The Long Road to Groundwater RODs on the ORR: Development of a Regional Groundwater Model – 15632

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ABSTRACT

This paper describes the first year of planning and development for the Oak Ridge Reservation (ORR) regional groundwater flow model (ORGFM). The first stage involved the creation of a groundwater model Technical Advisory Group (TAG), made up of local and national industry experts to support the model development. As a first step in the model development process, a smaller-scale model (a Test Case Model) is being developed to test the modeling tools and approach being considered for the regional model. The Test Case Model is allowing the team to identify and develop workflow processes on a small scale prior to developing the large, regional-scale model. The modeling team currently is testing the combined use of EarthVision®[1] and MODFLOW-USG (a modular finite-difference flow model using un-structured grids) to develop the regional-scale model. It is anticipated that the ORGFM will be completed by 2016. This paper presents the progress of the ORGFM model development.

INTRODUCTION

The complexity of the groundwater contamination issues on the U. S. Department of Energy's (DOE's) Oak Ridge Reservation (ORR) in East Tennessee has contributed to a long, methodical approach to Comprehensive Environmental Response, Compensation, and Liability Act of 1980 (CERCLA; [1]) decision-making related to groundwater in Oak Ridge. In 2011, the members of the ORR Federal Facility Agreement (DOE, U.S. Environmental Protection Agency [USEPA] Region 4, and the state of Tennessee) agreed to develop a formal, long-term Groundwater Strategy for the ORR. The resulting strategy included prioritization of 35 unique groundwater contaminant issues, identification of key data gaps and uncertainties related to groundwater on the ORR, and recommendations for implementing a strategy [2]. DOE began implementation of three of the recommendations in 2014, including: (1) set up an ORR Groundwater Program to implement the strategy; (2) implement an off-site groundwater quality assessment; and (3) develop and maintain an ORR-wide regional groundwater flow model to ensure a single, regional, calibrated model to support groundwater characterization, decision-making, and remediation.

Objectives of the ORGRM

Currently there are six final large watershed-scale groundwater Records of Decision (RODs) included in the ORR Environmental Management Program lifecycle baseline. The watersheds represent separate plant production areas with unique localized surface water-groundwater flow systems that all eventually drain to the Tennessee River drainage system. The ORGFM will provide a single, calibrated flow model

[1] Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof or its contractors or subcontractors.

for establishing flow boundary conditions for the individual plume models that will be necessary for the watershed RODs. A primary consideration for these watershed RODs will be the need to assess the potential for off-site deep groundwater flow, making this a primary objective for developing the regional model.

Technical Advisory Group

From the outset of the ORGFM project, it was determined that stakeholder involvement in planning and model development was critical to acceptance and long-term use of the model. It was also determined that independent technical expertise would help identify the best technical approach. To this end, the DOE established the ORR TAG, made up of stakeholders interested in the application of the model and industry experts experienced in the construction and calibration of large-scale flow models, specifically in fractured-flow environments. The Full TAG was made up of representatives from the DOE, USEPA Region 4, the state of Tennessee Department of Environment and Conservation (TDEC), URS|CH2MHill of Oak Ridge (UCOR) staff and subcontractors, and industry experts. The experts were also on a Technical Subcommittee, and included: Dr. Steve Haase, chairman and UCOR technical lead; Dr. Dan Goode of the U.S. Geological Survey (USGS); Dr. Barnard Kueper, an international karst model expert from Queen’s University, Ontario, Canada; Dr. Alauddin Khan, from Leidos, the lead modeler on the team with 20 years of experience modeling on the ORR; Nathan Voorhies, from Battelle, selected for experience applying EarthVision [3] at other DOE sites; and Gareth Davies, TDEC’s karst technical expert.

The full TAG met twice in fiscal year 2014 to agree on the model development approach. The Technical Committee of the TAG held additional meetings to tackle the technical details of the effort. This committee reviewed the available site conceptual model and past groundwater modeling projects on the ORR. Key findings from this review indicated that a regional flow model should be able to represent:

- The geologic structure of the model domain, including dipping beds with anisotropic flow
- Fractures with strong heterogeneity in a 3-D domain
- The influence of a hypothetical karst conduit on groundwater flow

The TAG developed a list of recommendations for designing and implementing the ORGFM (Table I). Key recommendations included:

1. Selection of the model code
2. Size of the model domain
3. The need for a Test Case Model, as well as construction and calibration requirements for the test.

Selection of Model Code

The TAG evaluated 14 model codes, several of which have been applied on ORR projects in the past. Based on the evaluation, three codes were seriously considered for selection: FEFLOW [4], Finite Element Heat and Mass (FEHM) [5], and the newest version of the USGS’s Modular Finite- Difference Flow Model (MODFLOW) code, MODFLOW-Un-Structured Grid (USG) [6]. The TAG recommended moving forward MODFLOW-USG, subject to presenting reasonable results in a test case. MODFLOW-USG was selected based on the following considerations:

TABLE I. 2014 Technical Advisory Group recommendations.

