Appendix G

Ground Water Flow and Transport Modeling

This page intentionally left blank

Technical Task Cover Sheet

Discipline Hydrology/Hydrogeology

Project:

UMTRA Ground Water Project

Site:

Durango, Colorado

Subject:

Durango Mill Tailings Site Ground Water Modeling Calculation

Sources of Data:

American Society for Testing and Materials (ASTM), 1993. *Standard Guide for Application of a Ground-Water Flow Model to a Site-Specific Problem*, ASTM D 5447-93,

———, 1995. *Standard Guide for Documenting a Ground-Water Flow Model Application*, ASTM D 5718-95.

Anderson, M.P., and W.W. Woessner, 1992. *Applied Groundwater Modeling Simulation of Flow and Advective Transport*, Academic Press, San Diego, California.

Baes, C.F., and R.D. Sharp, 1983. "A Proposal for Estimation of Soil Leaching and Leaching Constants for Use in Assessment Models," *Journal of Environmental Quality*, 12:1

Cleary, R.W., 2001. "Fate and Transport Process: Natural Attenuation Mechanisms in Contaminant Migration," notes from NGWA's Visual MODFLOW course.

Dixon, W.J., and F.J. Massey, Jr., 1957. *Introduction to Statistical Analyses*, Second Edition, McGraw-Hill Book Company, Inc., New York.

Environmental Simulations, Inc., 1997. *Guide to Using Groundwater Vistas, Advanced Model Design and Analysis*, Herndon, Virginia.

Gelhar, L.W., C. Welty, and K.R. Rehfeldt, 1992. "A Critical Review of Data on Field-Scale Dispersion in Aquifers," *Water Resources Research*, 28(7):1955–1974.

McDonald, M.G., and A.W. Harbaugh, 1988. *Techniques of Water-Resources Investigations of the United States Geological Survey,* Chapter A1: A Modular Three-Dimensional Finite-Difference Ground-Water Flow Model, Book 6, Modeling Techniques, U.S. Geological Survey Open-File Report.

Ruskauff, G.J., and Environmental Simulations, Inc., 1998. *Guide to Using Stochastic MODFLOW for Monte Carlo Simulation*, Herndon, Virginia.

Thronthwaite, C.W., and J.R. Mather, 1957. Instructions and tables for Computing Potential Evaporation and the Water Balance. *Climatology*, 10 (3).

U.S. Department of Energy (DOE), 2001. *Determination of Distribution Ratios, UMTRA Ground Water Project, Durango, Colorado, Site,* ESL-RPT-2001-02, prepared by MACTEC Environmental Restoration Services, LLC, for the U.S. Department of Energy, Grand Junction Office, Grand Junction, Colorado.

Zheng, C. and P. Wang, 1999. *MT3DMS: A Modular Three-Dimensional Multispecies Transport Model for Simulation of Advection, Dispersion, and Chemical Reactions of Contaminants in Ground Water Systems*, Documentation and User's Guide, Department of Geological Sciences, University of Alabama, Tuscaloosa, Alabama.

Task Order No. MAC02-05 **File Index No.** GWDUR13.02

Proj. No. UGW-511-0006-11 **Calc. No.** U0149900 **Supersedes Calc. No.** NA

Calculated by	Date	Checked by	Date	Approved by	Date	DOE Concurrence (if required)	Date
Ken Pill							

Contents

1.0 Introduction 1
- 1.1 Modeling Objective 1
- 1.2 Model Function 1
- 1.3 General Setting 1

2.0 Conceptual Model 3
- 2.1 Aquifer System Framework 3
- 2.2 Hydrologic Boundaries 3
- 2.3 Hydrologic Properties 5
- 2.4 Sources and Sinks 5
  - 2.4.1 Sources 5
  - 2.4.2 Sinks 5
- 2.5 Conceptual Water Budget 6

3.0 Computer Code Description 6
- 3.1 Assumptions 6
- 3.2 Limitations 8
- 3.3 Solution Techniques 8
- 3.4 Effects on Model 8

4.0 Model Construction 8
- 4.1 Model Domain 8
- 4.2 Hydraulic Parameters 11
- 4.3 Sources and Sinks 12
  - 4.3.1 Sources 12
  - 4.3.2 Sinks 12
- 4.4 Boundary Conditions 12

5.0 Calibration of Flow Model 15
- 5.1 Calibration Process 15
- 5.2 Calibration Goals 15
- 5.3 Flow Model Sensitivity Analysis 17
- 5.4 Stochastic MODFLOW 20
- 5.5 Qualitative and Quantitative Analysis 21

6.0 Transport Modeling 24
- 6.1 Development of the Transport Model 26
  - 6.1.1 Initial Contaminant Concentration Distribution 26
  - 6.1.2 Dispersivity 28
  - 6.1.3 Effective Porosity 28
  - 6.1.4 Bulk Density 32
  - 6.1.5 K_d 32
  - 6.1.6 Transport Parameter Summary 32
- 6.2 Transport Model Sensitivity Analysis 33

7.0 Steady State Stochastic Transport Modeling 35
- 7.1 Transport Model Development 35
- 7.2 Transport Modeling Results 36
  - 7.2.1 Cadmium 37
  - 7.2.2 Manganese 39
  - 7.2.3 Molybdenum 39
  - 7.2.4 Selenium 39
  - 7.2.5 Sulfate 43
  - 7.2.6 Uranium 43

8.0 Summary and Conclusions 47
8.1 Qualitative Analysis 47
8.2 Quantitative Analysis 47
8.3 Model Predictions 48

Figures

Figure 1. Durango Mill Tailings Site Location Map 2
Figure 2. Alluvial Aquifer Ground Water Surface Contour Map, Based on the Average Ground Water Elevation 4
Figure 3. Water Budget Flow Components for the Mill Tailings Site 7
Figure 4. Extent of the Mill Tailings Ground Water Model 9
Figure 5. Animas River Surface Elevation Measuring Point Locations 10
Figure 6. Surficial Aquifer Hydraulic Conductivity Zones 11
Figure 7. Boundary Conditions Assigned to the Model 13
Figure 8. Calibration Target Locations 14
Figure 9. Flow Model Development 16
Figure 10. Hydraulic Conductivity—Zone 1 Sensitivity Analysis Results 18
Figure 11. Hydraulic Conductivity—Zone 2 Sensitivity Analysis Results 18
Figure 12. Hydraulic Conductivity—Zone 3 Sensitivity Analysis Results 19
Figure 13. Recharge Sensitivity Analysis Results 19
Figure 14. Simulated Surficial Aquifer Ground Water Surface Contour Map 22
Figure 15. Comparison of Residual versus Observed Head 22
Figure 16. Target Residual Value 23
Figure 17. Comparison of Computed Head versus Observed Head 24
Figure 18. Procedure Used for Transport Modeling 25
Figure 19. Cadmium Initial Concentration Distribution 29
Figure 20. Manganese Initial Concentration Distribution 29
Figure 21. Molybdenum Initial Concentration Distribution 30
Figure 22. Selenium Initial Concentration Distribution 30
Figure 23. Sulfate Initial Concentration Distribution 31
Figure 24. Uranium Initial Concentration Distribution 31
Figure 25. Cumulative Average Residual Sum of Squares versus Realization Number 36
Figure 26. Residual Sum of Squares versus Realization Number 36
Figure 27. Predicted Average Cadmium Concentration at 10 Years 38
Figure 28. Predicted Average Cadmium Concentration at 100 Years 38
Figure 29. Probability of Cadmium Exceeding 0.01 mg/L After 100 Years 39
Figure 30. Predicted Average Manganese Concentration at 10 Years 40
Figure 31. Predicted Average Manganese Concentration at 50 Years 40
Figure 32. Probability of Manganese Exceeding 1.7 mg/L After 50 Years 41
Figure 33. Probability of Manganese Exceeding 1.7 mg/L After 60 Years 41
Figure 34. Predicted Average Selenium Concentration at 10 Years 42
Figure 35. Probability of Selenium Exceeding 0.05 mg/L after 25 Years 42
Figure 36. Predicted Steady State Sulfate Concentration at 25 Years 43
Figure 37. Predicted Steady State Sulfate Contamination at 50 Years 44
Figure 38. Predicted Steady State Sulfate Concentration at 70 Years 44
Figure 39. Predicted Average Uranium Concentration at 10 Years 45
Figure 40. Predicted Average Uranium Concentration at 25 Years 45
Figure 41. Predicted Average Uranium Concentration at 60 Years 46

Figure 42. Probability of Uranium Exceeding 0.044 mg/L After 60 Years 46
Figure 43. Probability of Uranium Exceeding 0.044 mg/L After 70 Years 47

Tables

Table 1. Water Budget Estimated Inflows and Outflows for the Mill Tailings Site 6
Table 2. Hydraulic Conductivity Values for the Surficial Aquifer..... 11
Table 3. Target Ground water Elevation Data 14
Table 4. Flow Model Calibration Objectives..... 17
Table 5. Flow Model Sensitivity Analysis Parameter Values 17
Table 6. Flow Parameter Coefficient of Variation Analysis..... 20
Table 7. Stochastic MODFLOW Parameter Ranges 20
Table 8. Comparison of Modeling Results Based on the Standard Devation/Range and RRS 21
Table 9. Parameter Values for the Statistically Best Realizations..... 21
Table 10. Calibration Objectives and Results..... 23
Table 11. Calibration Target Residuals 24
Table 12. Contaminant Ground water Concentrations from November 2000 Through August 2001 26
Table 13. Contaminant K_d Values 32
Table 14. Transport Parameter Value Ranges 32
Table 15. Sensitivity Parameter Values..... 33
Table 16. Transport Parameter Coefficient of Variation Analysis 34
Table 17. Ranges and Distribution Types Assigned to Longitudinal Dispersivity and Effective Posrosity Parameters 35
Table 18. Predicted Contaminant Maximum Average Concentrations (mg/L) at 5, 10, 15, 25, 50, 60, 70, 80, 90, and 100 Years 37

1.0 Introduction

1.1 Modeling Objective

As part of the final compliance strategy for the cleanup of contaminated ground water at the Durango, Colorado, Uranium Mill Tailings Remedial Action (UMTRA) Project Mill Tailings Site, it is necessary to develop a computer ground water model. This model, which consist of ground water flow and contaminant transport components, is designed to assist in forecasting whether natural flushing of various contaminants is a viable remediation alternative.

This document presents the development of steady state stochastic hydrologic flow and contaminant transport models to predict future contaminant concentrations. The various flow and transport parameters that affect the hydraulic head and contaminant distribution for the models are described. Contaminants that are modeled include cadmium, manganese, molybdenum, selenium, sulfate, and uranium.

The steps used for obtaining calibrated flow and transport models for the sites follow the ASTM Standard Guides D5447–93 and D5718–95. The specific steps are to: (1) evaluate the hydrogeologic setting and develop a conceptual model, (2) select the code to be used in the analysis, (3) establish the relationship between the conceptual and numerical models, (4) perform flow model calibration and sensitivity analysis on transport parameters, and (5) complete predictive simulations.

Stochastic simulations for the steady state models were performed, varying both flow and transport parameters, to evaluate the uncertainty in the predicted concentrations. These stochastic simulations were used to calculate mean concentrations and the probability of contamination remaining above acceptable levels across the site at specific times.

1.2 Model Function

This model will be used to investigate the steady-state ground water flow conditions and contaminant transport associated with the surficial aquifer at the Mill Tailings Site. In addition, the model can assess the impact of various hydraulic stresses on the surficial aquifer which may need to be examined, such as pumping, artificial recharge, and river stage elevation changes.

1.3 General Setting

The Durango UMTRA Project Site consists of two geographically contiguous, but hydrogeologically distinct, areas: The Mill Tailings Site and the Raffinate Ponds Site. Modeling was completed only for the Mill Tailings Site, and will be the focus of this document. Located on the west bank of the Animas River southwest of the city of Durango, in La Plata County, Colorado (Figure 1), the Mill Tailings Site lies immediately southwest of the intersection of Routes 160 and 550, at the confluence of Lightner Creek and the Animas River. The site encompasses an area of approximately 40 acres and lies at an elevation of approximately 6,500 feet (ft) above mean sea level (MSL). Surface remediation of tailings and mill related contamination was completed in 1991, with the contaminated material placed in the Bodo Canyon disposal cell located 1.5 miles southwest of the Durango sites.

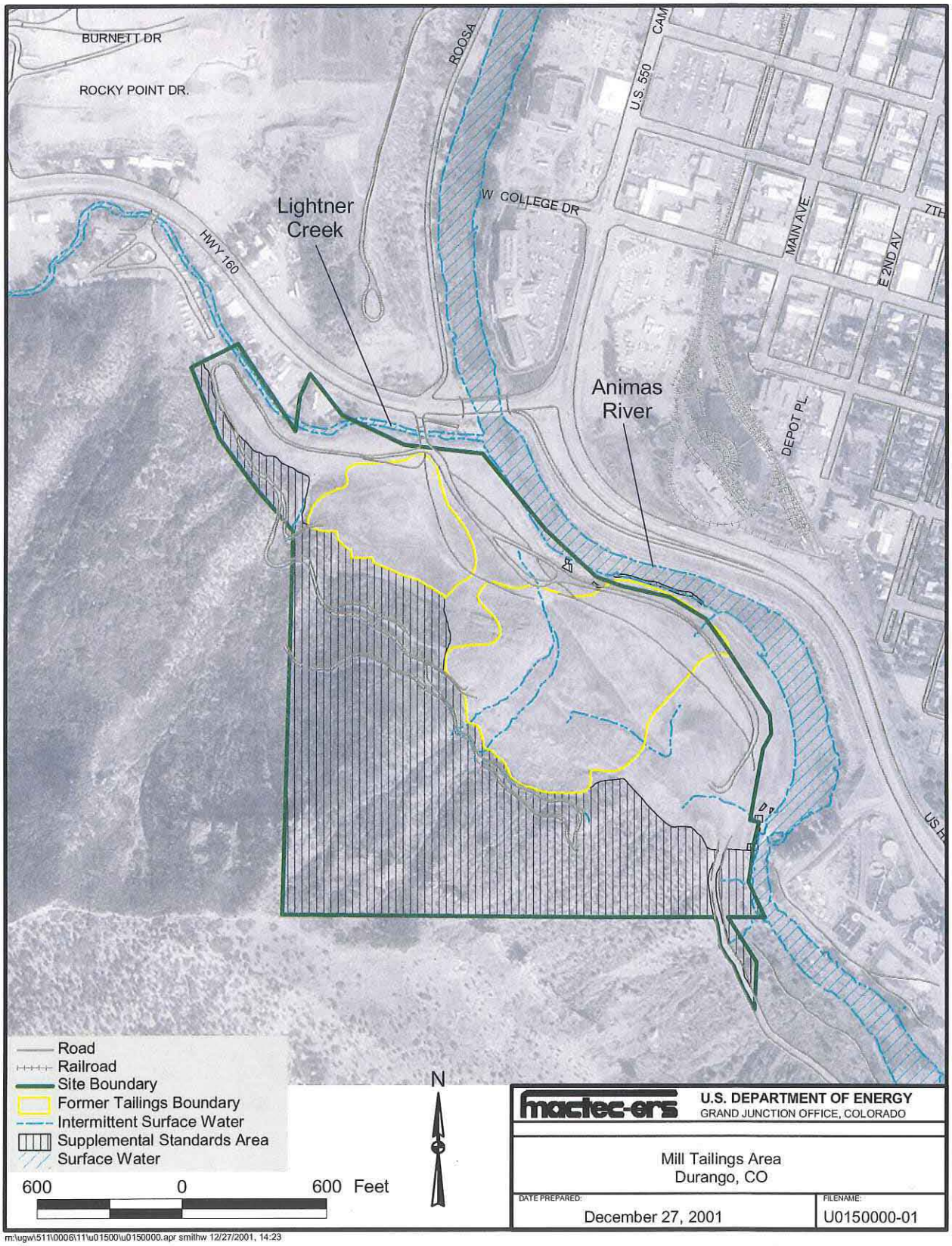


Figure 1. Durango Mill Tailings Site Location Map

2.0 Conceptual Model

2.1 Aquifer System Framework

The Mill Tailings Site hydrostratigraphic units include the Mancos Shale that is overlain by unconsolidated colluvial and alluvial deposits. In the vicinity of the site, the Mancos Shale is believed to be approximately 500 ft thick. None of the ground water monitoring wells drilled onsite have fully penetrated this bedrock unit.

Along the base of Smelter Mountain, which is located southwest of the site, the Mancos Shale is directly overlain by colluvium that consists of up to 25 ft of poorly sorted, silty soil that originated from Smelter Mountain. Closer to Lightner Creek and the Animas River, an alluvial deposit of river-lain sand and gravel up to 15 ft thick occurs between the colluvium and the Mancos Shale. These sands and gravels are well sorted and much more conductive compared to the colluvium. In addition to the alluvium and colluvium overlying the Mancos Shale, in the southeast corner of the site there is a layer of lead smelter slag (up to 25 ft thick in some locations) along the western bank of the Animas River.

The colluvium and alluvium combined comprise what will be referred to (for modeling purposes) in this document as the surficial aquifer. This aquifer is unconfined, while the Mancos Shale aquifer appears to be unconfined near the top of the unit and most likely semi-confined or confined near the bottom of the unit.

Average water level elevations measured in the wells screened in the surficial aquifer are displayed in Figure 2. This map shows that the ground water flow trends to the southeast, and generally follows the Animas River flow direction. The colluvium component of the surficial aquifer receives recharge from runoff from Smelter Mountain and infiltration of precipitation. The alluvium component receives recharge from Lightner Creek and the Animas River.

Water that migrates through the entire thickness of the colluvium, and reaches the surface of the Mancos, eventually discharges into the Animas River. Other sources of colluvium discharge include evapotranspiration. Discharge from the alluvium component includes ground water flow into the Animas River when the stage is low.

2.2 Hydrologic Boundaries

Due to the low hydraulic conductivity (K) of the Mancos Shale (estimated to be less than 0.01 ft/day), this underlying unit is considered to be impermeable. As a result, the ground water model for the Mill Tailing Site consists of only one layer representing the previously mentioned surficial aquifer.

Lightner Creek and the Animas River represent the dominant natural hydrologic boundaries associated with the site (Figure 1). In the case of the Animas River, the river channel cuts through the entire thickness of the surficial deposits, with the bed of the river on the surface of the Mancos Shale. In addition, the high topographic relief and associated high ground water elevations in wells located on the east side of the river indicate that the ground water on the east side flows toward and discharges into the Animas River. Such a flow pattern on the east side prevents ground water migration under the river to the other side.

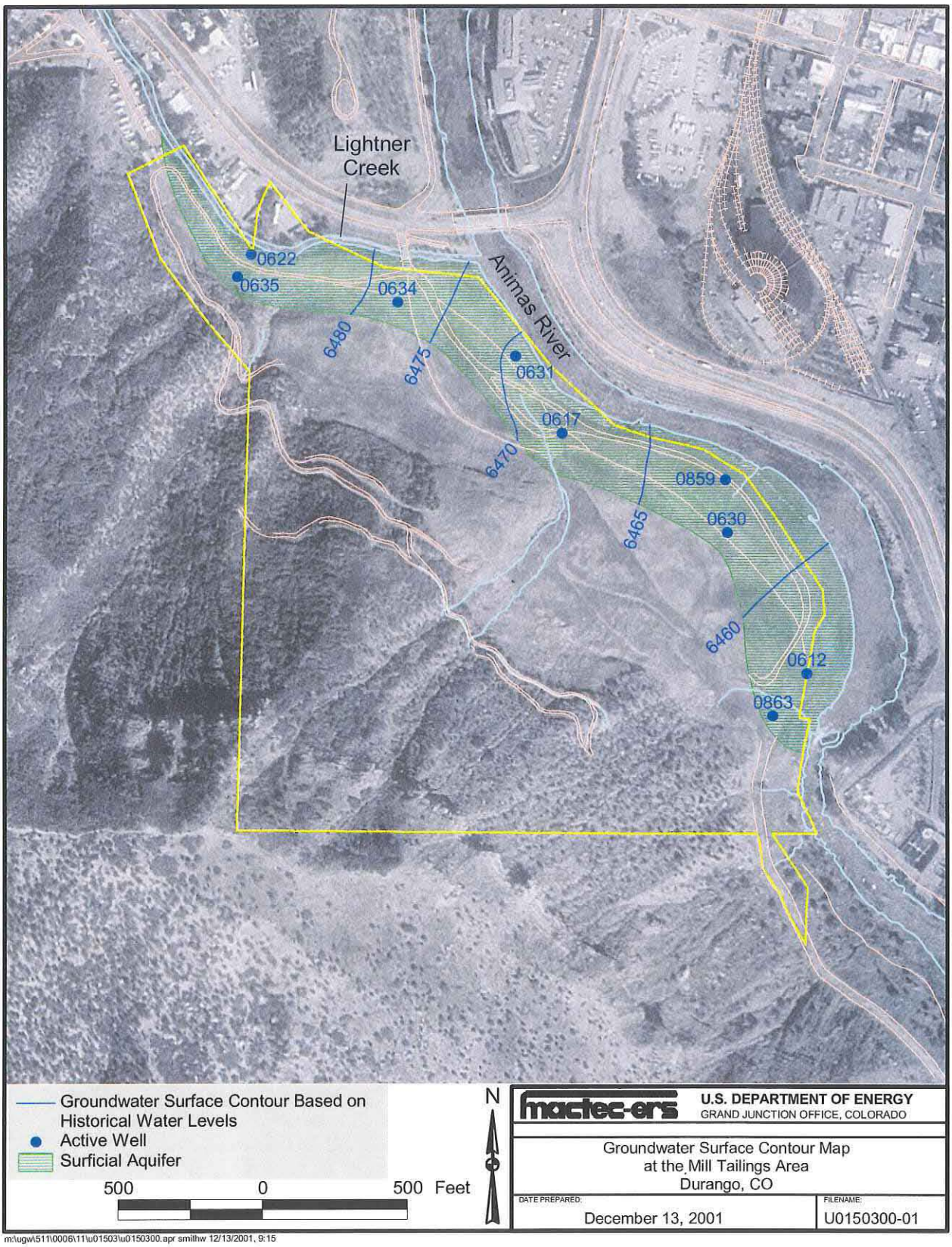


Figure 2. Alluvial Aquifer Ground Water Surface Contour Map, Based on the Average Ground Water Elevation

The extent of the alluvial aquifer in the southwest portion of the site is controlled by Smelter Mountain, where the colluvium component of the surficial aquifer pinches out.

