Appendix E

USGS Distribution Coefficient Analysis

1.0 Introduction

1.1 Distribution Coefficient (K_d) Analysis

The K_d is a bulk parameter that has been used with some success to describe the retardation of contaminant movement in an aquifer system. Laboratory measurements to determine the K_d for selected analytes were performed on alluvial material to support computer-modeling efforts in characterizing subsurface contaminant transport at the Naturita site.

1.1.1 Method of Solution

Laboratory analyses of the K_d were performed according to American Society for Testing and Materials (ASTM) procedure D 4646–87 (ASTM 1987), with slight modifications as detailed below, for two site-related contaminants of potential concern (COPCs): uranium and vanadium. Essentially, the procedure involves placing a sample representative of a location (e.g., soil, sediments, cuttings, core) into a solution of simulated contaminated ground water with which the material is likely to come in contact. The simulated ground water solution is agitated for 96 hours (uranium) or 24 hours (vanadium) and then centrifuged. The supernatant solution is analyzed and compared to the contaminant concentrations of the original solution. The difference between the two is assumed to be adsorbed to the sample. The linear adsorption isotherm distribution coefficient is generally defined as

$$C_{soil} = K_d \times C_{water}, \text{ which can be rearranged to } K_d = C_{soil}/C_{water},$$

or the ratio of the concentration of the contaminant in soil (or other material of interest) to the concentration of the contaminant in water at equilibrium. Therefore, the higher the K_d, the greater the retardation of contaminant movement in ground water.

The procedure requires analysis of only the solutions (and no actual soil samples) used in the experiments. Site samples collected from background areas or uncontaminated site samples are generally used, and all contaminant loss in the final solution is attributed to sample adsorption. However, for this study, uranium-contaminated alluvial samples were also collected, and uranium(VI) adsorption on these samples was determined by desorption in alkaline solutions and by uranium isotopic exchange in artificial ground water solution.

1.1.1.1 Sample Selection

A large sample of background alluvial material was collected by backhoe from the saturated zone of the aquifer at a location upgradient of the site on July 16 and 17, 1998. The sample was considered uncontaminated because concentrations of dissolved uranium at well 0547 (and decommissioned DOE wells nearby) were always very low, near the background uranium concentrations in the San Miguel River. The background sample of alluvium was screened in the field to remove cobbles larger than about 65 mm, and it was estimated visually that about 50 percent of the material scooped by the backhoe did not pass the 65-mm screen.

1.1.1.2 Preparation of the Sample of Background Alluvium

The sample was air dried at room temperature and sieved to separate the <3 mm fraction. Alluvial material totaling 190 kg passed a 3-mm screen and was mixed into a single composite

sample, representing 30 percent (by weight) of the material that had been sieved in the field through a 65-mm screen. The <3 mm sample represented approximately 15 percent of the total material sampled by backhoe in the field.

Synthetic solutions were prepared that simulated ground water at the Naturita site. Based on ground water analyses for several wells sampled in November 1998 and on preliminary batch experiments, a composition of synthetic ground water (AGW–3) was prepared for experiments equilibrated with air as follows (in mg/L): Na = 55.5, K = 2.5, Ca = 189, Mg = 36.8, SO_4 = 459, Cl = 171, C (inorganic) = 6.46, with pH adjusted to 7.9. The concentrations of C (inorganic) and Ca were expected to change somewhat during the batch experiments, because of the presence of calcite in the alluvial material. The AGW–3 solution equilibrated in the batch experiments with alluvial material and air without a significant change in pH (about 7.9) or alkalinity (37.5 mg/L as $CaCO_3$).

For uranium(VI), because of its tendency to form aqueous carbonate complexes, other synthetic solutions were prepared for experiments equilibrated with gas mixtures containing 0.5 percent CO_2/99.5 percent N_2 (AGW–7) and 2.0 percent CO_2/98 percent N_2 (AGW–5). The composition of AGW–7 was Na = 55.5, K = 2.5, Ca = 98.2, Mg = 36.8, SO_4 = 368.5, Cl = 8.2, and C (inorganic) = 30. This solution yielded a final pH of about 7.58 and an alkalinity of 152 mg/L as $CaCO_3$ after equilibration with the alluvial material and the gas mixture containing 0.5 percent CO_2. This alkalinity corresponds to a C (inorganic) concentration of 36.5 mg/L.

The composition of AGW–5 was Na = 55.5, K = 2.5, Ca = 257, Mg = 36.8, SO_4 = 459, Cl = 193, and C (inorganic) = 40. This solution yielded a final pH of about 7.18 and an alkalinity of 202 mg/L as $CaCO_3$, after equilibration with the alluvial material and the gas mixture containing 2.0 percent CO_2. This alkalinity corresponds to a C (inorganic) concentration of 48.4 mg/L. This latter solution was closer to the observed ground water pH and C (inorganic) concentrations observed in the alluvial aquifer than could be obtained by equilibrating experiments in the presence of air. Alkalinity in the alluvial aquifer ranges from 200 to 500 mg/L (as $CaCO_3$).

After equilibration of the synthetic solution with the alluvial material for 12 hours, either uranium or vanadium was then added from acidified nitrate stock solutions to study a range of target concentrations: 0.006 to 1.9 mg/L uranium or 1 to 16 mg/L vanadium.

1.1.1.3 Sample Analysis

The synthetic ground water solutions were analyzed to determine that the target concentrations were achieved by additions from the uranium(VI) and vanadium(V) stock solutions. These results are reported in Table 1.

Table 1. Laboratory Analytical Results for Synthetic Ground Water Solutions

Sample ID	Sample Description	Solution Volume (mL)	Target Concentration (mg/L)		Analyzed Concentration (mg/L)	
			U	V	U	V
AGW3–1	Synthetic ground water	30	0.0255	1.75	0.0267	1.73
AGW3–2	Synthetic ground water	30	0.241	5.25	0.0254	5.35
AGW3–3	Synthetic ground water	30	2.40	8.75	2.62	8.95

Aliquots of the synthetic ground water were first preequilibrated with each sample at a concentration of 25 g/L prior to use in the actual sample analyses, to preequilibrate the synthetic ground water with the sample surface. The preequilibrated synthetic ground water was filtered through a 0.45 micrometer (µm) filter prior to use in the sample analyses. For analysis with the ground water AGW–3, approximately 0.5 or 0.75 g of each sample was measured and placed in 50-milliliter (mL) polycarbonate centrifuge tubes with 20 or 30 mL of the filtered, preequilibrated synthetic ground water, resulting in sample suspension of 25 g/L. For analysis with the ground water AGW–7, approximately 3.75 g of each sample was measured and placed in 50-mL polycarbonate centrifuge tubes with 30 mL of the filtered, preequilibrated synthetic ground water, resulting in a sample suspension of 125 g/L. For analysis with the ground water AGW–5, approximately 7.5 g of each sample was measured and placed in 50 mL polycarbonate centrifuge tubes with 30 mL of the filtered, preequilibrated synthetic ground water, resulting in a sample suspension of 250 g/L.

Samples were rotated end over end at 14 revolutions per minute (rpm) for 24 hours, after which an aliquot of uranium(VI) or vanadium(V) stock solution was added to achieve the target contaminant concentration in the analysis. Samples were then rotated end-over-end at 14 rpm for 24 hours (V analysis) or 96 hours (U analysis). They were then centrifuged at 23,500 rpm for 30 minutes. The 5 mL aliquots of the resulting leachate samples were preserved with 50 µL concentrated HNO_3 in glass scintillation vials for analysis of U(VI) or vanadium. Analytical results are reported in Tables 2 through 4. Blank centrifuge tubes (with no solid sample) were included for each analysis to check for adsorption onto container walls; no adsorption on the container walls was observed. U(VI) was analyzed by kinetic phosphoresence analysis (KPA), and vanadium was analyzed by inductively coupled plasma optical emission spectrometry (ICP-OES).

Table 2. Analytical Results for Sample Leachate Solutions Using the Uncontaminated Alluvial Deposit Sample and Synthetic Ground Water AGW–3 (equilibrated with the partial pressure of CO_2 in air)

Sample ID	Sample Description	Solution Volume (mL)	Synthetic Solution Type	Sample Mass (g)	Concentration (mg/L)	
					U	V
Ex6S7	Alluvium composite leachate	30	AGW–3	0.75	0.00635	
Ex6S8	Duplicate	30	AGW–3	0.75	0.00584	
Ex6S9	Alluvium composite leachate	30	AGW–3	0.75	0.0167	
Ex6S10	Duplicate	30	AGW–3	0.75	0.0180	
Ex6S11	Alluvium composite leachate	30	AGW–3	0.75	0.0530	
Ex6S12	Duplicate	30	AGW–3	0.75	0.0514	
Ex6S13	Alluvium composite leachate	30	AGW–3	0.75	0.196	
Ex6S14	Duplicate	30	AGW–3	0.75	0.192	
Ex6S15	Alluvium composite leachate	30	AGW–3	0.75	0.412	
Ex6S16	Duplicate	30	AGW–3	0.75	0.420	
Ex6S17	Alluvium composite leachate	30	AGW–3	0.75	2.24	
Ex6S18	Duplicate	30	AGW–3	0.75	2.13	
ExVS5	Alluvium composite leachate	20	AGW–3	0.5		1.16
ExVS6	Duplicate	20	AGW–3	0.5		1.17
ExVS8	Alluvium composite leachate	20	AGW–3	0.5		4.34
ExVS9	Duplicate	20	AGW–3	0.5		4.32
ExVS11	Alluvium composite leachate	20	AGW–3	0.5		7.75
ExVS12	Duplicate	20	AGW–3	0.5		7.83
ExVS14	Alluvium composite leachate	20	AGW–3	0.5		11.8
ExVS15	Duplicate	20	AGW–3	0.5		12.0
ExVS17	Alluvium composite leachate	20	AGW–3	0.5		16.2
ExVS18	Duplicate	20	AGW–3	0.5		16.1

Table 3. Analytical Results for Sample Leachate Solutions Using the Uncontaminated Alluvial Deposit Sample and Synthetic Ground Water AGW–7 (equilibrated with 0.5 percent CO_2)

Sample ID	Sample Description	Solution Volume (mL)	Synthetic Solution Type	Sample Mass (g)	Concentration (mg/L)
					U
Ex11S107	Alluvium composite leachate	30	AGW–7	3.75	0.0178
Ex11S108	Duplicate	30	AGW–7	3.75	0.0182
Ex11S109	Alluvium composite leachate	30	AGW–7	3.75	0.0305
Ex11S110	Duplicate	30	AGW–7	3.75	0.0304
Ex11S111	Alluvium composite leachate	30	AGW–7	3.75	0.0644
Ex11S112	Duplicate	30	AGW–7	3.75	0.0657
Ex11S113	Alluvium composite leachate	30	AGW–7	3.75	0.188
Ex11S114	Duplicate	30	AGW–7	3.75	0.200
Ex11S115	Alluvium composite leachate	30	AGW–7	3.75	0.589
Ex11S116	Duplicate	30	AGW–7	3.75	0.574
Ex11S117	Alluvium composite leachate	30	AGW–7	3.75	1.95
Ex11S118	Duplicate	30	AGW–7	3.75	1.96

Table 4. Analytical Results for Sample Leachate Solutions Using the Uncontaminated Alluvial Deposit Sample and Synthetic Ground Water AGW–5 (equilibrated with 2.0 percent CO_2)

Sample ID	Sample Description	Solution Volume (mL)	Synthetic Solution Type	Sample Mass (g)	Concentration (mg/L)
					U
Ex10S7	Alluvium composite leachate	30	AGW–5	7.5	0.0252
Ex10S8	Duplicate	30	AGW–5	7.5	0.0225
Ex10S9	Alluvium composite leachate	30	AGW–5	7.5	0.0308
Ex10S10	Duplicate	30	AGW–5	7.5	0.0307
Ex10S11	Alluvium composite leachate	30	AGW–5	7.5	0.0566
Ex10S12	Duplicate	30	AGW–5	7.5	0.0621
Ex10S13	Alluvium composite leachate	30	AGW–5	7.5	0.180
Ex10S14	Duplicate	30	AGW–5	7.5	0.187
Ex10S15	Alluvium composite leachate	30	AGW–5	7.5	0.529
Ex10S16	Duplicate	30	AGW–5	7.5	0.535
Ex10S17	Alluvium composite leachate	30	AGW–5	7.5	1.87
Ex10S18	Duplicate	30	AGW–5	7.5	1.83

1.1.1.4 K_d Calculation

K_ds are calculated using the analytical data summarized in Table 5 through Table 7 and the following equation:

$$K_d = \frac{(A - B)V}{(M_s)B}$$

where

A = total initial concentration (mg/L) of the COPCs in the synthetic ground water,
B = final concentration of the COPCs in the leachate after 96 hours (uranium) or 24 hours (vanadium) in contact with the sediment sample (mg/L),
V = volume of solution (mL),
M_s = mass of sediment sample (grams), and
K_d = distribution coefficient (milliliters per gram [mL/g]).