Target	Considerations	TAG recommendation
	Regional Flow Model	
Regional Groundwater Flow Model Code	Fourteen potential candidate codes	MODFLOW-USG (*still being tested*)
Regional model domain area/flow boundaries	Can use the MODFLOW River Package (RIV) to represent the hydrologic boundaries and no-flow boundary to represent the boundary at the Kingston Fault	Clinch River to the northeast and south; Tennessee River to the southwest; and Kingston fault to the north
Regional model domain bottom depth	Incorporating brine layer at depth would require variable density modeling capabilities	Sea level (0 m amsl); justified on the basis that the brine layer represents a no-flow boundary to fresh water
	Hydrofracture injections were approximately 320 m bgs	Hydrofracture project will require a separate model that can handle variable density conditions
Conceptual model development	Need capability to develop 3-D, to-scale geologic framework to feed MODFLOW-USG	EarthVision® with capability to export spatial data output to other software, including ModelMuse (requested by EPA) [7]
	Test Case Model	
Test Case Model application	MODFLOW-USG has not been used on ORR to date	Start model development with a Y-12 Test Case using MODFLOW-USG with focus toward completion of a regional model
Test Case Model domain	Main purposes of test case: (1) Evaluate MODFLOW-USG applicability to ORR (2) Develop and test work flow processes looking toward regional model	Y-12 area included in the 1996 BCV FS MODFLOW-88 model: East - Scarboro Creek; west- topographic high west of State Highway 95; north - top of Pine Ridge; south - top of Chestnut Ridge; and bottom - sea level
Data sufficiency for Test Case Model	Focus on key model parameters such as formation dip, K, recharge, hydraulic head, and hydraulic head target calibration data	Y-12 data sufficient to test MODFLOW-USG
Test Case calibration requirements	Resource limitations on calibrating test case	Perform reasonable degree of calibration; review by TAG
Test Case Model sensitivity analysis scope	Resource limitations on sensitivity analysis for test case	Limited analysis on one or two model parameters
Option to perform a Phase 2 interim test case	Interim test case will delay regional model development	Move directly from test case to regional flow model

3-D = three-dimensional
BCV = Bear Creek Valley
bgs = below ground surface
EPA = U.S. Environmental Protection Agency
FS = feasibility study
MODFLOW-USG = Modular Finite-Difference Flow Model using Un-Structured Grids
ORR = Oak Ridge Reservation
TAG = Technical Advisory Group
Y-12 = Y-12 National Security Complex

- MODFLOW-USG has the necessary features to adequately represent regional groundwater flow within the ORR geologic environment – heterogeneous rock formations with dipping beds, anisotropic flow conditions, and karst features.
- MODFLOW-USG modular structure allows for integration with additional modules (e.g., the Connected Linear Network [CLN] package for modeling conduit flow, the river flow boundary package [RIV], and a total of > 50 additional packages that may be needed).
- MODFLOW-USG works with a large array of public and commercial pre- and post-processors.
- MODFLOW-USG is the industry standard, public domain groundwater model and, as such, has been continuously tested, verified, and validated. It has been used as the regional flow model code at major DOE sites.
- The modeling team has long experience with MODFLOW; free technical support is available, including model upgrades as requested.
- The model layers in MODFLOW-USG do not have to be continuous across the entire model domain.

MODFLOW-USG [6] is the newest version of MODFLOW and was developed to support a wide variety of structured and unstructured grid types, including nested grids and grids based on prismatic triangles, rectangles, hexagons, and other cell shapes. MODFLOW-USG is a 3-D control volume finite difference (CVFD) groundwater modeling package that simulates steady and unsteady flow through conduit and fracture network, aquifer materials as confined, unconfined, or a combination of confined or unconfined. External flow stresses such as wells, areal recharge, and flow through riverbeds and drains can be simulated. MODFLOW-USG has a modular structure that allows it to be easily modified to adapt the code for a particular application. Hydraulic conductivities or transmissivities for any layer may differ spatially and be anisotropic (restricted to having the principal directions aligned with the grid axes), and the storage coefficient may be heterogeneous. Specified head and flux boundaries can be simulated, as can a head dependent flux, across the model's outer boundary that allows water to be supplied to a boundary block in the modeled area at a rate proportional to the current head difference between a "source" of water outside the modeled area and the boundary block. Due to flexibility in grid design in MODFLOW-USG, it can be used to focus resolution along rivers, faults, inclined beds, and around wells, for example, or to sub-discretize individual layers to better represent hydrostratigraphic units. The grid in upper layers around rivers and drains can be refined and have coarser refinement in lower layers. Similarly, the grids around well screens in lower layers can be refined and the grid layers above the well screen can have coarser refinement. This unstructured grid design within MODFLOW-USG results with in fewer cells as compared to the traditional MODFLOW code [8 and9]. In MODFLOW-USG, the model layers do not have to be continuous across the entire model domain.