2.3 Hydrologic Properties

Slug tests were completed at eight different locations on the Mill Tailings Site to determine the hydraulic parameters of the surficial aquifer. These tests were performed on wells screened over the various deposits (both colluvium and alluvium) within the surficial aquifer. Test procedures, analysis of these data, and test results are presented in Calculation No. U0133300. Results indicate the horizontal hydraulic conductivity (K_x) of the colluvium ranges approximately from 1 to 10 ft/day. Data collected from wells completed in the Animas River alluvium suggest the K_x ranges from 10 to 28 ft/day, while the single test completed in a well screened in the Lightner Creek alluvium indicates the K_x is 66 ft/day.

2.4 Sources and Sinks

The Animas River, Lightner Creek, and precipitation are the main sources of recharge to the surficial aquifer. The Animas River is considered to be both a sink and a source (i.e., the surficial aquifer discharges water to the river along some reaches, and the river recharges the aquifer along other reaches). The discharge and recharge flows are seasonal in nature.

2.4.1 Sources

Three sources of recharge to the surficial aquifer have been identified. These include recharge from (1) precipitation and snowmelt, (2) Lightner Creek, and (3) the Animas River.

Historical meteorological data from the Fort Lewis Weather Station (station number 053016) located in Durango, Colorado, was used as a source of precipitation data for the site. Data collected from this station are the most representative because this station is within 5 miles of the site and has recorded monthly precipitation data more than 50 years. Data collected from 1948 through 2001 indicate there is on average 18.36 inches of annual precipitation in the Durango area, with July through October being the wettest months. Of this amount of precipitation, only a percentage is available to recharge the aquifer.

Lightner Creek is a main source of recharge to the alluvium component of the surficial aquifer along the banks of the creek during the spring runoff time period. Water flows from the creek into the conductive alluvium when the creek stage is high, generally between April through June.

The Animas River is the main source of recharge to the alluvium deposited along the banks of the river. Similar to the alluvium along Lightner Creek, the Animas River recharges the alluvium during time periods when the river stage is high.

2.4.2 Sinks

Two main sources of discharge from the surficial aquifer have been identified as evapotranspiration and ground water discharge into the Animas River.

Evapotranspiration is accounted for by the use of a net recharge estimate (which includes the loss due to evapotranspiration).

Ground water flows from the surficial aquifer into the Animas River during low river stage periods. Precipitation that migrates through the surficial aquifer and reaches the Mancos Shale also eventually discharges into the Animas River.

2.5 Conceptual Water Budget

A conceptual water budget that is estimated from the hydraulic properties of the alluvial deposits, interpolations of alluvial thickness from geologic logs, and projections of subcropping bedrock is presented in Calculation Set No. U0133800. This information is also presented in Section 5.1 of the site observational work plan. This document describes in detail each flow component associated with the Mill Tailings site, and their estimated inflows or outflows into or out of the modeled area. Table 1 presents the results of the water budget, while Figure 3 graphically shows the potential areas influenced by the flow components.

Table 1. Water Budget Estimated Inflows and Outflows for the Mill Tailings Site

Flow Component	Inflow (ft^3/day)	Outflow (ft^3/day)
Lightner Creek	990	840
Animas River	190	640
Areal Recharge	300	0
Total	1,480	1,480

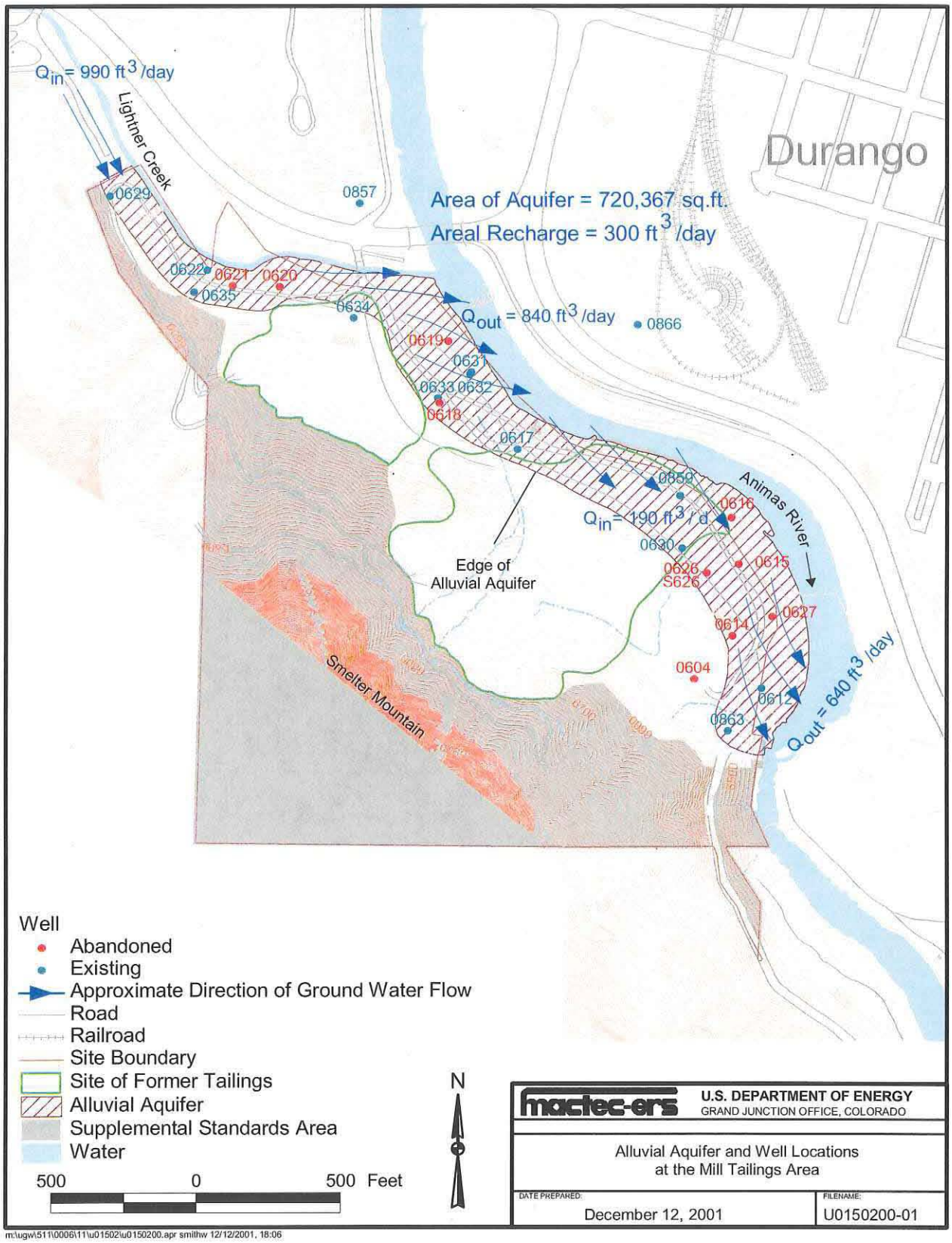
3.0 Computer Code Description

MODFLOW (McDonald and Harbaugh 1988), a modular three-dimensional finite-difference ground water flow model published by the U.S. Geological Survey (USGS) was selected as the flow code for this project. MT3DMS (Zheng and Wang 1999), a modular three-dimensional transport model for simulation of advection, dispersion, and chemical reaction of contaminants in ground water systems was selected as the transport code for this project. Each of these codes is divided into a main program and a group of independent subroutines called *modules*. Each module is made up of *packages* that deal with a single aspect of the simulation. The user of either MODFLOW or MT3DMS need only use those modules that simulate the stresses placed upon the flow and transport systems. This version of MT3DMS contains a new transport solver that is very efficient and makes multiple long simulation runs feasible.

Groundwater Vistas (Environmental Simulations, Inc. 1997), a Windows-driven, graphical, pre- and post-processor for MODFLOW and MT3DMS is used in conjunction with the site model to facilitate data entry, data-file modification, program execution, and analysis of modeling results.

3.1 Assumptions

A finite-difference model, such as MODFLOW, is based upon the continuity equation that states that the sum of all flows into and out of the cell is equal to the rate of change in storage in the cell, which relies on the assumption that the density of ground water is constant. Another assumption is that the numerical equations used by MODFLOW are good approximations to actual partial derivative equations. Other assumptions associated with MODFLOW include flow from a well is independent of head, and stream-aquifer interconnection is treated as a simple



m:\ugw\511\0006\11\u01502\u0150200.apr smithw 12/12/2001, 18:06

Figure 3. Water Budget Flow Components for the Mill Tailings Site

conductance term. A detailed description of the MODFLOW code formulation, approach, and assumptions is provided by McDonald and Harbaugh (1988).

3.2 Limitations

MODFLOW is based on the fundamental equation of ground water flow. For water table aquifers the head distribution along the exposed surface also equals or defines the upper physical boundary of the aquifer that may be rising or falling. As the head rises or falls, so does the physical boundary. This is described mathematically as a moving boundary value problem for which exact solutions are impossible due to the non-linear, quadratic head derivatives in the surface boundary condition (Cleary 2001).

In addition, MODFLOW is a finite difference model, where a continuous system as described by the fundamental equation is replaced by a finite set of discrete points in space and time. The partial derivatives are replaced by terms calculated from the differences in head values at these points. This process leads to a system of simultaneous linear algebraic difference equations which are solved for head at specific points and times (McDonald and Harbaugh 1988). As a result, an iterative process calculates the approximated head values.

Because we are dealing with a finite difference model, the model computes a value for the head at the node that is also the average head for the cell that surrounds the node. No assumption is made about the form of the variation of head from one node to the next (Anderson and Woessner 1992). As a result, in large cell areas (or areas of a high hydraulic gradient) the computed head will be an average value for the area within the cell. Groundwater Vistas, the graphic use interface software used for this modeling effort, does allow to interpolate between nodes; however, these resulting values should be considered an estimate.

3.3 Solution Techniques

MODFLOW offers several options for solving the flow equations, one of which is the Preconditioned Conjugate Gradient method, or PCG2. The PCG2 was the solver chosen for this model because of its ability to solve head matrices efficiently and generally converges quickly without oscillation problems.

3.4 Effects on Model

The use of a finite difference model may limit the representation of certain boundaries, such as stream or river traces. However, the use of the MODFLOW computer code for the Mill Tailings Site does not negatively influence the model representation because of the small scale of this model and the small grid size used.

4.0 Model Construction

4.1 Model Domain

The x-axis of the model is oriented in the east/west direction, centered over the location of the Mill Tailings Site. The modeled area consists of 160 rows and 160 columns of a 25 ft by 25 ft

orthogonal grid. Of the modeled 16,000,000 sq ft area, only 1,434 (or 896,250 sq ft) cells are active, with the remaining cells set as no-flow cells (Figure 4).

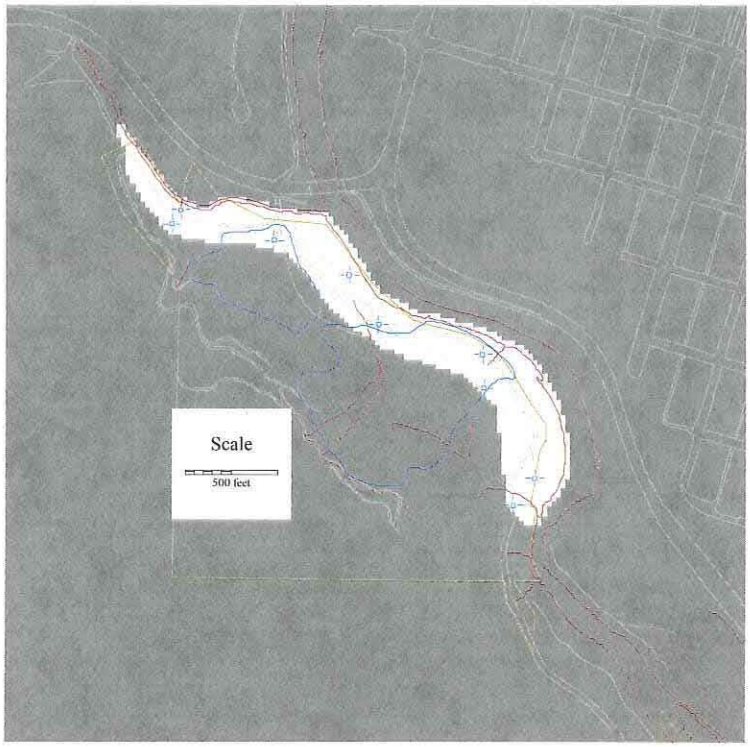


Figure 4. Extent of the Mill Tailings Ground Water Model

The western boundary of the grid was set arbitrarily and extended to a point west of the base of Smelter Mountain, which represents the extent of the surficial aquifer. Similarly, the eastern extent of the model grid was also set to include the Animas River. The northern boundary of the grid was set such that the modeled area included the extent of Lightner Creek, while the southern edge of the grid extended beyond the point where the surficial aquifer pinches out where the Animas River intersects the base of Smelter Mountain, in between the Mill Tailings and the Raffinate Ponds sites.

This model consists of a single layer representing the surficial deposits overlying the Mancos Shale. The Mancos Shale represents a no-flow boundary beneath the layer because of its low conductivity (less than 0.01 ft/day). The thickness of the surficial aquifer increases trending from the base of Smelter Mountain, where the surficial deposits pinch out, towards the river. In the vicinity of well 612, which is located in the very southern extent of the modeled area, the model layer reaches a maximum thickness of 55 ft.

Daily mean streamflow data (in cubic feet per second [cfs]) for the Animas River are collected at USGS Gaging Station #09361500, located 0.8 mile upstream from the Lightner Creek and Animas confluence. River elevation data are collected from two stilling wells located on the banks of the Animas River. Stilling well 868 is located just northeast of the 631/632 cluster, and stilling well 867 is located on the banks of the Animas River just northeast of well 859 (Figure 5). No streamflow or elevation data are available from Lightner Creek.

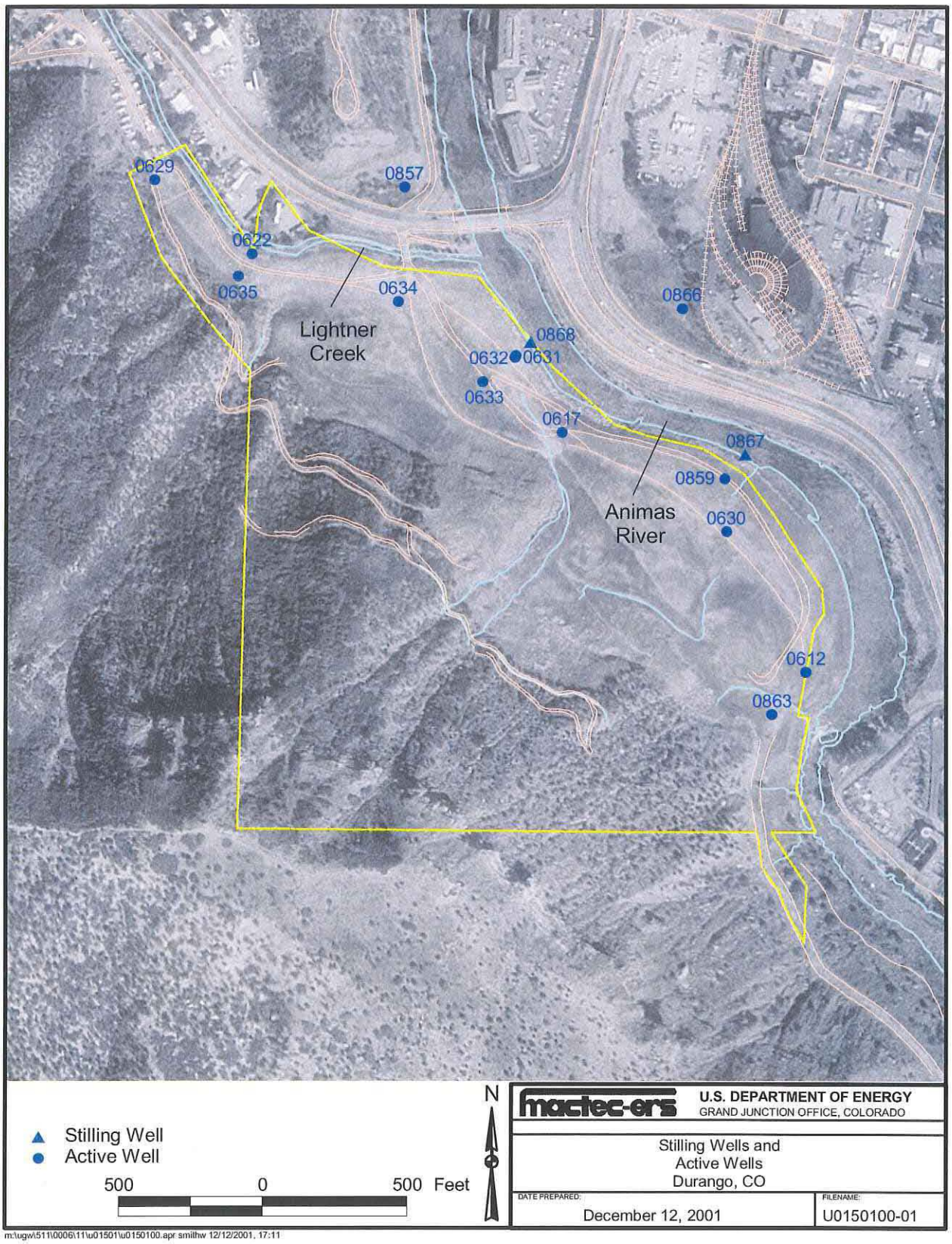


Figure 5. Animas River Surface Elevation Measuring Point Locations

4.2 Hydraulic Parameters

The surficial aquifer was divided into three hydraulic conductivity zones to reflect the various components of this layer (Section 2.1). The distribution of these zones is shown on Figure 6. Zone 1 represents the colluvium deposit originating from the slopes of Smelter Mountain. As previously discussed, this material has the lowest hydraulic conductivity measured during the Mill Tailings site field investigation. Zone 2 represents the alluvium deposited by the Animas River that overlies the colluvium, and Zone 3 represents the Lightner Creek alluvium and the alluvium located directly along the banks of the Animas River, which has the highest measured hydraulic conductivity.

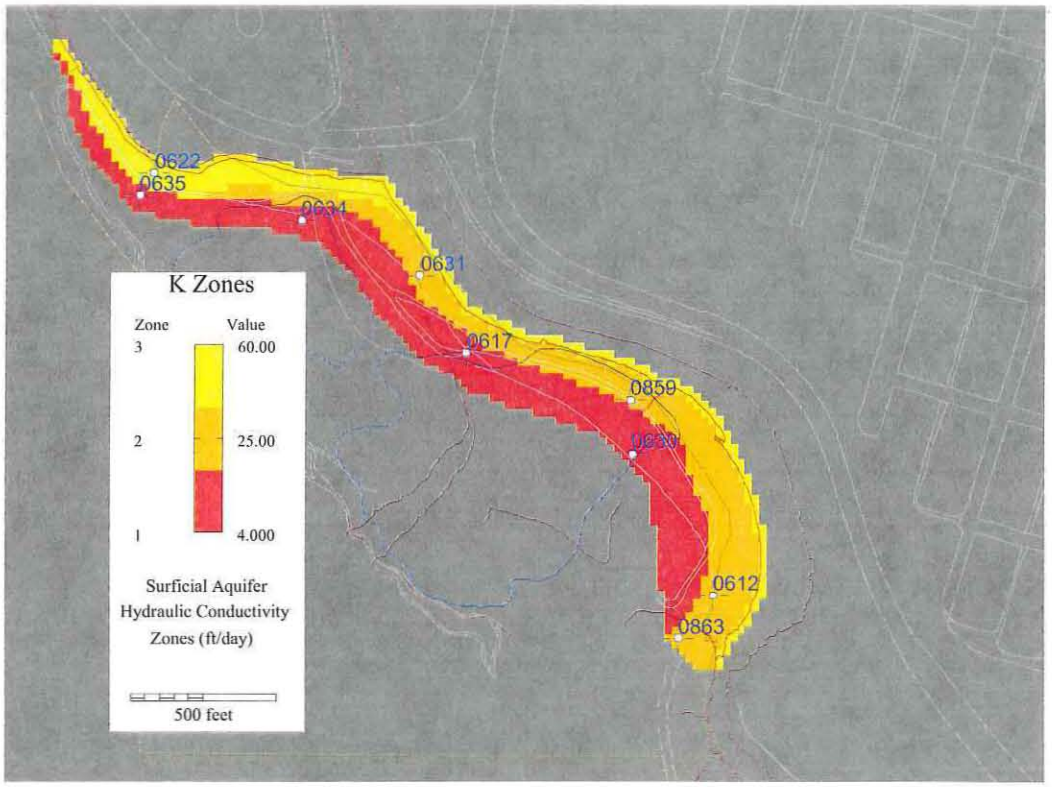


Figure 6. Surficial Aquifer Hydraulic Conductivity Zones

Based on the data collected in the field (including historical data), a range for the various hydraulic conductivity zones was established. These ranges are included in Table 2, which also presents the initial model input values.

