Development of a Regional Groundwater Flow Model for the U.S. Department of Energy Oak Ridge Reservation: Numerical Model using MODFLOW-USG –17368

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ABSTRACT

A regional scale groundwater flow model (GFM) has been developed for the U.S. Department of Energy (DOE) Oak Ridge Reservation (ORR). Development of the model implements a key recommendation of the ORR Groundwater Strategy. The model will be used as the single calibrated flow model for the ORR and as the framework for future, smaller scale, modeling efforts to support cleanup actions and decisions under the Comprehensive Environmental Response, Compensation, and Liability Act of 1980 (CERCLA).

The Oak Ridge site is located in a geologically complex region and encompasses three large government facilities, including the Y-12 National Security Complex (Y-12), Oak Ridge National Laboratory (ORNL), and the East Tennessee Technology Park (ETTP) (Fig. 1). An interagency approach for addressing legacy groundwater contamination from past operations at these facilities has been developed, resulting in an ORR Groundwater Strategy that was agreed to by DOE, the U.S. Environmental Protection Agency (EPA), and Tennessee Department of Environment and Conservation (TDEC). The ORR Groundwater Strategy provides a comprehensive approach to addressing and prioritizing groundwater issues across the DOE reservation. One component of the strategy is to "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."

As part of the cleanup plans for the Oak Ridge site under CERCLA and the Federal Facility Agreement (FFA), there are six final watershed-scale groundwater Records of Decision (RODs) currently planned. In preparation for future projects, the regional GFM has been constructed to serve as the single, calibrated regional flow model to be used as the hydrologic base for the groundwater plume-specific modeling developed for the RODs.

INTRODUCTION

This paper presents information about the development of a regional scale GFM for the U.S. DOE ORR. The up-front conceptual site model (CSM) development is addressed in a separate presentation; details of the numerical model are presented here. The modeling objectives, approach, and development process are described,

along with Technical Advisory Group (TAG) recommendations that guided the effort. Development of the model implements a key recommendation of the ORR Groundwater Strategy [1]. The draft report, *Regional Groundwater Flow Model Development – Fiscal Year 2016 Progress Report U.S. Department of Energy Oak Ridge Reservation, Oak Ridge, Tennessee* [2], and the associated FY 2014 [3] and FY 2015 Model Progress Reports [4] present detailed information about regional GFM development including a three-dimensional (3-D) representation of the conceptual site model (CSM) using EarthVision[®] software. The hydrogeologic framework developed by EarthVision[®] has been used as input to the numerical groundwater model. The numerical model, developed using USGS MODFLOW-USG software, is the first version of a completed, calibrated regional GFM based on available data. Updates of the model based on improved data are anticipated.

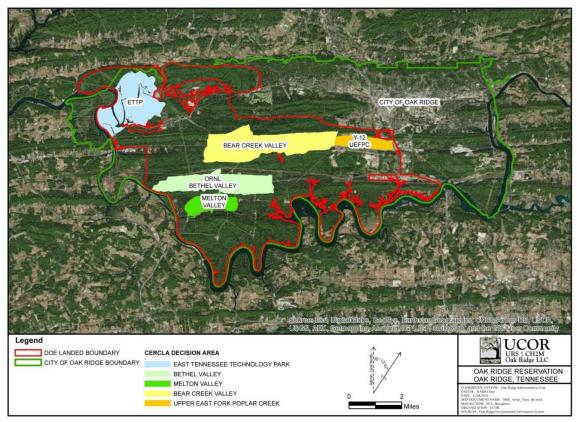


Fig. 1. Aerial view of the Oak Ridge Reservation and surrounding areas.

Construction of both the Test Case Model and the regional scale model required significant testing of the ability of MODFLOW-USG to work with various graphical user interfaces (GUIs) and modular finite difference flow model (MODFLOW) modules. The suite of tools that were ultimately selected includes:

- EarthVision[®] (EV) [5] Develop spatially referenced, 3-D computer model of the ground surface and subsurface geology.
- MODFLOW-USG [6] develop the regional scale GFM.