MODFLOW-USG is based on an underlying CVFD formulation in which a cell can be connected to an arbitrary number of adjacent cells. To improve accuracy of the CVFD formulation for irregular grid-cell geometries or nested grids, a generalized Ghost Node Correction Package that uses interpolated heads in the flow calculation between adjacent connected cells is an optional addition to MODFLOW-USG. MODFLOW-USG includes a Groundwater Flow (GWF) Process, based on the GWF Process in MODFLOW 2005, as well as a new Connected Linear Network (CLN) Process to simulate the effects of multi-node wells, karst conduits, and tile drains, for example. The CLN Process is tightly coupled with the GWF Process in that the equations from both processes are formulated into one matrix equation and solved simultaneously. This robustness results from using an unstructured grid with unstructured matrix storage and solution schemes. MODFLOW-USG also contains an optional Newton-Raphson formulation (MODFLOW-NWT) for improving solution convergence and avoiding problems with the drying and rewetting of cells. MODFLOW-USG uses a new solver, Sparse Matrix Solver (SMS) Package, which provides several methods for resolving nonlinearities and multiple symmetric and asymmetric linear solution schemes to solve the matrix arising from the flow equations and the Newton Raphson formulation, respectively.

Because MODFLOW-USG allows for new emphasis on the underlying geologic framework of the model area, the TAG also agreed to use the EarthVision® software package [3] as the tool for developing the 3-D geologic model. EarthVision® was selected due to the fact that it has functions and visualization capabilities that outpace all other similar software. Some stakeholders expressed concern that EarthVision® is an expensive commercial software that requires significant training and experience to run, resulting in a limited number of people and organizations who would be able to use the EarthVision® software. The TAG agreed that the model development team should identify approaches that will allow the data sets developed and stored in EarthVision® to be exported to other similar tools. The model development team identified the following data file export capabilities in EarthVision®: Z-MAP (either pre- or post-R98), American Standard Code for Information Interchange (ASCII), SEG-Y, DXF ("Drawing Interchange" file format), Gocad (.gp), Simulator Preprocessor, and Environmental Systems Research Institute (ESRI) Shapefile format files. Members of the TAG agreed that with the ability to export ASCII format files and Geographic Information System (GIS) shapefiles generated in EarthVision®, it should make the information transportable to most graphical user interface (GUI) software tools.

The modelers recommended using Groundwater Vistas (GV) [10] as the GUI to process information from EarthVision® to MODFLOW-USG, and perform additional model pre- and post-processing tasks.

Model Domain Boundaries

Fig. 1 shows the approximate boundaries of the regional-scale model as further described in Table I. The boundaries of the regional flow model to the north, east, and south were relative easy to identify. To the east and south, the boundary will be the Clinch River (the hydrologic boundary). To the north the boundary will be the Kingston Fault line (a no-flow boundary), which is also an approximate topographic high line north of ETTP.

The west, southwestern boundary of the model is not as certain and may move as model development occurs. The two options evaluated for the southwestern boundary were: (1) the hydrologic boundary, the Tennessee River; and (2) a slight topographic divide between I-40 and the Tennessee River. TDEC representatives pointed out that the Tennessee River may not be the true downgradient flow boundary for waters flowing under the ORR and that the boundary could be further to the southwest. However, TDEC agreed that the Tennessee River would be an acceptable boundary. The modelers indicated that taking the model to the Tennessee River would not cause computational stresses on the model runs if a computer with increased random-access memory (RAM) is available to the team. The team also agreed that since it is not known if the slight topographical high point southwest of I-40 is a true groundwater flow divide, it should not be a forced boundary. Several team members pointed out that although the river stage data can be used for calibration purposes for both the scenarios, it will be easier to communicate and explain the Tennessee River serving as the boundary. Based on these considerations, the TAG recommended the Tennessee River as the southwestern boundary of the regional flow model.