Table 2. Hydraulic Conductivity Values for the Surficial Aquifer

K Zone Number	K Initial Model Input Value (ft/day)	K Initial Model Range (ft/day)
1	4	1 to 14
2	25	5 to 50
3	60	40 to 100

4.3 Sources and Sinks

4.3.1 Sources

Weather Service data indicate there is an average of 18.36 inches per year of precipitation in the vicinity of the site. The amount of precipitation available for recharge can be estimated by the Thronthwaite method (Thronthwaite and Mather 1957). This method, which provides a range of potential recharge, takes into account the mean monthly air temperature, annual precipitation, potential evaporation, and potential runoff to determine the amount of precipitation available for recharge to the aquifer.

Of the 18.36 inches per year of precipitation, an estimated 0.01 to 6.61 inches per year is available for aquifer recharge. This translates into a net recharge flux of 0.000002 to 0.00151 ft/day. The potential runoff parameter is based on the rock type in the vicinity of the site. With the site located at the base of Smelter Mountain, which has the potential to provide a large volume of recharge to the site, the actual recharge flux is expected to be near the higher end of this range.

Lightner Creek and the Animas River are the main sources of recharge to the surficial aquifer alluvium deposited along the banks of the creek and river.

4.3.2 Sinks

The main sources of discharge from the surficial aquifer have been identified as evapotranspiration and ground water discharge into the Animas River. The amount of potential evapotranspiration has been accounted for by the use of the Thronthwaite method.

Ground water discharges from the surficial aquifer in various areas into the Animas River during low river stage periods.

In addition, any recharge from precipitation that migrates through the surficial aquifer and reaches the Mancos Shale is expected to eventually discharge into the Animas River.

4.4 Boundary Conditions

As previously mentioned, the surficial deposits within the model are limited to the area between the base of Smelter Mountain, Lightner Creek, and the Animas River. No-flow cells are assigned to areas beyond the extent of the surficial deposits (Figure 7).

Along the northern extent of the surficial aquifer, Lightner Creek is represented as a constant head boundary. As a result of the lack of streamflow or elevation data associated with Lightner Creek, the head values assigned to the constant head cells representing Lightner Creek were based on the surface topography. Based on the topography, along the extent of the alluvium, the head drops from an elevation of approximately 6,495 ft MSL to 6,470 ft MSL in the area adjacent to the active model cells.

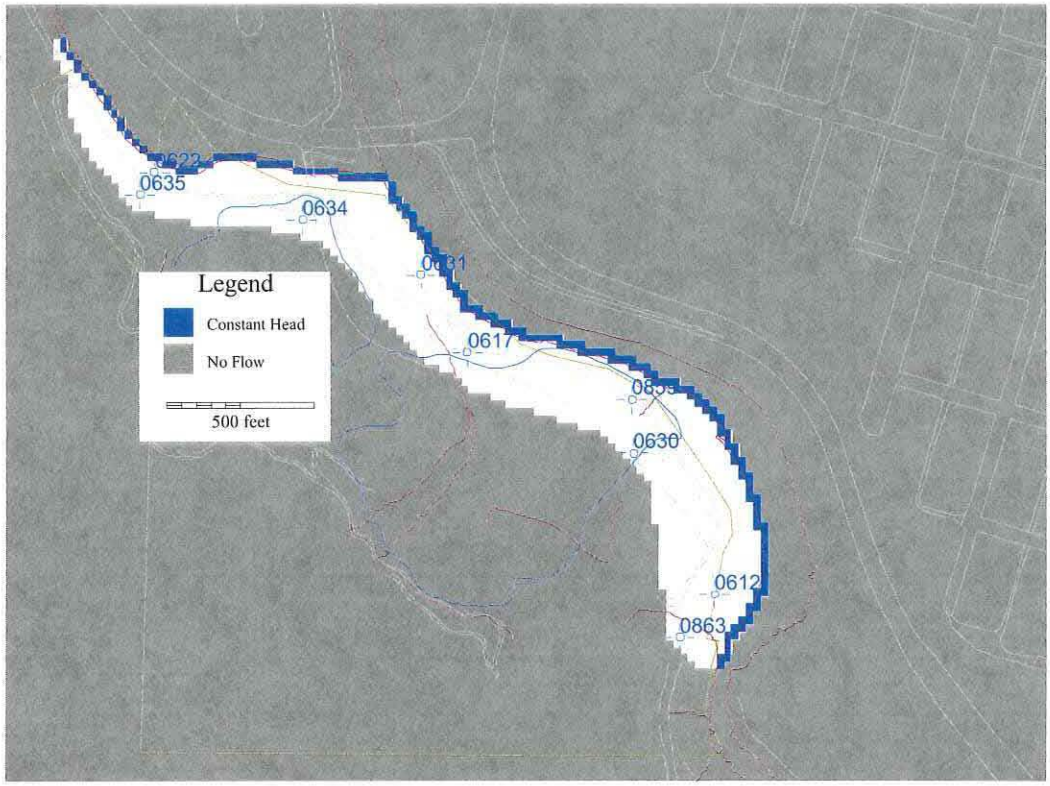


Figure 7. Boundary Conditions Assigned to the Model

The Animas River is also represented by a constant head boundary. River elevation survey data were collected during March 16, 2001, at the two stilling well locations. Based on this data the river has a hydraulic gradient of 0.0058 ft/ft. Over the past 10 years, the Animas River daily streamflow statistical mode was 250 cfs, and on March 16, 2001, the streamflow was 258 cfs. As a result, the survey data collected at this time are representative of the gradient typically encountered during the year.

The river elevations measured during the survey were assigned to the two stilling well locations, and the remaining constant head cells were assigned elevations based on a linear interpolated gradient. As a result, the elevation assigned to the constant head cells associated with the Animas River range from 6,470 ft MSL at the confluence of Lightner Creek to 6,455 ft MSL to the south of well 863, where the surficial deposits pinch out where the Animas River intersects the base of Smelter Mountain.

4.5 Selection of Calibration Targets

Despite the fact that 15 wells are associated with the Mill Tailings Site, only nine wells were chosen as calibration targets within the modeled area. Wells were either eliminated because they were (1) located outside of the modeled area, (2) not screened entirely over the surficial aquifer, or (3) the standard deviation based on the historical water level data was excessively high. The locations of the nine wells used for calibration targets are shown on Figure 8.

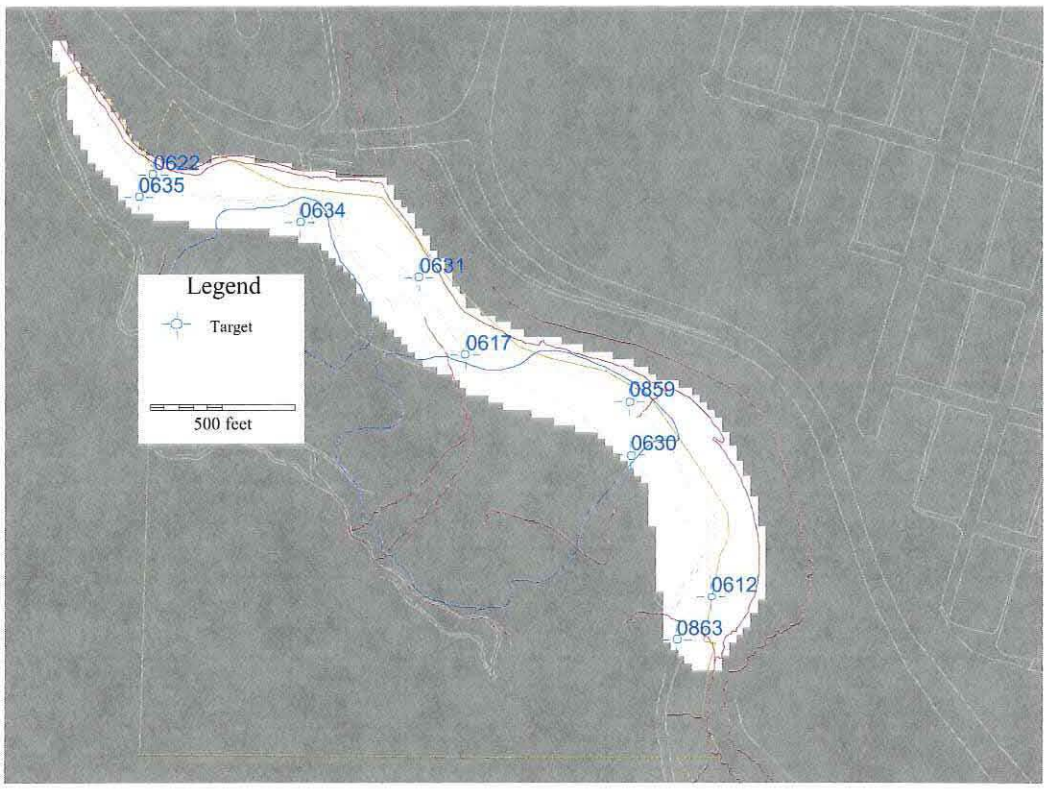


Figure 8. Calibration Target Locations

The target values are based on historical average water level data, as shown in Table 3. This table also provides the standard deviation and the number of measurements contained within the database used to determine the average ground water elevation.

Table 3. Target Ground water Elevation Data

Well	Historical Average Ground Water Elevation (ft MSL)	Standard Deviation	Number of Measurements
0612	6,459.67	1.41	36
0617	6,469.64	4.15	36
0622	6,484.83	0.86	35
0630	6,461.41	1.15	15
0631	6,468.97	1.55	15
0634	6,478.46	0.59	15
0635	6,484.59	0.74	16
0859	6,463.39	1.12	4
0863	6,455.57	1.75	4

Wells 0612, 0617, and 0622 (installed in 1983), and wells 0630, 0631, 0634, and 0635 (installed in 1993) were installed prior to the 2000 field investigation, and as a result the average water level for these locations was based on a larger database. The remaining two targets (0859 and 0863) were installed in September or October 2000, with the average water level based on the available data since installation.

5.0 Calibration of Flow Model

The steps required to develop the flow model and subsequent calibration are presented in the flow chart in Figure 9. Section 5.1 addresses the calibration process, while Sections 5.2, 5.3, 5.4, and 5.5 discuss the calibration goals, sensitivity analysis, stochastic MODFLOW results, and the qualitative and quantitative analysis, respectively.

5.1 Calibration Process

The initial flow model was based on the parameter input values presented in Section 4.2, Table 2. A sensitivity analysis for the four flow model parameters (hydraulic conductivity of zones 1, 2, and 3, and recharge) was completed to determine if the parameter is sensitive and the optimal value for each parameter based on calibration statistics.

Once the sensitivity analysis of the flow model is complete, the sensitive parameters are assigned a range of values. This range is based on the sensitivity analysis as well as field observations. For example, if the sensitivity analysis results indicate that the optimal recharge value is greater than the amount of precipitation available to the site, then the range assigned will only reflect the data that is most representative of actual site conditions.

The flow model is then re-run, using a stochastic version of MODFLOW (Ruskauff and Environmental Simulations, Inc. 1998). This version allows the user to assign a range of values to each sensitive parameter (or any parameters in which the value was obtained from the literature) as opposed to a single value. Results obtained from a stochastic run address the uncertainty associated with simulations in which parameters are assigned only a 'best guess' value.

Once the stochastic MODFLOW results are analyzed, a base flow model is generated which is compared to the calibration goals. If the calibration goals are achieved, this base flow model is used to develop the transport model for each of the contaminants, and provide the final simulation results.

5.2 Calibration Goals

Prior to beginning model calibration, it is important to decide upon the acceptance criteria for the calibration process. The acceptance criteria chosen for this project are:

- The model must be able to simulate the general flow directions observed at the site.
- The numerical model should not have any inherent bias. In other words, because the model will either over or under predict the measured hydraulic heads, the arithmetic mean of the residuals should be as close to 0.0 as possible and fairly evenly distributed above and below 0.0.
- The mass balance error should be less than 5 percent.

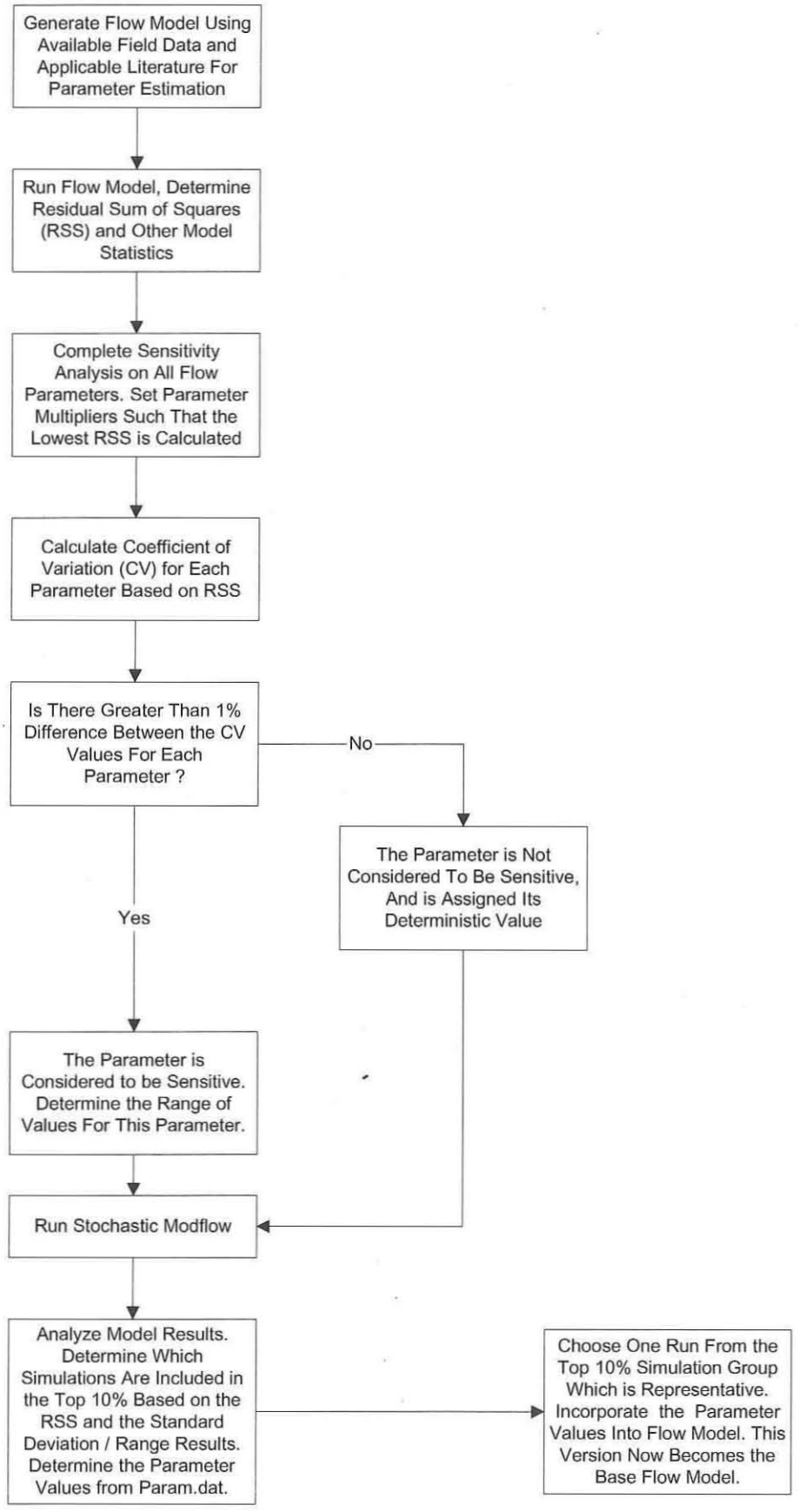


Figure 9. Flow Model Development

In addition, several flow model calibration objectives based on the result statistics were set prior to calibrating the model. The objectives for the steady state model are shown in Table 4.

Table 4. Flow Model Calibration Objectives

	Residual Mean (ft)	Absolute Residual Mean (ft)	Sum of Squares (ft^2)	Minimum Residual (ft)	Maximum Residual (ft)	Standard Deviation/Range (%)
Objective	0	< 1.	< 20.	> -2.0	< 2.0	< 5.0

5.3 Flow Model Sensitivity Analysis

A sensitivity analysis is useful to evaluate the effects that variations in flow parameters have on the final predicted results. Highly sensitive parameters can be treated as uncertain for stochastic simulations. GWVistas contains an auto sensitivity package that allows the user to run the flow model using up to fifteen different values for the parameter to be tested, and compares the residual sum of squares (Section 5.4) result from each run. Generally, only the results from five variations of the parameter are adequate in order to determine if the parameter is sensitive. The flow parameters selected for the sensitivity analysis are horizontal hydraulic conductivity of zones 1, 2, and 3, and recharge. Table 5 presents the initial values assigned to each flow parameter for the sensitivity analysis.

Table 5. Flow Model Sensitivity Analysis Parameter Values

Parameter (units)	Flow Parameter Values				
Kx, Zone 1 (ft/day)	0.4	0.8	4	6	12
Kx, Zone 2 (ft/day)	0.75	1.25	2.5	12.5	25
Kx, Zone 3 (ft/day)	0.3	0.6	1.2	3	6
Recharge (ft/day)	0.001142	0.002284	0.003426	0.004568	0.00571

The criteria used for the sensitivity analysis for these flow parameters is the residual sum of squares, (i.e., the difference between the computed head and observed head at the 9 target wells). The results of the sensitivity analysis for these four parameters are shown in Figure 10 through Figure 13. Visually, this qualitative (subjective) analysis indicates that the model is sensitive to changes in each of the four parameters.

It should be noted that the range assigned to the sensitivity analysis parameters may fall outside the initial range. This is a result of the attempt to determine the optimal value of the parameter. For all four of these flow parameters, the optimal value was encountered outside of the initial range.

