6-month update for SN 480E. ed

Initial entries made 3/27/2001 by James Winterle JRW

3-Dimensional, Site-Scale Groundwater Flow Model for Yucca Mountain, Nevada

CNWRA

Center for Nuclear Waste Regulatory Analyses

Scientific Notebook #480E

Principal Investigator:

Jim Winterle

Dated entries reviewed and approved by James Winterle are followed by electronic initials: JRW

Project contributors to this scientific notebook will include but not be limited to the following individuals:

Chandrika Manepally	(conceptual model development and modeling results)
Melissa Hill	(conceptual model development and modeling results)
Darrell Sims	(data and graphics from Earth-Vision Hydrogeologic Framework Model)

About this Notebook

This electronic scientific notebook is intended to comply with CNWRA Operating Procedure QAP-001. Many graphics and data files will be referenced throughout this notebook. To keep the size of this notebook manageable, these graphics and data files will be kept as separate electronic files in a platform-independent format (e.g., JPEG and ASCII text) that will be archived with this notebook on a data storage disk. All cited references will be recorded at the end of this notebook, so the page numbers of the references section may change as entries are made to the notebook. Thus, if more than one printing of this notebook is required for the Quality Assurance archive, the entire reference section will need to be placed in the archive for each printing. For in-process entries only pages that are new since the last archive need to be printed.

Project Objectives

The objective of this effort is to develop a 3-D, site scale, saturated zone groundwater flow model of the Yucca Mountain area in Southern Nevada. The main purpose is to develop a tool that will allow CNWRA and NRC staff to evaluate different conceptual models of geologic structure, boundary conditions, and hydrologic properties, and their effects on potential groundwater flow and contaminant transport pathways in the saturated zone between the Yucca Mountain project area and potential receptor locations. Other uses for the model may include abstraction of flow paths for the Total Performance-Assessment (TPA) code, development of boundary conditions for smaller-scale detailed models, development of flow vectors for use in geochemical or radionuclide transport modeling.

Project Approach

The foundation of this groundwater flow model is the Hydrogeologic Framework Model (HFM) that was developed by CNWRA using the Earth Vision code Sims et al., 1999). The spatial layer data from the HFM was output from Earth Vision and used as input to assign properties to the flow model grid. The Groundwater Modeling System (GMS), version 3, interface will be used to view and edit the grid (Grid Module), and to run flow models (MODFLOW module). At this writing the Grid and MODFLOW modules of the GMS interface were in the process of being validated in accordance with the latest version of operating procedure TOP-18. Documentation of the GMS modules and demonstration versions of the code can be found at the EMS-i Internet site: http://www.ems-i.com. CNWRA maintains two licensed copies of GMS version 3, which also contain all codes and documentation and are archived by IMS staff. To achieve consensus regarding methods and assumptions among the various potential users of this model, a saturated zone modeling workshop was held on August 7-9, 2001 with participation from CNWRA, NRC and consultants.

IN-PROCESS ENTRIES BEGIN HERE

Following entries made 9/28/01 JRW

Model Domain and Grid

The rectangular lateral boundaries of the model domain are shown in figure 1 (Figures\figure1). Using the UTM NAD-27 coordinate system, the Southwest corner of the model occurs at Easting 535000 m, Northing 4049000 m; the Northeast corner occurs at Easting 563000 m, Northing 4090000 m. The bottom of the 3-D model domain is at a constant elevation of 1500 m below sea level (-1500 masl). The top of the model domain occurs at 1200 masl, however, all of the model grid cells that are entirely above the water table elevation were flagged as inactive. The water table elevation used to assign inactive cells is based on a previous interpretation (Winterle et al, 2000, Figure 4-1) similar to the more recent interpretation shown in figure 1.