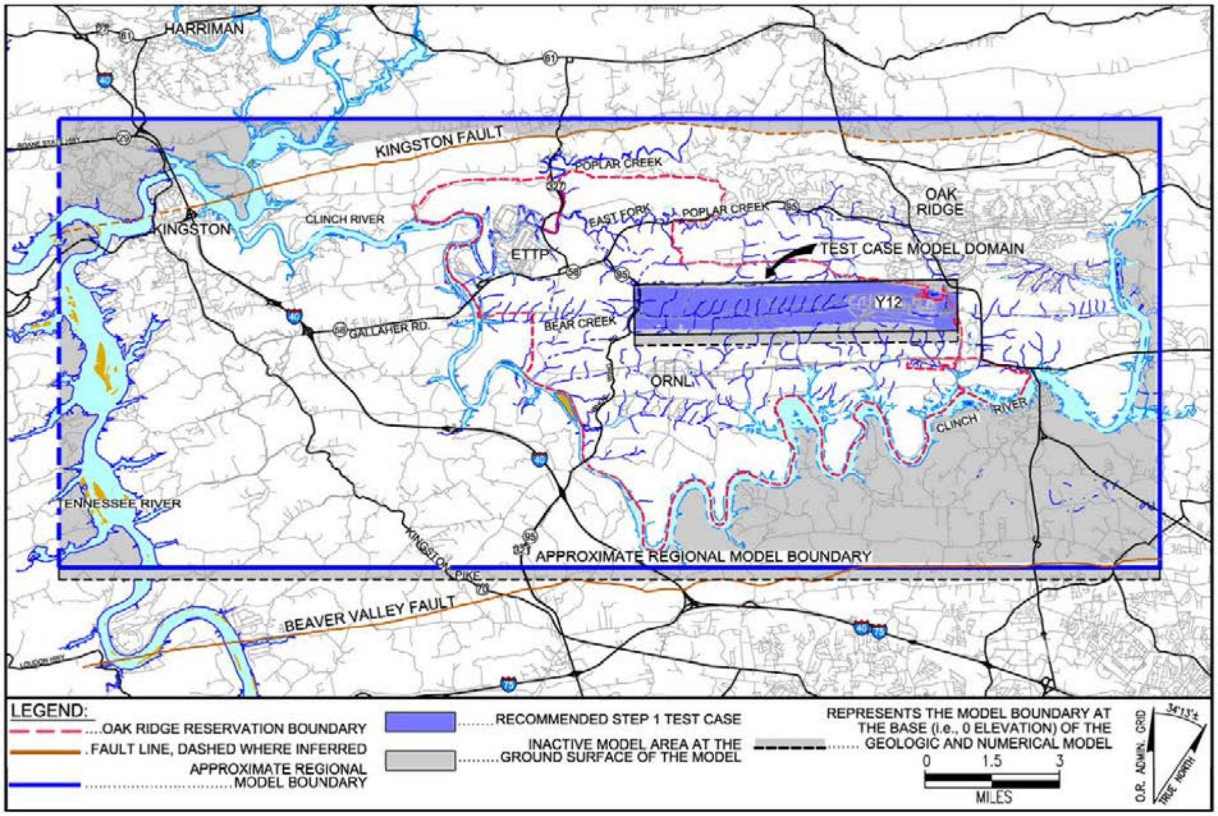

Fig. 1. Oak Ridge groundwater flow model domain

Test Case Model

Members of the Technical Committee of the TAG agreed that a test of MODFLOW-USG was needed prior to full-scale regional application. The goals of a Test Case Model were to 1) allow the modeling team to become familiar with the selected model code, MODFLOW-USG, which is relatively new and untested on the ORR; 2) establish work flow processes for moving from the conceptual site model to the numerical model; and 3) test MODFLOW-USG's ability to model a stratified, heterogeneous aquifer with a high degree of anisotropy, dipping beds and conduit flow. The TAG recommended limited but sufficient calibration for the test, mostly to show using particle tracts that the model was simulating proper flow directions, thereby accounting for the anisotropic conditions on the ORR.

Model development activities performed in 2014 and described below focus on the development of the Test Case Model.

2014 TEST CASE MODEL DEVELOPMENT ACTIVITIES

Test Case Model Domain

The Y-12 Plant site in the Bear Creek Valley watershed was selected as the area for the test because of the large amount of geologic and hydrologic data available for this area. In addition, a historical MODFLOW model was developed and calibrated for this area in the mid to late 1990s and could be used as the starting framework for testing MODFLOW-USG. The Test Case area is identified in Fig. 1.

Test Case Conceptual Model Development

The conceptual site model (CSM) for the Test Case Model was developed in two steps: 1) identification, compilation, analysis, and interpretation of available data for the entire regional model domain; and 2) population of selected data into a 3-D, to-scale depiction of the geologic framework using EarthVision®.

Numerous field studies and data analysis activities have been performed on the ORR since the 1950s. Much of the information generated is pertinent to developing the CSM. The historical data were in a variety of forms including electronic spreadsheets, American Standard Code for Information Interchange text files, electronic information stored in the Oak Ridge Environmental Information System, electronic data available from the USGS, electronic data available from the Tennessee Valley Authority, published geologic maps available from the Tennessee Division of Geology, an unpublished geologic map of the ORR, published USGS reports, numerous published and unpublished DOE ORR documents, and electronic files from previous groundwater modeling efforts on the ORR. The model team has developed a separate report documenting all data collection activities, analysis, and references and plans to update the report throughout the model development period.

Test Case Model Geology

The Y-12 Plant site and associated waste disposal areas are located in BCV (Fig. 2). The geology is shale-dominated aquitard units of the Conasauga Group in the northern portions of the valley and the Knox Group/Maynardville Limestone aquifer in the central/southern portion of the valley. Bedding strike is generally N55°E, with dips averaging about 38° southeast. The unconsolidated zone consists of soil and weathered bedrock, ranging from 0 to 25 m thick. The Maynardville and Knox Group rocks exhibit significant karst development. Details of BCV geologic descriptions can be found in *Groundwater Strategy for the U.S. Department of Energy Oak Ridge Reservation, Oak Ridge, Tennessee* [2].

- The hydrostratigraphic units underlying BCV are characterized by anisotropic hydraulic conductivities that are higher in the direction of geologic strike. The highest anisotropy is observed in the Nolichucky Shale ranging between 3 and 38 based on either aquifer or tracer test. The observed average value for Maynardville Limestone is 14.9 while Maryville Limestone is 5 and the Conasauga Group varies between 2 and 4.