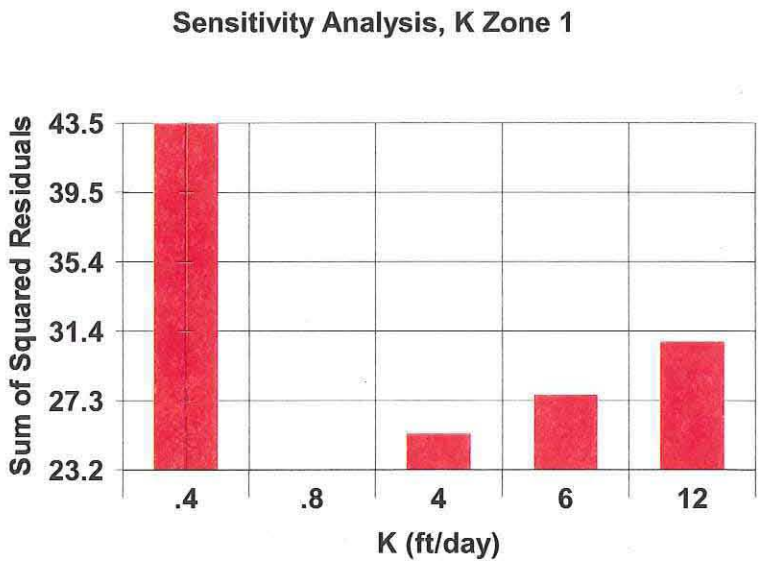


Figure 10. Hydraulic Conductivity—Zone 1 Sensitivity Analysis Results

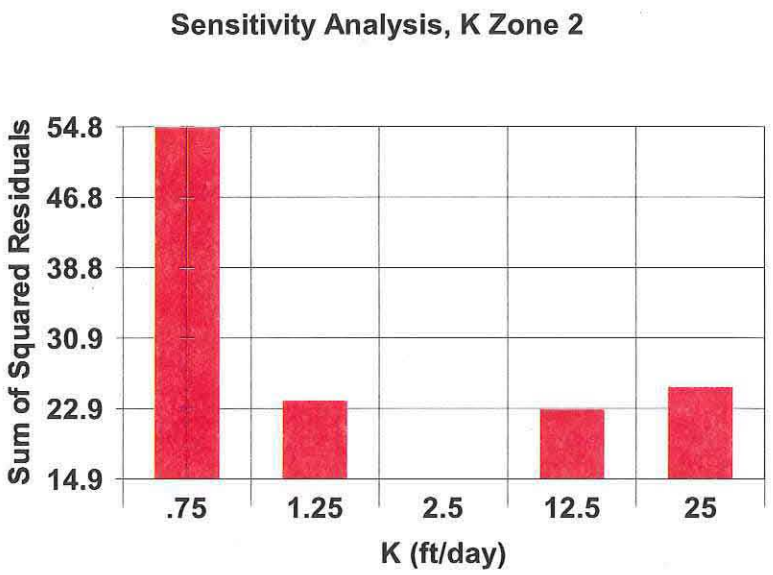


Figure 11. Hydraulic Conductivity—Zone 2 Sensitivity Analysis Results

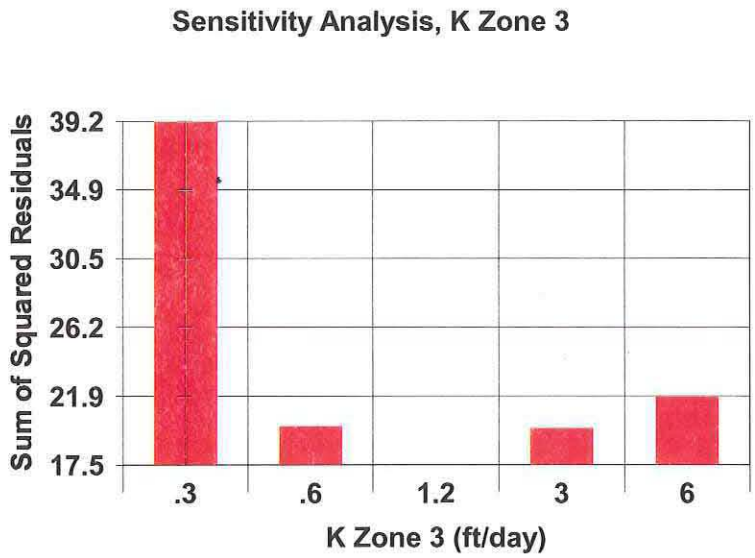


Figure 12. Hydraulic Conductivity—Zone 3 Sensitivity Analysis Results

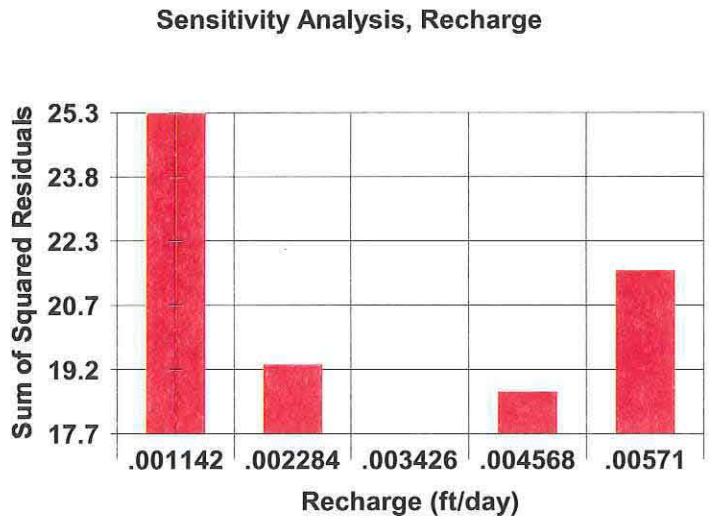


Figure 13. Recharge Sensitivity Analysis Results

As an additional quantitative (objective) check, the coefficient of variation (CV) of the residual sum of squares was calculated for each of these parameters. The CV is defined as the standard deviation (σ) divided by the mean ($\bar{x}$). Parameters resulting in a CV greater than 1 percent are considered sensitive. The CV has been calculated using an unbiased estimate of the standard deviation (σ) adjusted for sample size (Dixon and Massey 1957). The results of the CV analysis are shown in Table 6. Based on these criteria, the model is shown to be sensitive to each of the four parameters.

Table 6. Flow Parameter Coefficient of Variation Analysis

Flow Parameter	Mean	Standard Deviation	Adjusted Standard Deviation	Coefficient of Variation
Horizontal Hydraulic Conductivity, Zone 1	30.10	8.01	8.50	0.2827
Horizontal Hydraulic Conductivity, Zone 2	28.32	15.34	16.28	0.5747
Horizontal Hydraulic Conductivity, Zone 3	23.68	8.81	9.35	0.3947
Recharge	20.52	3.03	3.22	0.1568

5.4 Stochastic MODFLOW

Table 7 presents the flow parameters and associated ranges assigned to each parameter for the stochastic MODFLOW run. These ranges were established based on the sensitivity analyses results and the available field data. The model was designed to perform a total of 100 realizations.

Table 7. Stochastic MODFLOW Parameter Ranges

Flow Parameter	Determinsitic Value (ft/day)	Stochastic Range (ft/day)	Distribution
Horizontal Hydraulic Conductivity, Zone 1	4	1 to 14	Triangular
Horizontal Hydraulic Conductivity, Zone 2	25	5 to 50	Uniform
Horizontal Hydraulic Conductivity, Zone 3	60	40 to 100	Uniform
Recharge	0.001142	0.001 to 0.002	Triangular

The results were analyzed by reviewing the output files and the param.dat file that is produced by stochastic MODFLOW to provide the value of each parameter for each of the 100 realizations. The output file was exported into a spreadsheet and the data were sorted to determine which of the 100 simulations provided the statistically best model.

The data generated by the results were analyzed to determine the statistically optimal run using two criteria: (1) the residual sum of squares, and (2) the standard deviation divided by the range. The top ten percent statistically best realizations were determined for each criteria. These realizations are shown in Table 8 for comparison. Any realizations that were included in the top ten percent based on each criterion are considered to be acceptable base flow models.

Realizations 20, 85, 23, 10, 39, and 34 are found in the upper 10 percent of the results based on both criteria. The param.dat file was reviewed to determine the flow parameter values for each of these realizations. This information is presented in Table 9.

Comparing these values to the parameter value of the deterministic flow model (prior to the sensitivity analysis), the results in Table 9 suggest realization #23 provides a statistically acceptable model based upon flow parameter values that are representative of the data collected during the field investigation.

Table 8. Comparison of Modeling Results Based on the Standard Devation/Range and RRS

Top 10% Realizations Based On the Standard Deviation / Range		Top 10 % Realizations Based on the Residual Sum of Squares	
Realization #	Result	Realization #	Result
20	0.042933	34	15.0434
85	0.043033	85	15.5846
23	0.043266	20	16.552
10	0.043426	80	17.6201
39	0.043556	79	17.9399
34	0.043569	38	18.0679
24	0.043616	10	18.3879
60	0.043626	23	19.1843
12	0.04363	14	19.4009
76	0.043711	39	19.4155

Table 9. Parameter Values for the Statistically Best Realizations

Realization #	K Zone 1 (ft/day)	K Zone 2 (ft/day)	K Zone 3 (ft/day)	Recharge (ft/day)
20	5.3	6.6	40.7	0.001636
85	5.9	5.9	52.9	0.001821
23	4.6	11.4	49.6	0.001541
10	6.1	5.4	68.9	0.001255
39	9.1	8.5	86.7	0.001736
34	4.6	5.1	91.5	0.001847

5.5 Qualitative and Quantitative Analysis

As a result, the steady state base model contains the following flow parameter values:

- Hydraulic Conductivity of Zone 1 = 4.6 ft/day
- Hydraulic Conductivity of Zone 2 = 11.4 ft/day
- Hydraulic Conductivity of Zone 3 = 49.6 ft/day
- Recharge = 0.001541 ft/day

The calibration goals presented in Section 5.1 were compared to the results obtained from the model based on these parameter values. Figure 14 presents the ground water surface contour map generated by the flow model. When comparing this map to Figure 2 (the ground water contour map based on the observed water level data), the ground water flow directions are similar.

Figure 15 displays the observed hydraulic heads versus residuals for the steady state model. The plot shows there is a positive bias, in other words, the model tends to underestimate the water levels compared to the measured water levels.

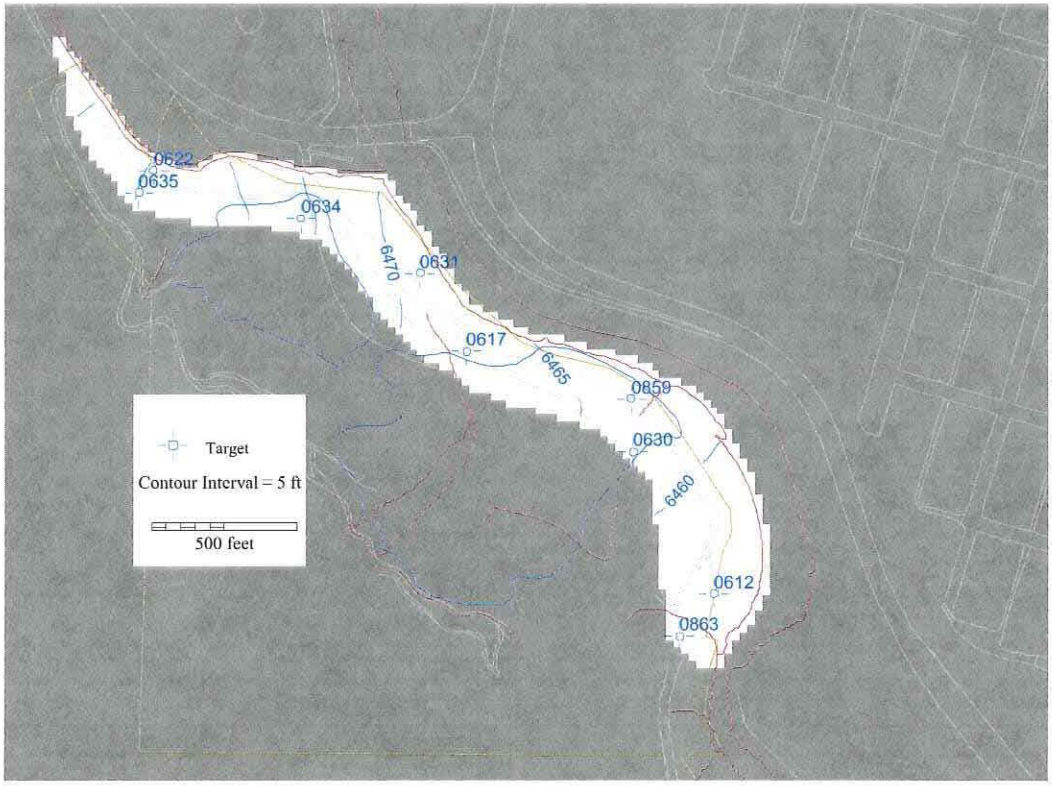


Figure 14. Simulated Surficial Aquifer Ground Water Surface Contour Map

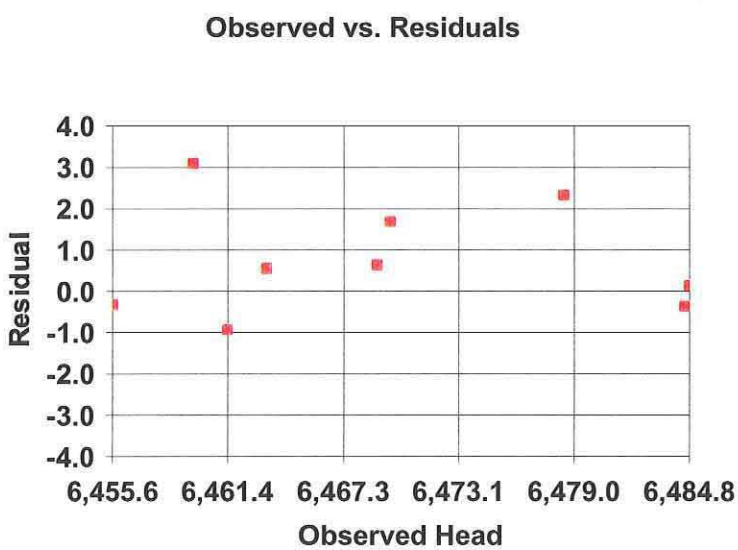


Figure 15. Comparison of Residual versus Observed Head

The mass balance error for the steady state model is 0.00015 percent, which is well below the 5 percent goal. Additional calibration goals and results are presented in Table 10. Although some of the criteria are not met (residual mean, absolute residual mean, and maximum residual), they are not exceeded by a significant amount.

Table 10. Calibration Objectives and Results

	Residual Mean (ft)	Absolute Residual Mean (ft)	Sum of Squares (ft^2)	Minimum Residual (ft)	Maximum Residual (ft)	Standard Deviation/Range (%)
Objective	0	< 1.	< 20.	> -2.0	< 2.0	< 5.0
Results	0.77	1.12	19.8	-0.92	3.10	4.3

The target residual values are shown on Figure 16. A positive residual value indicates the simulated head is less than the observed head.

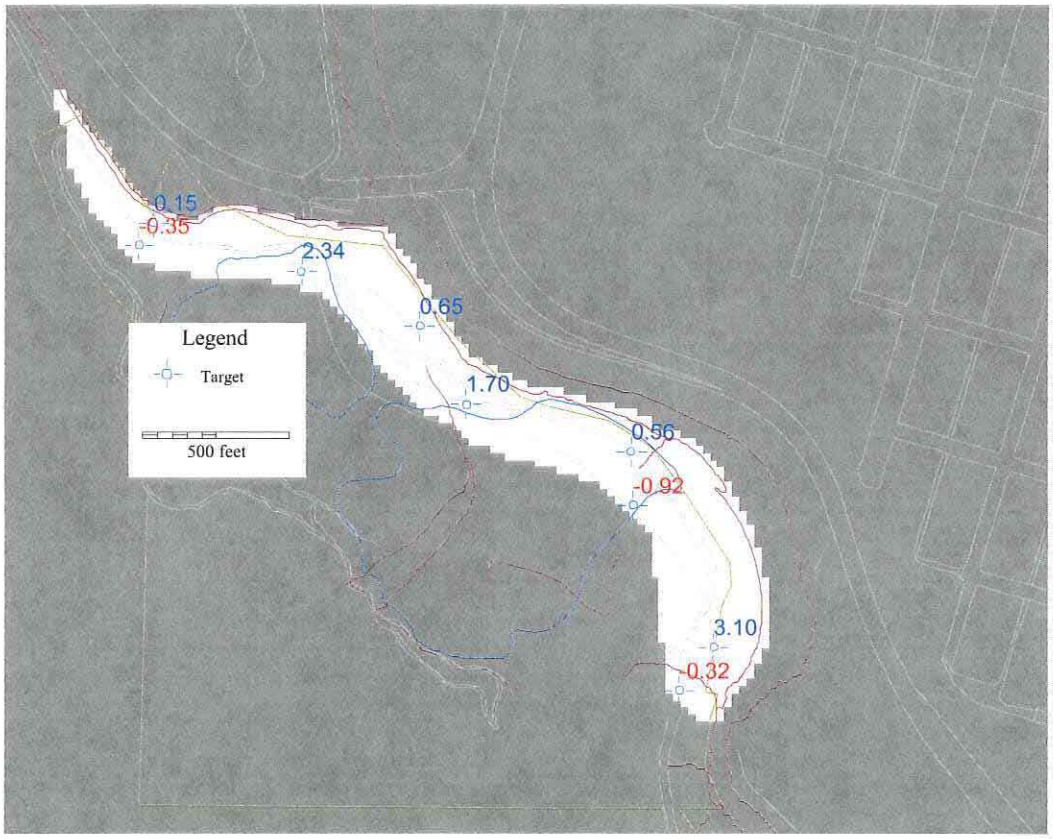


Figure 16. Target Residual Value

The steady state calibrated model results and the residual at each target are shown in Table 11. A plot of predicted (computed) hydraulic head versus observed hydraulic head would fall on a straight line for a calibrated model. Figure 17 demonstrates that the model accurately predicts field measurements.

Table 11. Calibration Target Residuals

Well	Observed Head (ft MSL)	Computed Head (ft MSL)	Residual (ft)
612	6459.67	6456.63	3.04
617	6469.64	6467.43	2.20
622	6484.83	6484.67	0.16
630	6461.41	6461.83	-0.42
631	6468.97	6468.37	0.60
634	6478.46	6475.80	2.66
635	6484.59	6484.83	-0.24
859	6463.39	6462.73	0.66
863	6455.57	6456.00	-0.43

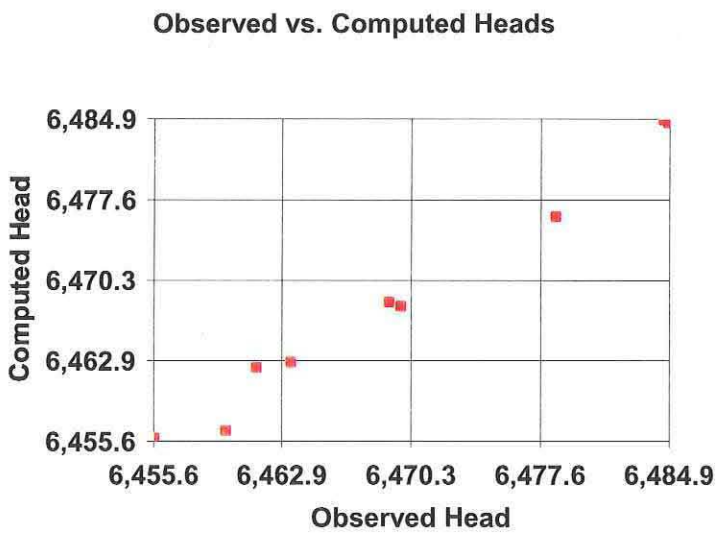


Figure 17. Comparison of Computed Head versus Observed Head

6.0 Transport Modeling

As shown in Figure 18 subsequent to the completion of the calibration of the flow model is the development of the transport model. Initial concentration files are generated from the data, and the transport parameters are assigned values based on the field data or the literature. The computer code MT3DMS allows for the predictive simulations to be computed at various time intervals in the future. Another sensitivity analysis to determine which of the transport parameters are sensitive is completed, and ultimately a stochastic transport model is created to predict the contaminant concentrations. Section 6.1 describes the steps followed to develop the transport model, and Section 6.2 details the transport model sensitivity analysis.

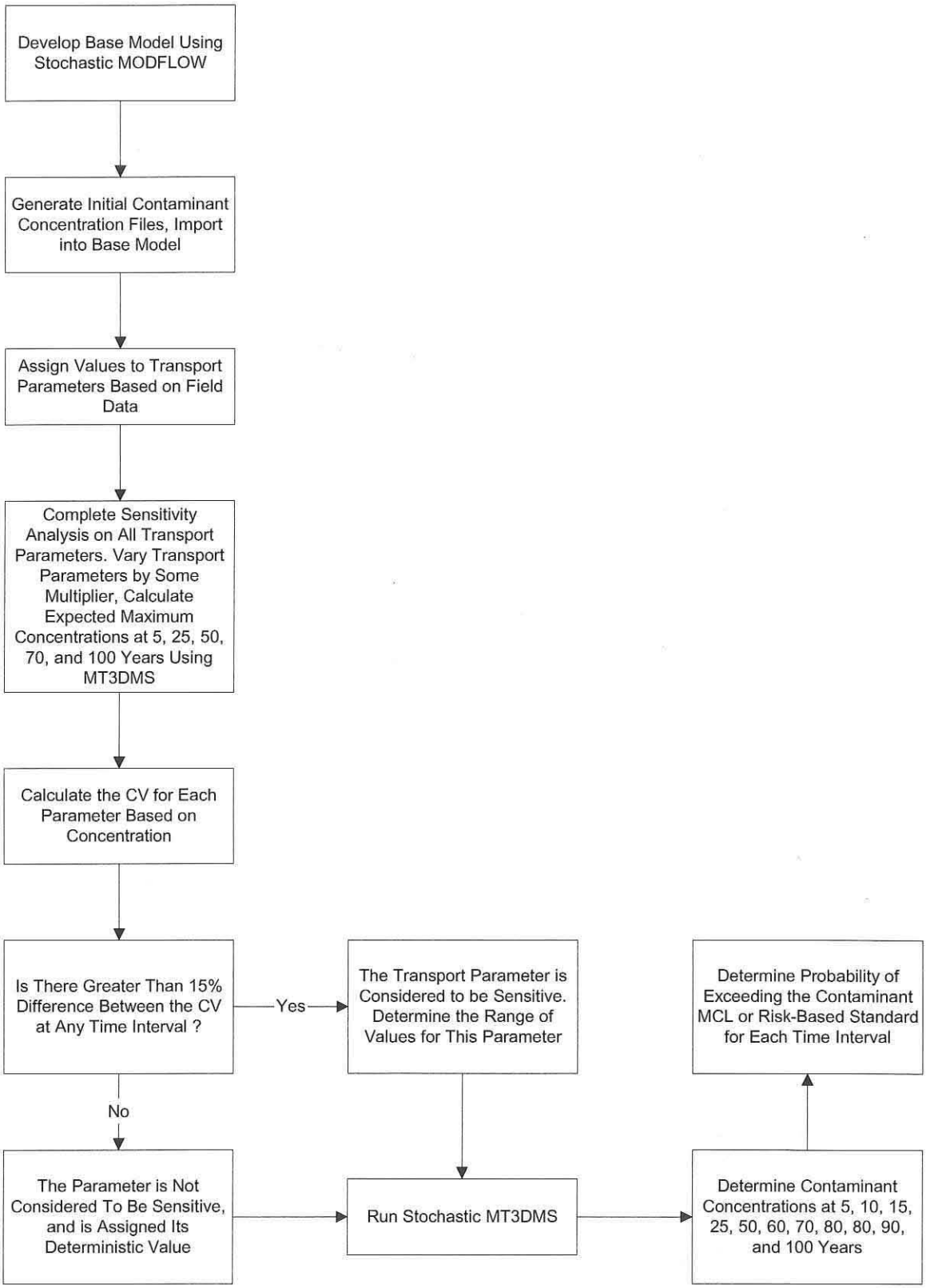


Figure 18. Procedure Used for Transport Modeling

6.1 Development of the Transport Model

The contaminant transport parameters of interest are the initial contaminant concentration distribution, longitudinal, transverse, and vertical dispersivity, effective porosity, bulk density, and the distribution coefficient (K_d). Each parameter and the source of the parameter values are discussed separately.