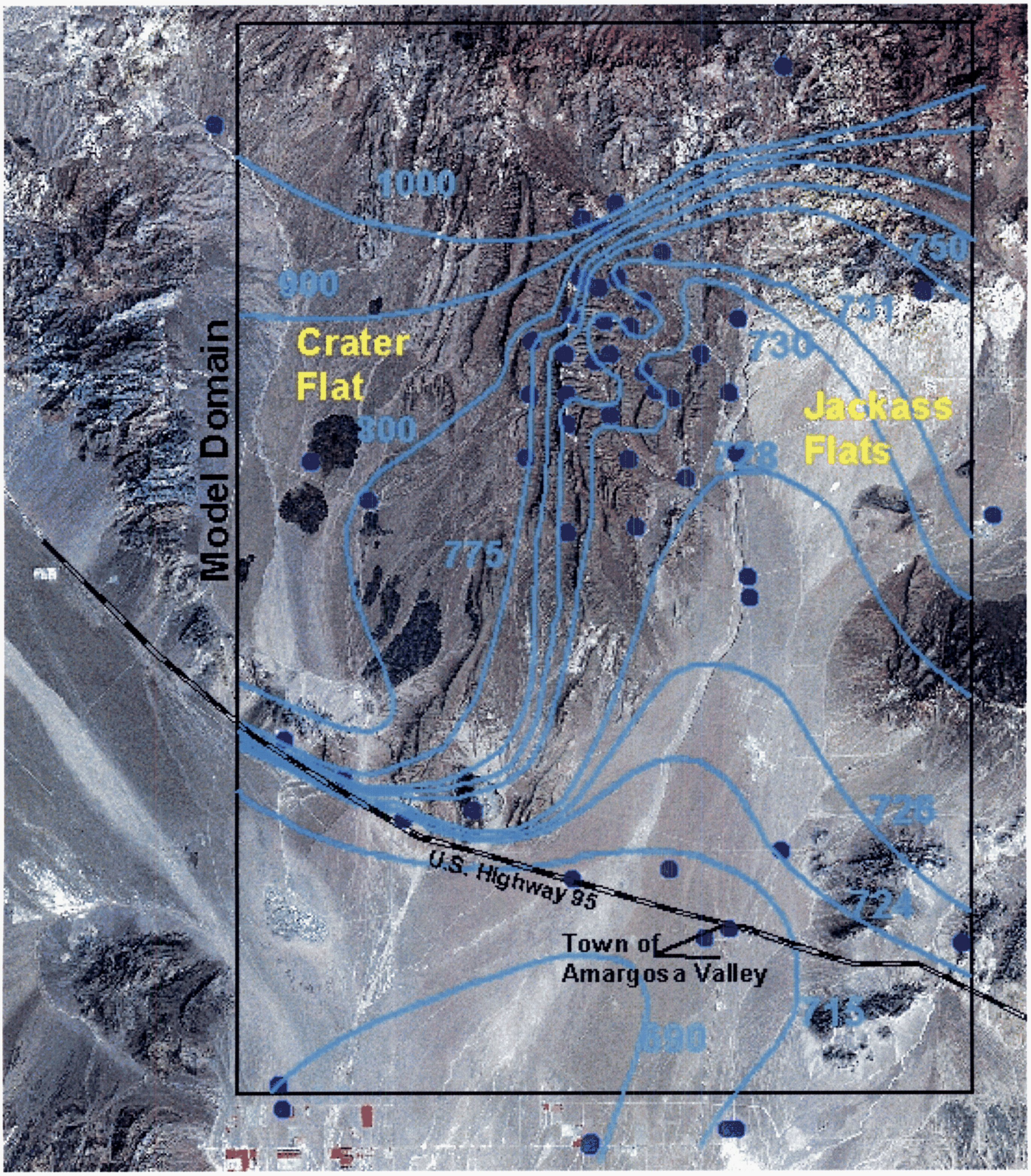

Figure 1 - Satellite map of the Yucca Mountain region showing the site-scale flow model lateral boundaries, interpreted water table elevations within the model boundaries, and locations of wells with available water level measurements.

Selection of the model domain and the discretization of the model into the MODFLOW finite-difference grid blocks required several considerations. The first consideration was to center the model around potential flow paths from Yucca Mountain to the 18 km compliance boundary. In deciding the lateral and vertical extent of the model, it was necessary to strike a balance between keeping the computational grid small enough to achieve reasonable model run times, yet large enough so that the model boundaries are far enough from the area of interest (i.e., potential flow paths) so that the error caused by uncertainty in model boundary conditions is mitigated. For horizontal discretization, it was decided that uniform 300-m square grid blocks would be sufficiently small to incorporate the major structural features (i.e., layers and faults) of the model. (Note that the DOE saturated zone flow model uses a 500-m square horizontal grid discretization).

Note that the North, East, and West boundaries coincide with the extent of HFM (Sims et al., 1999) boundaries.

Following Entries made 2/07/2002 JRW

Hydrogeologic Framework

The hydrogeologic framework that underlies this site-scale flow model was developed by Sims et al. (1999).

To assign material properties to the GMS model grid, an data processing script was written to process output data from the Sims et al. framework model into an output that can be read by the GMS grid module. This script is a file called "*mk3gd_1.sh*" archived in the DISK 1 data disk that accompanies this notebook in a directory called *Documentation/Scripts/*. This script is written in the nawk language, which is standard on unix and linux operating systems. Instructions to run the script are written directly into the script file, which can be read on any text browser.

Boundary Conditions

*****(begin text from C. Manepally to Jim Winterle on 9/27/01, pasted into notebook on 2/7/2002)*****

The constant head values were assigned to the boundary cells based on the map developed using head data shown in Figure 1. The following steps describe the details.

The Map Module of GMS can be used to create arcs between two constant head locations on the boundary and GMS will interpolate the constant head values along the arc, which can then be read into MODFLOW for constant-head boundary conditions. The location of the nodes that were used to create arcs and the head assigned are as follows:

Left Boundary Nodes					Right Boundary Nodes			
x	y	Constant Head (m)			x	y	Constant Head (m)	
535000	4049000	697	SW		563000	4049000	719	SE
535000	4060384	700			563000	4054192	724	
535000	4062534	724			563000	4061582	731	

Left Boundary Nodes					Right Boundary Nodes			
535000	4064713	775			563000	4079094	750	
535000	4085500	1010			563000	4083206	800	
535000	4089018	1100			563000	4086795	1000	
535000	4090000	1130	NW		563000	4088913	1100	
					563000	4090000	1130	NE
Bottom Boundary					Top Boundary			
x	y	Constant Head (m)			x	y	Constant Head (m)	
550237.8	4049000	700	Bottom		538250	4090000	1200	
555742.2	4049000	715	Bottom		543000	4090000	1300	
					551900	4090000	1300	
					557100	4090000	1200	

These values were applied to all the layers in the z direction. This implies that the vertical gradient was neglected. The software interpolates the heads for the cells located along the arc based on the values at the nodes. The Map→Modflow command transfers this information to the Modflow module. The corresponding cells will be declared at constant head and the interpolated value will be assigned to the cell.

************ (end of text provided by C. Manepally to Jim Winterle on 9/27/01) *****************

Following entries by Jim Winterle

Change to constant-head boundary condition – after playing with some model runs I adjusted some of the constant head values on the right side of the model by hand editing (it was just easier than playing with the map module). Basically I wasn't completely happy with the interpolation between the 724 and 732 m constant head values on the east model boundary. So, I just changed it by hand editing to make the gradient between these points steeper to the north and shallower to the south. The boundaries are still consistent with the figure 1 above.

Following Entries Made 2/8/2002 JRW

Model Runs

The model runs are described in the February, 2002, intermediate milestone report that came out of this effort. The report is titled "Concepts of Saturated Zone Modeling for Development of a Site-Scale Groundwater Flow Model for Yucca Mountain" (Winterle et al., 2002). A copy of this report is saved on DISK1 that accompanies this notebook. Since the concepts that went into the model runs are described in the report, they are not repeated here.

Following is a Table listing the model grids and MODFLOW model runs that were developed as part of this effort using the GMS 3.1 Groundwater Modeling System. All files needed to repeat the model runs are archived on DISK1 that accompanies this report.

Table listing models and documentation contained on DISK1 that accompanies this report.