- The flow paths in the near surface storm-flow zone are active only during and immediately following storms; most water drains to nearby streams.

- The water table interval (comprising the saturated zone of the regolith and the weathered bedrock) is the most active part of the groundwater system and accounts for most of the groundwater component of the flow in the streams during storms and most of the baseflow during high-flow periods. Groundwater flow in this interval can be as fast as 40 m/day.

- Flow along strike and across strike in the deep bedrock interval occurs at a much slower rate, accounting for < 1% of the total flow in the aquitard formations. However, groundwater modeling suggests that migration pathways along strike can cross tributary watershed boundaries and eventually discharge directly to the Maynardville Limestone where flow is dominated by fractures and karst conduits.

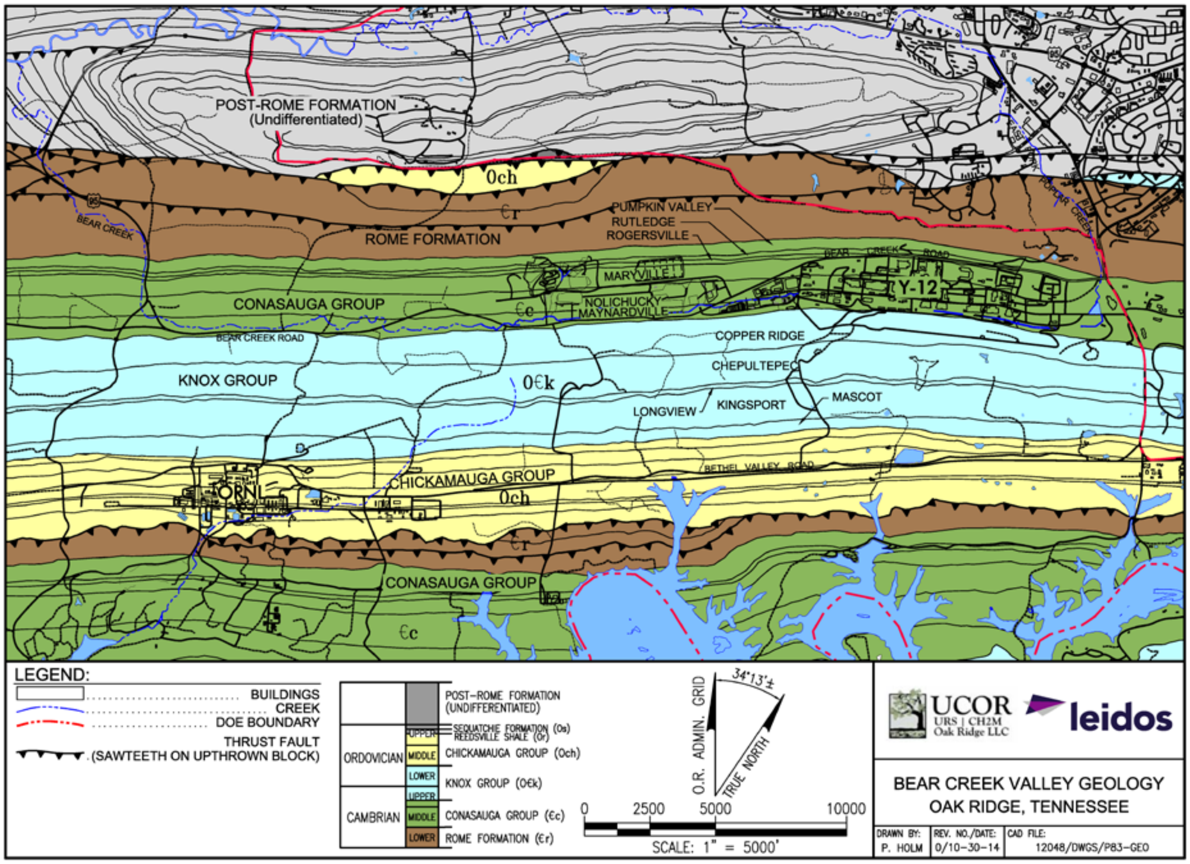

Fig 2. Stratified geology of Bear Creek Valley

- Because active fractures occur at greater depth in the Knox Group and the Maynardville Limestone, active groundwater circulation is deeper in these formations. Contaminant plumes in the Knox and Maynardville (Conasauga) carbonate-dominated formations (i.e., plumes in BCV and the UEFPC) have migrated further and deeper than the plumes in adjacent clastic-dominated formations.

- In the shale formations of the Conasauga Group, there is generally an upward hydraulic gradient at depths ranging from 14 to 150 m below ground surface (bgs). However, at shallow depth the vertical gradients reverse in response to recharge events.

- The hydraulic conductivity of the subsurface materials has been observed to decrease rapidly with increasing depth causing significantly higher groundwater flux rates in the shallow portion of the flow system.