Results of the calculations are presented in Table 5 through Table 7. The K_d values are consistent with R_d values in the ASTM procedure; this value only represents a true K_d if equilibrium conditions were attained during the test period.

Table 5. Measured K_d Values for the Uncontaminated Alluvial Deposit Sample and Synthetic Ground Water AGW–3 (equilibrated with the partial pressure of CO_2 in air)

Sample ID	Sample Description	Initial Concentration (mg/L)		Final Concentration (mg/L)		K_d (mL/g)	
		U	V	U	V	U	V
Ex6S7	Alluvium composite leachate	0.0108		0.00635		28.1	
Ex6S8	Duplicate	0.0107		0.00584		33.9	
Ex6S9	Alluvium composite leachate	0.0279		0.0167		27.1	
Ex6S10	Duplicate	0.0280		0.0180		22.5	
Ex6S11	Alluvium composite leachate	0.0791		0.0530		19.8	
Ex6S12	Duplicate	0.0794		0.0514		21.9	
Ex6S13	Alluvium composite leachate	0.255		0.196		12.2	
Ex6S14	Duplicate	0.256		0.192		13.2	
Ex6S15	Alluvium composite leachate	0.533		0.412		11.7	
Ex6S16	Duplicate	0.534		0.420		10.8	
Ex6S17	Alluvium composite leachate	2.59		2.24		6.1	
Ex6S18	Duplicate	2.59		2.13		8.6	
ExVS5	Alluvium composite leachate		1.73		1.16		20.0
ExVS6	Duplicate		1.73		1.17		19.5
ExVS8	Alluvium composite leachate		5.35		4.34		9.3
ExVS9	Duplicate		5.35		4.32		9.5
ExVS11	Alluvium composite leachate		8.95		7.75		6.2
ExVS12	Duplicate		8.95		7.83		5.7
ExVS14	Alluvium composite leachate		13.3		11.8		5.2
ExVS15	Duplicate		13.3		12.0		4.5
ExVS17	Alluvium composite leachate		17.8		16.2		4.0
ExVS18	Duplicate		17.8		16.1		4.3

Table 6. Measured Uranium K_d Values for the Uncontaminated Alluvial Deposit Sample and Synthetic Ground Water AGW–7 (equilibrated with 0.5 percent CO_2)

Sample ID	Sample Description	Initial Concentration (mg/L)	Final Concentration (mg/L)	K_d (mL/g)
		U	U	U
Ex11S107	Alluvium composite leachate	0.0304	0.0178	5.8
Ex11S108	Duplicate	0.0304	0.0182	5.4
Ex11S109	Alluvium composite leachate	0.0466	0.0305	4.3
Ex11S110	Duplicate	0.0454	0.0304	4.2
Ex11S111	Alluvium composite leachate	0.0904	0.0644	3.5
Ex11S112	Duplicate	0.0940	0.0657	3.6
Ex11S113	Alluvium composite leachate	0.273	0.188	3.7
Ex11S114	Duplicate	0.274	0.200	3.0
Ex11S115	Alluvium composite leachate	0.756	0.589	2.3
Ex11S116	Duplicate	0.756	0.574	2.6
Ex11S117	Alluvium composite leachate	2.42	1.95	2.0
Ex11S118	Duplicate	2.40	1.96	1.8

Table 7. Measured Uranium K_d Values for the Uncontaminated Alluvial Deposit Sample and Synthetic Ground Water AGW–5 (equilibrated with 2.0 percent CO_2)

Sample ID	Sample Description	Initial Concentration (mg/L)	Final Concentration (mg/L)	K_d (mL/g)
		U	U	U
Ex10S7	Alluvium composite leachate	0.0430	0.0252	3.0
Ex10S8	Duplicate	0.0429	0.0225	3.8
Ex10S9	Alluvium composite leachate	0.0570	0.0308	3.6
Ex10S10	Duplicate	0.0570	0.0307	3.6
Ex10S11	Alluvium composite leachate	0.0974	0.0566	3.1
Ex10S12	Duplicate	0.0979	0.0621	2.5
Ex10S13	Alluvium composite leachate	0.283	0.180	2.4
Ex10S14	Duplicate	0.282	0.187	2.2
Ex10S15	Alluvium composite leachate	0.772	0.529	2.0
Ex10S16	Duplicate	0.777	0.535	1.9
Ex10S17	Alluvium composite leachate	2.55	1.87	1.5
Ex10S18	Duplicate	2.54	1.83	1.6

Measured K_d values obtained for the alluvial aquifer samples were adjusted on the basis of aquifer grain size analysis. It was found in collecting the uncontaminated alluvial material that only 15 percent of the aquifer material was in the <3 mm fraction and that most of the material was gravel to cobble size. Therefore, the measured K_d values for the alluvial aquifer, which were

performed on the <3 mm fraction, were adjusted by multiplying by 0.15. This assumes that the gravel- and cobble-sized materials are insignificant in terms of contaminant adsorption. The adjusted values are reported in Table 8 through Table 10.

Table 8. Results for K_d Values Adjusted for Grain-Size Distribution for the Uncontaminated Alluvial Deposit Sample and Synthetic Ground Water AGW–3 (equilibrated with the partial pressure of CO_2 in air)

Sample ID	Sample Description	K_d (mL/g)	
		U	V
Ex6S7	Alluvium composite leachate	4.2	
Ex6S8	Duplicate	5.1	
Ex6S9	Alluvium composite leachate	4.1	
Ex6S10	Duplicate	3.4	
Ex6S11	Alluvium composite leachate	3.0	
Ex6S12	Duplicate	3.3	
Ex6S13	Alluvium composite leachate	1.8	
Ex6S14	Duplicate	2.0	
Ex6S15	Alluvium composite leachate	1.8	
Ex6S16	Duplicate	1.6	
Ex6S17	Alluvium composite leachate	0.92	
Ex6S18	Duplicate	1.3	
ExVS5	Alluvium composite leachate		3.0
ExVS6	Duplicate		2.9
ExVS8	Alluvium composite leachate		1.4
ExVS9	Duplicate		1.4
ExVS11	Alluvium composite leachate		0.93
ExVS12	Duplicate		0.86
ExVS14	Alluvium composite leachate		0.77
ExVS15	Duplicate		0.67
ExVS17	Alluvium composite leachate		0.59
ExVS18	Duplicate		0.64

Table 9. Results for K_d Values Adjusted for Grain-Size Distribution for the Uncontaminated Alluvial Deposit Sample and Synthetic Ground Water AGW–7 (equilibrated with 0.5 percent CO_2)

Sample ID	Sample Description	K_d (mL/g) U
Ex11S107	Alluvium composite leachate	0.87
Ex11S108	Duplicate	0.81
Ex11S109	Alluvium composite leachate	0.65
Ex11S110	Duplicate	0.63
Ex11S111	Alluvium composite leachate	0.52
Ex11S112	Duplicate	0.54
Ex11S113	Alluvium composite leachate	0.56
Ex11S114	Duplicate	0.45
Ex11S115	Alluvium composite leachate	0.35
Ex11S116	Duplicate	0.39
Ex11S117	Alluvium composite leachate	0.30
Ex11S118	Duplicate	0.27

Table 10. Results for K_d Values Adjusted for Grain-Size Distribution for the Uncontaminated Alluvial Deposit Sample and Synthetic Ground Water AGW–5 (equilibrated with 2.0 percent CO_2)

Sample ID	Sample Description	K_d (mL/g) U
Ex10S7	Alluvium composite leachate	0.45
Ex10S8	Duplicate	0.58
Ex10S9	Alluvium composite leachate	0.54
Ex10S10	Duplicate	0.54
Ex10S11	Alluvium composite leachate	0.46
Ex10S12	Duplicate	0.37
Ex10S13	Alluvium composite leachate	0.36
Ex10S14	Duplicate	0.32
Ex10S15	Alluvium composite leachate	0.29
Ex10S16	Duplicate	0.28
Ex10S17	Alluvium composite leachate	0.23
Ex10S18	Duplicate	0.25

The data show that the K_d values are somewhat dependent on the concentration of the COPC, under otherwise constant chemical conditions (Figure 1 through Figure 3). In addition, the data show that the uranium K_d values are greatly decreased by increasing alkalinity (or partial pressure of carbon dioxide gas), due to the formation of weakly adsorbing, aqueous uranyl-carbonate complexes (Figure 4).

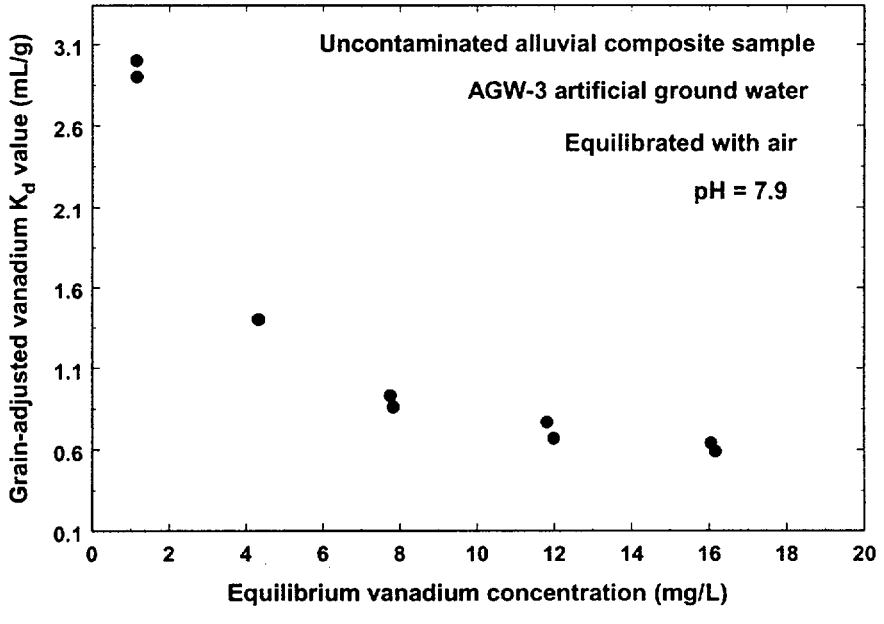

Figure 1. Grain-Adjusted K_d Values for Vanadium as a Function of Vanadium Concentration Vanadium Concentrations in the Alluvial Aquifer Vary from Below Detection to 7 mg/L

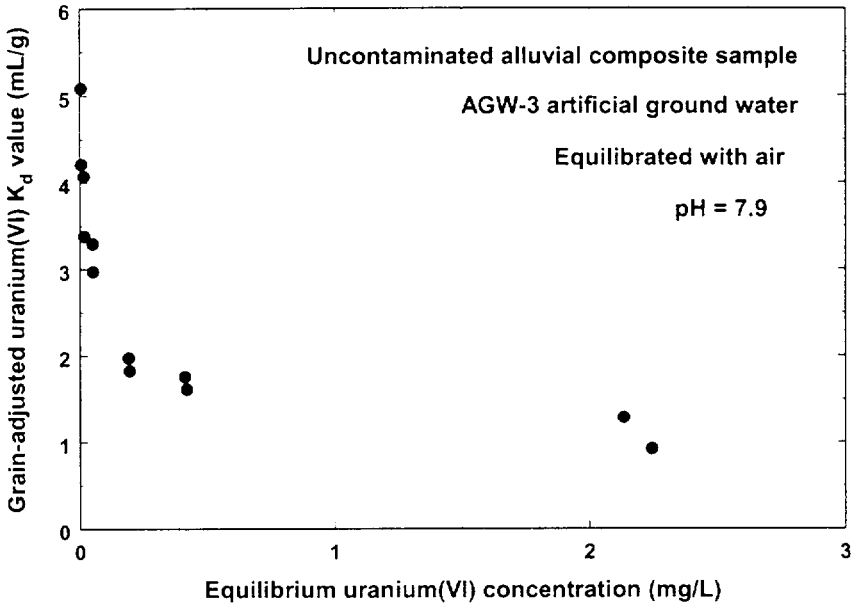

Figure 2. Grain-Adjusted K_d Values for Uranium as a Function of Uranium Concentration Uranium Concentrations in the Alluvial Aquifer Vary from 0.005 to 2.6 mg/L