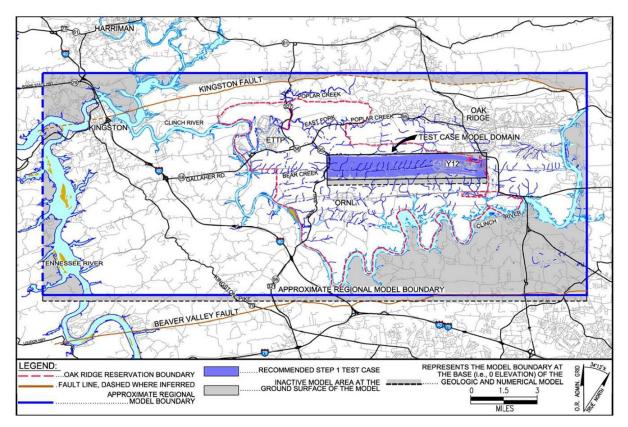


Fig. 2. Approximate area of the regional GFM and the Test Case Model

- Groundwater Vistas (GV) [7] Pre- and post-data processor.
- MODFLOW River & Drain Packages [8] Account for water leaving and entering the groundwater system via interactions with surface water.
- MODFLOW Conduit Flow Package (Connected Linear Network) [9] Simulate conduit flow network.
- mod-PATH3DU [10] Particle track simulation.
- PEST [11, 12] Parameter estimation code for model sensitivity analysis and calibration.

At several points in the process of testing MODFLOW-USG, members of the technical model team, several of whom have extensive knowledge of the ORR and have experience with smaller scale models in the area, have observed that MODFLOW-USG is significantly more appropriate for addressing the complex geologic subsurface environment in Oak Ridge than the previously used codes. The primary reason the code was selected was its ability to incorporate unstructured grids, thereby allowing the ORR model to accurately reflect the inclined subsurface geologic layering across the region.

MODELING OBJECTIVES

The two main objectives of the regional GFM are to: (1) provide a single, calibrated flow model for establishing flow boundary conditions (BCs), and (2) provide the

framework to support future smaller scale models and groundwater characterization, monitoring, actions, and decisions. The GFM, in conjunction with smaller scale modeling, is expected to play a role in the following:

- Analysis of regional flow systems and simulation of changes,
- Additional characterization and placement of monitoring wells to delineate the extent of plumes, including optimization of the long-term monitoring network,
- Visualization of extent and movement of groundwater and contaminants,
- Conducting "what-if" testing to evaluate potential on-site and off-site migration flow paths,
- Engineering studies to identify remediation alternatives, as well as the follow-on engineering design work,
- Assessment of potential short- and long-term risks, and
- Final watershed groundwater decisions that may include monitored natural attenuation or Technical Impracticability waivers.

MODELING APPROACH AND PROGRAM SELECTION

Prior to development of an initial Y-12 centered Test Cast Model and build out of the full regional scale model, a selection process for the CSM and numeric model program (code) was performed primarily by the Technical Committee of the TAG. The goal was to select programs that would be consistent with the modeling objectives and be applicable to the ORR site-wide scale, and meeting as many of the desirable attributes as possible including representation of the stratified heterogeneous aquifer system with dipping beds, conduit flow, etc., that are present at the ORR. The software also needed to have the ability to model sufficient details (i.e., finer grids to include all the features including dipping beds, faults, rivers, creeks and tributaries, etc.) and stay within memory limitation of the computer platform chosen for simulations.