6.1.1 Initial Contaminant Concentration Distribution

Initial contaminant concentration plumes were developed in **Surfer®** for the model using the average concentration based on the November 2000, March 2001, June 2001, and August 2001 data (Table 12).

Table 12. Contaminant Ground water Concentrations from November 2000 Through August 2001

Cadmium					
well no	**Nov-00**	**Mar-01**	**Jun-01**	**Aug-01**	**avg**
0612	0.0435	0.0434	0.0266	0.0369	0.0376
0617	0.0010	0.0002	0.0004	0.0008	0.0006
0622	0.0002	0.0007	0.0004	0.0009	0.0006
0629	0.0002	0.0002	0.0004	0.0007	0.0004
0630	0.0167	0.0019	0.0004	0.0007	0.0049
0631	0.0002	0.0002	0.0004	0.0007	0.0004
0633	0.0002	0.0009	0.0004	0.0008	0.0006
0634	0.0002	0.0003	0.0004	0.0007	0.0004
0635	0.0002	0.0003	0.0004	0.0008	0.0004
0859	0.0002	0.0004	0.0004	0.0007	0.0004
0863	0.0002	0.0002	0.0004	0.0007	0.0004
Manganese					
well no	**Nov-00**	**Mar-01**	**Jun-01**	**Aug-01**	**avg**
0612	5.4000	5.2700	2.8600	4.3100	4.4600
0617	0.0068	0.0138	0.0070	0.0097	0.0093
0622	0.0159	0.0023	0.0025	0.0050	0.0064
0629	0.1790	0.1370	0.0731	0.1260	0.1288
0630	0.8750	1.7100	0.9450	2.6800	1.5525
0631	0.2600	0.2390	0.3880	0.4840	0.3428
0633	0.1680	0.0169	0.0050	0.0962	0.0715
0634	0.1800	0.1670	0.0861	0.0397	0.1182
0635	0.0954	0.0215	0.0032	0.0545	0.0437
0859	1.4100	1.5000	1.2500	0.8030	1.2408
0863	0.1830	0.0614	0.0980	0.0941	0.1091

Table 12 (continued). Contaminant Ground water Concentrations from November 2000 Through August 2001

Molybdenum					
well no	**Nov-00**	**Mar-01**	**Jun-01**	**Aug-01**	**avg**
0612	0.1330	0.1160	0.1020	0.1160	0.1168
0617	0.0014	0.0017	0.0030	0.0030	0.0023
0622	0.0021	0.0021	0.0030	0.0030	0.0026
0629	0.0009	0.0004	0.0030	0.0030	0.0018
0630	0.0033	0.0067	0.0030	0.0034	0.0041
0631	0.0108	0.0119	0.0030	0.0068	0.0081
0633	0.0012	0.0017	0.0030	0.0030	0.0022
0634	0.0016	0.0027	0.0030	0.0030	0.0026
0635	0.0027	0.0021	0.0030	0.0030	0.0027
0859	0.0032	0.0038	0.0030	0.0030	0.0033
0863	0.0074	0.0025	0.0030	0.0030	0.0040
Selenium					
well no	**Nov-00**	**Mar-01**	**Jun-01**	**Aug-01**	**avg**
0612	0.0060	0.0059	0.0009	0.0004	0.0033
0617	0.0577	0.0515	0.0643	0.0501	0.0559
0622	0.0001	0.0325	0.0003	0.0003	0.0083
0629	0.0002	0.0003	0.0003	0.0003	0.0003
0630	0.0003	0.0033	0.0178	0.0003	0.0054
0631	0.0003	0.0005	0.0035	0.0003	0.0012
0633	0.0362	0.1080	0.1230	0.0445	0.0779
0634	0.0001	0.0016	0.0003	0.0003	0.0006
0635	0.0092	0.0145	0.0200	0.0155	0.0148
0859	0.0001	0.0003	0.0003	0.0003	0.0003
0863	0.0001	0.0003	0.0003	0.0003	0.0003
Sulfate					
well no	**Nov-00**	**Mar-01**	**Jun-01**	**Aug-01**	**avg**
0612	2280	2370	2030	2300	2245
0617	1980	2030	1960	1810	1945
0622	204	379	132	205	230
0629	2120	2090	2070	2190	2118
0630	2280	1930	1830	1990	2008
0631	409	354	945	981	672
0633	3250	2990	2670	3510	3105
0634	2110	1840	2070	2090	2028
0635	980	924	1280	1470	1164
0859	878	1110	NS	723	904
0863	662	544	678	656	635

Table 12 (continued). Contaminant Ground water Concentrations from November 2000 Through August 2001

Uranium					
well no	Nov-00	Mar-01	Jun-01	Aug-01	avg
0612	2.1200	2.1200	1.5600	1.9700	1.9425
0617	0.2440	0.2440	0.2150	0.2110	0.2285
0622	0.0171	0.0290	0.0176	0.0173	0.0203
0629	0.0008	0.0007	0.0010	0.0006	0.0008
0630	0.0819	0.1970	0.2140	0.2030	0.1740
0631	0.2310	0.2570	0.3310	0.3440	0.2908
0633	1.2200	0.9420	0.8900	1.2700	1.0805
0634	0.0334	0.1840	0.0597	0.0585	0.0839
0635	0.0062	0.0065	0.0079	0.0076	0.0071
0859	0.0477	0.0547	0.0437	0.0439	0.0475
0863	0.0005	0.0016	0.0014	0.0007	0.0010

Each set of data were kriged in **Surfer®** and interpolated to approximately a 12.5 ft grid spacing, or one-half of the model grid size. This surface was then interpolated to all active model grid cell centers and imported as the initial concentration plume into the model. The plots presented in Figure 19 through Figure 24 show the initial concentration plumes for cadmium, manganese, molybdenum, selenium, sulfate, and uranium, respectively.

It should be noted that the highest average concentration values for each contaminant listed in Table 12 (far right column) do not exactly match the maximum concentration presented on Figure 19 through Figure 24. Even with the 12.5 ft grid spacing used in the kriging process, the values do not match up exactly; however, they are very close. Because the maximum concentrations are within 98 percent of each other, the impact on the final results is negligible.

6.1.2 Dispersivity

The literature on dispersivity as it relates to large-scale models is vague and often contradictory (Gelhar, Welty, and Rehfeldt 1992), with longitudinal values ranging from 2 percent to 30 percent of the length of the plume or maximum flow path length. In addition, dispersivity is almost impossible to measure in the field for large sites.

The primary (or longitudinal) flow direction for this site is to the southeast. The flow direction generated from the MODFLOW model dictate the longitudinal and transverse dispersivity directions. The length of the flowline that the contaminant follows is dependent upon the location on the site. As a result, the longitudinal dispersivity was assigned values that ranged from 5 to 80 ft for the stochastic simulation.

6.1.3 Effective Porosity

No data were collected to measure the effective porosity in the field. Based on the soil type, the literature suggests the effective porosity may range from 15 to 55 percent. This range was assigned to this transport parameter.