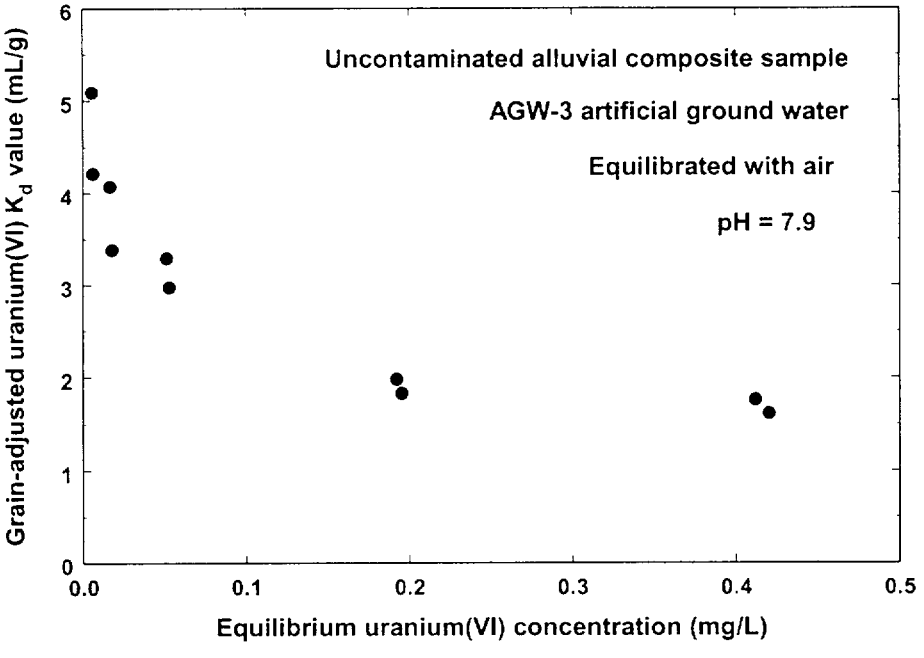

Figure 3. Grain-Adjusted K_d Values for Uranium as a Function of Uranium Concentration at Low Uranium Concentrations
Uranium Concentrations in the Alluvial Aquifer Vary from 0.005 to 2.6 mg/L

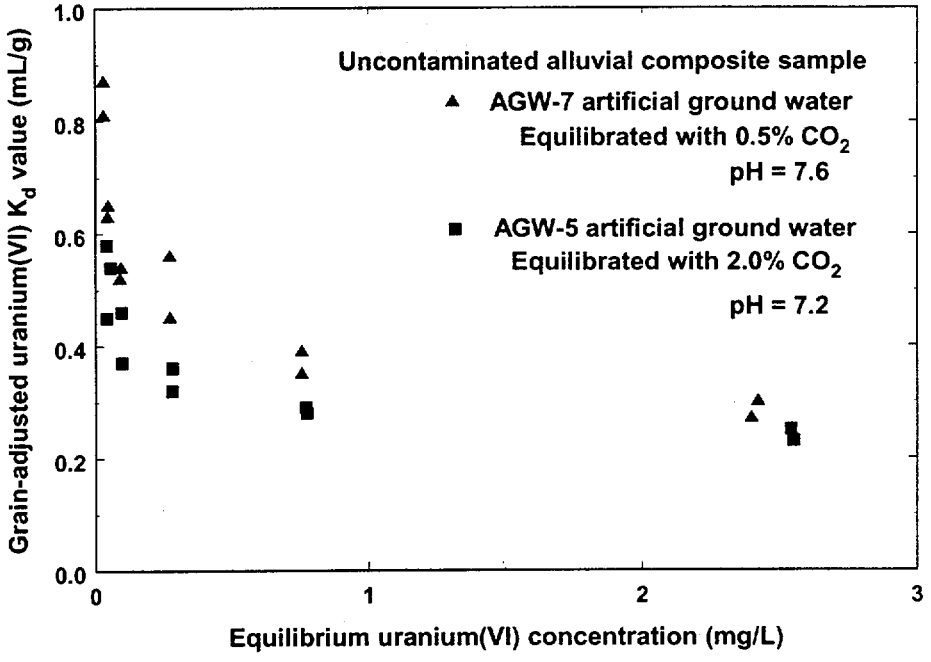

Figure 4. Grain-Adjusted K_d values for Uranium as a Function of Uranium Concentration in Waters Equilibrated with 0.5 or 2 percent CO_2
Each System Reaches a Different Equilibrium pH Value Due to Equilibration with Carbonate Minerals in the Alluvial Sediments. Partial Pressures of CO_2 in the Alluvial Aquifer Range from 1 to 10 percent CO_2

If left undisturbed, the trailing edge of the contaminant plume will probably leave the site with low uranium concentrations and an alkalinity closer to background conditions. This would be near the conditions represented by the sample analysis with 0.5 percent CO_2, although alluvial ground water usually has a lower pH (7.0 to 7.2). Based on the range of K_d values indicated by the sample analysis, it is recommended that K_d values in the range of 1–3 mL/g be used for both uranium and vanadium in the contaminant transport modeling of alluvial ground water.

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Appendix F

Contaminant Transport Modeling

1.0 Introduction

1.1 General Setting

The Naturita site is located in Montrose County in the southwestern portion of Colorado, about 2 miles northwest of the town of Naturita along Colorado State Highway 141 (Figure 1). Most of the site is on the west bank of the San Miguel River, between the river and the highway. The former ore storage area is west of the highway. The site (Figure 2) covers 53 acres which includes the former tailings pile area (27 acres), the former mill yard and former ore-buying station (14 acres), and the adjacent former ore storage area (12 acres). A brief operating history of the site can be found in page 2-1 through 2-4 of the BLRA (DOE 1995). A gravel mining operation upgradient of the former site is not considered in the U.S. Geological Survey (USGS) flow model. The future expansion of this operation could significantly impact the ground water flow and the transport of contaminants.

1.2 Study Objective

1.2.1 Natural Flushing

As part of the compliance strategy for the cleanup of contaminated ground water at the Naturita UMTRA Project site it is necessary to develop a computer ground water flow model and a subsequent contaminant transport model to assist in forecasting whether natural flushing of the contaminants of potential concern (COPC) is a viable remediation alternative.

This document presents the use of the steady state deterministic flow model, developed by the USGS, the steady state stochastic flow model, and the development of the contaminant transport models (deterministic and stochastic) to predict future COPC concentrations. The various flow and transport parameters that affect the hydraulic head and contaminant distribution for the steady state deterministic and steady state stochastic models are described below.

The steps used for obtaining a calibrated flow and transport model for the site 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 codes to be used in the analysis, (3) establish the relationship between the conceptual and numerical models, and (4) perform calibration and sensitivity analysis on the flow model parameters and sensitivity analysis on transport parameters.

Stochastic simulations for uranium were performed for both the flow or transport models even though the deterministic model indicated that neither uranium or vanadium come close to achieving the clean-up standard by natural flushing within 100 years.

1.2.2 Pumping Followed by Natural Flushing

The purpose of this modeling was to determine if pumping specified wells (unknown) at specified rates (unknown) for a specified number of years (unknown) followed by natural flushing for 100 years would result in achieving the clean-up standard for uranium and vanadium. This is a classical optimization problem and could probably be formulated as such. However, a much simpler approach is taken here.