Directory on DISK1	Description of Model or directory contents
Grids\Original project file: *YM.gpr*	The files in this directory represent the original model grid that was generated from the HFM data (Sims et al. 1999) using the script *mk3dg_1.sh*. The script, which was described previously creates a grid file (in a format that can be read by GMS) that identifies the material type for each cell and whether cells are active or inactive. After reading the grid file into GMS, colors were assigned to material types and then the whole thing was saved as a GMS project that can be viewed by opening the file *YM.gpr*. This grid was used to check quality or the script by comparing the resulting grid to HFM cross sections as described by Winterle et al (2002). No MODFLOW runs were created for this grid.
Grids\Calico project file: *Calico.gpr*	The files in this directory represent modifications made to the *Original\YM.gpr* project described above. Basically, the Calico hills layer in the grid was manually edited to make it continuous in areas where it was missed by the *mk3dg_1.sh* script because it was too thin and did not pass through the center of at least one grid cell. This editing process is also described in Winterle et al (2002). No MODFLOW runs were created for this grid.
Grids\Scenario1 project file: *Scenario1.gpr*	The files in this directory represent modifications made to the *Calico\Calico.gpr* project file described above. Starting with the Calico project, fault zones were added to the model by hand editing. This hand editing was aided by obtaining several cross sections from the HFM model and using them as visual aids to decide where to put the faults. The *HFM slices* are archived on DISK1. MODFLOW runs were conducted for this model grid and a rough calibration was obtained by trial and error. The results are described in Winterle et al. (2002) in the section on "Calibration Approach 1."
Grids\Scenario2 project file: *Scenario2.gpr*	The files in this directory represent modifications made to the *Scenario1\Scenario1.gpr* project file described above. A zone to represent the caldera complex in the northernmost portion of the model was added by hand editing. The approach is described in Winterle et al., (2002). MODFLOW runs were conducted for this model grid and a calibration was obtained by trial and error. The results are described in Winterle et al. (2002) in the section on "Calibration Approach 2."
Grids\geot.tif	This is a tiff image of a satellite map of the model area that is read by the Model grids described above.

Directory on DISK1	Description of Model or directory contents
Documentation	This directory contains the following files and subdirectories *SNB480.wpd* This file is an electronic copy of this notebook *HFM slices* directory containing the HFM cross sections that were used to visually aid the editing of the grid to include fault features. *Figures* directory containing .jpg file of figures in this notebook. *Scripts* directory contains the *mk3dg_1.sh* script and the associated data file *allhorizons_mod.dat* that has the HFM output data provided by Darrell Sims, and a *header* file. Also included is a script called *mkstarthead.sh* which was used to get initial starting heads from the water table surface in the HFM; these starting heads were just used to get the initial model running and are not the starting heads that are currently in the MODFLOW runs described above.

Alphabetical Listing of References

Sims, D.W., J.A. Stamatakos, D.A. Ferrill, H.L. McKague, D.A. Farrell, A. Armstrong. *Three Dimensional Structural Model of the Amargosa Desert, Version 1.0: Report to Accompany Model Transfer to the Nuclear Regulatory Commission*. CNWRA Letter Report. San Antonio, TX: Center for Nuclear Waste Regulatory Analyses. 1999.

Winterle, J.R., N.M. Coleman, W.A. Illman, and D. Hughson. *Review of Permeability Estimates Obtained from the Yucca Mountain Project.* February, 2000 Letter Report. San Antonio, TX: Center for Nuclear Waste Regulatory Analyses. 2000.

Winterle, J.R., M.E. Hill, and C. Manepally. "Concepts of Saturated Zone Modeling for Development of a Site-Scale Groundwater Flow Model for Yucca Mountain." February, 2002 Letter Report. San Antonio, TX: Center for Nuclear Waste Regulatory Analyses. 2002.

Copy of SNB 480E up to this point was printed for records on 4/1/2002.

Following Entries Made 1/28/2003 JRW

Table listing versions and descriptions of changes made to the Site-Scale Flow model since last entries were made in this notebook

Project File	Description of Model or directory contents
S3.gpr	The files in this directory represent modifications made to the *Scenario2.gpr* project file, which was archived on disc 1. The modification was to extend the Fortymile Wash fault laterally westward to make it a fault zone that abuts the Bow-Ridge Paintbrush fault zone.
S4.gpr	The files in this directory represent modifications made to the *S3.gpr* project file described above. The modification was to change the geometry of the south end of the Fortymile Wash and Bow-Ridge fault zones to see if it affects how far east flow paths from the repository can go before being diverted south in the high-permeability fault zones.
S5.gpr	The files in this directory represent major modifications made starting with the *S3.gpr* project file described above. The modification was a substantial increase in the size of the Caldera zone at the north end of the model and an increase in the heads at the north boundary.
S6.gpr	S6, includes the following changes starting from model version S5: 1. Increased slightly the size of the Caldera-altered zone at the north end of the model, extending it slightly further south compared to version 5 (see directory S5). 2. Made slight changes to fault zones, making the SC-IR zone wider by one cell-width at the very northern end; modified the BR-PB zone so it doesn't go quite so far north. 3. S6 version is run in Confined/Unconfined mode to allow the calculated water table elevation to be the same as the calculated heads. 4. The recharge package is used to evaluate the effects of recharge to the entire the top layer (layer 1), which represents the higher elevations to the north. 5. The constant head boundary at the north end was increased to a head value of 1250m. Notes: The model was initially calibrated using the PEST code to vary calibration parameters, including layer-1 recharge, north boundary head, and ten hydraulic conductivity values. The observations wells used in the calibration are from the DOE saturated zone process model report. I wasn't completely satisfied with the PEST calibration, however, so I tweaked some of the hydraulic conductivity values to get a better fit in the area of the flow paths east-southeast of Yucca Mountain. So, I can't really call this a PEST calibration

Following entries made 3/1/2003 JRW

S6_1.gpr is an alternative model developed by Antoine Claisse. This model began with the S6.gpr model listed in the above table, but Antoine made some modifications to existing structural features and

added several new features, and adjusted some of the boundary heads. The purpose of his model was to improve calibration as much as possible.
S6.gpr and S6_1.gpr are both documented in a paper written for the proceedings of the 2003 IHLRWM conference — full citation is as follows.

Winterle, J.R., A. Claisse, H.D. Arlt. "An Independent Site-Scale Groundwater Flow Model for Yucca Mountain." In: Proceedings of the 10th International High-Level Radioactive Waste Management Conference. La Grange Park, IL: American Nuclear Society. 2003.

This paper is archived on my computer (Amon) in directory D:/GMS/30-Layer/Documentation and will eventually be archived to disk with this notebook.

The model input files and results are archived in folders S6 and S6_1 of D:/GMS/30-Layer/Grids/. These files will also be archived to disk with this notebook, eventually.