The steps followed for selecting the numerical code included identification of a set of code attributes, development of a preliminary list of potentially viable codes, evaluation of a short list of codes that incorporate key code attributes, and finally testing of the candidate codes. This process is described in the FY 2014 Model Progress Report [3]. Based on this evaluation, MODFLOW-USG was selected for testing via a test case. The primary features to address in the test case application were: (1) ORR representative lithologic and structural features, including groundwater flow in stratified heterogeneous aquifer system with dipping beds; and (2) conduit flow. Based on review of the capabilities of modeling codes and supporting programs, the suite of tools (presented in the earlier paragraphs) were tested using the Test Case Model [3] and finally, selected for the regional GFM development.

GENERAL CSM AND NUMERIC MODEL CONSTRUCTION

A CSM and numerical groundwater model is the quantitative transformation of a physical system representing complex hydrogeologic conditions of a site. Therefore, it represents a modeler's understanding of the subsurface flow system, which may deviate from the actual system. The 3-D geologic CSM represents an area

approximately 39.62 Km long by 16.61 Km wide (24.62 mile long by 10.32 mile ft wide), and retains the lower cut-off at sea-level. Fig. 2 shows the approximate boundaries of the regional-scale model. The TAG recommended the areal extent of the regional flow model was based primarily on the Tennessee Valley river system. As shown in Fig. 2, the eastern and southern boundaries of the model are the Clinch River, which circles three sides of the ORR. The western boundary of the model is not the Clinch River, but rather the Tennessee River. This was a key decision, acknowledging that the Clinch River may not serve as a flow boundary for groundwater leaving the ORR. The only model boundary not defined by a river is the northern boundary. In this case, the Kingston Fault serves as the northern boundary of the regional model domain. The geologic model constructed in EarthVision[®] provides the geologic framework for the numerical groundwater flow model constructed in MODFLOW-USG.

The GV GUI, a groundwater modeling pre- and post-processing platform for MODFLOW-USG, was used to develop all the numerical model layers (the regolith, the weathered bedrock, and inclined continuous (34) and discontinuous (6) bedrock formations exported from EV). The surfaces used to construct the EV 3-D geologic model were exported to files that were directly imported into MODFLOW-USG in GV GUI. EV data were provided in 152.4 m x 30.48 m (500 ft × 100 ft) spacing for all geological formations, including the regolith and the weathered bedrock. Therefore, numerical model grid spacing was also designed at 152.4 m x 30.48 m (500 ft × 100 ft) so that each numerical cell has actual EarthVision[®] data imported and no data interpolation was necessary while developing the numerical geometric grids. The top two horizontal formations (regolith and weathered bedrock), the 34 continuous inclined formations, and 6 discontinuous formations in the vicinity of ETTP were assimilated into the numerical model (Fig. 3). Each of the exported geologic grids consisted of 546 rows x 261 columns and was rotated clockwise so the XY axes were oriented in cardinal directions.

Based on the TAG recommendations [3], it was decided to enhance the model construction by dividing the inclined geologic layers in the existing model to additional sub-layers based on the distribution of hydraulic conductivity (K) values, water level elevations, etc., by depth. To maximize resources the subdivision was limited to the two most important formations in Bear Creek Valley (i.e., Maynardville Limestone and Nolichucky Shale) in the Y-12 portion of the model domain. Both units were divided into three horizontal layers based on the hydraulic conductivity distributions. These inclined layer subdivisions were at approximately 0 to 61 m (0 to 200 ft) below average ground surface (bgs), 61 to 122 m (200 to 400 ft) bgs, and 122 m (400 ft) bgs and below. A lesson from this effort is that vertical discretization within the inclined layers is not currently supported by GV. Therefore, the most efficient way to discretize vertically was to create those layers in EarthVision[®] before importing the CSM into GV for construction of the MODFLOW- USG model.