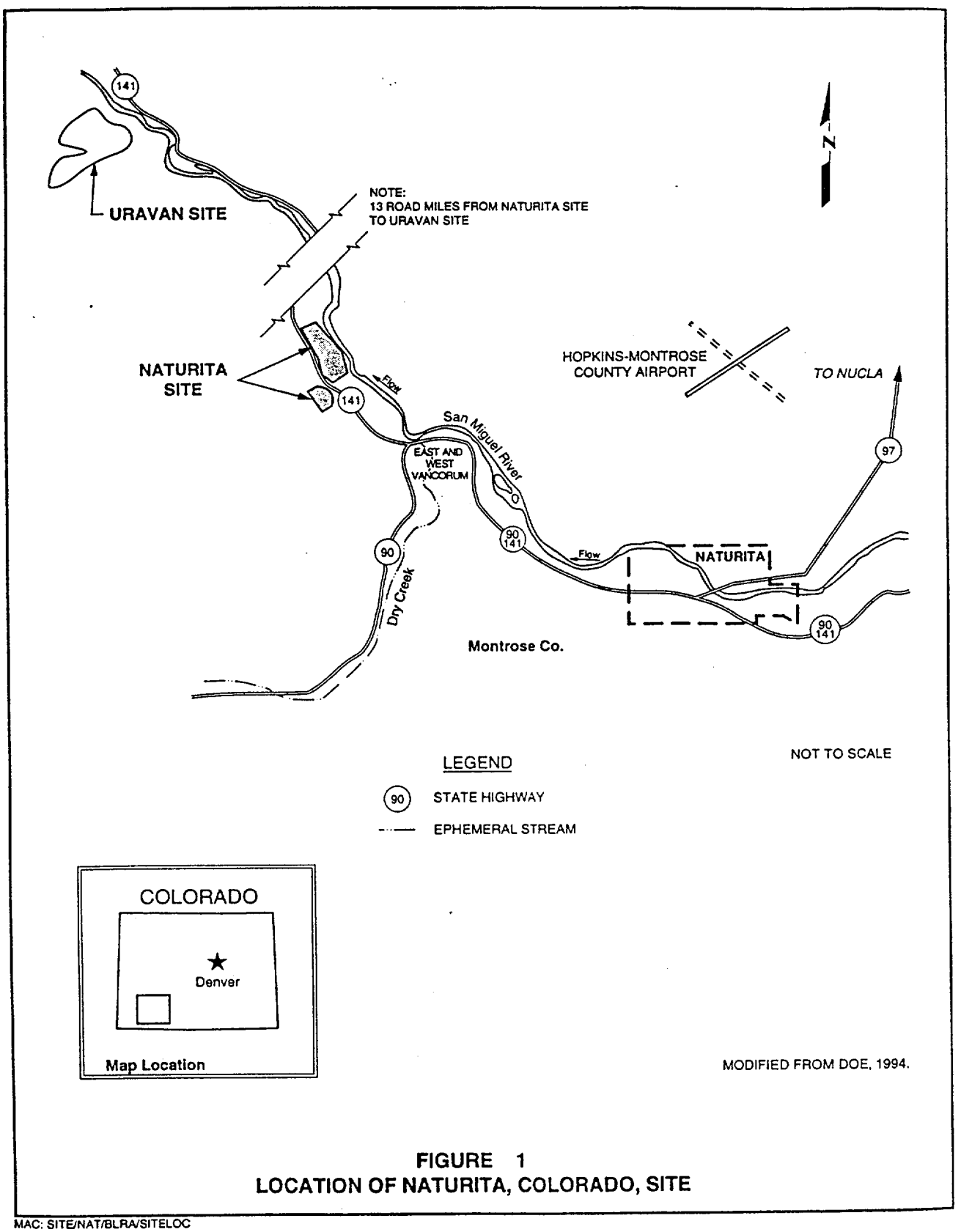

FIGURE 1
LOCATION OF NATURITA, COLORADO, SITE

MAC: SITE/NAT/BLRA/SITELOC

Figure 1. Location of the Naturita Site

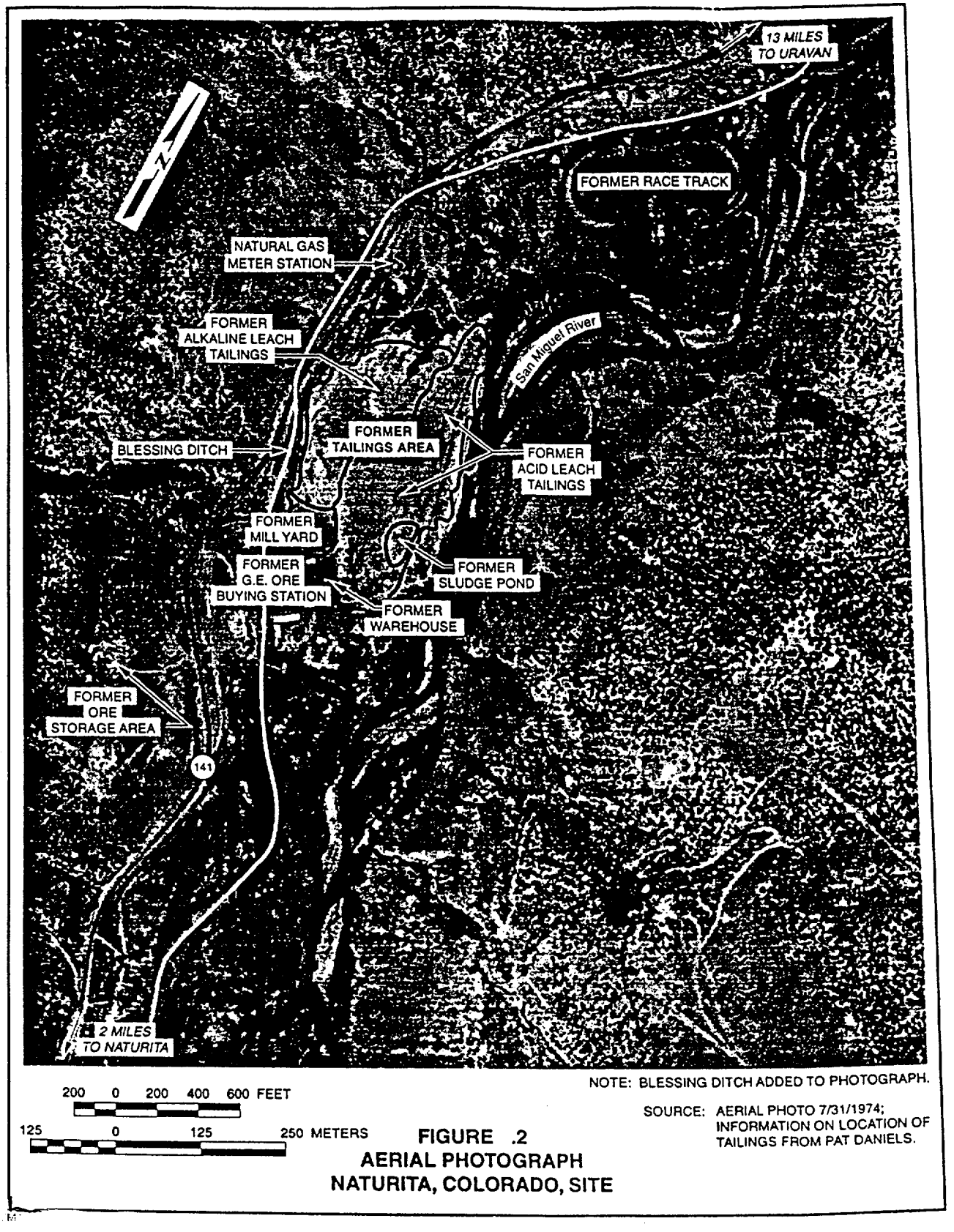

Figure 2. Aerial Photograph of the Naturita Site, July 1974

2.0 Conceptual Model

2.1 Aquifer System Framework

The Naturita processing site rests on Quaternary surficial deposits that include unconsolidated alluvial sediment composed of river gravel and cobbles in a silty-to-clayey sand matrix, and fill material. These deposits range in thickness from 11 to 34 feet (ft) with an average thickness of 20 ft. The alluvium is underlain by the Morrison Formation. The Morrison Formation is subdivided into the Brushy Basin Member and the Salt Wash Member. The Brushy Basin Member lies directly beneath the alluvium at the site and has a maximum thickness of 490 ft. The top of the Salt Wash Member is encountered at depths of 130 to 165 ft. Both units dip two to four degrees to the northeast. The Brushy Basin Member is not a significant water-bearing unit and is considered the bottom of the aquifer. The alluvial aquifer is unconfined and is treated as such in the model.

2.2 Ground Water Flow System

Two aquifers are present in the vicinity of the Naturita site. The shallow upper, or alluvial aquifer, is approximately 3 to 18 ft below land surface. The lower, or Salt Wash aquifer, is at a depth of about 170 ft below land surface. These two aquifers are separated by the Brushy Basin Member, which is primarily a low permeability rock unit. The alluvial aquifer receives recharge from subsurface flow along the San Miguel River and precipitation. During high river stage, the alluvial aquifer is recharged by the river along the southern and eastern boundary. Likewise, during low river stage, water in the alluvial aquifer discharges to the river. Occasional recharge occurs from localized storms via unnamed ephemeral streams that drain the uplands to the west and transect the site north and west of the former tailings pile area. North of the site the river channel crosses from the east side to the west side of the valley. This creates a natural discharge zone for the alluvial aquifer water to the San Miguel River.

2.3 Hydrologic Boundaries

The alluvial aquifer is bounded to the west by the rocks of the Brushy Basin Member that forms the lower canyon wall, and may be regarded as a no-flow boundary. To the east and north of the site, the San Miguel River dissects the valley alluvium and constitutes a hydrologic boundary for the alluvial aquifer.

2.4 Hydraulic Properties

The USGS developed a steady state deterministic flow model for the Naturita site. The flow model hydraulic properties of interest that influence the aquifer system are the hydraulic conductivity of the alluvial aquifer, areal recharge due to precipitation, and recharge from and discharge to the San Miguel River via riverbed hydraulic conductance.

2.5 Contaminant Transport Properties

The contaminant transport properties of interest are the initial concentration distributions of the COPC, the effective porosity, the aquifer bulk density, the distribution coefficients (K_d) of the COPC, and dispersivity.

2.6 Sources and Sinks

The San Miguel River is a source of water to the aquifer. Areal recharge over the area is an annual source of water to the site. The San Miguel River is considered to be both a sink and a source (i.e., the alluvial aquifer discharges water to the river along some reaches and the river recharges the alluvial aquifer along other reaches). Discharge and recharge are seasonal in nature.

2.6.1 Sources

Two sources of recharge to the alluvial aquifer have been identified: precipitation and recharge from the San Miguel River.

The model surface area is represented by one recharge zone, with recharge being solely from precipitation. The calibrated USGS model uses a recharge value of 0.0 inches per year (in/yr). Site-specific meteorological data indicate there is approximately 13 inches of annual precipitation (0.00297 ft per day [ft/day]) in the Naturita area. However, the estimated amount available for recharge based on the Thornthwaite equation (Thornthwaite and Mather 1957) is 1.99 to 2.79 in/yr (0.00045 to 0.00064 ft/day).

2.6.2 Sinks

Several sources of discharge from the alluvial aquifer have been identified. These include evapotranspiration and ground water discharge from the alluvial aquifer into the San Miguel River. Evapotranspiration is accounted for by the use of a net recharge estimate (which includes the loss due to evapotranspiration).

3.0 Computer Code

3.1 Code Selection

MODFLOW (McDonald and Harbaugh 1988), a modular three-dimensional finite-difference ground water flow model published by the 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.

The USGS was tasked with developing a steady state deterministic flow model for the Naturita site. The USGS uses the Argus Open Numerical Environments (Argus ONE) family of product for the pre- and post-processing for MODFLOW. The calibrated MODFLOW files created by the Argus ONE products were then converted to a format compatible with the version of MODFLOW in GWVistas. The output from MODFLOW is used as input to MT3DMS.

GWVistas (Environmental Simulations, Inc. 1997) is a Windows-driven, graphical, pre- and post- processor for MODFLOW and MT3DMS. It is used in conjunction with the site model to facilitate data entry, data-file modification, program execution, and analysis of modeling results. GWVistas was used to complete additional flow model simulations for sensitivity analysis of flow parameters and for all the transport modeling using MT3DMS.

3.2 Code Description

These codes are fully described in the references cited. They have been verified, benchmarked, and approved for use by most government and regulatory agencies.

4.0 Steady State Deterministic Flow Model

The USGS was contracted with and tasked to develop a steady state deterministic flow model for the Naturita site. This effort is described and documented in a separate document.

4.1 Model Grid and Model Boundary Conditions

The San Miguel River flows in a north-northwest direction in the vicinity of the Naturita site, therefore the model grid was rotated 30 degrees counterclockwise so that the y-axis of the model is oriented along the length of the site. An orthogonal grid, consisting of 263 rows and 69 columns, was designed to encompass the site and an extensive area surrounding the site. The grid size is approximately 25 ft by 25 ft. The alluvial aquifer is bounded to the west by the rocks of the Brushy Basin Member which forms the lower canyon wall (which is approximately the location of Highway 141) and is considered a no-flow boundary. To the east, south, and north of the site the San Miguel River dissects the valley alluvium and constitutes a hydrologic boundary for the alluvial aquifer. This boundary is represented as a river boundary. Many of these hydrological/geological features are visible in Figure 2. Figure 3 shows the model extent and some natural physical features.

4.2 Hydraulic Parameters

Aquifer tests were conducted by the USGS and are described in a separate document.

4.3 Sources and Sinks

The model surface area is represented by a single recharge zone. The steady state recharge value assigned to this zone is 0.0 ft/day as recommended by the USGS.

Discharge from the ground water system consists of subsurface flow from alluvial aquifer into some sections of the San Miguel River on a seasonal basis. Discharge also occurs at the north end of the site where the San Miguel River crosses from the east side to the west side of the valley.

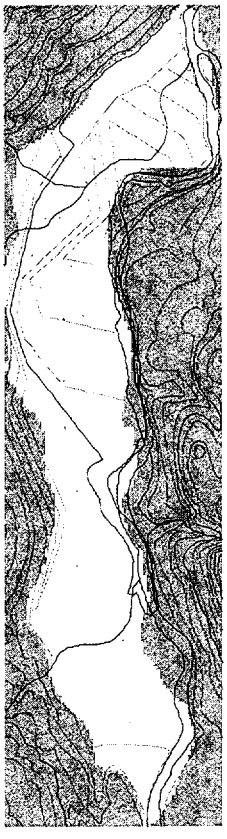

Figure 3. Model Extent and Site Features

4.4 Boundary Conditions

The west side of the model is represented as a no-flow boundary where the Brushy Basin Member geological unit forms the lower canyon wall and rises above the alluvium. The east, south, and north of the model is defined by the San Miguel River and is represented as a river boundary. The southeast part of the model is represented by a head-dependent flux boundary (GHB source) to account for upgradient subsurface flow into the alluvial aquifer.

4.5 Calibration Objectives and Results

Although the steady state deterministic flow model was developed and calibrated by the USGS, it is important to determine if the model meets the acceptance criteria that would be considered realistic for this site. The acceptance criteria chosen for this project are:

1) The model must be able to simulate the general flow directions observed at the site. Measured ground water elevations in February 2000 are represented as a potentiometric surface in Figure 4. Simulated steady state ground water elevations are presented in Figures 5 and 6.