Following entries made 3/13/2003 JRW

I am now working on a milestone report for the USFIC KTI which is supposed to look at a range of alternative conceptual models for flow at Yucca Mountain. I started this effort with the model S6.gpr, which is described just above, and made a few minor, and saved all files in folder D:/GMS/30-Layer/Grids/**S6a.gpr**. Changes from S6 are simply a change in material properties near the north end of the Solitario Canyon fault feature (SC-IR). This change was necessary because we had this feature curving too far to the east and passing under the northern repository area, which is not consistent with area maps. The change was simply to reassign the SC-IR cells that were too far east as Cald_VR material type. Recall that Cald_VR represents volcanic rock that conceptually was altered by whatever processes during the period of caldera activity, causing it to have lower permeability.

In the milestone report, I plan to look at several conceptualizations of infiltration rates using the S6a model. I don't necessarily plan to save each infiltration case as a separate model grid, so I will try to describe the changes made for each case that goes into the report, so someone could repeat the process by making minor changes to the S6a GMS and MODFLOW input files.

I will probably also present some variations of the S6_1 model in the milestone report, but haven't yet decided to what extent I will run with that model version.

New pages since last printing printed for QA records on 3/13/2003. Next printing should begin with page 10.

6-month update
ECP 9/26/03

Following Entries Made 9/26/2003

Latest and Greatest: the following is a description of the most recent version of the 3-D site scale model. The runs described are documented in an USFIC milestone report dated April, 2003:

Winterle, J.R. "Evaluation of Alternative Concepts for Saturated Zone Flow: Effects of Recharge and Water Table Rise on Flow Paths and Travel Times from Yucca Mountain, Nevada." CNWRA Letter Report. April, 2003.

This model is contained in Directory **S6a** on Disk 2 attached to this notebook.

This directory, created by Jim Winterle Mar 10, 2003, contains GMS groundwater model files for the version 6a of the cnwra site-scale 3D groundwater flow model for Yucca Mountain.

Top 7 layers are run in Confined/Unconfined mode (MODFLOW BFC package), the remaining layers use the Confined mode.

Changes for this version since original version 6:

1. Modified slightly the size of the Caldera-VR zone, extending it slightly further south compared to version 5 (see directory S5).

2. Made slight change to the SC-IR zone so that it stays on the west side of the repository footprint, consistent with geo maps of the area

3. Recharge in layer 1 in the north model area was increased from 1mm/yr to 10 mm/yr and I had to increas Ksat of the Caldera_VR unit to keep a decent calibration.

4. I reduced all of the calibration Ksat values to 1/2 of what they were in the original S6 model version so that I can keep the BR-PB zone at 5 m/d, which is consistent with the c-holes test data.

5. Made grid cells active above the current water table so that I could evaluate water table rise and flow paths during future wetter conditions.

MODFLOW and MODPATH Simulation input and output files are in those subdirectories, the different runs named run1, run2, etc. So, for example, run1 results in the MODPATH directory are based on the corresponding run1 steady-state solutions in the MODFLOW directory. Depending on how how you came to be reviewing this README file, you may of may not have been provided with all of the different model runs, since they take up a lot of memory.

Here are descriptions of the Runs produced I have so far for this grid:

Run1 -- boundary conditions based on present-day water table interpretation
-- 10 mm/yr recharge in northern model area; 5 mm/yr above Yucca Mtn area
-- Note: this run 1 was presented as "Case 2" in the Winterle, 2003, USFIC milestone report

Run 2 -- Same as run 1 but with no recharge in the Yucca Mtn area; used to evaluate importance of considering recharge in source area.
-- Note: Run 2 was presented as "Case 1" in the Winterle, 2003, USFIC milestone report, so hopefully no confusion.

Run 3 -- Started with Run 1 and raised the constant head boundary conditions on the model sides by 5% around the whole model; double recharge to 20 mm/yr in the north model area and to 10 mm/yr in the Yucca Mtn area. Added a drain cell at location of well EWDP-9S and used this to constrain the amount of water table rise.

Run 4 -- Same as Run 3 but with 200 mm/yr recharge rate added to the Fortymile Wash Channel area to account for more streambed recharge during future climate.

Run 5 -- This was run as special request from Hans Arlt at NRC. Same as Run 4, but no recharge over Yucca Mtn area. Hans wanted to see if the effects of recharge on flow paths from YM were still as pronounced for future climates. Hans used these results in his poster for the 2003 Devil's Hole workshop.

DATA SETS: there are a few GMS Data Sets saved into the S6a grid that the user should know about (these can be selected from the tool bar on top of GMS interface:

elevation -- this is a default GMS grid data set that you can't get rid of. It just has the elevation data for each of the model grid cells

aq_poros -- this is a file with porosity values for each grid cell that I used for the MODPATH simulations presented in Winterle, 2003 milestone report; each material type is given a porosity of either 0.1, 0.01, or 0.001, as listed in the Winterle 2003 report. Use this data set to construct new MODPATH files if you want to use the same porosities. Otherwise, you'll have to build your own porosity data set. The easiest way to build a porosity data set is to cheat using the MODFLOW menu Material Properties dialog -- for each material type, you just assign a porosity value where it says "vertical hyd. conductivity", check the box, select the option for "assign values to cells with highlighted material only", then click "Assign Values to Cells." Do this for each material type listed then quit the menu and go to the MODFLOW BCF Package menu and select Vert. Hyd. Conductivity, this brings up the hyd. conductiviy data, which is now the porosity values you have assigned; from here click the Grid->3D data set option, give the data set a name, and now you have a data set that can be read into MODPATH. Don't forget to go back to the MODFLOW materials properties menu and change the porosity values back to hydraulic conductivity values -- or, if you have not saved the MODFLOW run, you can quit and reopen and it should have back the conductivity.

tpa_porosity -- this is a porosity data set I created to do MODPATH simulation for development of the TPA code version 5 abstraction. TPA only has two kinds of porosity -- tuff and alluvuim. So I assigned all tuff porosity at 0.001 and alluvium at 0.1. Units like the Carbonate aquifer system don't occur on flow paths from Yucca Mtn and are not in TPA, so I just left those at a value of 0.1. Using this data set gives me a basis for comparing the MODPATH travel time estimates with the TPA "gwtt" output, so I can see if the abstraction in TPA is consistent with the model.

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Disk 2 Data Archive, Attached to this notebook, contains the following directories:

S3\, S4\, S5\, S6: these are all versions that contain sequential changes and improvements as described in the table on page 8 of this notebook. The only one of these that was ever used was S6, which I provided to Antoine Claisse for his development of the S6_1 case.