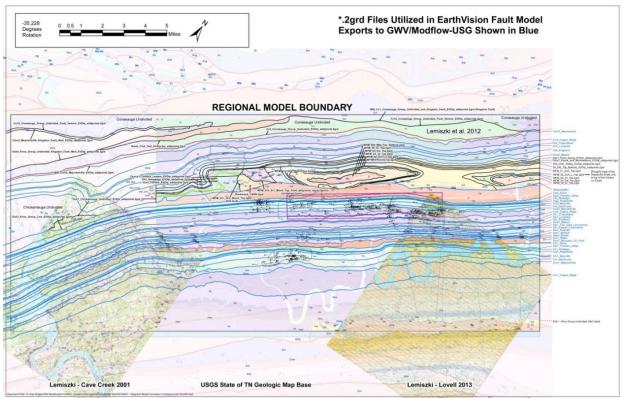


Fig. 3. EV exports to GV/MODFLOW-USG showing GFM boundary and geologic contacts.

BOUNDARY CONDITIONS

A critical aspect of developing a groundwater model is defining the water flows that enter and leave the model domain at the model boundaries. The development of inflow and outflow is 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 regional GFM outer boundaries consist of the following:

- Constant head boundaries along the Tennessee River on the western side of the model domain and along the Clinch River on the eastern and southern sides of the model domain indicating head at the boundary does not vary (provide an inexhaustible source of water).
- Precipitation recharge on the top of the model at Layer 1 (regolith).
- River and Drains on the top two layers of the model in regolith and weathered bedrock formations.
- The no flow boundary on the northern side and a portion of the southern side of model domain indicating head at the boundary does not vary (flux across the boundary is zero).

Fig. 4 shows the GFM domain, the inactive cells, and BCs for the top two horizontal layers (Layer 1 and Layer 2) of the model.

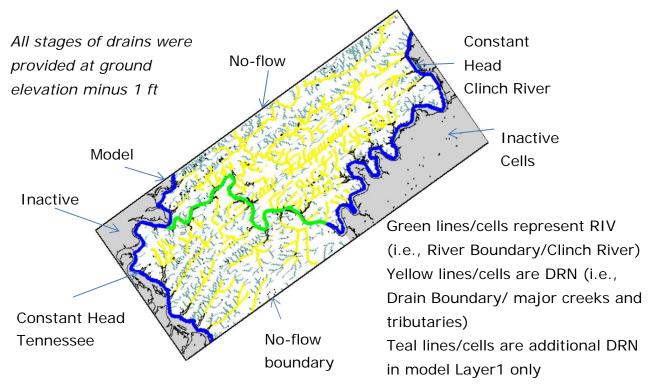


Fig. 4. ORR Regional GFM model domain and BCs – Layers 1 and 2.

MODEL CALIBRATION

Model calibration was performed in two steps: initial manual calibration through trialand-error and (2) final auto calibration using PEST [11] a software developed for performing the model run iterations necessary to fine tune parameters.

The manual calibration step was conducted in order to check whether the model is working properly and to perform a parameter sensitivity analysis using PEST to determine which input parameters have the greatest influence on the calibration and, thus, were needed to be optimized during the auto-calibration. During the manual calibration process, several problems were identified with the calibration targets and the CSM as utilized in the model construction. These problems and corresponding resolutions are discussed below:

- Because all stages of rivers were set at ground elevations based on the topography provided by EV (i.e., top of Layer 1), significant errors were introduced in the Constant Heads and RIV BCs. To resolve this problem, the USGS elevations for the river/stream centerlines were back interpolated and the points and associated elevations were posted in the map. The key points of the rivers (from the map) were selected and correct BCs for RIV and Constant Heads were provided.
- Initially the layer or layers assigned to a target well were based on the midscreen and top and bottom elevations of the screen. However, the thickness