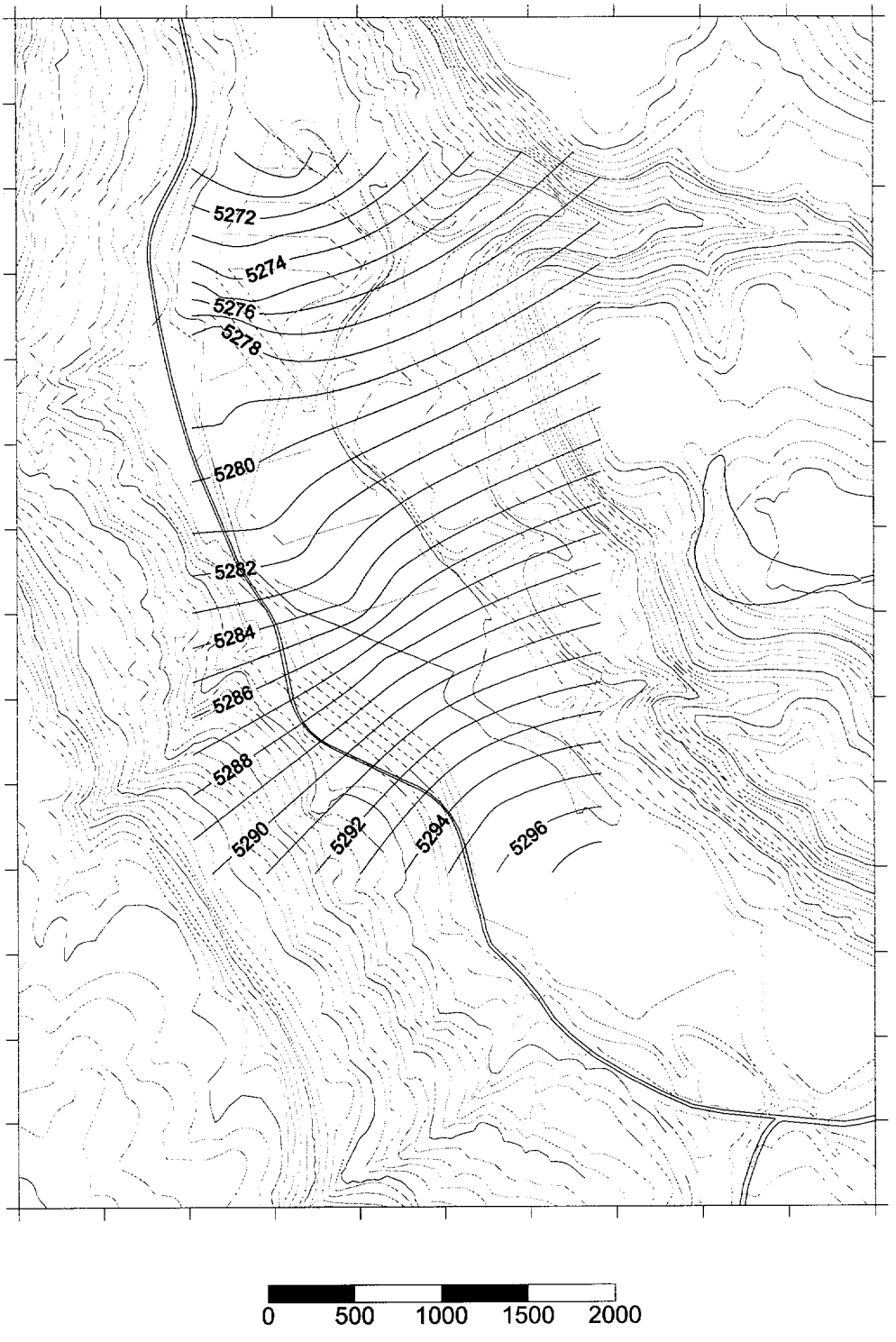

Figure 4. Potentiometric Surface (in feet above MSL)—February 2000

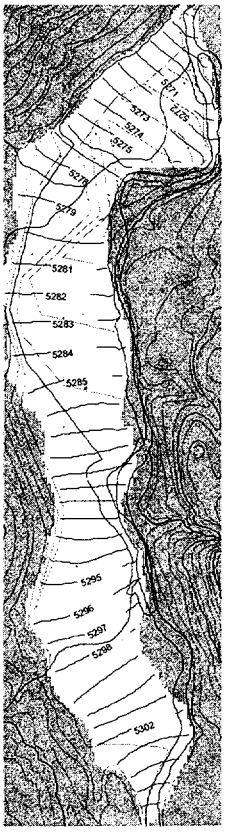

Figure 5. Simulated Steady State Ground Water Elevations (in feet above MSL)

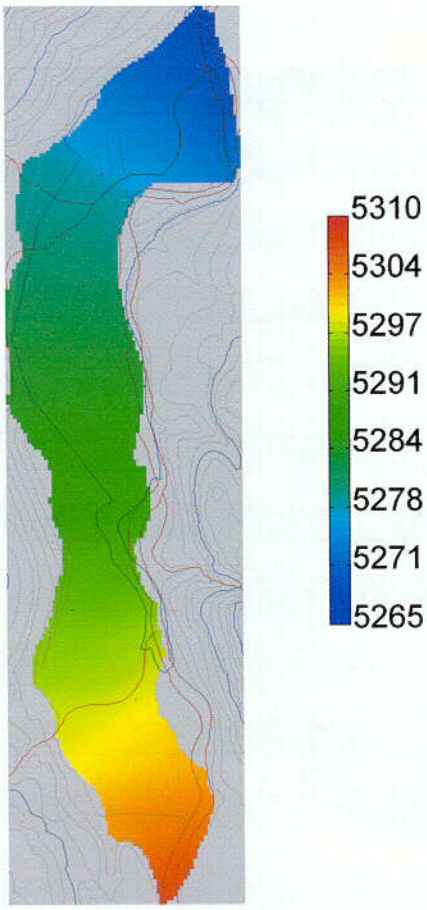

Figure 6. Simulated Steady State Ground Water Elevations (in feet above MSL)

2) The numerical model should not have any inherent bias. In other words, since 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. Figure 7 displays the observed hydraulic heads versus residuals for the steady state model. The plot shows a slight bias of underestimating water levels at the higher elevations.

3) Forty-one calibration targets were selected for the steady state model based on the February 2000 water level measurements. Several flow model calibration objectives were set prior to receiving the calibrated model from the USGS. The objectives and the calibrated model results for the steady state model are shown in Table 1. Although some of the criteria are not met, none of the criteria is exceeded by a significant amount.

4) The mass balance error must be less than 1 percent. The mass balance error for the steady state model is -0.27443 percent.

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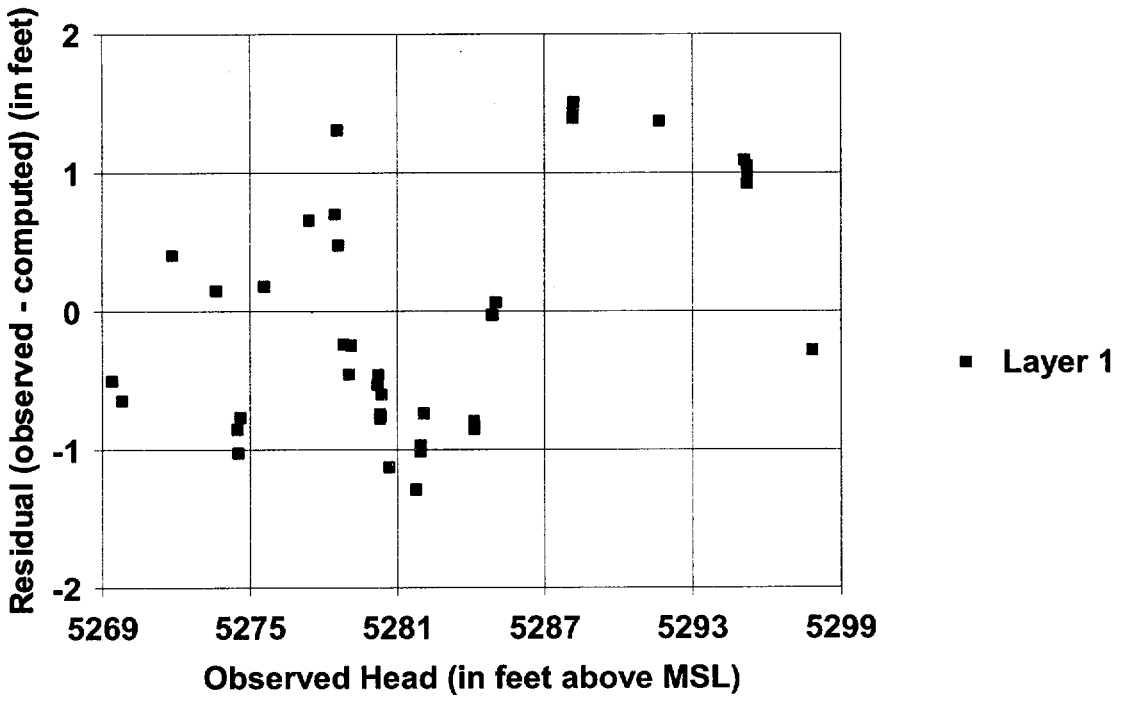

Figure 7. Comparison of Residual versus Observed Head

Table 1. 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.	< 30.75	> -2.0	< 2.0	< 5.0
Actual	-0.067	0.737	28.878	-1.284	1.511	2.940

4.6 Calibration and Residual Analysis

The steady state deterministic calibrated model results and the residual at each target are shown in Table 2. The results satisfy the specified criteria. A plot of predicted (computed) hydraulic head versus observed hydraulic head demonstrates that the model accurately predicts field measurements (Figure 8).

Table 2. Calibration Target Residuals

Well ID	Observed Head (ft)	Predicted Head (ft)	Residual (observed – predicted)
NAT01-1	5279.10	5279.34	-0.24
NAT02	5282.06	5282.80	-0.74
NAT03	5280.27	5281.04	-0.77
NAT04-1	5281.92	5282.93	-1.01
NAT05	5280.17	5280.70	-0.53
NAT06-1	5281.73	5283.01	-1.28
NAT07-1	5280.32	5280.92	-0.60
NAT08	5280.30	5281.06	-0.76
NAT09	5280.28	5281.02	-0.74
NAT10	5280.64	5281.76	-1.12
NAT11	5284.12	5284.97	-0.85
NAT12-1	5279.01	5279.46	-0.45
NAT13-1	5284.12	5284.94	-0.82
NAT14-1	5284.11	5284.90	-0.79
NAT15-1	5280.21	5280.67	-0.46
NAT16-1	5281.93	5282.90	-0.97
NAT17-1	5288.16	5286.65	1.51
NAT18-1	5288.14	5286.69	1.45
NAT19	5288.13	5286.74	1.39
NAT20	5295.18	5294.25	0.93
NAT21-1	5295.20	5294.20	1.00
NAT22-1	5295.19	5294.14	1.05
NAT23	5277.38	5276.72	0.66
NAT24	5278.53	5277.22	1.31
NAT25	5278.44	5277.73	0.71
NAT26	5278.79	5279.03	-0.24
NAT27-1	5284.84	5284.86	-0.02
NAT28-1	5284.87	5284.89	-0.02
NAT29	5285.00	5284.93	0.07
NAT30-1	5291.64	5290.27	1.37
MAU01	5274.59	5275.36	-0.77
MAU02-1	5274.50	5275.52	-1.02
MAU03	5271.82	5271.41	0.41
MAU04	5269.77	5270.41	-0.64
MAU05	5274.47	5275.32	-0.85
MAT06	5273.60	5273.45	0.15
MAU07	5269.37	5269.87	-0.50
MAU08	5275.56	5275.38	0.18
547	5295.08	5293.99	1.09
548	5278.58	5278.10	0.48
DM-1	5297.83	5298.11	-0.28
n	41		
Mean	-0.067		
Absolute Mean	0.737		
Sum of Squares	28.878		
Standard Deviation	0.837		
Minimum	-1.284		
Maximum	1.511		

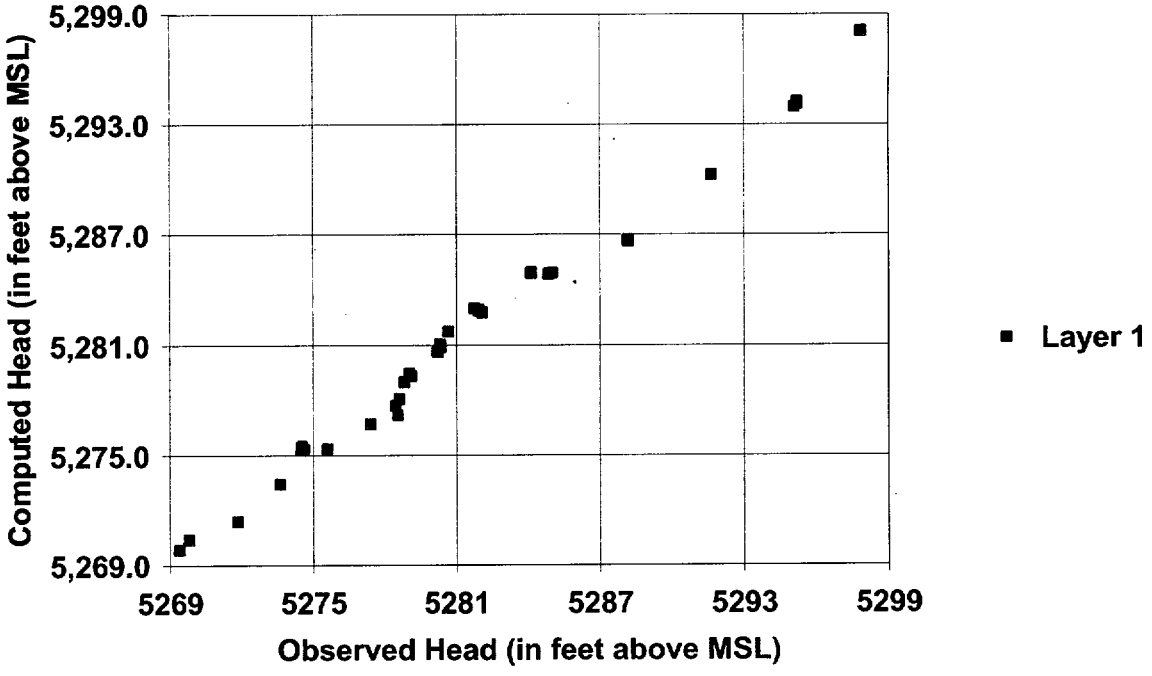

Figure 8. Comparison of Computed Head versus Observed Head

4.7 Flow Model Sensitivity Analysis

A sensitivity analysis is useful to evaluate the effects that variations in flow and transport parameters have on the final predicted contaminant concentration results. Highly sensitive parameters can be treated as uncertain for stochastic simulations. The flow parameters selected for the sensitivity analysis are hydraulic conductivity, recharge, river bed conductance, GHB conductance, river stage, and GHB head. The criteria used for sensitivity analysis of the flow model to these flow parameters is the residual sum of squares, (i.e., the difference between the computed head and observed head at the 41 target wells). The results of the sensitivity analysis for these six parameters are shown in Figures 9 through 14. Visually, this qualitative (subjective) analysis indicates that the flow model is not sensitive to hydraulic conductivity, river bed conductance, GHB conductance, or GHB head. The model does appear to be sensitive to recharge and river stage.