S6_1 : This directories is a modification to the S6 model by Antoine Claisse. This model adds additional structural features, which have a conceptual basis but are not necessarily supported by data. The model calibration is excellent with only 0.8 m of mean absolute error. See pp. 8-9 of this notebook and *Readme.txt* file in directories for additional explanation.

S6a: This is the most recent version of the model as of 9/26/03. Check future notebook entries to see if it is superceeded. This directory contains several runs which are described on pp. 10-12 of this notebook and *Readme.txt* file in the directory. Basis for USFIC April, 2003 milestone report.

====================end disk 2 archive list=========================

Notebook pages 10-12 printed for QA records on 9/26/03 along with Disk 2. Next printing should begin with page 13.

Following Entries made 1/11/2005

Since initial development of the site scale model, much new water level data has been collected by the Nye County well drilling program. I now update the model to ***Version S6b*** to include an updated new water-level observation coverage that includes these new well data and to compare the calibrated *run 1* from model version *S6a* to see how it matches the new data.

Before getting into the model discussion, let's talk about the updated observation well coverage. Here are some key steps I followed to update the coverage:

- Obtain the latest Nye County well water level data: The www.nyecounty.com website has links to Excel spreadsheets with well water levels; however, the latest file, with data through June 2004, did not have location data for all of the wells. Two other file with summaries of well completion had the necessary location data. I sent an email to Dale Hammermeister at Nye County to ask him if these were good data sets. In return he sent me a more recent file that had everything in one place. I cross checked locations and water levels against the QA-approved files on the Nye website and everything looked good. The name of the file is "*EWDP data thru Oct2004.xls*" and is archived with this notebook (probably on data disk 3).

- Convert well locations to UTM NAD-27 coordinates. All of the well locations in the Nye County data base are in latitude and longitude units of degrees, but all the older DOE data used in the CNWRA site-scale model calibration are in UTM, Zone 11, NAD-27 coordinates. I used a USGS freeware program called Corpscon to convert the units for well locations. I checked a couple of the coordinate points against UTM NAD-27 locations already calculated by DOE and got the same values to within a meter, so I consider these calculations to be checked IAW QAP-14. Check was done using locations in table 7 of the DOE analysis/model report "Calibration of the site-scale SZ Flow model, Rev. 00."

Below is the revised table that can be exported to GMS for an observation coverage.

Name	x	y	z	head	Std._Dev.
1	555753	4088350	990.8	1187.7	50
2	534069	4086110	859.2	1008	5
3	549352	4083100	983.2	1034.6	20
4	548143	4082540	371.5	1020.2	20
5	551146	4081230	714.1	738.3	1
6	548032	4080260	793.4	779	0.5
7	549468	4080240	722.1	730.8	1
8	548306	4080020	125.7	754.2	1
9	561084	4079700	681.4	748.3	0.5
10	550439	4079410	709	730.8	0.5
11	554034	4078690	698.7	729.2	0.5
12	548933	4078600	542.2	730.1	0.5
13	549925	4078330	584	731	0.5
14	552630	4077330	703.6	729.7	0.5
15	548595	4077030	702	730.7	0.5
16	550955	4075930	473.2	730.3	0.5
17	550930	4075900	474.3	730.3	0.5
18	550955	4075870	553.2	730.2	0.5
19	553730	4075830	703.8	729.1	0.5
20	546151	4075470	740.9	775.8	0.5
21	549152	4074970	708.4	730.4	0.5

22	547543	4074620	318.1	730.5	0.5	
23	554017	4073520	354.8	728.4	0.5	
24	545964	4073380	734.2	776	0.5	
25	549905	4073310	705.4	729.7	0.5	
26	537738	4073210	282.8	810.5	0.75	
27	552090	4072550	705.8	729.6	0.5	
28	539976	4071710	490.5	779.4	0.75	
29	550168	4070660	702.6	729.5	0.5	
30	547542	4070430	691.9	730.7	0.5	
31	554444	4068770	659.6	727.9	0.75	
32	554498	4067970	662.7	727.8	0.75	
33	544027	4059810	710.2	729.8	1	
34	553704	4056230	697.4	718.4	1	
35	553808	4055460	675.6	702.8	1	
36	553883	4055400	682	704.1	1	
37	554131	4055400	698	705.6	1	
38	554008	4055340	679.3	701.7	1	
39	553685	4055240	682.1	705.3	1	
40	549863	4054910	664.3	706.7	1	
41	552818	4054930	636.5	705.5	1	
42	562604	4054690	688.7	725.1	5	
43	549746	4053650	669.9	707.7	1	
44	549679	4052320	675.3	704.4	1	
45	543481	4050070	638.6	694.4	2	
46	536350	4050010	673.8	691.9	2	
47	540673	4049990	676.7	694.3	2	
48	541518	4049940	654.7	694.4	2	
49	553471	4049850	699.2	722.1	2	
50	545596	4049400	667.6	697.8	2	
51	536552	4049330	672	690.2	2	
52	538889	4049000	678.6	707.4	2	
53	542194	4048890	651.6	698.1	2	
54	536903	4048620	685.1	691	2	
55	546718	4048670	686.7	693.6	2	
56	538196	4048440	685.7	706.9	2	
57	540035	4048450	669.5	699	2	
58	536655	4048400	671.1	691.3	2	
59	540608	4048080	662.8	695.2	2	
60	534967	4047970	677	689.2	2	
61	547120	4047960	664.6	686.4	2	
62	547941	4047780	673.3	696.2	2	
63	537727	4047670	654.5	691.4	2	
64	552390	4047680	667.2	709	2	
65	541778	4047600	664	690.4	2	
66	541381	4047560	677.1	705.7	2	
67	553609	4047630	690.2	717.2	2	
68	554006	4047630	693.4	718.8	2	
69	548466	4047260	715.4	690.1	2	
70	548492	4047080	668.3	688.9	2	
71	550431	4047060	615.4	691.2	2	
72	553612	4047080	702.5	717.4	2	
73	553687	4047080	688.7	714.8	2	
74	548393	4046950	673.9	701.4	2	
75	539147	4046840	672.1	696.5	2	
76	539968	4046820	664.7	694.2	2	
77	540788	4046820	686.2	694	2	
78	552097	4046880	678.9	699.5	2	
79	548727	4079930	-495.5		785.5	0.5
80	548727	4079930	193	736	0.5	
81	548727	4079930	562.5	730.6	0.5	
82	548727	4079930	680.5	730.9	0.5	
83	547668	4078840	704.2	775.5	0.5	
84	547668	4078840	446.4	775.6	0.5	
85	549949	4078420	-8.8	729.7	0.5	