of the weathered bedrock (Layer 2) throughout the model domain is set at 16.5 ft, and the thickness of the regolith (Layer 1) throughout the model domain is set at 18.3 ft. Therefore, for the wells where the actual thicknesses of the regolith and weathered bedrock are greater than the uniform thickness values used in the model, the inclined formation top elevation provided from EV is raised in the model. This caused a number of water level target wells from Layer 1 and Layer 2 (regolith and weathered bedrock) to fall into the inclined fresh bedrock formations. Similarly, if the actual thicknesses of the regolith and weathered bedrock are less than the average values used in the model, then the inclined formation top elevation provided from EV is lower in the model, which caused some bedrock wells to fall into Layer 2 (even into Layer 1 in some cases). To resolve this problem, the wells that do not have correct layer allocations (i.e., an unconsolidated well screen is in inclined bedrock formation in the model, or an inclined fresh bedrock well is in Layer 1 [regolith] or Layer 2 [weathered bedrock]) were removed from the list of target wells for calibration. It should be noted here that this is a temporary solution. It is proposed, in the future when site scale models are developed, that the CSM be revised to match the actual site topography (based on new light detection and ranging [LiDAR] data), and the regolith thickness as well as the weathered bedrock thickness should be nonuniform as applicable to the site so that the well screen intervals and the targets fall within the correct formations. This option would require refining the top of the fresh bedrock elevations for all three major target areas.

- Except for the Cmn2 and Cn2 formations, none of the inclined model layers are subdivided; thus these inclined layers are very thick (i.e., approximately 1000 ft). Therefore, for the multiple screened wells, there is more than one screen for a single well in one of these inclined layers, producing multiple water level targets for the same location within an inclined layer. In order to resolve this problem, these multiple targets in an inclined layer at the same location were consolidated by using the average of these multiple target water levels as the final calibration target for PEST calibration. For example, because of this action of consolidation, 48 water level targets for MV Picket Wells were reduced to only 14 water level targets.
- Several water level targets with significantly different water levels (> 30 ft) were identified in the adjacent cells or in the same cell because of the coarser grid size (i.e., 500 ft × 100 ft). In order to resolve this problem, the well with the significantly different water level (> 30 ft) from the nearby wells within the same formation was taken out of the list of target wells for calibration.

Calibration Targets

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 or monitoring wells, with monitoring wells being the most common targets. Groundwater levels based on

steady-state average of measured values for the 20-year dry period conditions are the primary calibration targets for the GFM development. July through November was considered as the dry period for model calibration. Statistical analysis was performed using groundwater level data for the ORR sites to develop the dry period water level targets that are presented in the yearly progress reports [3, 4] and the draft FY 2016 model report [2]. Similarly, work was performed for finalizing other calibration targets including representation of the lakes and ponds, dry period seeps and springs, stream discharges, and offsite wells, with water level targets as available. Fig. 5 shows the water level target locations including seeps and springs used for the final calibration of the GFM. Initially, a total of 1,175 monitoring wells, and 95 seep/springs were selected as preliminary calibration targets. However, additional work was performed for finalizing the calibration targets based on problems encountered during the calibration process that are discussed above.

It should be noted here that the offsite target locations (red dots in Fig. 5) with water level results obtained from the 1975 U.S. Nuclear Regulatory Commission's report on the Clinch River Breeder Reactor (CRBR) plant environmental investigation [13] were not very reliable as there were no well construction data and no information about whether the water levels in the wells were stabilized. Therefore, these data were not used in the calibration; instead they were utilized for model verification purpose.

Calibration Results

For the final calibrations using PEST, a total of 1091 monitoring stations were selected for developing the water level targets, including 84 springs and seeps discharge elevations, and seven lakes and ponds. PEST parameter sensitivity analysis provided the relative extent to which each adjustable parameter affected the overall model calibration. The parameter sensitivity values calculated by PEST were utilized to guide the selection of parameters to be used for final model calibration. Four sets of key model input parameters were used for the sensitivity analysis: (1) Kx values for multiple zones; (2) Ky/Kx in the X and Y direction for the regolith and weathered bedrock layer (i.e., Layers 1 and 2) as well as the inclined formations; (3) Kz values for multiple zones; and (4) precipitation recharge values. Detailed discussion of parameter sensitivity analysis is provided in the draft FY 2016 model report [2].