- The hydraulic conductivities in BCV range from 1E-05 m/day to 50 m/day with most of the higher conductivities observed in the shallow groundwater interval. However, conductivities in the range of 0.003 to 0.3 m/day have been observed in the deeper interval of the Maynardville Limestone (183 to 396 m bgs) and Knox Group (61 to 152 m bgs).

A key component of the CSM is the description of the water balance, necessary for estimating recharge to the aquifer. Precipitation recharge is the major source of water for the groundwater system beneath the BCV. The modeling effort performed for the Bear Creek Valley RI/FS evaluated historical efforts to quantify recharge rates [11 and 12]. Estimated recharge rates ranged from 13 to almost 50 centimeters (cm)/year. The BCV RI/FS calibrated flow model [12] resulted in a recharge rate of 27 and 18 cm/year for the carbonate and shales, respectively.

As indicated, there is considerable variation in historical estimates of recharge to the bedrock groundwater flow system, and thus recharge becomes a major uncertainty in model development that will need to be addressed in the calibration and sensitivity analysis stages.

Natural groundwater discharge in the BCV occurs through seeps and springs, streams, and evapotranspiration. Bear Creek, its tributaries, and the solution cavity system along Bear Creek are the major discharge areas for groundwater moving through the interbedded strata of BCV. UEFPC is the major discharge stream in the eastern part of BCV.

Population of EarthVision®

Working in MODFLOW-USG places additional emphasis on a quantitative 3-D representation of the site geology since model layers can more accurately mimic the site geology. The team elected to first build the 3-D, to-scale geologic model in EarthVision® and export/import the EarthVision® model to MODFLOW-USG.

The workflow process in EarthVision® for construction of the 3-D geologic model primarily consists of assembling American Standard Code for Information Interchange (ASCII) text files, which contain space- or tab-delimited data for input into gridding, annotation (display), and 3-D model-generation routines. Experienced users rely on scripting routines to both manipulate/structure files and to build the 3-D models. A graphical user interface (GUI) is available for each EarthVision® module (e.g., Workflow Manager, Geologic Structure Builder, etc.). These GUIs can be used to build scripts that can subsequently be saved, modified as part of process automation, and iteratively re-used. EarthVision® accepts a variety of specialized file formats associated with seismic data collection and petroleum industry standards but does not natively handle more common file types in use by the environmental business such as Excel and Access. The same holds true for EarthVision® output intended for other external programs such as those used for groundwater modeling; most exports are shapefiles or ASCII text format with x,y,z and attribute information.

Key datasets used for the development of the 3-D model included:

- An Excel spreadsheet containing depth to weathered bedrock and depth to competent bedrock for approximately 1130 wells drilled over 50 years on the ORR.
- A geologic pick data set from ORR reports and data sources for the Y-12 Test Case model area. This includes the top depth/elevation for geologic picks (contacts) identified in 337 drill holes in this area

of the ORR, as well as other information associated with the screen, screen placement, depth to water, depth to weathered bedrock

- The *2012 Preliminary Detailed Geologic Map of the Oak Ridge, Tennessee, Area* by Peter J. Lemiszki (Tennessee Division of Geology); Robert D. Hatcher, Jr. (University of Tennessee, Knoxville); and Richard H. Ketelle (UCOR, Oak Ridge). This map is not available in a form that can be referenced at this time. This map covers roughly 90+% of the regional ORR model space and includes detailed surface geology. Geology maps from the State were also used.
- USGS NED tiles from the National Map Viewer for generating the topographic surface in the model space.
- The USGS High-Resolution National Hydrography Dataset (1:24,000 scale) for Stream/Water Bodies

A separate report of the data and detailed approach to building the conceptual geologic model in EarthVision® has been developed by the team. Fig. 3 shows a cross section slice through the Test Case EarthVision® model looking down Bear Creek Valley from the northeast to the southwest.

The layer surfaces used to construct the EarthVision® 3-D geologic model were exported to Groundwater Vistas/MODFLOW-USG. These surfaces, shown in the foreground of Fig. 3, include the eight surfaces that define the top of the eight dipping bedrock units included in the geologic model area, plus three surfaces that are laid on top of these eight dipping grids (top of competent bedrock, top of weathered bedrock, and topography). In broad terms, export of the EarthVision® surfaces to MODFLOW-USG involved nulling (truncating) the surfaces in areas beyond the numerical model domain and then exporting the nulled surfaces to x,y,z ASCII data files.

Test Case Numerical Model Development

Although model development continues as of the writing of this paper, enough Test Case model construction activities have occurred to test various functions of MODFLOW-USG. After numerous attempts the team was successful at the export-import of the 3-D geologic model framework from EarthVision®. In addition the following data has been populated into the Test Case MODFLOW-USG model:

- Hydraulic Conductivities: Hydraulic conductivity values applied for the initial model setup were obtained from the site-specific measurements data (see below).

- Recharge: The average recharge during dry season based upon site-specific water balance was used to set up the initial numerical model. For the initial test case runs, the following recharge rates have been used: 18 cm/year in the valley; 5 cm/year on the ridges, 0.5 cm/years in capped areas, and 1.1 cm/year in the plant area..