86	549949	4078420	366.2	730.7	0.5
87	546188	4077820	662.9	776	0.5
88	546188	4077820	315.8	775.9	0.5
89	549188	4077310	395.5	730.4	0.5
90	549188	4077310	45	730.5	0.5
91	547562	4075760	576.9	731.5	0.5
92	547562	4075760	343.2	755.9	0.5
93	551501	4075660	-410.3	752.4	0.5
94	547578	4077550	725.9	731.2	0.5
95	548384	4076500	637.7	727.6	0.5
96	548550	4079260	678.3	731.1	0.5
97	548492	4077420	696.7	730	0.5
98	548697	4081910	734.8	839.8	0.5
107	563799	4071060	687.2	732.2	1
108	534386	4062600	673.4	715.9	1
109	549529	4052570	739.9	704.1	1
110	551348	4047430	704.1	713.3	2
115	555680	4088200	1180.6	1186.8	50
120(SD7)	547484	4077310	731.5	731.5	1
Nye1DXs	536768	4062500	784.2	787.2	0.5
Nye1DXd	536768	4062500	132.6	749.2	0.5
Nye1Sz1	536771	4062500	751.0	781.5	1.0
Nye1Sz2	536771	4062500	730.0	781.5	1.0
Nye3Sz2	541268	4059445	704.0	719.9	1.0
Nye3Sz3	541268	4059445	662.0	719.8	1.0
Nye_3D	541272	4059445	572.0	719.3	2.0
Nye4PA	553166	4056766	687.3	718.1	0.5
Nye4PB	553201	4056768	582.5	723.6	0.5
Nye5SB	555676	4058419	706.7	723.5	0.5
Nye7S	539557	4064318	826.5	830.3	1.0
Nye7SCz1	539551	4064311	812.0	830	5.0
Nye7SCz2	539551	4064311	778.0	830	5.0
Nye7SCz3	539551	4064311	740.0	821	5.0
Nye7SCz4	539551	4064311	704.0	792	5.0
Nye9SXz1	539038	4061004	765.0	766.4	1.0
Nye9SXz2	539038	4061004	751.0	767.2	1.0
Nye9SXz3	539038	4061004	714.0	767.2	1.0
Nye9SXz4	539038	4061004	695.0	767.2	1.0
Nye10Ps	553069	4064910	695.3	726.9	0.5
Nye10Pd	553069	4064910	650.4	726.9	0.5
Nye10Sz1	553060	4064894	696.0	727.0	0.5
Nye10Sz2	553060	4064894	651.0	726.9	0.5
Nye12Pa	536904	4060767	666.6	722.8	0.5
Nye12Pb	536872	4060794	666.5	722.9	0.5
Nye12Pc	536871	4060809	713.5	720.8	0.5
Nye15P	544847	4058158	716.4	722.4	0.5
Nye16P	545585	4064258	723.0	729.4	0.5
Nye18P	549335	4067227	702.4	727.5	0.5
Nye19P	549249	4058287	694.5	707.3	0.5
Nye19PBd	549257	4058311	660	708.0	1.0
Nye22Pas	551940	4062033	700.9	724.8	0.5
Nye22Pad	551940	4062033	652.1	724.9	0.5
Nye22Pbs	551958	4062033	584.9	724.8	0.5
Nye22Pbd	551958	4062033	514.9	724.8	0.5
Nye22Sz1	551939	4062015	701.0	724.9	0.5
Nye22Sz2	551939	4062015	652.0	724.9	0.5
Nye22Sz3	551939	4062015	585.0	724.9	0.5
Nye22Sz4	551939	4062015	515.0	724.9	0.5
Nye23Ps	553843	4059870	704.1	724.2	0.5
Nye23Pd	553843	4059870	649.3	724.3	0.5
Nye2DB	547720	4057187	-76.6	712.5	2.0
Nye28P	545665	4062388	719.0	729.3	0.5
Nye29P	549316	4059601	719.0	724.8	0.5
Nye24P	549305	4062050	723.0	727.1	0.5

```
Nye27P      544855     4065270     724.0 728.6 0.5
Wshbn1Xd    551464     4057564     686.0 714.4 0.5
```

Notes on above list:

- The numbered values at the beginning are the same as the numbers reported in table 7 of the DOE analysis/model report "Calibration of the site-scale SZ Flow model, Rev. 00." Toward the end of the list, the wells identified by name are the ones that I updated using the recent Nye County data – the updated wells that were pre-existing in the DOE table were removed, as can be noticed from the gaps in the numeric sequence in this list. Several of the wells are new and were not on the previous list.
- I also deleted from the list wells 111 through 114 from the DOE table in which the reported measurement elevation was higher than the reported water level, as this is not physically possible – these were all agricultural or municipal wells that I do not considered reliable for calibration.
- After importing to model version S6b, I deleted all of the wells outside of the model area. These can easily be re-imported as the entire list is archived with model version S6b in a file called "*obs-nad27.tob*".

The next step is to compare calibration with old observation versus new observation data.

Comparison of old versus new observation coverage. Using run1 of model version 6a the following is an error summary of the run1 calculated heads versus the observation data.

	Old observation coverage – *"obswells.tob"* in S6a directory	New Observation coverage – "*obs-nad27.tob*" in S6b directory
Mean error	2.82	0.46
Mean absolute error	8.84	8.45
Root mean square error	17.35	15.48

It can be seen that the calibration error is less with the new observation coverage.

Notebook pages 13-16 printed for QA records on 3/29/05. Next printing should begin with page 17.

Following Entries made 4/12/05

New Task to Update the Site Scale Model to run on GMS Version 5.1 and MODFLOW - 2000

Starting with model version S6b grid described on the preceding pages, I read the grid and the "Run 1" set of MODFLOW input parameters and boundary conditions. The goal here is to run this version, which was initially calibrated with MODFLOW-96, with the newer MODFLOW-2000, then check to make sure the calibration and flow paths do not significantly change as a result of running the model with a different version of MODFLOW. The following bullets describe the procedure I followed.