A map of the target residual heads for the calibrated GFM is shown in Fig. 6. A plot of overall observed versus model-calculated heads is shown on Fig. 7. Target residual statistics and plots of observed versus model-calculated heads for the individual areas (e.g., ETTP area, ORNL area, Y-12 area, MV Westbay wells, offsite OMW wells, and seeps and springs) were also generated and in general, these target residual statistics and plots of observed versus model calculated values appear to be quite reasonable and meet the criteria for GFM calibration. However, calibration results for MV Westbay

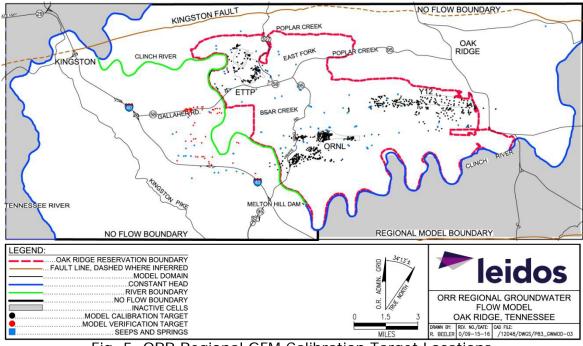


Fig. 5. ORR Regional GFM Calibration Target Locations.

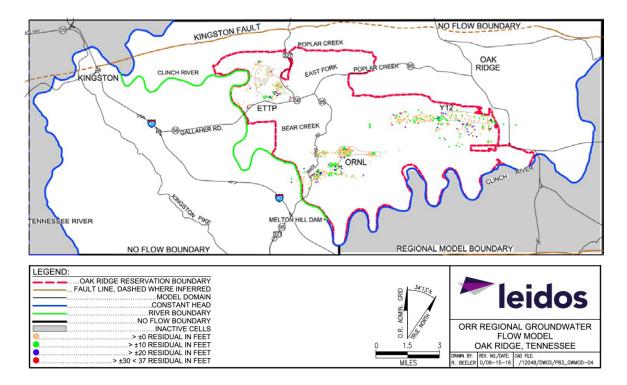


Fig. 6. Target residual heads for the calibrated GFM.

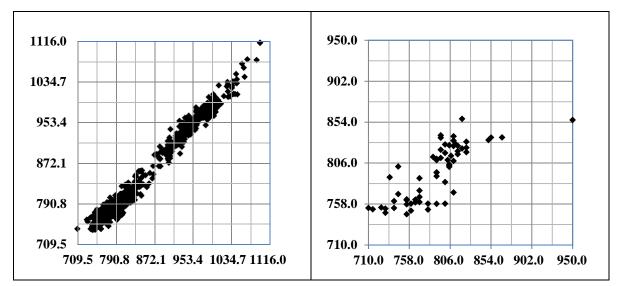


Fig.7. Target plot of observed (x-axis) versus model-predicted heads (y-axis) for overall model (left), and CRBR verification wells (right).

wells and offsite OMW wells, respectively, did not meet the calibration criteria which could be explained due to the fact that these two locations are very small in area, compared to the regional scale, with significantly lower head range indicating a regional scale model will not generally meet site scale hydrologic conditions.

MODEL VERIFICATION

Model verifications were performed by predicting the water level elevations for the CRBR wells, and the results of this analysis are shown in Fig. 7. As can be seen in this figure, except for a few data points, in general, good agreement between the observed and simulated values is achieved. Model verification was also performed qualitatively by examining the predicted head conditions around some major boundaries such as:

- The Clinch River near Melton Hill Dam,
- Beneath the channel from Melton Hill Dam to downstream of ETTP,
- The East End Volatile Organic Compound (EEVOC) extraction at well GW-845,
- The Rogers Quarry groundwater capture zone, and
- Comparison of predicted water table surface elevations to ground surface near streams (i.e., are stream boundaries sufficient to shape the groundwater surface and discharge patterns).