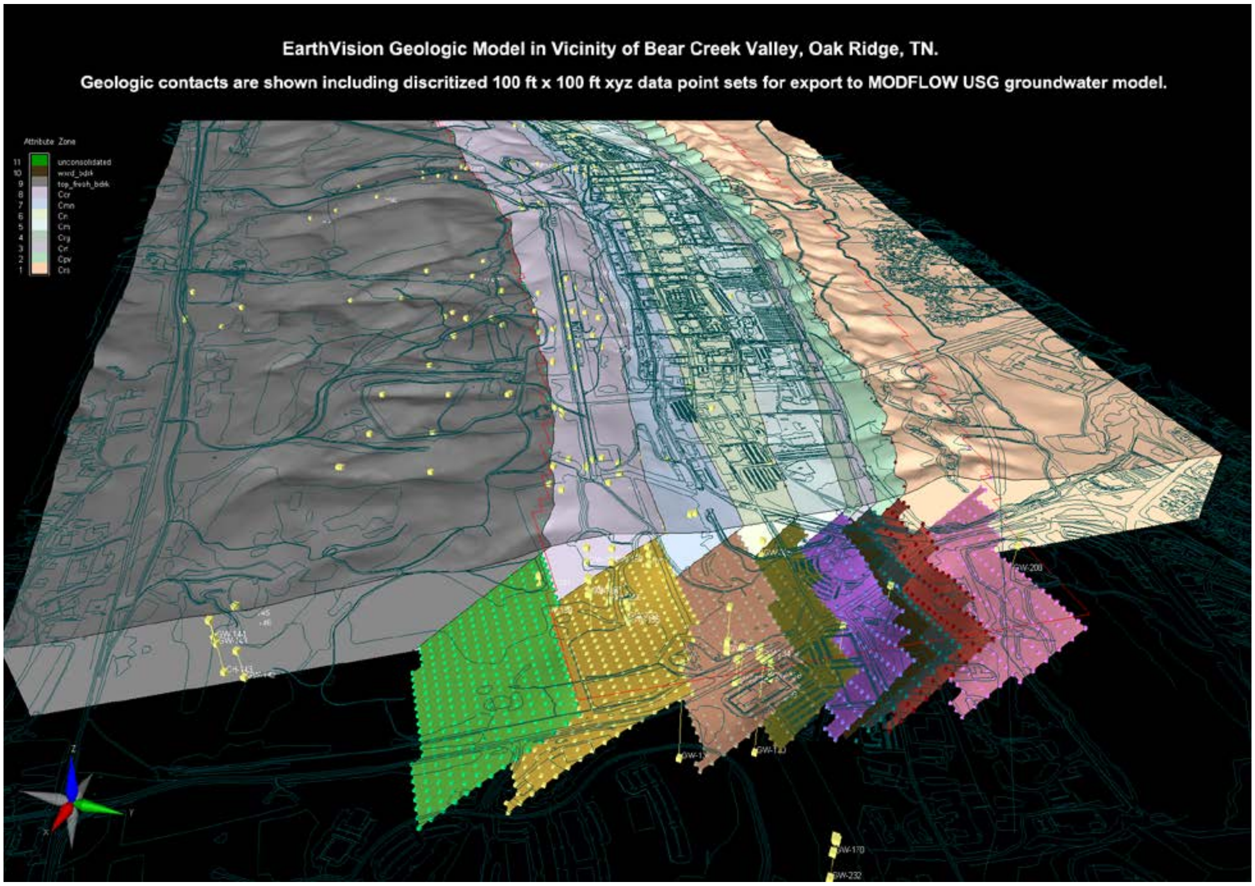

Fig. 3. Test Case EarthVision® slices in the Numerical Model Domain. Closeup of geologic model at eastern end of Y-12 Complex.

Hydraulic Conductivity

The assignment of K values (per model layer) was based on evaluations of K-data for wells within each formation for the Y-12 area. All test wells screened in a particular geologic formation were grouped to develop the hydraulic conductivity statistics for that formation with mean, median, range, expected value for the probability density function, etc.

Based on TAG recommendations it was decided to further enhance the model construction by dividing the inclined geologic layers to additional sub-layers based on the distribution of hydraulic conductivity (K) values and water level elevations by depths. It was determined to limit this test to only the two most important formations (i.e., Maynardville Limestone and Nolichucky Shale) in the Test Case Model domain. Both the Maynardville Limestone and the Nolichucky Shale were divided into three horizontal layers based on the hydraulic conductivity distributions. Once the addition of the three layers was completed, MODFLOW-USG was simulated with the existing hydraulic conductivity parameter values in the model (i.e., without revising the hydraulic conductivity values for the sub-layers) in order to test the stability of the model to reproduce similar results given the additional grid discretization. Similar results were produced without any parameter revisions. Therefore, it can be concluded that MODFLOW-USG inclined layers could be divided into multiple horizontal sub-layers in order to improve the resolutions when needed, and will be incorporated into the Test Case Model by populating discrete hydraulic conductivity values for each sub layer. A lesson from this test is that vertical discretization within the MODFLOW-USG inclined layers is not currently supported by Groundwater Vistas (the groundwater modeling pre- and post-processing platform used by MODFLOW-USG) and has to be performed outside Groundwater Vistas. Therefore, the most efficient way to discretize vertically would be to create those layers in EarthVision before importing the conceptual model into Groundwater Vistas for construction of the MODFLOW-USG model.