- Copied the S6b grid files to a new directory: D:/GMS/GMS-5
- Initiated the GMS version 5.1 software, which successfully read in the S6b grid input files with only an error message that the plot file was not compatible — this is not a problem as new plot settings were automatically generated by GMS-5 when I saved the file.
- Checked grid coordinates in the old and new GMS versions. For some reason, GMS 5.1 assigns the grid node coordinate that is a fraction of a millimeter different than the X and Y coordinates defined in the old GMS 3.1 version. For example, the at i,j,k = 1,1,1 the in the old version, X = 535000 m and Y = 4049000 m; however, in GMS 5.1, the same cell is assigned X = 534999.99616 and Y = 4089999.99496. Not sure why it does this, but it is not enough to make any difference.
- With the S6b grid loaded, I opened the old "run1.mfs", which is the calibrated MODFLOW-96 run for grid S6b. GMS-5 read in the file, but queried if I wanted to convert the BCF format to LPF format. LPF is an input format that can be used by MODFLOW 2000 instead of BCF. I told GMS-5 to convert and the simulation was read in with no errors.
- After reading in the run 1 simulation, I opened the MODFLOW menu for the LPF package and set the option to "use material IDs" for assigning properties to cells. Also selected "Specified Kv" as the method for assigning vertical conductivity. Checked that top 7 layers were set to "convertible" mode, which allows a switch to an unconfined solution if water level is below top of the cell.
- Checked recharge package to make sure 10 mm/yr recharge in northern area and 5 mm/yr recharge over YM area were read in correctly. All recharge cells were properly assigned.
- First attempt to run MODFLOW-2000 did not work; an error message was generated saying something about observation input was selected, but no observation was read in. I spend some time playing with the observation coverage menus in the map module. I am not sure what I did to fix the problem, but I think it was right clicking on the "Observation coverage" icon in the directory tree in the upper right pane; from that menu, I selected "Properties..." which gives a menu of options: I de-selected "transport" and selected "LPF" as the flow package option. A test run of MODFLOW-2000 ran fine after this.

- After MODFLOW-2000 ran successfully, I started a new run with the starting heads in the model set to 1101 m for the top 7 layers. I then ran the model again and checked the residual observation errors. They were slightly different than the error for run 1 using GMS 3.1. I then saved the calculated heads as the new starting heads, ran the model again, and again checked the residual error. It changed slightly. A couple of more iterations of saving the new starting heads and re-running the model were done until the residual observation error no longer changed significantly. I saved this as the new calibrated model version. A comparison of the residual errors for the GMS version 3.1 (Modflow 96) and version 5.1 (Modflow 2000) are in the table below.

Comparison of residual errors for the GMS version 3.1 (Modflow 96) and version 5.1 (Modflow 2000).

	GMS version 5.1 (Modflow 2000)	**GMS version 3.1 (Modflow 96)**
Mean error	0.230	0.46
Mean absolute error	9.098	8.45
Root mean square error	16.197	15.48

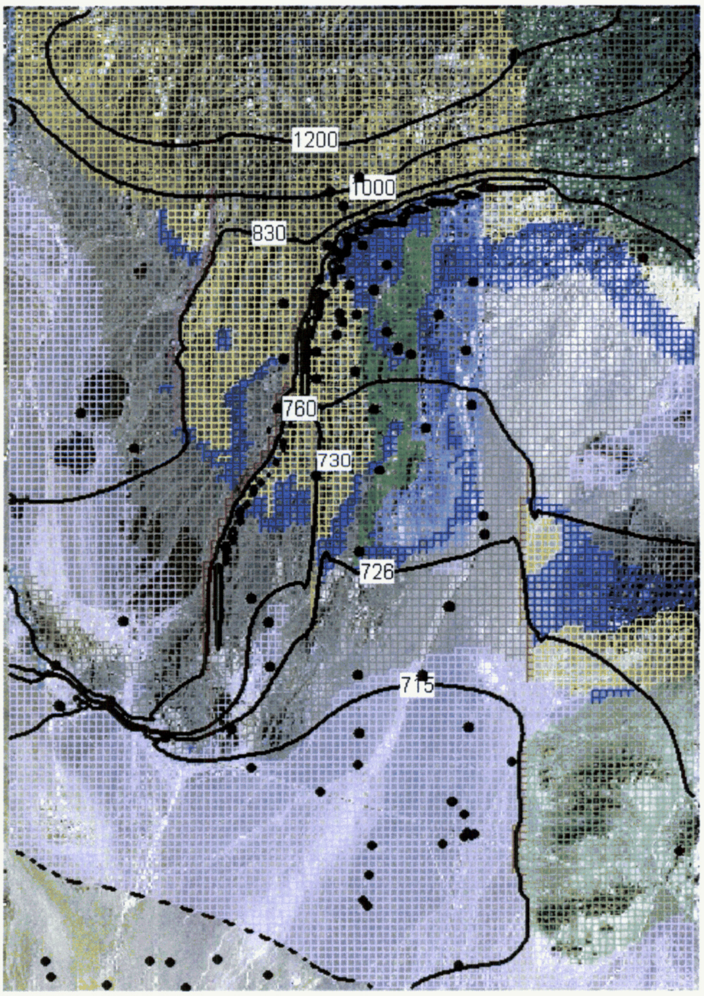
In general, I consider this a good match to the calibrated values from the old GMS 3.1 version of the model. Differences could be due to different interpolation routines used by GMS to calculate head values for observations that lie in between nodes. Or, it could just be differences in how MODFLOW-2000 converges on its final solution.

To gain additional confidence that the model has been properly converted to the MODFLOW 2000 format, I compare on the next page figures showing the active cells and the hydraulic head contour lines obtained from layer 6 of both models. The two figures are virtually identical to the naked eye. I consider this exercise to provide sufficient validation that MODFLOW 2000 works properly and the procedure described in the preceding paragraphs has successfully updated the flow model to the GMS 5.1 and MODFLOW-2000 formats.