The predicted groundwater elevations at every node within the active model domain were exported to EV to generate 3-D potentiometric surfaces and were qualitatively evaluated near the boundaries discussed above. Illustrations of these evaluations are provided in the draft FY 2016 model report [2] with an example figure presented here (Fig. 8), which represents the head pressures in the vicinity of EEVOC extraction well GW-845. The elliptical shape of the head pressures indicates Ky/Kx anisotropy in this area associated with a strike parallel groundwater flow regime and

25 gallons per minute pumping that is maintained as part of the treatment system. It also shows the impact from low head pressures at Rogers Quarry.

MODEL APPLICATION

The model applications–evaluation of conduit flow and particle track analysis–were conducted after model calibration was completed. The planned locations of conduits and particle track analysis were discussed with the TAG Technical Committee.

Conduit Flow

It had previously been tested [3, 4] that MODFLOW-USG can effectively simulate conduit flow using its MODFLOW-USG CLN Package. However, due to time limitations, it was proposed that only two conduits be added to the regional GFM. One of these conduits represents the SS-5 Spring: in BCV near Bear Creek, with the conduit inflow point near Bear Creek kilometer 11.54 and a conduit discharge near SS-5 Spring (see Fig. 9). It was assumed that the conduit passes through the weathered bedrock model layer on top of the inclined competent bedrock model layers. The results of the conduit flow simulation are shown in Fig. 9. As can be seen in this figure, there are many cells either near or in the conduits that are dry, thereby limiting the groundwater flow into or out of the conduit.

Particle Tracking

Verification of groundwater flow through particle tracking was performed at three locations by developing submodels using telescopic mesh refinement (TMR) technique. The only particle tracking software available at the time of analysis that worked with MODFLOW-USG with some limitations was the earlier version of mod-PATH3DU [10]. Because the particle tracking method in mod-PATH3DU is head-gradient-based, it is more dependent on model grid resolution relative to a flux based solution like the Pollock method in MODPATH [14]. The head gradient based version of mod-PATH3DU was used with refined discretization around the particle track locations to try to avoid the unexpected particle track patterns observed during the model testing [4].

Particles are expected to terminate at streams or active drain cells, or at the submodel boundaries. In general, the velocity of particles in the bedrock portion of the submodels (with an effective porosity of 0.005 used for this analysis) is significantly faster than that in the unconsolidated/weathered bedrock (with an effective porosity of 0.04 used in this analysis). Figure 10 presents the particle tracks from the S-3 Ponds area with the particles released in Layer 2, which corresponds to weathered bedrock. Two particles were released in this simulation in the Nolichucky Formation (Cn) with migration occurring in a southerly direction into the Maynardville Limestone (Cmn). The western of the two particle tracks immediately started a down valley pathway along the Maynardville, and after a

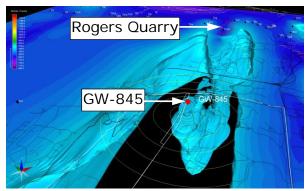


Fig. 8. View up-valley to the northeast in the vicinity of GW-845 pumping well. Head pressures shown are 680 ft to 890 ft with horizontal slice at elevation 795 ft MSL. Note the head pressure effect running along strike to the northeast toward Rogers Quarry.

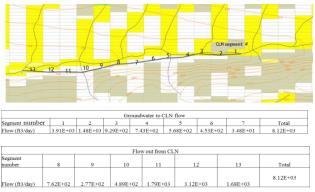


Fig. 9. Application of MODFLOW CLN Package to MODFLOW-USG GFM – SS-5 Spring. Tan shading represents dry cells, where the water table is below weathered bedrock.

simulated time of 19 years, ended its track at the first active drain cell. The second particle track also migrated southeast toward the Cmn but did not start an along-strike change in direction. After 62 years of simulated time, the particle ended at a dry cell (Fig. 10). The particle tracking code appears to have worked well for the western of the two tracks, but the more eastern particle release resulted in an unexpectedly slow and erratic path toward the middle of the Cmn.