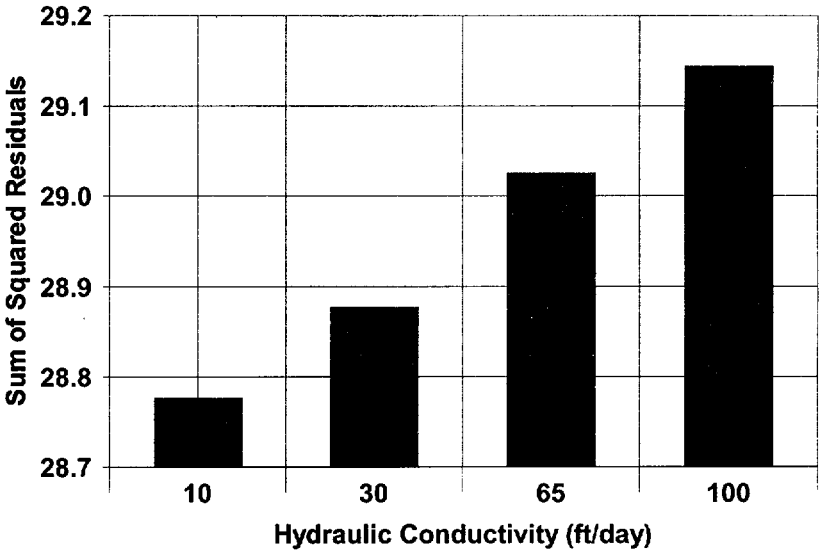

Figure 9. Hydraulic Conductivity Sensitivity Analysis Results

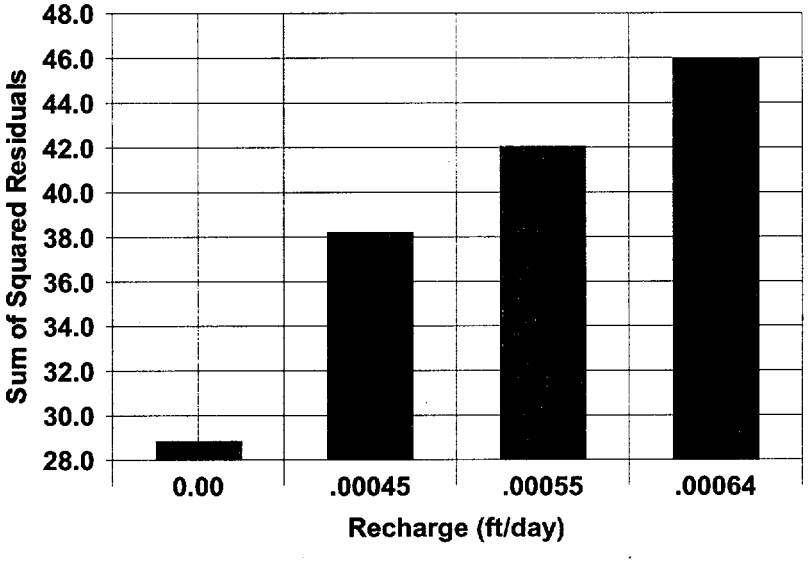

Figure 10. Recharge Sensitivity Analysis Results

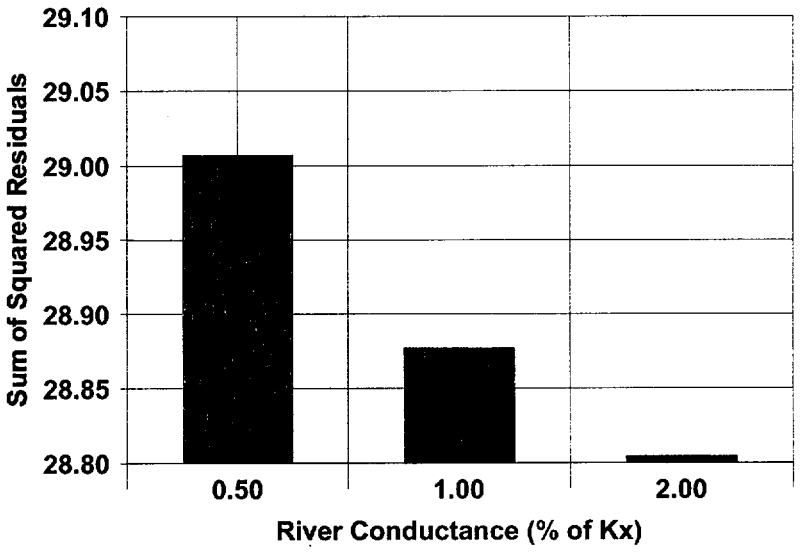

Figure 11. River Conductance Sensitivity Analysis Results

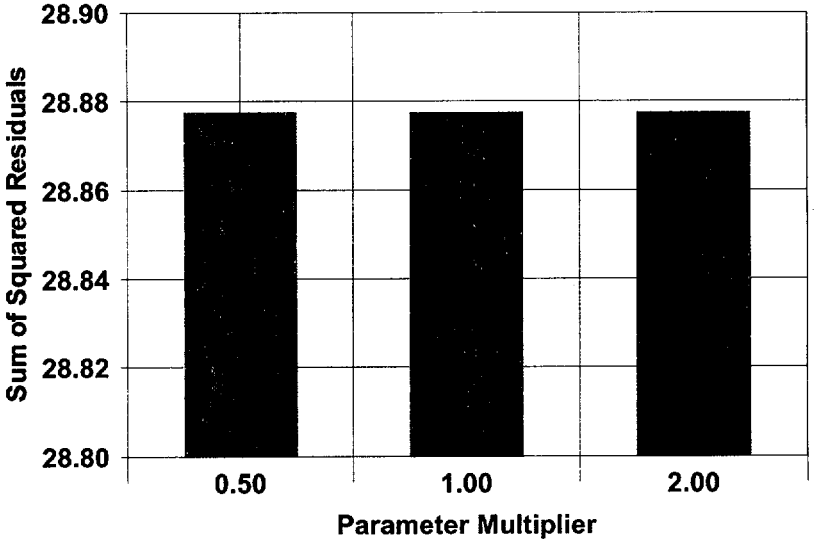

Figure 12. GHB Conductance Sensitivity Analysis Results

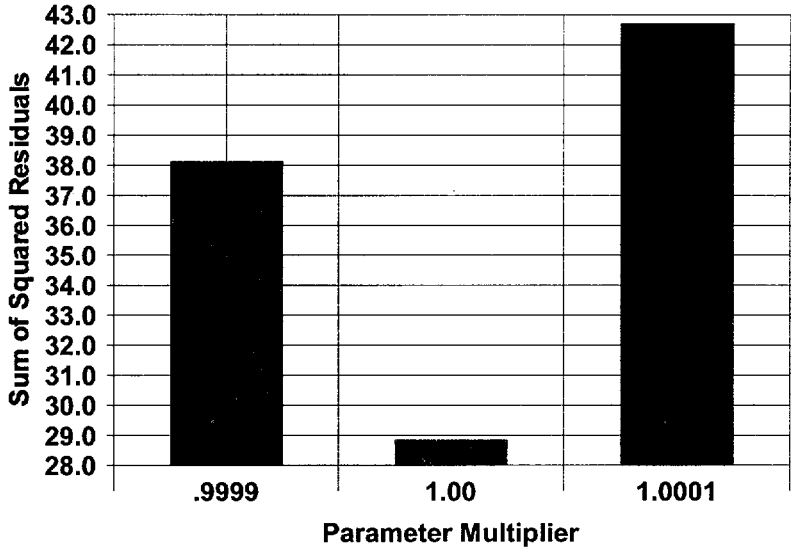

Figure 13. River Stage Sensitivity Analysis Results

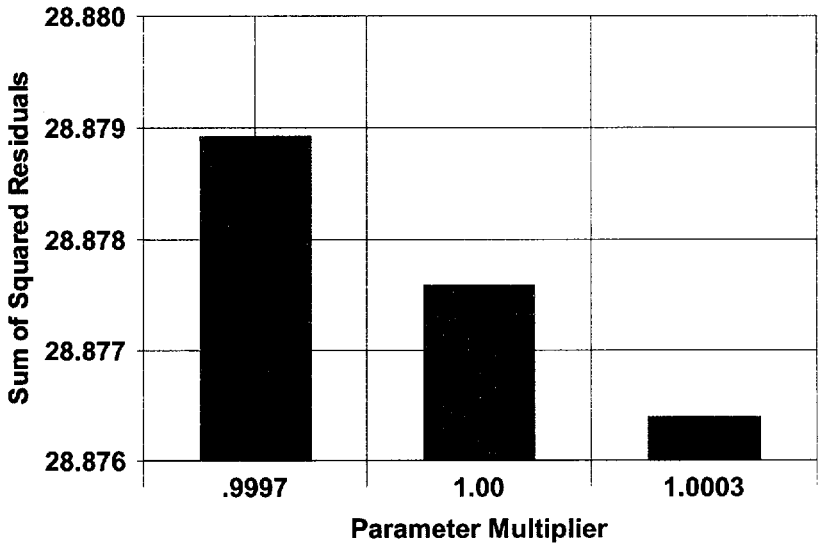

Figure 14. GHB Head Sensitivity Analysis Results

As an additional quantitative (objective) check, the coefficient of variation (CV) of the residual sum of squares can be calculated for each of these flow parameters. The residual sum of squares for GHB conductance does not vary for different parameter values, therefore the CV cannot be calculated for this parameter. The CV was calculated for hydraulic conductivity, recharge, river bed conductance, river stage, and GHB head. The CV is defined as the standard deviation (σ) divided by the mean ($\bar{x}$). Flow parameters resulting in a CV greater than 1 percent between the predicted residual sum of squares for different parameter values can be 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 3. These results indicate recharge and river stage appear to be sensitive, and are in agreement with qualitative visual residual sum of squares sensitivity analysis.

Table 3. Flow Parameter Coefficient of Variation Analysis

Flow Parameter	Mean	Standard Deviation	Adjusted Standard Deviation	Coefficient of Variation
Hydraulic Conductivity	28.95643	0.16221	0.17590	0.00607
Recharge	38.79988	7.34060	7.96014	0.20516[a]
River Conductance	28.89681	0.10245	0.11557	0.00400
River Stage	36.58345	7.05642	7.95964	0.21757[a]
GHB Head	28.87764	0.00127	0.00143	0.00005

[a]indicates parameter is sensitive per this criteria

The criteria used for sensitivity analysis of the transport model to these flow parameters is the CV. This quantitative (objective) check was made on each of the flow parameters in Table 3. For this sensitivity analysis, each of these flow parameters was simulated at three or four different parameter values. These values are shown in Table 4. The approach taken here is to calculate the coefficient of variation (CV) of the difference in predicted concentration at each selected time interval (5, 10, 15, 25, 50, 60, 70, 80, 90, and 100 years). Any parameter resulting in a CV greater than 15 percent between the predicted concentration at any time interval is considered sensitive and will be treated as stochastic.