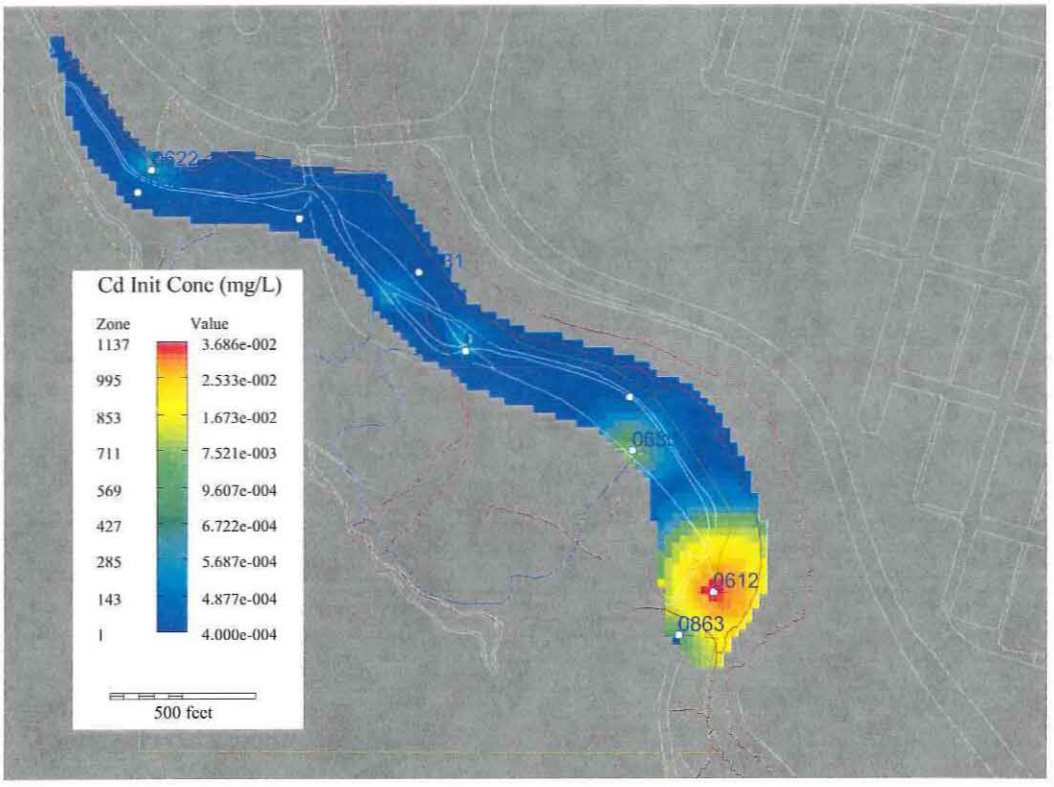


Figure 19. Cadmium Initial Concentration Distribution

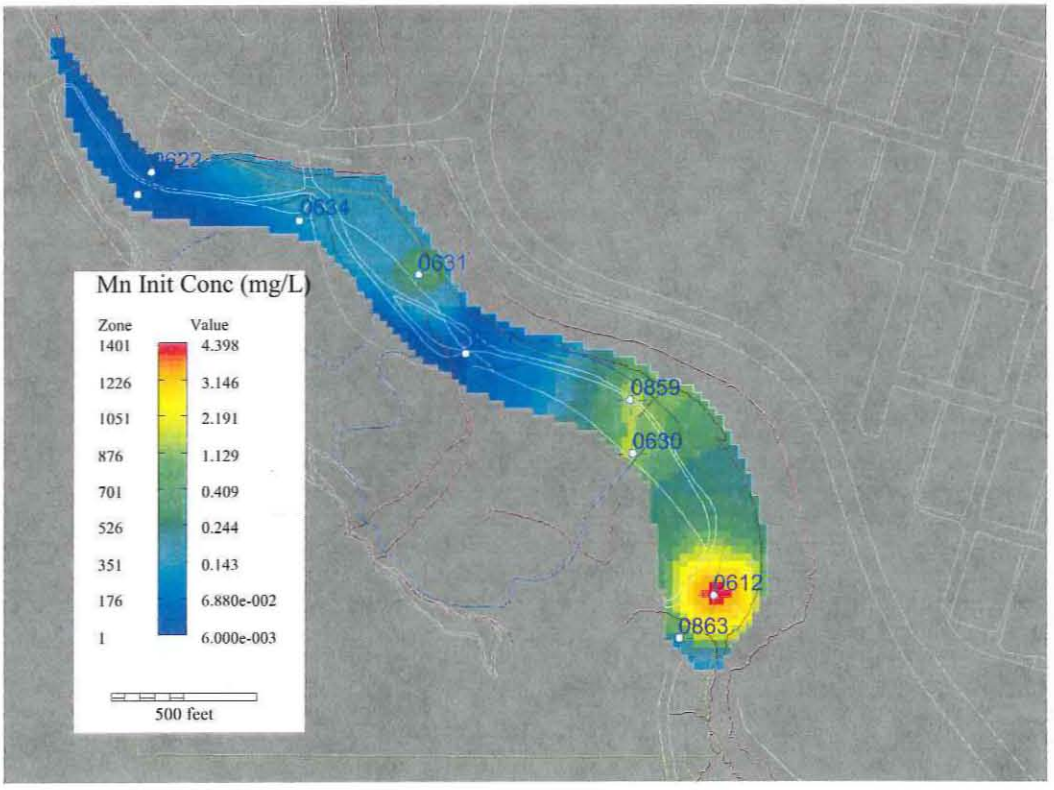


Figure 20. Manganese Initial Concentration Distribution

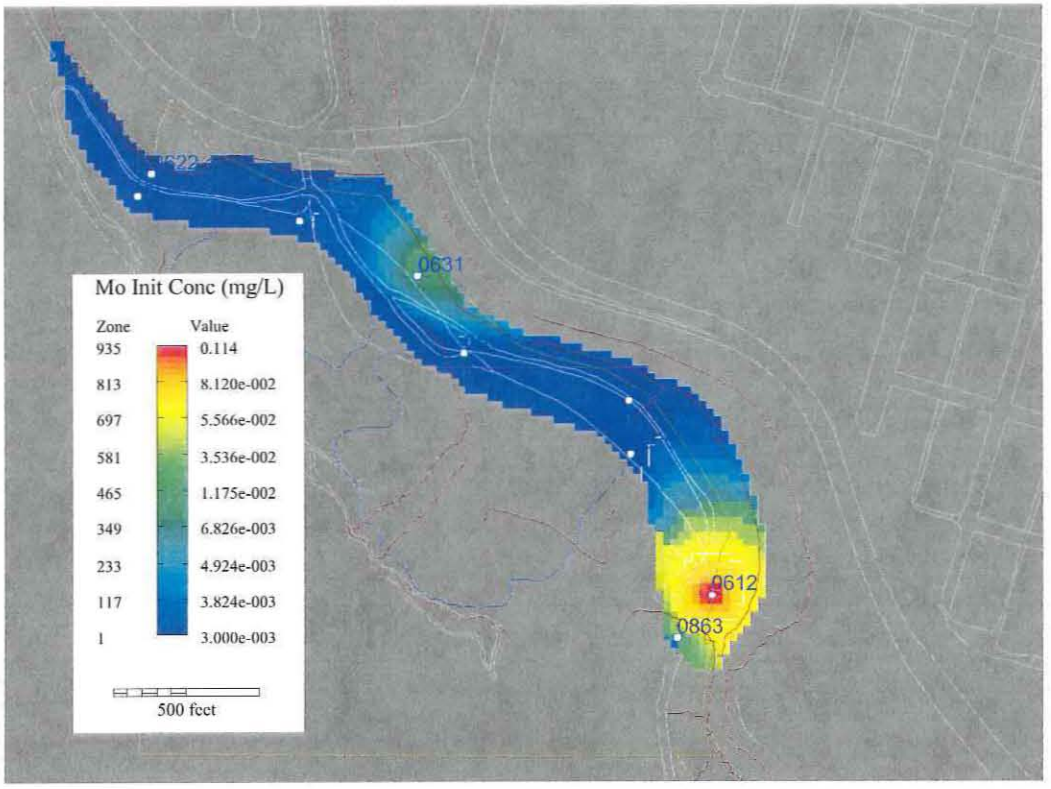


Figure 21. Molybdenum Initial Concentration Distribution

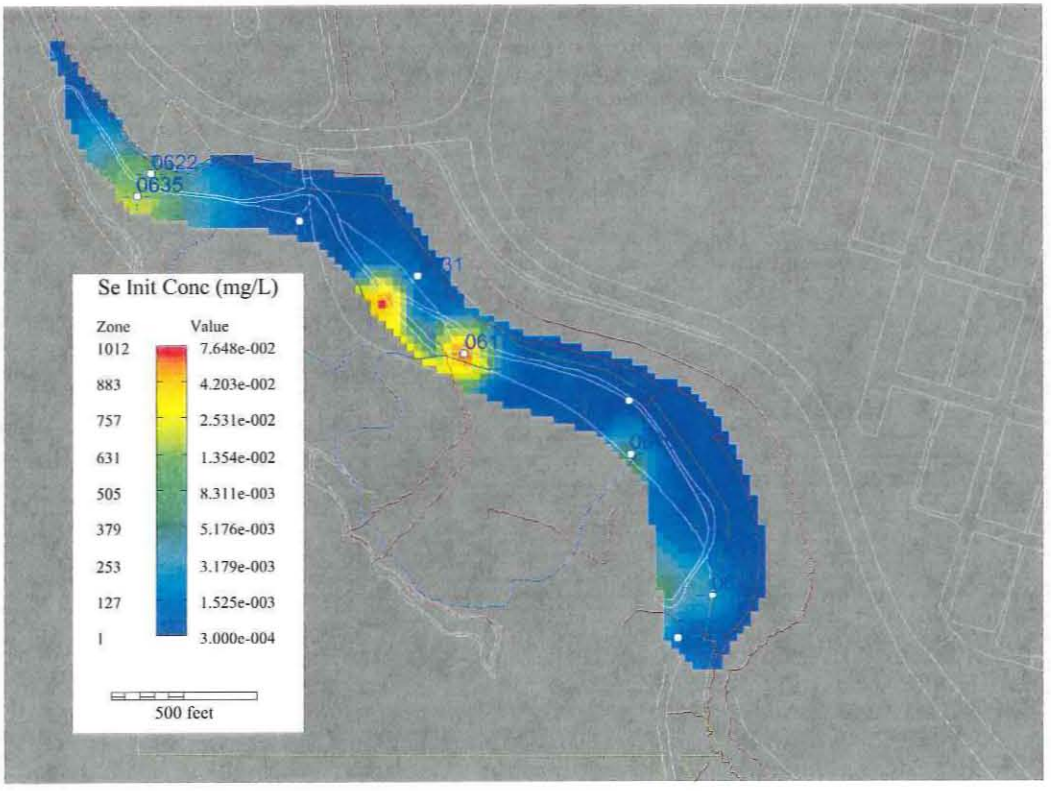


Figure 22. Selenium Initial Concentration Distribution

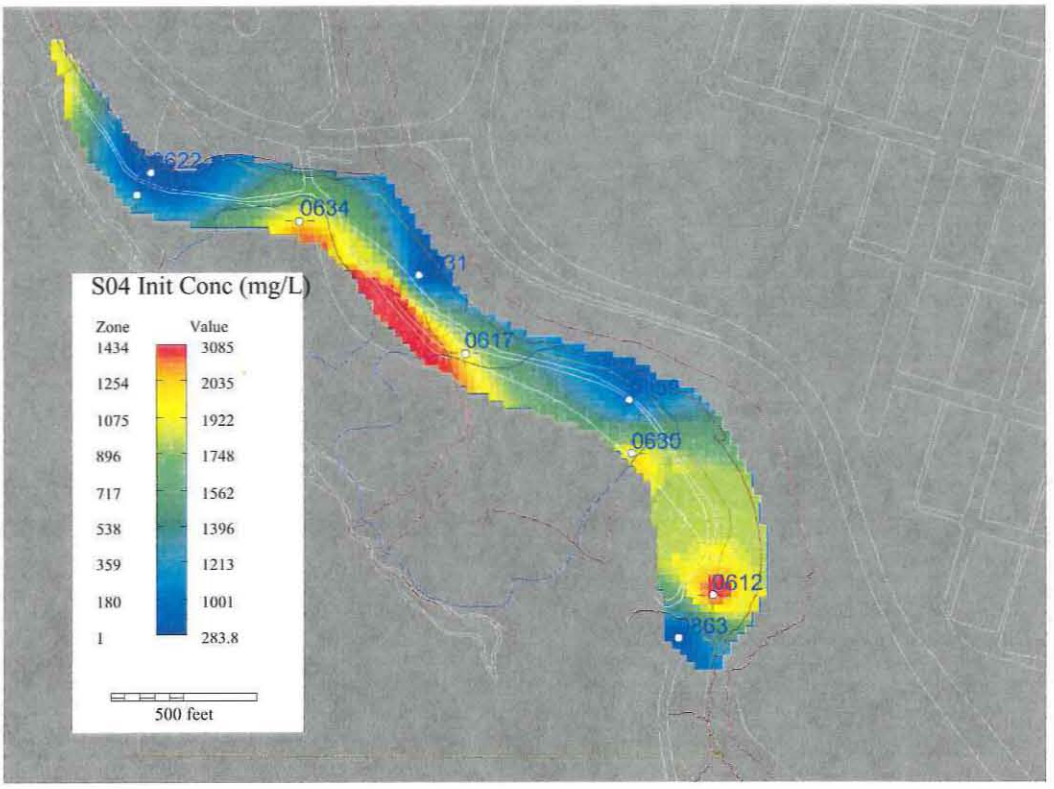


Figure 23. Sulfate Initial Concentration Distribution

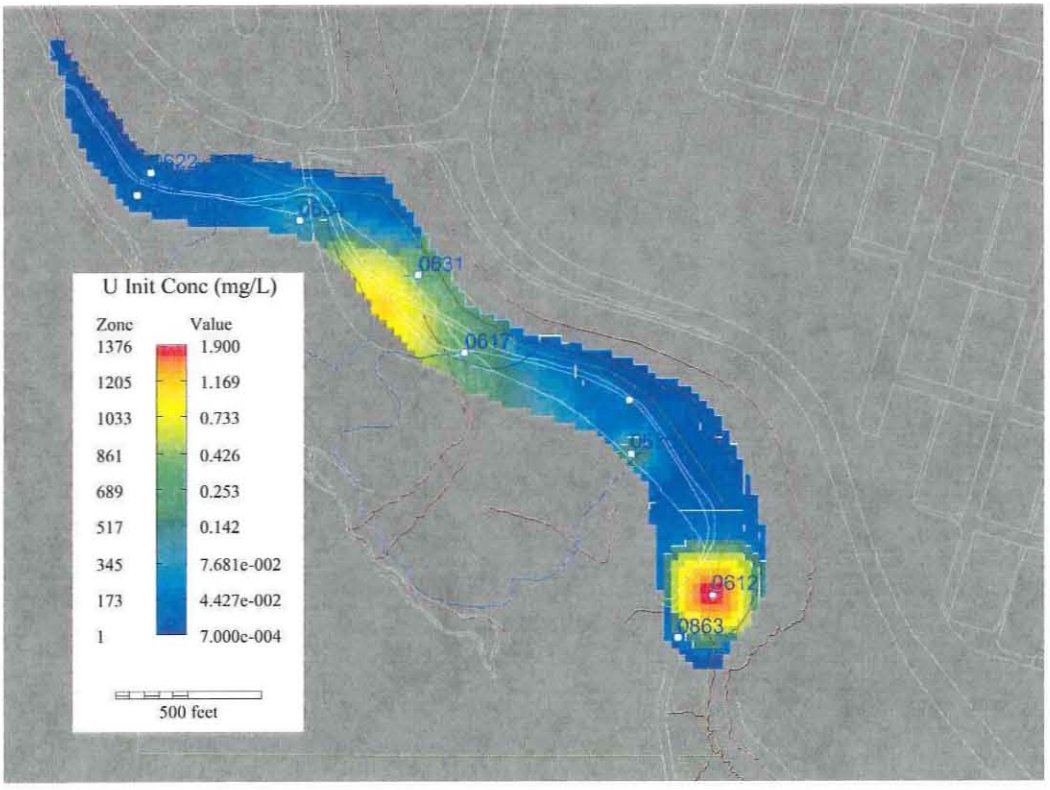


Figure 24. Uranium Initial Concentration Distribution

6.1.4 Bulk Density

Similar to the effective porosity, this parameter was not measured in the field and was assigned a value from the applicable literature based on the soil type. For the stochastic transport modeling, this parameter was assigned a value of 1.55 grams per cubic centimeter (g/cc). The bulk density parameter was not assigned a range because it is not considered to be a stochastic parameter in the stochastic MT3DMS code.

6.1.5 K_d

The distribution coefficient (K_d) will have the greatest impact on the amount of time required for natural flushing to reduce the contamination level below the required standard. Average values and associated ranges for cadmium, molybdenum, selenium, and uranium were obtained from the Environmental Sciences Laboratory (ESL) (DOE 2001).

Of the reported values for the Mill Tailings site, only those associated with locations 857, 859, 863, and 866 are considered to be representative of the surficial aquifer. As a result, the range of K_d values associated with these locations was used for parameter inputs.

The K_d values for manganese were obtained from the literature, and there are no values reported for sulfate in the literature due to the complex geochemical reactions associated with sulfate in groundwater. Table 13 presents the average K_d value, range, and data source for each of the contaminants.

Table 13. Contaminant K_d Values

Contaminant	K_d Average value / Range (mL/g)	Source
Cadmium	60.4 / 17 to 418	ESL Report (DOE 2001)
Manganese	5 / 0.2 to 10,000[a]	Baes and Sharp 1983
Molybdenum	0.86 / 0.19 to 3.01	ESL Report (DOE 2001)
Selenium	14.8 / 6.3 to 50.6	ESL Report (DOE 2001)
Sulfate	1 / 1 to 10	[b]
Uranium	1.4 / 0.69 to 3.2	ESL Report (DOE 2001)

[a]Even though the literature reports a range of 0.2 to 10,000, simulations were completed using a range of 1 to 10.
[b] No K_d values associated with sulfate are reported in the literature

6.1.6 Transport Parameter Summary

Table 14 provides a summary of the transport parameters and associated values assigned to each parameter for the stochastic simulations.

Table 14. Transport Parameter Value Ranges

Parameter (units)	Range of values	Source
Initial Conc. (mg/L)	See Table 12	Ground water Sampling Results
Dispersivity (ft)	5 to 80	Literature / Field Conditions
Effective Porosity	0.15 to 0.55	Literature
Bulk Density (g/cc)	1.55[a]	Literature
K_d (mL/g)	See Table 13	ESL Report (DOE 2001), Literature

[a]No range assigned to parameter, not considered a stochastic parameter by the MT3DMS code.

6.2 Transport Model Sensitivity Analysis

The sensitivity analysis procedure for the transport parameters is not as straight forward compared to the sensitivity analysis associated with flow model and flow parameters. The sensitivity analysis for the flow model is based on the residual sum of squares of observed head minus computed head. Similarly, the sensitivity analysis for the transport model could be based on the residual sum of squares of observed concentration minus computed concentration.

The sensitivity analysis for the transport modeling parameters was completed using selenium as the contaminant. The transport parameters selected for sensitivity analysis are effective porosity, K_d, longitudinal dispersivity, transverse dispersivity, and vertical dispersivity. Transport parameters were simulated at five different values that range from the lowest to the highest expected value.

The sensitivity analysis for the longitudinal, transverse, and vertical dispersivity was accomplished in such a manner that the sensitivity of the individual parameters could be evaluated. As shown in Table 15, when determining the sensitivity of the longitudinal dispersivity, the values for the transverse and vertical dispersivity did not change. The same procedure was used to determine the sensitivity of the transverse and vertical dispersivity parameters.

Parameter values for the sensitivity analyses are contained in Table 15.

Table 15. Sensitivity Parameter Values

Parameter (units)	Flow Parameter Values				
Effective Porosity	0.15	0.25	0.35	0.45	0.55
K_d (mL/g)	6.3	14.8	28.5	39.5	50.6
Long. Disp. (ft) (long / transv / vert)[a]	5 / 2 / 0.2	20 / 2/ 0.2	40 / 2 / 0.2	60 / 2 / 0.2	80 / 2 / 0.2
Trans. Disp. (ft) (long / transv / vert)[a]	20 / 0.5 / 0.2	20 / 2 / 0.2	20 / 4 / 0.2	20 / 6 / 0.2	20 / 8 / 0.2
Vert. Disp. (ft) (long / transv / vert)[a]	20 / 2 / 0.05	20 / 2 / 0.2	20 / 2 / 0.4	20 / 2 / 0.6	20 / 2 / 0.8

[a]long / transv / vert represents longitudinal, transverse, and vertical dispersivity estimates, respectively

A quantitative procedure similar to the one described for flow model parameters (Section 5.3) was also used to determine if the parameter tested is sensitive. As a result, the coefficient of variation (CV) of the difference in predicted selenium concentration at each selected time interval (5, 25, 50, 70, 100 years) was calculated. Any parameter resulting in a CV greater than 15 percent between the predicted selenium concentration at any time interval is considered sensitive and will be treated as stochastic. The results are presented in Table 16.

Table 16. Transport Parameter Coefficient of Variation Analysis

Effective Porosity				
Year	**Mean**	**Stdev**	**Adj Stdev**	**CV**
5	0.0688	0.0001	0.0001	0.0009
25	0.0476	0.0001	0.0001	0.0029
50	0.0336	0.0001	0.0001	0.0036
70	0.0268	0.0002	0.0002	0.0063
100	0.0191	0.0001	0.0001	0.0072
K_d				
Year	**Mean**	**Stdev**	**Adj Stdev**	**CV**
5	0.0698	0.0056	0.0059	0.085
25	0.0531	0.0142	0.0151	**0.2841**
50	0.0412	0.0164	0.0174	**0.4225**
70	0.0349	0.0164	0.0175	**0.5007**
100	0.0281	0.0157	0.0166	**0.5917**
Longitudinal Dispersivity				
Year	**Mean**	**Stdev**	**Adj Stdev**	**CV**
5	0.0655	0.0051	0.0054	0.0822
25	0.0438	0.0078	0.0083	**0.189**
50	0.031	0.0059	0.0062	**0.2014**
70	0.0251	0.005	0.0053	**0.2104**
100	0.0183	0.0036	0.0039	**0.2105**
Transverse Dispersivity				
Year	**Mean**	**Stdev**	**Adj Stdev**	**CV**
5	0.0683	0.0007	0.0007	0.0106
25	0.0465	0.0016	0.0017	0.0369
50	0.0323	0.0019	0.0021	0.0634
70	0.0257	0.0018	0.0019	0.0746
100	0.0187	0.0012	0.0012	0.066
Vertical Dispersivity				
Year	**Mean**	**Stdev**	**Adj Stdev**	**CV**
5	0.0688	0	0	0
25	0.0476	0	0	0
50	0.0336	0	0	0
70	0.0268	0	0	0
100	0.0191	0	0	0

Notes: Mean = mean Se concentration for each time interval
Stdev = Standard Deviation
Adj Stdev = Adjusted Standard Deviation
CV = Coefficient of Variation

The results indicate that the transport model is not sensitive to effective porosity, transverse dispersivity, or vertical dispersivity. However, the transport model is highly sensitive to K_d and longitudinal dispersivity.

7.0 Steady State Stochastic Transport Modeling

Based on the results of the sensitivity analysis, the K_d, and longitudinal dispersivity transport parameters were assigned ranges of values for the stochastic transport modeling. The effective porosity value assigned to the deterministic model was derived from the literature; therefore it was also treated as a sensitive parameter and assigned a range of values for the stochastic modeling, despite the fact it is an insensitive parameter.

Table 17 provides the range of values and distribution assigned to the longitudinal dispersivity and porosity for the stochastic transport modeling. The MT3DMS code automatically assigns the transverse and vertical dispersivity values a percentage of the longitudinal dispersivity, as set by the user in the deterministic transport model. In the Durango Mill Tailings Site deterministic transport model, the longitudinal, transverse, and vertical dispersivity parameters were assigned values of 20, 2, and 0.2 ft, respectively. As a result, during the stochastic transport modeling when the code randomly chooses a value to assign to the longitudinal dispersivity, the code will automatically assign transverse and vertical dispersivity values that are 10 percent and 1 percent of the longitudinal dispersivity, respectively.

Table 17. Ranges and Distribution Types Assigned to Longitudinal Dispersivity and Effective Posrosity Parameters

Parameter	Range	Distribution
Longitudinal Dispersivity	5 to 80 ft	Triangular
Effective Porosity	0.15 to 0.55	Uniform

Table 13 presents the K_d range assigned for each of the contaminants, and the source for each range.

7.1 Transport Model Development

One of the problems associated with stochastic simulations is to determine how many realizations (individual simulations) are sufficient. From a strict mathematical standpoint, hundreds or even thousands of realizations may be necessary to truly represent the uncertainty when random samples are drawn from distributions for a number of parameters. A qualitative or subjective justification to determine if enough realizations were simulated can be obtained by looking at a plot of cumulative average residual sum of squares versus realization number.
If there is limited change in the cumulative average as the number of realizations increases, then it can be safely concluded that enough simulations have been run. The plot in Figure 25 indicates that the cumulative average residual sum of squares becomes relatively stable at approximately 25 square feet (ft^2) after 50 realizations. Therefore, 100 realizations should be adequate to account for the uncertainty in the stochastic parameters.

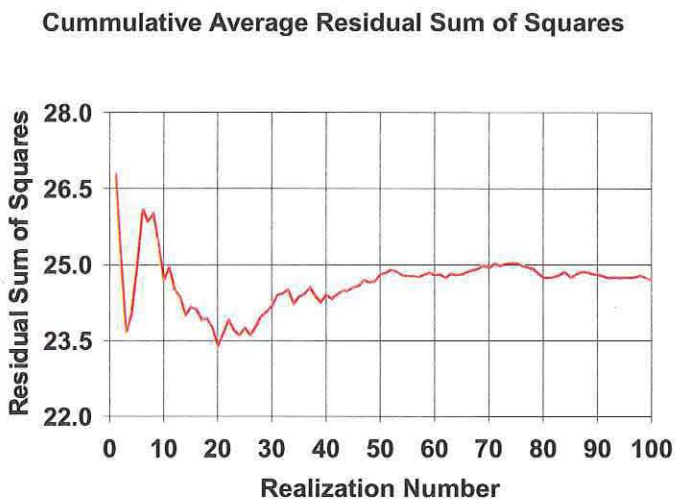


Figure 25. Cumulative Average Residual Sum of Squares versus Realization Number

Another useful evaluation tool is to look at how the individual realizations compare to the calibrated flow model results. The plot in Figure 26 shows the residual sum of squares for each of the 100 realizations. About 12 percent of the realizations are below the calibrated model residual sum of squares value of 19.8 ft^2.

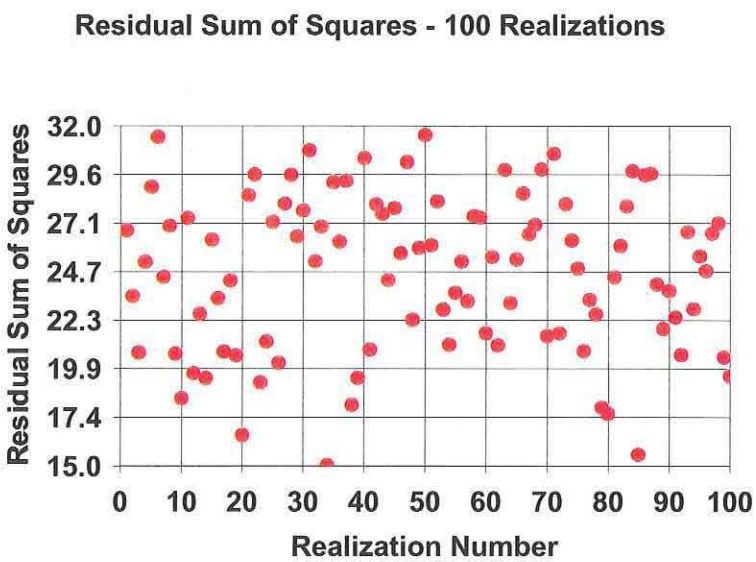


Figure 26. Residual Sum of Squares versus Realization Number

7.2 Transport Modeling Results

Average contaminant concentration results are provided by stochastic MT3DMS. The computer code calculates the contaminant concentration of each active cell for each realization, and then calculates an average concentration based on the 100 realizations. The code calculates the probability of exceeding a standard in a similar fashion. Once the model is finished, the code allows the user to calculate the number of times a standard was exceeded within the total number of realizations. For example, within a single cell, if a standard is exceeded 22 times within a total

of 100 realizations, then a 22 percent probability exists that this standard will be exceeded in that particular cell. The computer code provides both results in tabular and graphical forms.

As a result, even though the maximum average contaminant concentration (at a specific time) may not exceed the standard, there may still be some probability that the standard will be exceeded at that same time period. In addition, the areas within the model where the results indicate a standard is exceeded and the area where the probability of exceeding a standard may occur not coincide.

Table 18 presents the predicted maximum average concentrations (milligrams per liter [mg/L]) for cadmium (Cd), manganese (Mn), molybdenum (Mo), selenium (Se), sulfate (SO_4), and uranium (U) at 5, 10, 15, 25, 50, 60, 70, 80, 80, 90, and 100 years into the future. The distribution and probability of exceeding the applicable standard are discussed separately for each contaminant. These average concentrations and associated uncertainty at each time period of interest are based on 100 computer simulations

Table 18. Predicted Contaminant Maximum Average Concentrations (mg/L) at 5, 10, 15, 25, 50, 60, 70, 80, 90, and 100 Years

	Contaminant											
	Cadmium		**Manganese**		**Molybdenum**		**Selenium**		**Sulfate**		**Uranium**	
Concentration Goal	0.01 mg/L		1.7 mg/L		0.1 mg/L		0.05 mg/L		1,276 mg/L		0.044 mg/L	
Source	MCL		Risk-based		MCL		EPA–SDWS[c]		Background		MCL	
Time (yrs)	**Conc[a] (mg/L)**	**Prob[b] (%)**	**Conc[a] (mg/L)**	**Prob[b] (%)**	**Conc[a] (mg/L)**	**Prob[b] (%)**	**Conc[a] (mg/L)**	**Prob[b] (%)**	**Conc[a] (mg/L)**	**Prob[b] (%)**	**Conc[a] (mg/L)**	**Prob[b] (%)**
5	0.0365	100	3.848	100	0.0812	0	0.0686	100	2,792	100	1.3650	100
10	0.0363	100	3.505	100	0.0652	0	0.0625	100	2,537	100	1.0820	100
15	0.0362	100	3.234	100	0.0519	0	0.0576	86	2,310	100	0.8628	100
25	0.0357	100	2.794	100	0.0318	0	0.0500	54	1,919	100	0.5311	100
50	0.0347	100	1.916	99	0.0094	0	0.0379	2	1,571	100	0.1301	100
60	0.0343	100	1.630	17	0.0061	0	0.0345	0	1,471	100	0.0726	100
70	0.0340	100	1.388	0	0.0038	0	0.0315	0	1,374	99	0.0442	51
80	0.0336	100	1.167	0	0.003	0	0.0289	0	1,280	54	0.0287	1
90	0.0333	100	0.973	0	0.003	0	0.0266	0	1,190	2	0.0185	0
100	0.033	100	0.815	0	0.003	0	0.0246	0	1,105	0	0.0118	0

[a]Value represents the predicted maximum average contaminant concentration (mg/L)
[b]Value represents the probability (%) the applicable standard will be exceeded
[c]EPA Safe Drinking Water Standard

7.2.1 Cadmium

As a result of the high K_d associated with cadmium (average K_d of 60.4 milliliters per gram [mL/g] and a range from 17 to 418 mL/g), the concentration only reduces 0.0039 mg/L (from a starting concentration of 0.0369 mg/L) over 100 years. Figure 27 and Figure 28 present the average cadmium concentration distribution at 10 and 100 years. After 100 years the probability of exceeding the 0.01 mg/L UMTRA standard is 100 percent (Figure 29).