Fig. 11 presents the particle tracks from the S-3 Ponds area in Layer 24 (i.e., the inclined fresh bedrock layer [Cmn2]). Both of the particle tracks appear to have progressed in directions consistent with the CSM, with one headed east of the groundwater divide in this area and the second heading along strike to the west. The eastern particle ended its track at the edge of the submodel boundary (an expected result). However, the western particle shows some evidence of "stair-stepping" at the contact with Layer 23 (Ccr2). There is a significant (six orders of magnitude) difference in K values between Layer 24 and Layer 23. Therefore, it may be concluded that the flow along and across high K value Cmn2 (Layer 24) encounters an interface (i.e., the region of geologic contact between Cmn2 and Ccr2) and the sharp variation of K values. This sharp variation of properties may have caused discontinuity in the domain. These effects can be studied by the methodologies described in Dynamics of Fluids in Porous Media [15] that deal with flow in a strongly heterogeneous medium with discontinuities in properties. Some specific and special conditions are required to deal with such a system, and it may be that the modPATH3DU code is ineffectively resolving this boundary issue. Both particle tracks progressed rapidly through their movement in about one half year, which is consistent with the hydraulic parameters in this formation.

From this analysis it was observed that the previous version of mod-PATH3DU used in the analysis can produce the expected particle paths for a simple groundwater

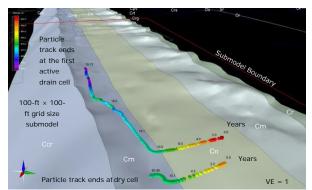


Fig. 10. Particle tracks from S-3 Ponds area shallow zone, Layer 2.

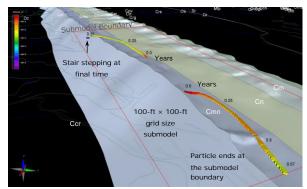


Fig. 11. Particle tracks from S-3 Ponds area in Layer 24, Cmn.

system, but fails for a highly complex groundwater system (i.e., highly heterogeneous system with sharp variation of hydraulic conductivities). Future analysis to address remaining particle tracking issues may be performed using recently developed software (e.g., the updated version of mod-PATH3DU [10, 16] or MODPATH 7 [17]) or other software that becomes available.

SUMMARY AND CONCLUSION

The GFM reasonably matches water levels, and reproduces the flow paths as expected based on the CSM. Overall the model honors the ORR CSM. The regional GFM may be used for establishing flow BCs for the smaller-scale efforts. This model may serve as the single, calibrated flow model for the region and can be used as the hydrologic base for the groundwater plume-specific modeling developed for the RODs. This model, in conjunction with site scale modeling, is anticipated to play a role in future characterization, analysis of remedial alternatives, decision making, remediation design, and monitoring for the ORR.

Construction of the CSM in MODFLOW-USG was successfully achieved and model runs completed with incorporation of highly variable geologic unit hydraulic properties, which provided challenging solutions at associated formation interfaces. In addition, the simulation time for the GFM has been reduced significantly with MODFLOW USG due to its unique feature of using pinch out layers that are inactive in the model and not requiring the model layers to be continuous across the entire model domain. After working within the MODFLOW-USG framework for two years, the project team's assessment is that this was the right choice for construction of the ORR regional GFM. Third-party software tools that tie into and support MODFLOW-USG will continue to advance and provide additional functionality and enhancements for future refinements to the GFM. Future improvements to the model may include more refined, site-specific models in support of decision making and remediation projects. Updates may address dry cells and model flooding via fixed regolith and weathered bedrock thicknesses, refined river/creek discretization, use of wet season and/or transient data, increased vertical and horizontal model discretization, addition of conduit networks, and evaluation of "what-if" scenarios.

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