Table 4. Flow Model Sensitivity Parameter Values

Parameter	Low Value and Low Stochastic Value	Mid-Range Value		High Value and High Stochastic Value
Hydraulic Conductivity (ft/day)	10	30[a]	65	100
Recharge (in/yr)	0.[a]	1.99	2.39	2.79
Recharge (ft/day)	0.[a]	.00045	.00055	.00064
Parameter	**Low Value**	**Mid-point Value**	**High Value**	
River Bed Conductance	5% of Kx = 30	10% of Kx = 30	20% of Kx = 30	
Parameter	**Low Multiplier**	**Multiplier**	**High Multiplier**	
River Stage	.9999 (~ -0.5 ft)	1.0000[a]	1.0001(~ +0.5 ft)	
GHB Head	.9997(~ -1.5 ft)	1.0000[a]	1.0003(~ +1.5ft)	

[a]USGS recommended value

The results of this analysis are presented in Table 5. This analysis shows that the flow model is sensitive to hydraulic conductivity at 10, 15, 25, 50, 60, 70, 80, 90, and 100 years. Recharge is sensitive at 10, 15, 25, 50, 60, 70, 80, 90, and 100 years. The model is not sensitive to river bed conductance, river stage, or GHB head. Because the primary concern is to determine which parameters have an effect on the results of the transport simulations, both hydraulic conductivity and recharge are treated as stochastic in the flow model.

Table 5. Flow Model Coefficient of Variation Analysis Results at Specific Times (Years)

Flow Parameter	Year	Mean	Standard Deviation	Adjusted Standard Deviation	Coefficient of Variation
Hydraulic Conductivity					
	5	2.37900	0.10600	0.11494	0.04832
	10	2.17518	0.31611	0.34279	0.15759[a]
	15	1.95590	0.51102	0.55415	0.28332[a]
	25	1.53273	0.83991	0.91080	0.59424[a]
	50	0.93843	1.06031	1.14980	1.22523[a]
	60	0.82181	1.02828	1.11507	1.35684[a]
	70	0.72194	0.97968	1.06237	1.47154[a]
	80	0.63412	0.93164	1.01027	1.59317[a]
	90	0.55950	0.88796	0.96291	1.72101[a]
	100	0.49854	0.84654	0.91799	1.84136[a]
Recharge					
	5	2.12215	0.20761	0.22513	0.10609
	10	1.79180	0.39132	0.42434	0.23682[a]
	15	1.53165	0.51960	0.56345	0.36787[a]
	25	1.36029	0.71144	0.77149	0.56715[a]
	50	0.56471	0.49696	0.53890	0.95430[a]
	60	0.41401	0.42247	0.45813	1.10657[a]
	70	0.29102	0.33167	0.35966	1.23587[a]
	80	0.19514	0.24164	0.26203	1.34278[a]
	90	0.12487	0.16488	0.17879	1.43185[a]
	100	0.07676	0.10682	0.11584	1.50909[a]
River Bed Conductance					
	5	2.42667	0.00012	0.00013	0.00005
	10	2.36820	0.00017	0.00020	0.00008
	15	2.29923	0.00060	0.00068	0.00030
	25	2.02543	0.00201	0.00227	0.00112
	50	1.30473	0.00275	0.00310	0.00238
	60	1.04387	0.00215	0.00243	0.00232
	70	0.78606	0.00190	0.00214	0.00272
	80	0.55615	0.00145	0.00164	0.00294
	90	0.37135	0.00089	0.00100	0.00270
	100	0.23655	0.00051	0.00058	0.00243
River Stage					
	5	2.42710	0.00161	0.00182	0.00075
	10	2.36733	0.00433	0.00489	0.00206
	15	2.29927	0.01035	0.01167	0.00508
	25	2.02740	0.02519	0.02842	0.01402
	50	1.30627	0.01412	0.01592	0.01219
	60	1.04597	0.01600	0.01805	0.01726
	70	0.78872	0.01508	0.01701	0.02157
	80	0.55830	0.01356	0.01530	0.02740
	90	0.37308	0.01137	0.01282	0.03436
	100	0.23794	0.00876	0.00988	0.04153

Table 5 (continued). Flow Model Coefficient of Variation Analysis Results at Specific Times (Years)

Flow Parameter	Year	Mean	Standard Deviation	Adjusted Standard Deviation	Coefficient of Variation
GHB Head					
	5	2.42660	0.00000	0.00000	0.00000
	10	2.36830	0.00000	0.00000	0.00000
	15	2.29930	0.00000	0.00000	0.00000
	25	2.02570	0.00000	0.00000	0.00000
	50	1.30470	0.00000	0.00000	0.00000
	60	1.04390	0.00000	0.00000	0.00000
	70	0.78606	0.00001	0.00001	0.00001
	80	0.55613	0.00002	0.00002	0.00004
	90	0.37135	0.00001	0.00001	0.00004
	100	0.23655	0.00001	0.00001	0.00003

[a]indicates parameter is sensitive at this time (year) per this criteria

5.0 Steady State Deterministic Contaminant Transport Model

5.1 Transport Parameters

The contaminant transport parameters of interest are longitudinal and transverse dispersivity, effective porosity, bulk density, K_d (distribution coefficient), and the initial concentration distribution for each of the COPC.

The K_d typically has the greatest impact on the amount of time required for natural flushing to reduce the contamination level below the required standard. For uranium the estimated range of values for this site is from 0.3975 to 1.1225 milliliters per gram (mL/g). An average value of 0.6078 mL/g was used as the K_d value for uranium. For vanadium the estimated range of values for this site is from 4.445 to 20.6575 milliliters per gram (mL/g). An average value of 12.46 mL/g was used as the K_d value for vanadium. A site specific arsenic K_d value is not available for the Naturita site, therefore a K_d value of 5.45 mL/g (from another UMTRA site with an alluvial aquifer) was used. Since this value is higher than the literature values, the results are considered conservative.

The literature on dispersivity as it relates to large-scale models is vague and often contradictory, 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. Commonly a value of 10 percent of the length of the plume is used for longitudinal dispersivity. With a maximum flow path length of approximately 2,500 ft, the longitudinal dispersivity could be as much as 250 ft. However, this is considered unrealistic for this site because the width of the site (transverse distance) is small relative to the length of the site (longitudinal distance), consequently a value of 100 ft was used. This value is approximately 4 percent of the length and considered a conservative estimate. For this transport model transverse dispersivity is 10 percent (10 ft) of longitudinal dispersivity (100 ft).

Bulk density was set at 1.55 g/mL (approximately 97 lbs/ft^3). The effective porosity was set to 25 percent.

Initial concentration plumes were developed in Surfer® for each of the COPC. The set of data for each COPC was kriged in Surfer® and interpolated to approximately a 25 ft grid spacing which corresponds to the model grid size. Each resulting surface was then interpolated to all active model grid cell centers and imported as the initial concentration plume. The plots presented in Figures 15, 16, and 17 show the initial concentration plumes for each of the COPCs. The range of concentration is shown on the color bar in each figure.

5.2 Transport Calibration and Parameter Sensitivity Analysis

The calibration and sensitivity analysis of the transport model is not as straightforward as the flow model. The calibration and sensitivity analysis of the flow parameters to the flow model is based on the residual sum of squares of observed head minus computed head. Similarly, the calibration and sensitivity analysis of the transport parameters to the transport model could be based on the residual sum of squares of observed concentration minus computed concentration. Since GWVistas does not yet have the capability to calibrate on concentration, only sensitivity analysis was used.

The transport parameters selected for sensitivity analysis are porosity, bulk density, K_d (for uranium and vanadium), longitudinal dispersivity, and transverse dispersivity. For the sensitivity analysis, each of the transport parameters (except transverse dispersivity) were simulated at three parameter values that correspond to the lowest expected value, the most likely value, and the highest expected value. Transverse dispersivity was simulated at three parameter values that are a percentage of the longitudinal dispersivity. These values are shown in Table 6. The approach taken here is to calculate the coefficient of variation (CV) of the difference in predicted concentration at each selected time interval (5, 10, 15, 25, 50, 60, 70, 80, 90, and 100 years). Any parameter resulting in a CV greater than 15 percent between the predicted concentration at any time interval is considered sensitive, and will be treated at stochastic if possible. GWVistas does not allow some transport parameters to be stochastic.

Table 6. Transport Model Sensitivity Parameter Values

Parameter	Lowest Expected	Most Likely (unless otherwise noted)	Highest Expected
Porosity	0.25[a]	0.30	0.40
Bulk Density (g/mL)	1.13	1.55	1.99
Uranium K_d (mL/g)	0.3975	0.6078	1.1225
Vanadium K_d (mL/g)	4.445	12.46	20.6575
Long. Disp. (ft)	50	100	200
Parameter	**% of Long. Disp.**	**% of Long. Disp.**	**% of Long. Disp.**
Trans. Disp.	10[a]	20	50
Parameter	**Low Value**	**Mid Value**	**High Value**
Trans. Disp. (ft)	10[a]	20	50

[a]Most Likely

The results are shown in Table 7. This analysis shows that the transport model is sensitive to porosity, bulk density, uranium K_d, longitudinal dispersivity, and transverse dispersivity. Porosity, uranium K_d, and longitudinal dispersivity are treated as stochastic. GWVistas does not allow bulk density and transverse dispersivity to be stochastic. Transverse dispersivity will show some variability because it is a percent of longitudinal dispersivity, which is stochastic.

