any connections to cross material interfaces by adding nodes on interfaces when a connection crosses an interface, thereby increasing the number of nodes and elements. The final step is to ensure that there are no negative-coupling coefficients. This is done by calculating the area vectors associated with all elements, and if any are negative, the element is divided until the coupling coefficients are positive. This step also adds nodes and elements to the mesh.

Further enhancement of the final mesh is also possible. Increased resolution may be required in some parts of the model. This is done with the grid refinement utilities of GEOMESH. Meshes corresponding to different areas can be joined together using mesh merging utilities, which allows a large model to be constructed from smaller and simpler pieces.

MODEL CALIBRATION STRATEGY

Several steps remain in achieving a model calibrated against field observations (such as water levels, permeability measurements, and flux measurements). The first step is the construction of a new 3D finite-element mesh of the study area using the add-mesh capabilities of GEOMESH. The new mesh will be based on an HFM sampling of the entire model area at a cell spacing of 1500 meters. An outer band of elements surrounding the lateral edges of the model domain might be added to accommodate the specification of fluxes that will be extracted from a larger finite-difference model of the regional ground-water flow system. This outer band of elements will correspond exactly to the top two layers of the regional finite-difference model to facilitate the specification of fluxes.

In the northeastern segment of the model domain, which includes all of Yucca Mountain, a separate mesh will be constructed on the basis of an HFM sampling at a cell spacing of 500 meters. This separate finer mesh will be added to the coarser mesh using the add-mesh capability of GEOMESH. Additional nodes corresponding to water levels in wells in three-dimensional space will be added to this combined mesh, providing points for water-level calibration.

General flux boundary conditions will be derived from the regional finite-difference model and assigned to the appropriate nodes of the 3D finite-element mesh. In addition, recharge fluxes will be specified along Fortymile Wash, Amargosa River, and an unnamed wash in Crater Flat, and discharge fluxes will be specified along Carson Slough and Franklin Lake playa. Areal recharge and discharge elsewhere in the model domain is considered minor. This forward-model configuration will be used to obtain a steady-state model run of the flow system.

The configuration of the forward FEHMN model will be modified to provide input to a model-independent parameter estimation routine, PEST[3] (Watermark Computing, 1994). The routine will be used to optimize permeability values using observations of water levels. Because FEHMN simulates pressures and saturations, water levels at the observation nodes (which were added to the finite-element mesh) will be identified as having a pressure head of 0.0 and a saturation of 1.0, thus providing two observations at each node against which PEST may calibrate the model permeability values. If low correlations between permeability parameter zones and fluxes can be achieved, PEST will be used to optimize both permeability values and fluxes. Some permeability estimates from hydraulic testing in the study area will be used to constrain optimized model values.

FEHMN was successfully coupled with PEST and used in trial parameter estimation runs. PEST returned flux and permeability estimates within 2 percent of those specified for a previous steady-state simulation, using only seven pressure observations located at the corners of a simple cubic domain comprised of 1331 nodes.

SUMMARY

This paper presents the development of a preliminary three-dimensional model of the ground-water flow system at Yucca Mountain, Nevada. The model required interfacing of the following processes: (1) complex three-dimensional hydrogeologic framework modeling; (2) fully three-dimensional, unstructured, finite-element mesh generation; and (3) ground-water flow, heat, and transport simulation. The framework-model data were used to feed an automated mesh generator (GEOMESH), designed to discretize irregular three-dimensional solids, and to assign material properties from the hydrogeologic framework model to the tetrahedral elements. GEOMESH facilitated the addition of nodes corresponding to the exact three-dimensional position of the potentiometric surface based on water-levels from wells, which are used for model calibration. A finite-element ground-water flow and heat simulator (FEHMN) was run with the resulting 3D finite-element mesh, within a parameter-estimation program (PEST). The PEST program was applied to provide optimal values of permeability and specified fluxes over the model domain to minimize the residual between observed and simulated water levels. Application of the calibrated model could be extended to examine radionuclide transport using FEHMN.

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