Additional Test Case Model Parameters

Additional key hydraulic parameters that have been used in the Test Case Model are described below.

An arbitrary anisotropy ratio of 10:1 for both transverse (Ky) and vertical (Kz) hydraulic conductivity values was used throughout the model domain (i.e., one-tenth of Kx values were used for the both Ky and Kz). The development of water flow inflow and outflow was performed by assigning water level values at the model boundaries **-** if the water level is higher at the boundary than within the model, then the flow at that boundary will be inward. The Test Case Model outer boundaries consist of the following:

- No flow boundary on all sides of the model.
- Recharge on the top of the model at regolith formation.
- Rivers and drains on the top two layers of the model in regolith and weathered bedrock formations.

Initially, the Test Case Model was setup using either DRAIN or RIV package cells for addressing Bear Creek and Upper East Fork Poplar Creek and their tributaries. The DRAIN package only allows water to be removed from the groundwater system if the head computed by the model is greater than the head in the boundary (drain); however, if the head computed by the model is less than the head in the boundary (drain), the boundary condition is turned off. The RIV package also allows water to be removed from the groundwater system when the simulated head is above the river boundary but it also allows recharge to the groundwater system when the simulated head is below the head in the boundary (river), and the boundary condition is turned off when the aquifer head drops below the bottom of the river.

The TAG suggested that the model team should replace the DRAIN and RIV package with the stream package for MODFLOW (STR7), which is a modification of the MODFLOW RIV package that allows flow to route through streams (i.e., rivers, canals, creeks, etc.) in addition to computing leakage between the streams and the groundwater system. The network of streams defined in the STR7 package is divided into reaches and segments. A stream reach is the portion of the stream associated with a finite-difference cell used in the model. A segment is a group of reaches that have (1) uniform rates of overland flow and precipitation to them; (2) uniform rates of evapotranspiration from them; (3) uniform or linearly changing properties (for example; streambed elevation, thickness, and hydraulic conductivity, and stream depth and width); (4) tributary flows or specified inflow or outflow (only in the first reach); and (5) diversions (only from the last reach).

The initial attempt to apply the STR7 package quickly resulted in the realization that this effort would require significant data inputs and model construction efforts to populate a substantial amount of flow inputs along all segments and reaches of Bear Creek, UEFPC, and their tributaries. In most cases, measured flow data were not available and assumptions would have to be made. Based on this finding the test of the STR7 package was limited to just testing the applicability of the package in order to demonstrate that the stream package can be used with MODFLOW-USG. A small-scale simulation along UEFPC was successful and demonstrates that the STR7 package does work with MODFLOW-USG and should be considered as the best tool for performing small-scale modeling in areas where there is significant recharge and discharge between streams and groundwater, but that the RIV and DRAIN package may be more optimal for the regional scale.

Calibration Efforts

The model calibration will be performed by comparing measured water levels at selected monitoring stations (i.e., calibration targets) to computed water levels and adjusting model parameters as appropriate to reduce errors to an acceptable level for the steady-state average condition based on 20-year dry period conditions. The PEST software developed by Doherty (2004) will be used for performing the model run iterations necessary to fine tune parameters [13]. PEST is a parameter estimation code that automatically determines the best parameter values for a model as configured. The model parameters will include but are not limited to hydraulic conductivities, recharge rates, river cell conductance, anisotropic ratios (e.g., Kx:Ky, Kx:Kz, and Ky:Kz), etc.

A calibration water level target represents a point within the model domain at which measured water level data are available and at which the model output should closely replicate those data. Such locations can be springs and monitoring wells, with monitoring wells being the most common targets. A total of 356 target groundwater well locations will be used for the calibration of the Test Case Model. Average water level data are available for these well from 1994 through 2013 for the dry period (i.e., August, September, and October). Currently, only the water levels from the monitoring wells will be used as the calibration targets for the Test Case Model because the goals of this model is not to develop a fully-calibrated model, rather to test the modeling tools. However, in the future, springs and groundwater flux will also be included as calibration targets for the regional flow model.

PATH FORWARD

The groundwater model team will continue to perform the following Test Case Model activities:

- Complete the model construction
- Perform particle tracking to test the ability of the model to handle the anisotropic conditions on the ORR
- Test conduit flow capability. The model team will simulate a known conduit in Bear Creek Valley to test the ability of MODFLOW-USG to interact with the CLN package.
- Perform calibration and sensitivity analysis. The model team will perform limited calibration and sensitivity work as discussed above in order to proceed quickly to the development of the regional flow model.
- Develop the test case report

Once the Test Case Model effort affirms that MODFLOW-USG is a viable model code to use in the Oak Ridge area, construction of the regional-scale flow model will commence.

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