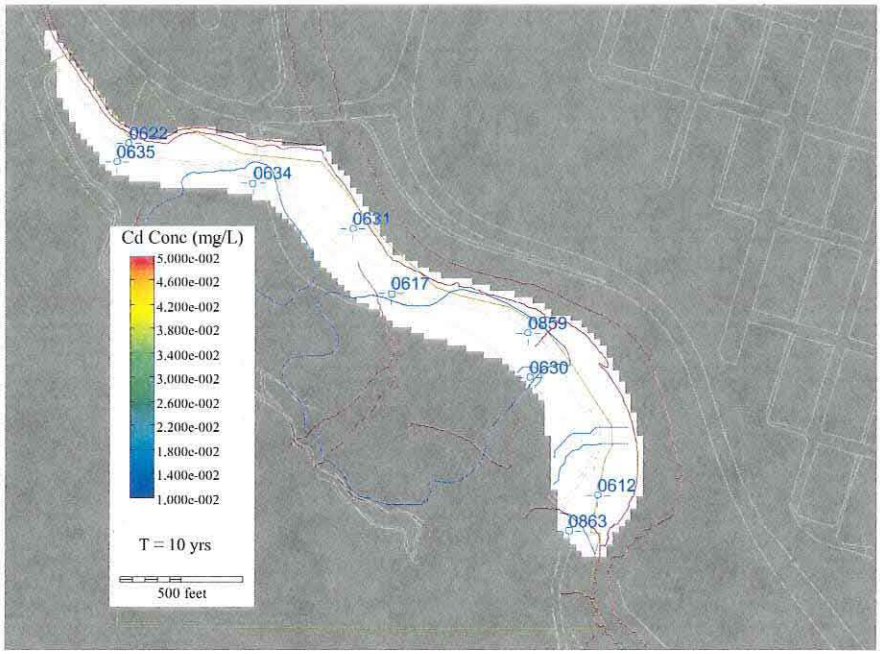


Figure 27. Predicted Average Cadmium Concentration at 10 Years

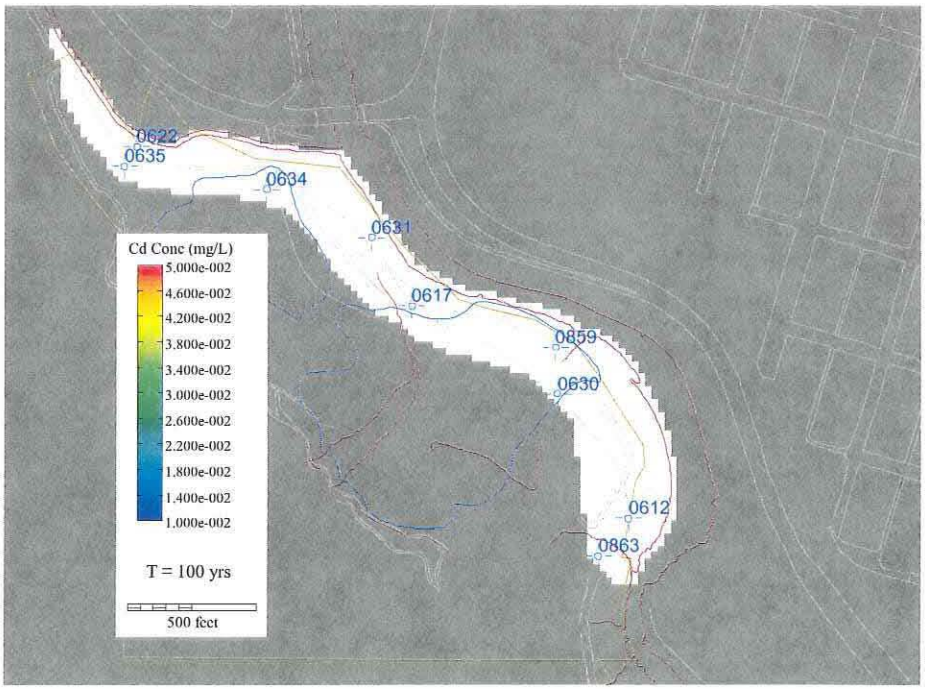


Figure 28. Predicted Average Cadmium Concentration at 100 Years

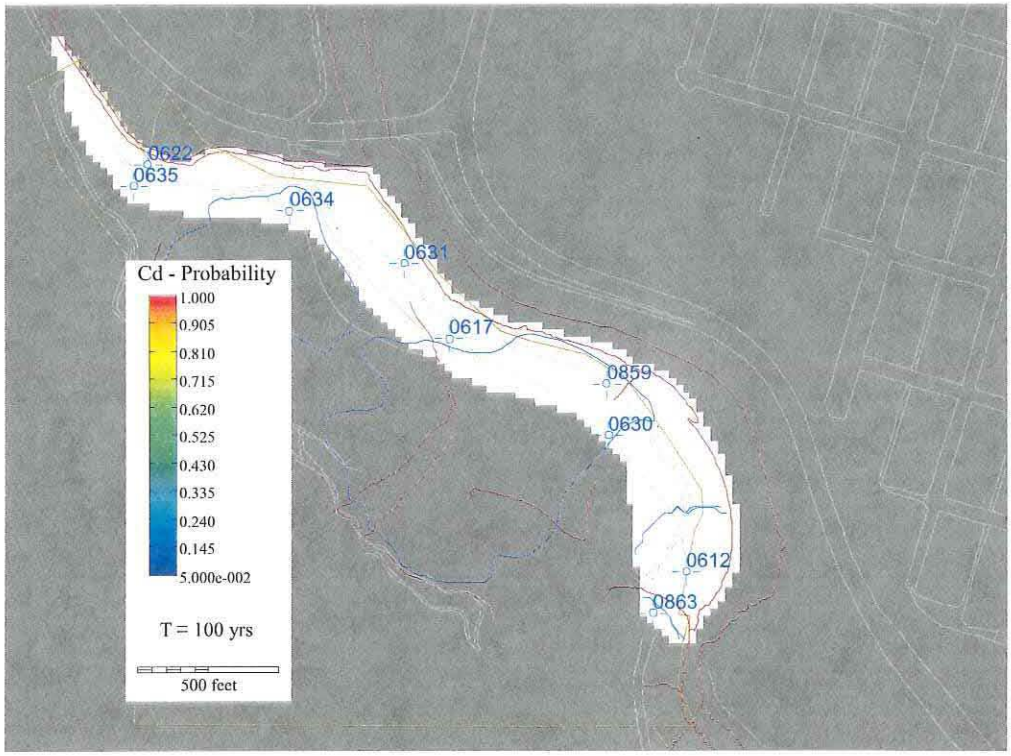


Figure 29. Probability of Cadmium Exceeding 0.01 mg/L After 100 Years

7.2.2 Manganese

As shown in Table 18 the maximum average manganese concentration falls below the risk-based standard of 1.7 mg/L between 50 and 60 years. Figure 30 and Figure 31 present the manganese distribution and at 10 and 50 years, respectively.

The probability of exceeding the 1.7 mg/L risk-based standard is 99 percent after 50 years (Figure 32) and drops to 17 percent after 60 years (Figure 33). At 70 years the probability of exceeding the standard drops to 0 percent

7.2.3 Molybdenum

As shown on Figure 21, the initial concentration maximum is just above the UMTRA Project standard of 0.1 mg/L. Having a low initial concentration, in conjunction with a low K_d, results in the maximum average concentration falling below the standard prior to 5 years. The probability of exceeding the standard after 5 years is 0 percent.

7.2.4 Selenium

A high K_d range (6.3 to 50.6 mL/g) measured onsite for selenium resulted in this contaminant's inability to naturally flush below the UMTRA Project standard of 0.01 mg/L within the 100-year timeframe. As a result, DOE defers to the EPA Safe Drinking Water standard of 0.05 mg/L. As shown in Table 18, the maximum average selenium concentration drops below this 0.05 mg/L standard after 25 years.

After 10 years of flushing, the model predicts that selenium concentrations above the standard will be limited to one cell southwest of well 631 (Figure 34). At 25 years, there is a 54 percent

probability the maximum average selenium concentration will exceed 0.05 mg/L (Figure 35), with the probability dropping to 0 percent after 60 years.

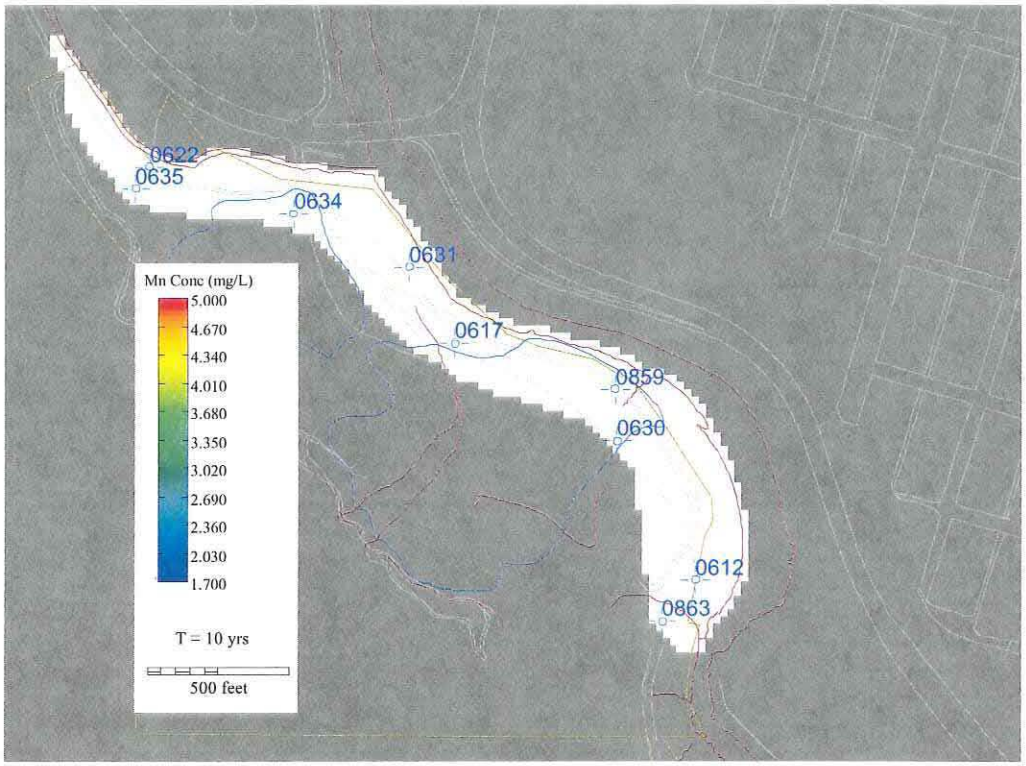


Figure 30. Predicted Average Manganese Concentration at 10 Years

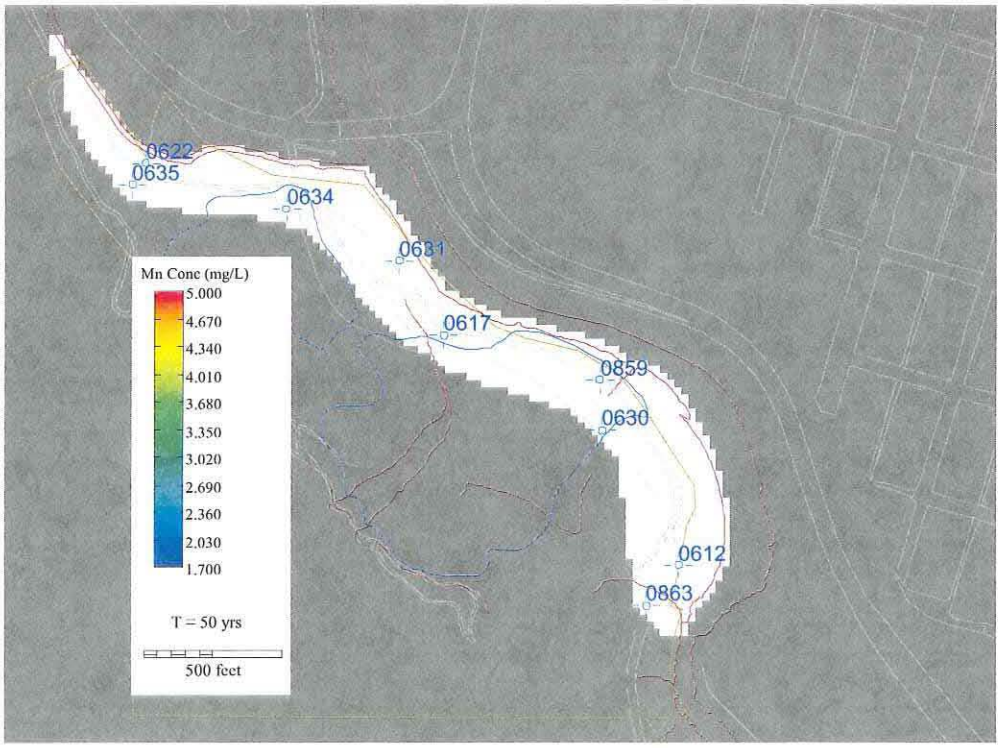


Figure 31. Predicted Average Manganese Concentration at 50 Years

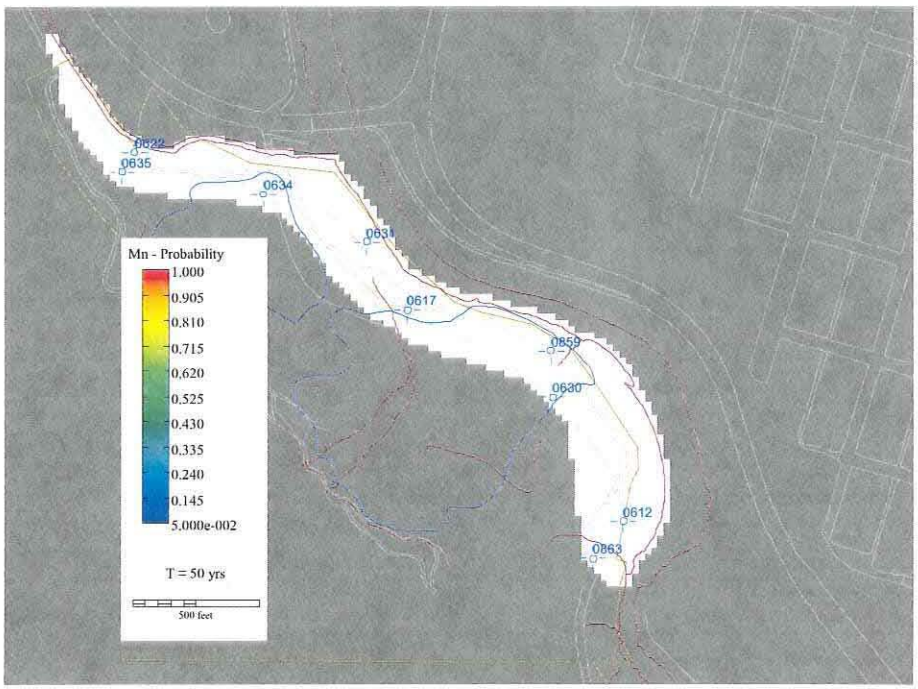


Figure 32. Probability of Manganese Exceeding 1.7 mg/L After 50 Years

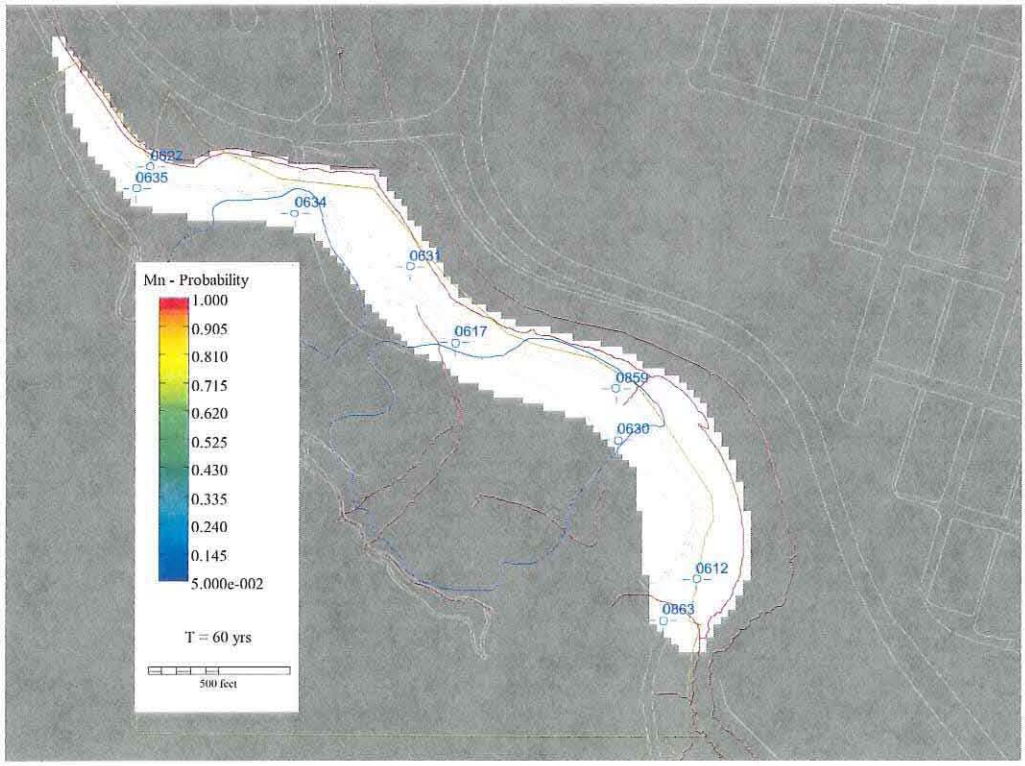


Figure 33. Probability of Manganese Exceeding 1.7 mg/L After 60 Years

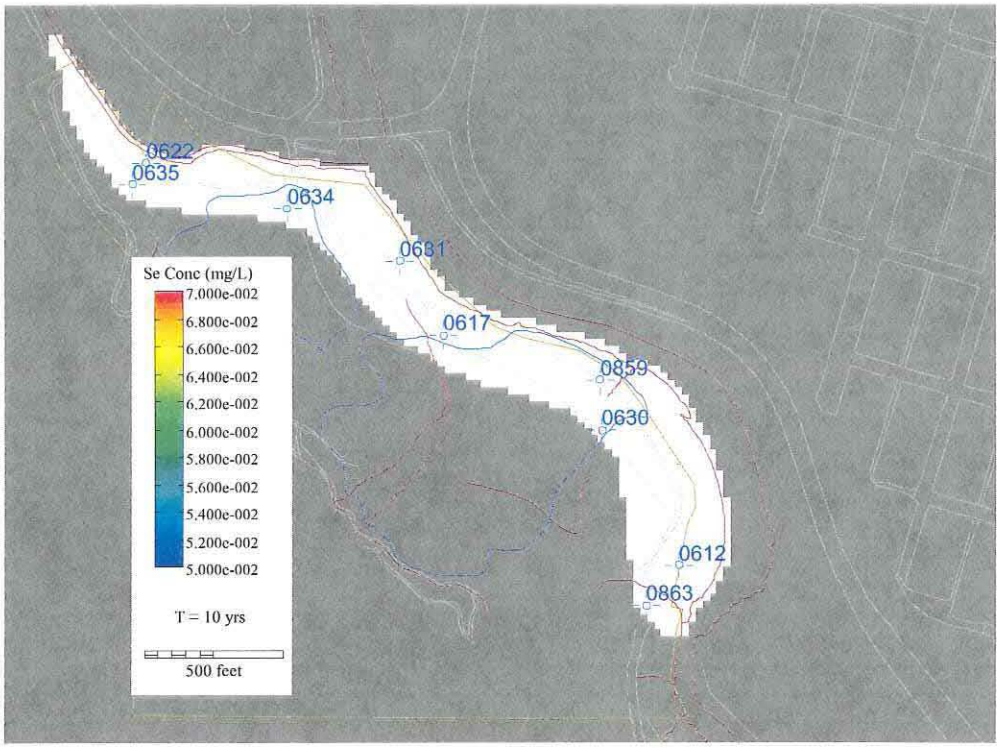


Figure 34. Predicted Average Selenium Concentration at 10 Years

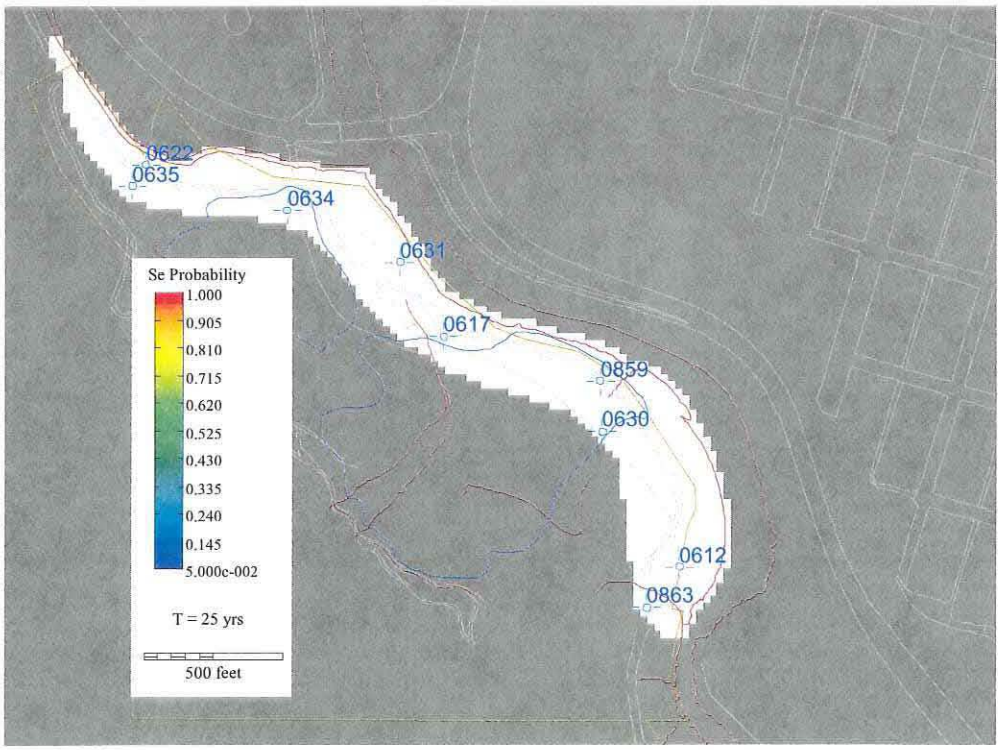


Figure 35. Probability of Selenium Exceeding 0.05 mg/L after 25 Years

7.2.5 Sulfate

The predicted sulfate distribution at 25, 50, and 70 years is shown as Figure 36, Figure 37, and Figure 38, respectively. Modeling results indicate the maximum average sulfate concentration will drop below the mean background concentration of 1,276 mg/L between 80 and 90 years. At 80 years there is a 54 percent probability the maximum average concentration will exceed 1,276 mg/L (Figure 39). By 100 years, there is 0 percent probability the background concentration will be exceeded.