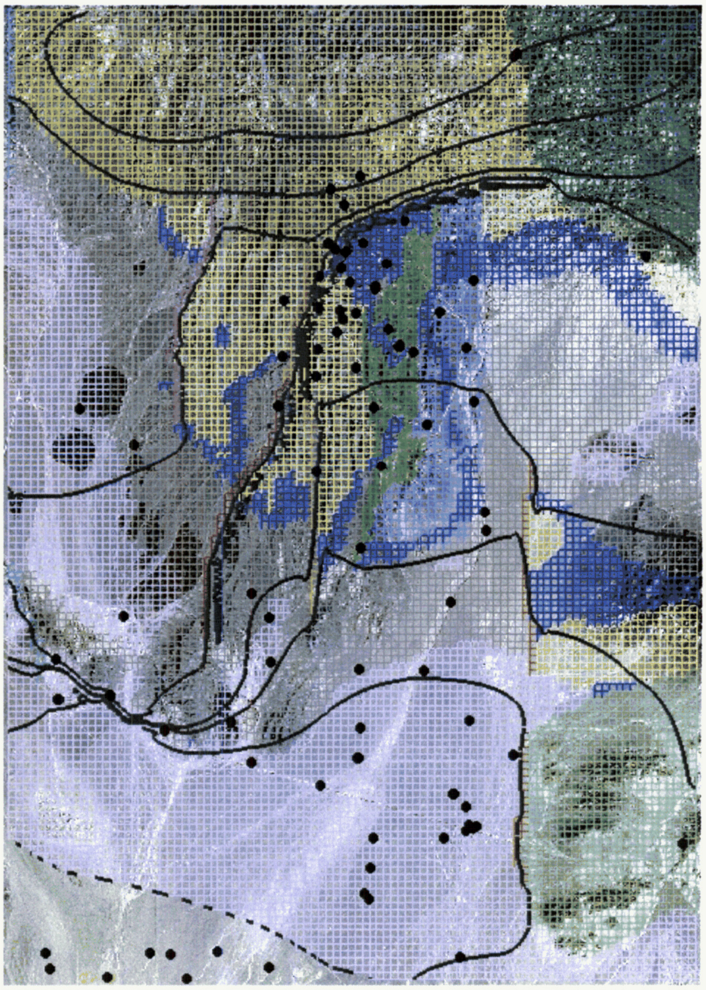
--------------no more entries this page----------

Figures below show calculated hydraulic head contours for grid S6b, run-1, using GMS 3.1/MODFLOW-96 (on left) and GMS 5.1/MODFLOW-2000 (on right).

GMS 3.1/ MODFLOW-96



GMS 5.1/MODFLOW-2000



– No more entries this page –

Following Entries Made 8/08/2005

New Task: Flow Modeling to Evaluate Effects of Spring Flows South of Yucca Mountain

The following entries document work that I performed during the last several months. This work was summarized in my presentation at Devils Hole Workshop in May, 2005; and is documented in greater detail in a project milestone report 06002.01.272.521. Entries below summarize the purpose and where model input and output files can be located prior to archiving on a CD.

Data Files:

Model Input and Output files for this analysis of spring flow effects on flow paths can be found on J. Winterle's desktop computer in the following folder: **D:\GMS\30-Layer\GMS-5\S6b\S6b-Run4**. Opening the model project S6-Run4.gpr will allow user to view model with the GMS, Version 5 Interface.

Purpose:

The CNWRA site-scale saturated zone flow model previously has been used to evaluate the potential effects on flow paths of a higher water table that might result from future wetter climate conditions (Winterle, 2003). During that exercise, a higher water table was simulated by increasing the constant-head model boundary values by a fixed 5 percent. This approach was successful in predicting that a rising water table would first intersect the land surface in an area where thick evaporite mineral deposits are present. These mineral deposits are the result of evaporating spring flows that occurred when the water table intersected the land surface in the past. This previous work suggested that the modeled increase in water table elevation resulted in increased hydraulic gradients but did not significantly affect flow paths from beneath Yucca Mountain. A limitation of the analysis by WInterle (2003), however, is that spring discharge was included in the model at only a single model cell with a spring discharge rate of only 0.3 m^3/d [10^{-4} cfs]. In this analysis, the effect of potential spring flows that occur over a larger area and at higher flow rates is explored.

Winterle, J.R. "Evaluation of Alternative Concepts for Saturated Zone Flow: Effects of Recharge and Water Table Rise on Flow Paths and Travel Times at Yucca Mountain." San Antonio, Texas: CNWRA. 2003.

Abstract:

The Center for Nuclear Waste Regulatory Analyses (CNWRA) developed an independent, three-dimensional, saturated-zone flow model for the Yucca Mountain region using the MODFLOW code. This model has proven useful as an independent means of evaluating parameter uncertainties and alternative interpretations of hydrogeologic conditions. In this presentation, we show results of analyses used to evaluate the effects of water-table rise during potential wetter climate conditions. Water table rise was included in the model by increasing potentiometric head values at the model side boundaries by a fixed percentage and doubling the rate of surface recharge. A five-percent increase in boundary heads from the estimated present-day values caused the calculated water table elevation to first reach the land surface in the in an area coincident with evaporite deposits that

indicate the past occurrence of spring flows. To model their effect on flow paths, spring discharges were simulated using the MODFLOW Drain package; total spring discharge was varied by using different values for drain conductance and elevation. Particle-tracking analyses of flow paths from beneath Yucca Mountain were then performed for different spring discharge rates using the MODPATH code. A maximum spring discharge in excess of 3,000 acre-ft per year was evaluated at this location. Results suggests that calculated flow paths from beneath Yucca Mountain do not change appreciably as a result of spring discharges at this location. Reverse particle tracking indicated that the simulated discharges at this location originate from the Crater Flat area, west of Yucca Mountain.

— End of entries for 8/08/2005 —

Following Entries Made 11/18/2005

I am preparing to close this notebook out and submit for QA records. Relevant model files created since 1/11/2005 are archived to Disk 3, to be attached to this scientific notebook.

Disk 3 Data Archive, Attached to this notebook, contains the following directories:

***S6b*:** Contains the model version S6b described in 1/11/2005 entries; this version runs with GMS version 3.1. A readme.txt file also describes what is contained in this directory

GMS5\\: Contains the model version S6b that was converted to run with GMS version 5.0. This folder contains the model runs described by entries beginning 4/ 2/2005. A readme.txt file also describes what is contained in the S6b subdirectory.

Notebook closed on 11/18/2005.

I have reviewed this scientific notebook and find it in agreement with QAP–001.

James Winterle
Manager, Performance Assessment Group

11-18-05
Date

No more entries.