7.2.6 Uranium

Predicted uranium average concentrations above the UMTRA Project standard of 0.044 mg/L at 10, 25, and 60 years into the future are presented in Figure 39 through Figure 41, respectively. After 70 years, the model predicts the maximum average concentration is at the standard concentration. Prior to 80 years, the maximum uranium average concentration present will be below the 0.044 mg/L standard. At 60 year, the probability is 100 percent that the maximum average concentration exceeds the standard (Figure 42), and at 70 years the model predicts the probability drops to 51 percent (Figure 43). At 80 years the probability is only 1 percent and is 0 percent at 90 years.

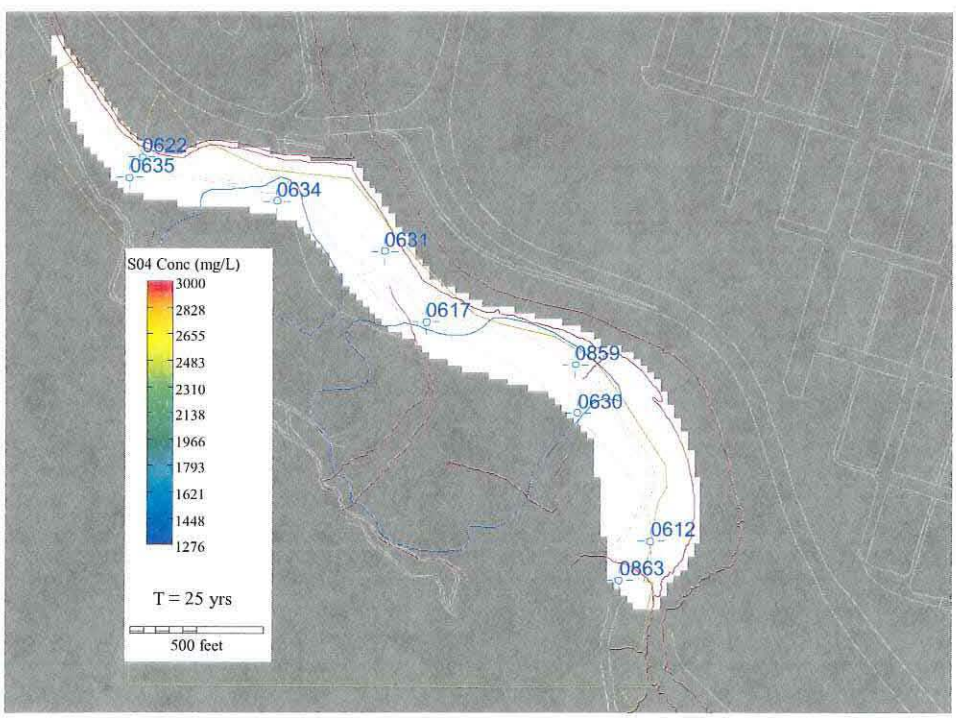


Figure 36. Predicted Steady State Sulfate Concentration at 25 Years

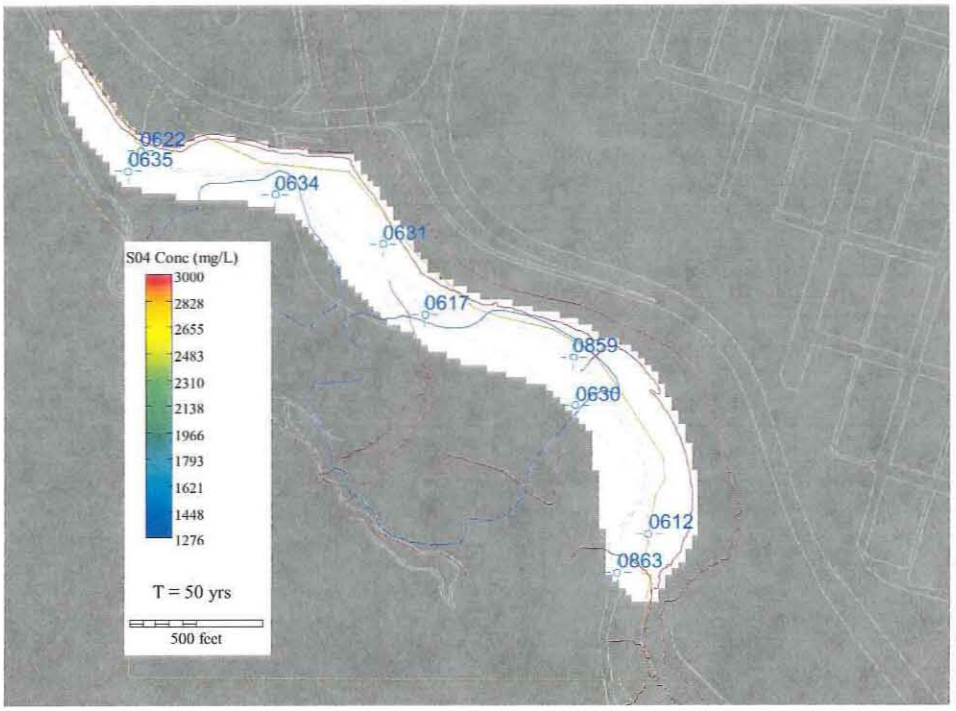


Figure 37. Predicted Steady State Sulfate Contamination at 50 Years

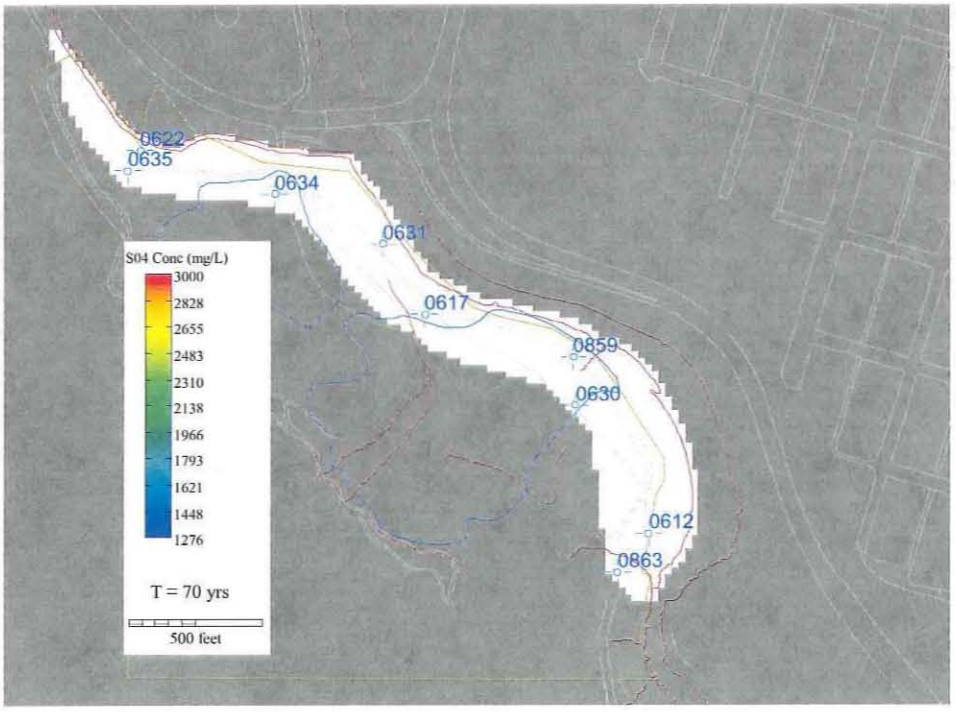


Figure 38. Predicted Steady State Sulfate Concentration at 70 Years

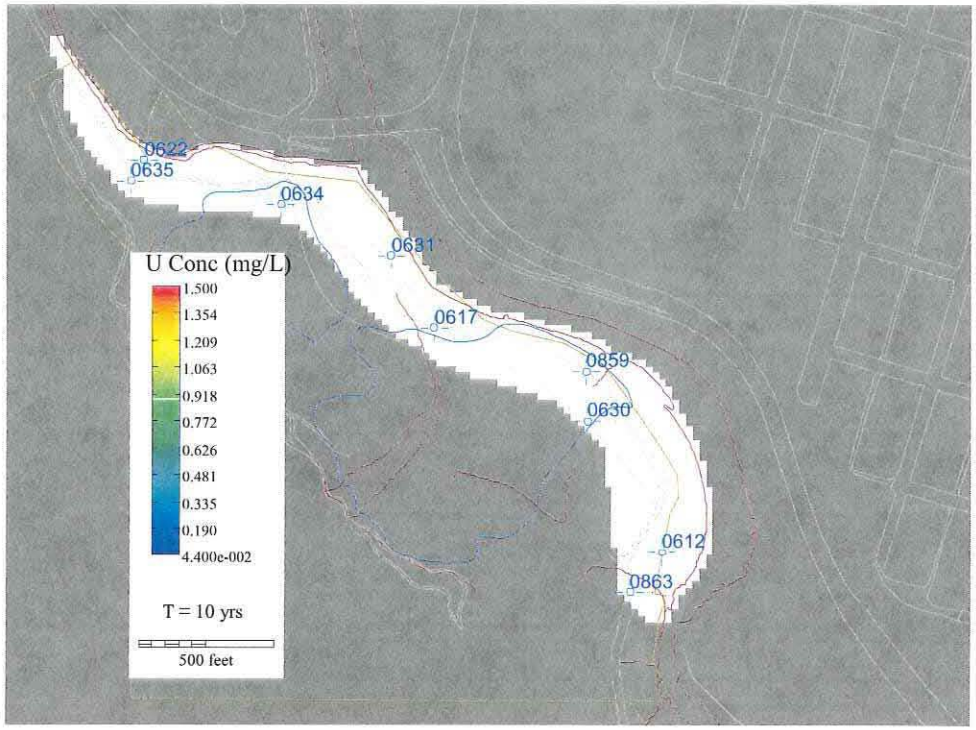


Figure 39. Predicted Average Uranium Concentration at 10 Years

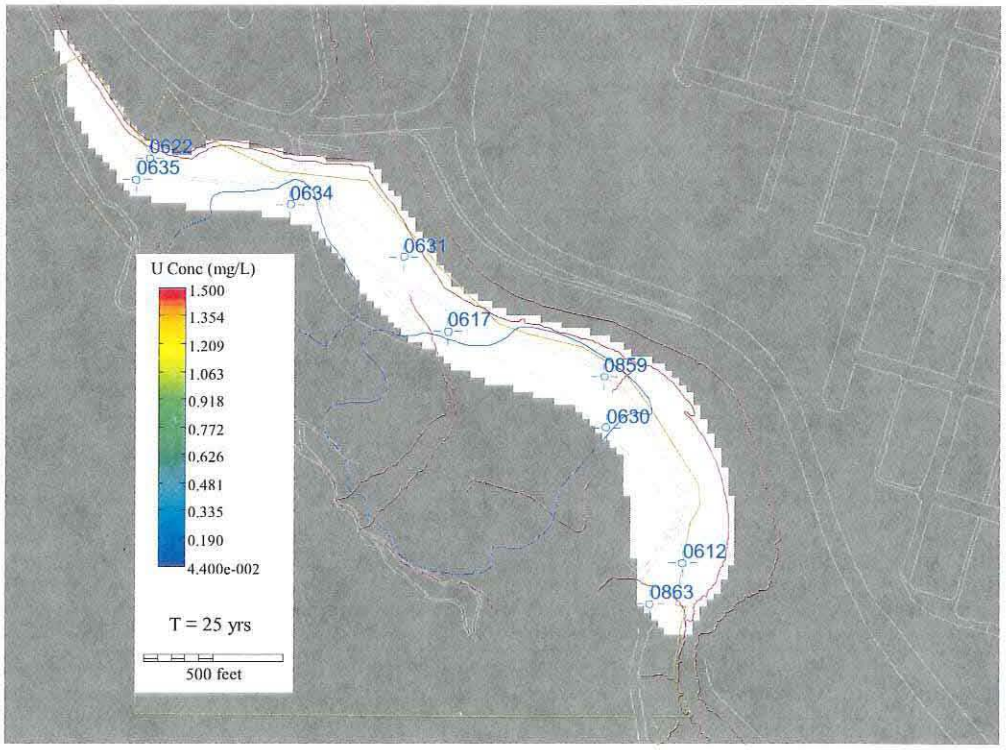


Figure 40. Predicted Average Uranium Concentration at 25 Years

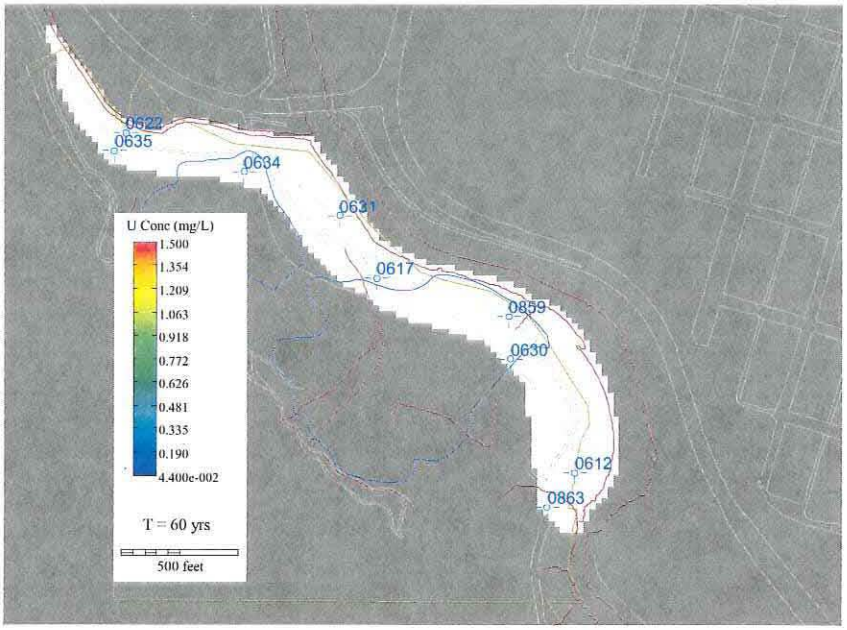


Figure 41. Predicted Average Uranium Concentration at 60 Years

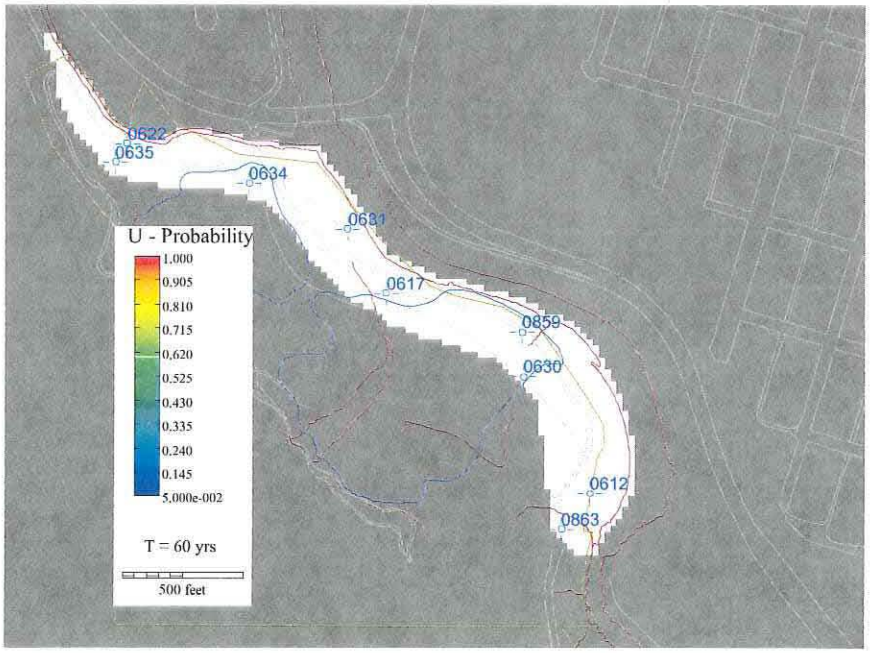


Figure 42. Probability of Uranium Exceeding 0.044 mg/L After 60 Years

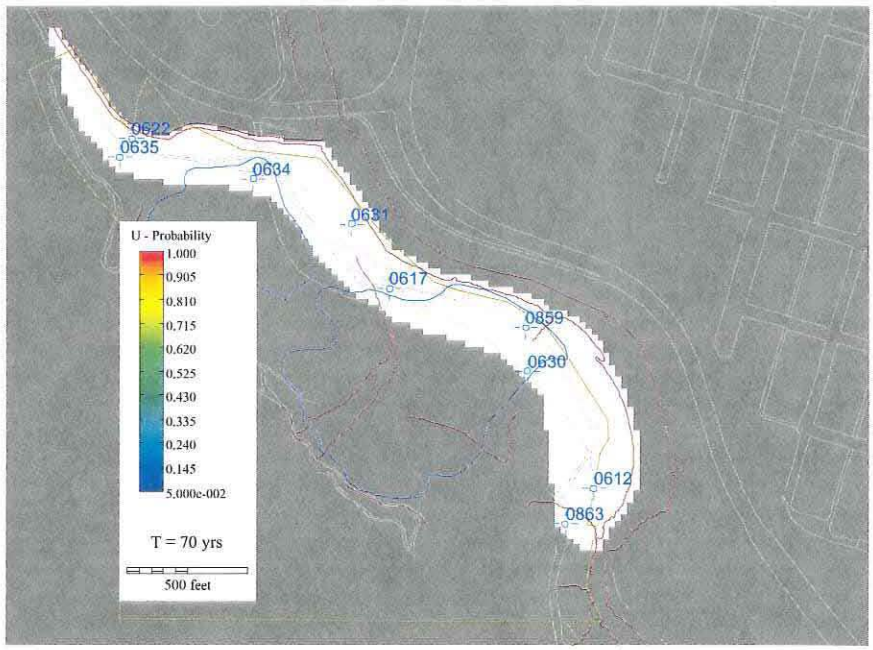


Figure 43. Probability of Uranium Exceeding 0.044 mg/L After 70 Years

8.0 Summary and Conclusions

A ground water flow and transport model was developed to evaluate if natural processes will reduce site-related contaminant concentrations to regulatory levels in the alluvial aquifer within 100 years. Contaminants modeled during this investigation include cadmium, manganese, molybdenum, selenium, sulfate, and uranium. A steady state stochastic flow and transport model was used to quantify the uncertainty in flow and transport parameters. Based on modeling results, natural flushing appears to be an acceptable compliance strategy which results in contaminant concentrations below applicable standards, risk-based standards, or background concentrations after the 100 year time frame for cadmium, manganese, molybdenum, selenium, sulfate, and uranium.

8.1 Qualitative Analysis

Ground water flow patterns predicted by the steady state stochastic flow model (Figure 14) closely resemble the ground water gradient measured in April 2001 (Figure 2). This visual analysis suggests that the calibrated flow model adequately and accurately predicts the observed water level elevations.

8.2 Quantitative Analysis

Data presented in Table 10 and Figure 15 and Figure 17 indicate that the calibrated steady state flow model satisfies the acceptance criteria and calibration objectives established prior to the modeling process. Calibration results presented in Figure 15 demonstrate that the flow model has a slight bias of underestimating water levels across the site. However, this bias is not large

enough to influence the modeling results, as shown by a mean residual of 0.77 ft and an absolute mean residual of 1.12 ft. Results presented in Figure 17 demonstrate that the predicted hydraulic heads versus the observed heads fall on a straight line, as expected. According to the flow model results, the total inflow and outflow for the surficial aquifer of the model is 1,926 ft^3/day. These values are higher compared to the estimated flow from the conceptual water budget (1,480 ft^3/day). Modifications to the conceptual model during the modeling process can explain this difference.

8.3 Model Predictions

- After 100 years of natural flushing, the maximum average cadmium concentration decreases only 0.0039 mg/L. A K_d range from 17 to 418 mL/g (average 60.4 mL/g) is the main factor contributing to the ineffectiveness of natural flushing for this contaminant. The maximum average cadmium concentration does not drop below the 0.01 mg/L standard after 100 years.

- After 60 years, the maximum predicted manganese concentration is 1.63 mg/L, which is below the risk-based standard of 1.7 mg/L.

- Molybdenum concentrations drop below the 0.1 mg/L UMTRA Project standard prior to 5 years of natural flushing.

- Initial selenium concentrations are below the 0.18 mg/L risk-based standard. The maximum predicted selenium concentration after 100 years is 0.0246 mg/L, which is above the 0.01 mg/L UMTRA Project standard.

- After 60 years of natural flushing the maximum average sulfate concentration drops below the risk-based standard of 1,500 mg/L.

- Uranium concentrations drop below the UMTRA Project standard of 0.044 mg/L prior to 80 years of natural flushing.