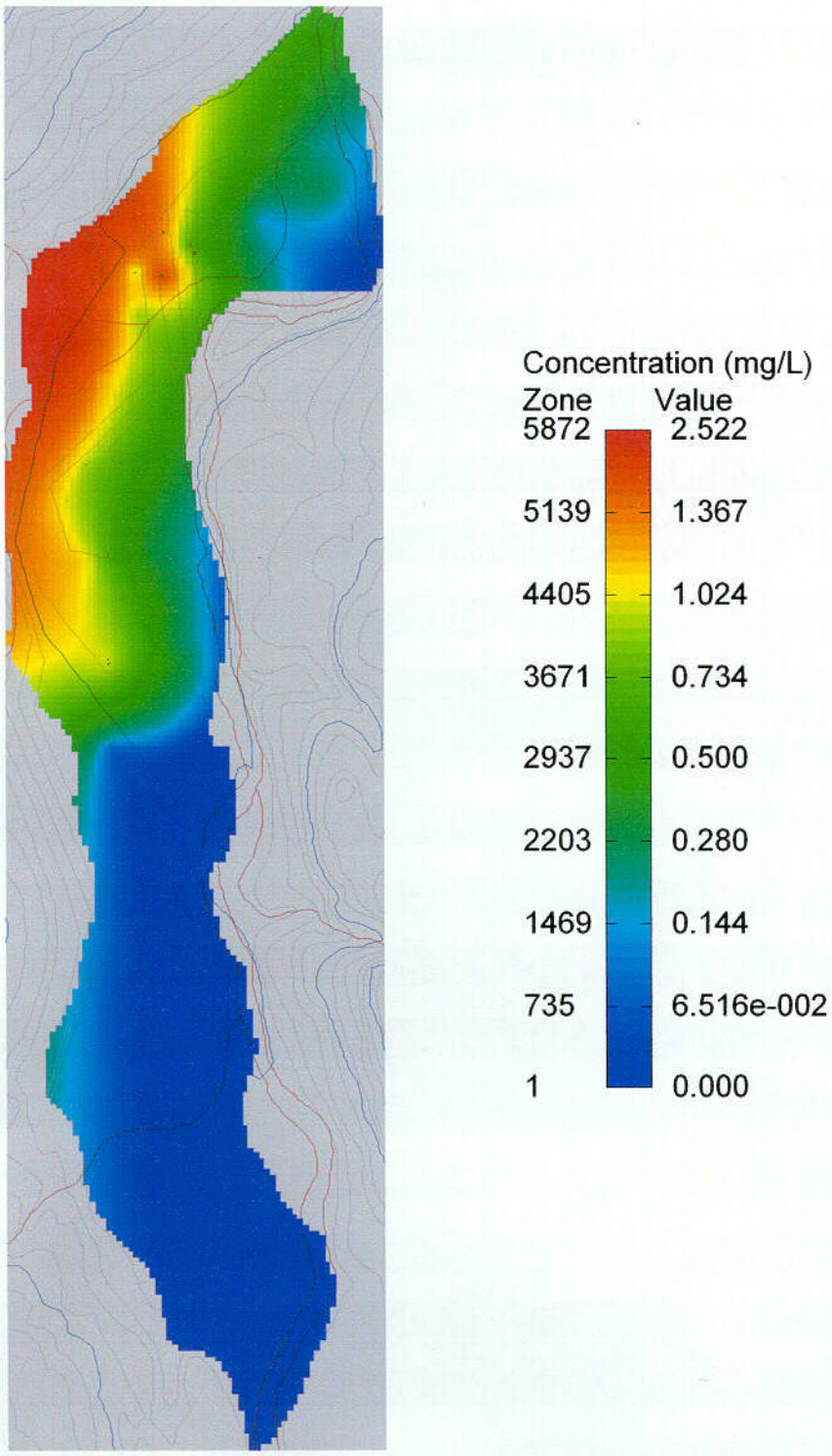

Figure 15. Initial Uranium Concentration

C02

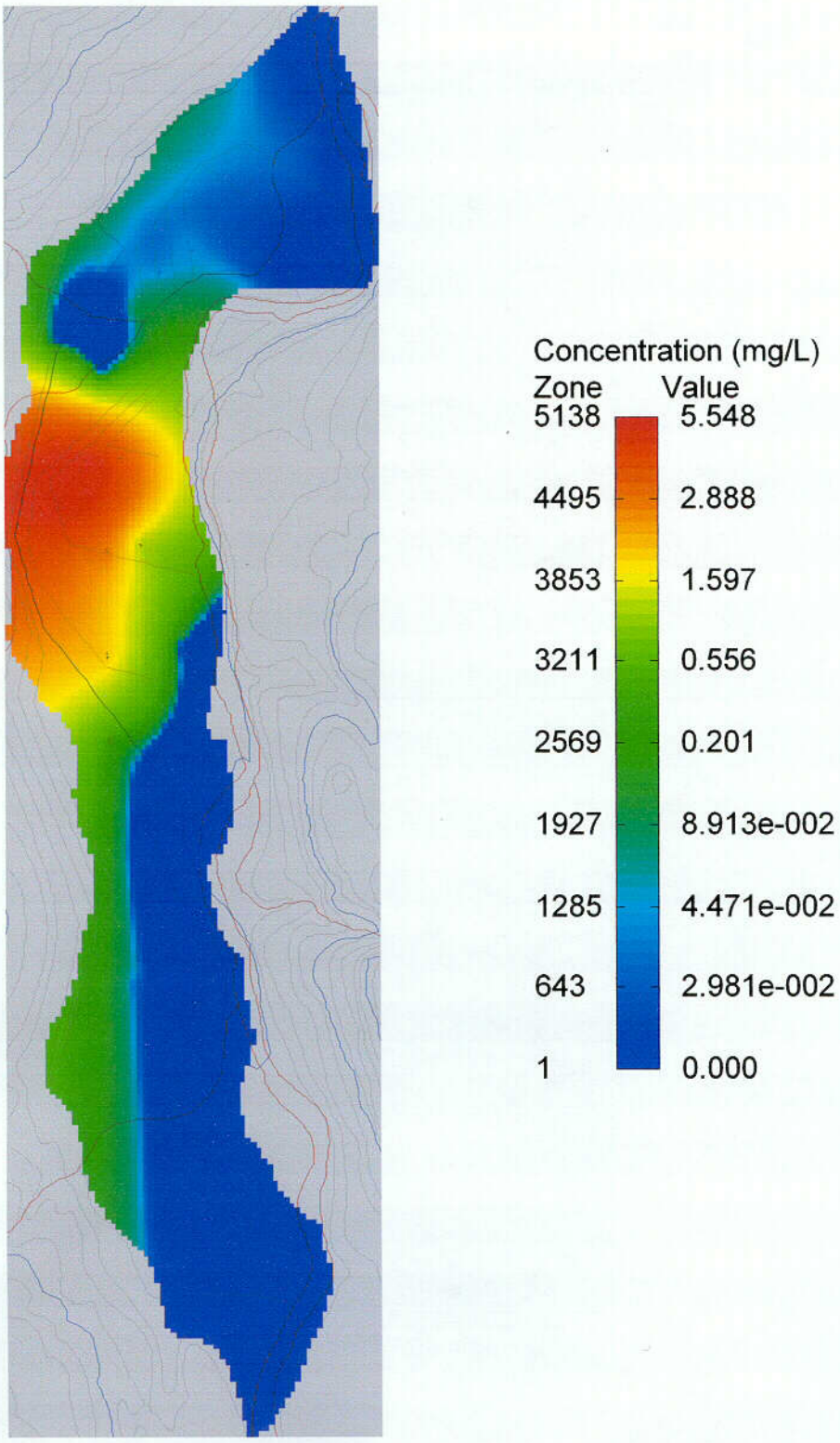

Figure 16. Initial Vanadium Concentration

C03

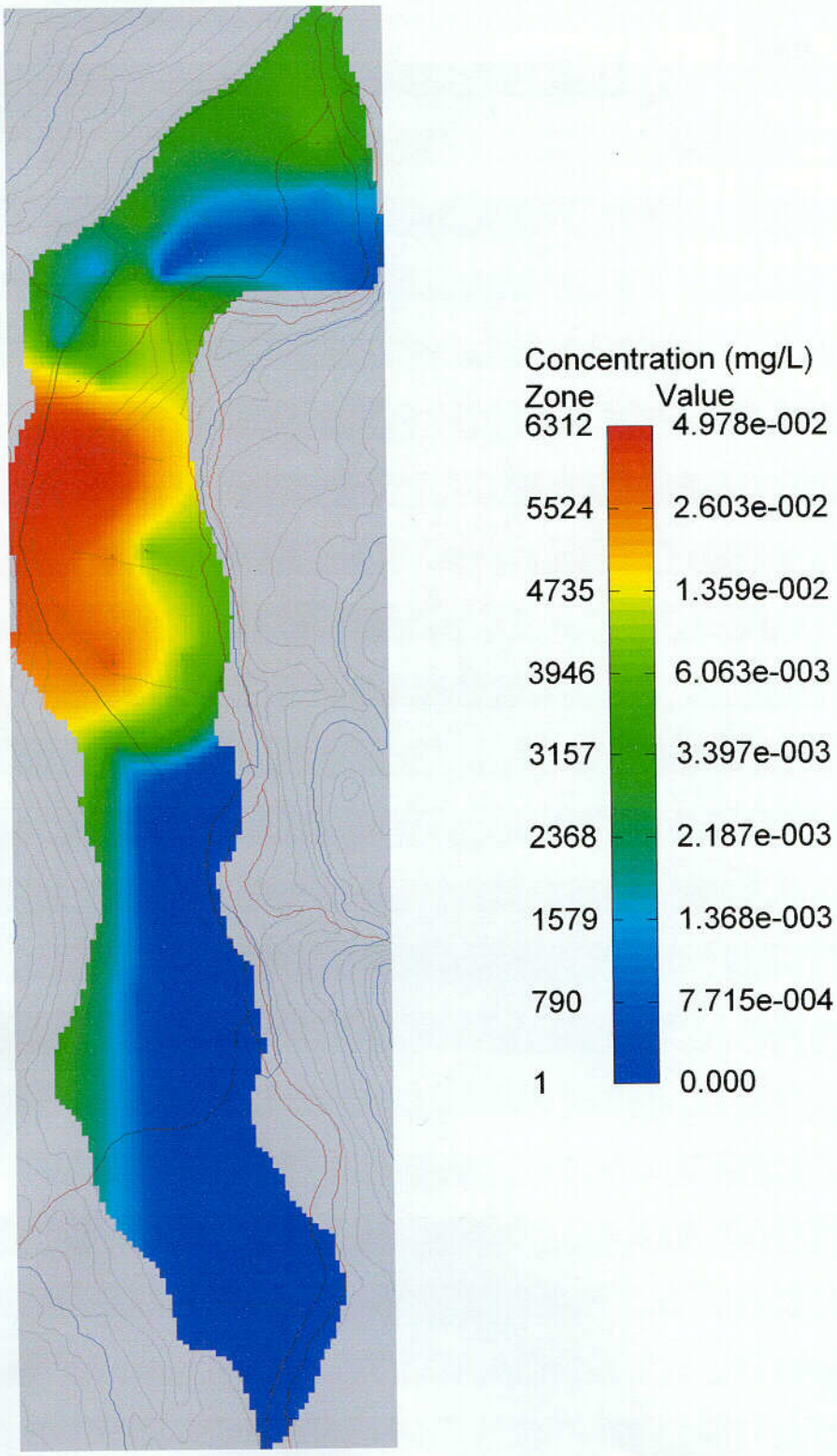

Figure 17. Initial Arsenic Concentration

C04

Table 7. Transport Model Coefficient of Variation Analysis Results at Specific Times (Years)

Flow Parameter	Year	Mean	Standard Deviation	Adjusted Standard Deviation	Coefficient of Variation
Porosity					
	5	2.43020	0.00412	0.00465	0.00191
	10	2.37330	0.00538	0.00607	0.00256
	15	2.31230	0.01411	0.01591	0.00688
	25	2.06630	0.04513	0.05091	0.02464
	50	1.36847	0.07095	0.08004	0.05849
	60	1.12363	0.08897	0.10036	0.08931
	70	0.87625	0.10144	0.11442	0.13058
	80	0.64690	0.10319	0.11640	0.17993[a]
	90	0.45318	0.09423	0.10629	0.23455[a]
	100	0.30344	0.07805	0.08804	0.29013[a]
Bulk Density					
	5	2.42543	0.01518	0.01713	0.00706
	10	2.36177	0.02739	0.03090	0.01308
	15	2.28133	0.07127	0.08039	0.03524
	25	1.99947	0.18396	0.20750	0.10378
	50	1.26196	0.29326	0.33079	0.26213[a]
	60	1.00384	0.34752	0.39200	0.39050[a]
	70	0.76447	0.36471	0.41139	0.53814[a]
	80	0.55966	0.34156	0.38528	0.68841[a]
	90	0.39607	0.29176	0.32911	0.83093[a]
	100	0.27218	0.23178	0.26145	0.96056[a]
K_d – Uranium					
	5	2.43187	0.03222	0.03635	0.01495
	10	2.36727	0.04996	0.05635	0.02380
	15	2.27933	0.11209	0.12644	0.05547
	25	2.01690	0.29130	0.32859	0.16292[a]
	50	1.32897	0.52352	0.59053	0.44435[a]
	60	1.07465	0.58288	0.65749	0.61182[a]
	70	0.85851	0.61359	0.69213	0.80620[a]
	80	0.68685	0.61510	0.69383	1.01017[a]
	90	0.54906	0.58576	0.66074	1.20340[a]
	100	0.43888	0.53506	0.60355	1.37522[a]
K_d – Vanadium					
	5	5.31613	0.11290	0.12735	0.02396
	10	5.18977	0.19229	0.21690	0.04179
	15	5.08167	0.24534	0.27675	0.05446
	25	4.90573	0.32142	0.36257	0.07391
	50	4.59133	0.41699	0.47036	0.10245
	60	4.51227	0.41008	0.46257	0.10251
	70	4.43793	0.41200	0.46474	0.10472
	80	4.35900	0.42313	0.47730	0.10950
	90	4.28047	0.45270	0.51064	0.11930
	100	4.20683	0.47929	0.54064	0.12852

Table 7 (continued). Transport Model Coefficient of Variation Analysis Results at Specific Times (Years)

Flow Parameter	Year	Mean	Standard Deviation	Adjusted Standard Deviation	Coefficient of Variation
Longitudinal Dispersivity					
	5	2.41797	0.05348	0.06032	0.02495
	10	2.34723	0.09163	0.10336	0.04404
	15	2.26457	0.15054	0.16980	0.07498
	25	1.99683	0.22181	0.25021	0.12530
	50	1.29265	0.29686	0.33486	0.25905[a]
	60	1.02913	0.28894	0.32592	0.31670[a]
	70	0.77957	0.25304	0.28543	0.36614[a]
	80	0.55403	0.19039	0.21476	0.38764[a]
	90	0.36997	0.12134	0.13687	0.36994[a]
	100	0.23652	0.06955	0.07845	0.33168[a]
Transverse Dispersivity					
	5	2.40037	0.03229	0.03643	0.01518
	10	2.31553	0.06763	0.07628	0.03294
	15	2.19827	0.12686	0.14309	0.06509
	25	1.84983	0.20988	0.23674	0.12798
	50	1.06217	0.25712	0.29003	0.27305[a]
	60	0.79107	0.25576	0.28850	0.36470[a]
	70	0.55676	0.22893	0.25823	0.46381[a]
	80	0.37173	0.18380	0.20733	0.55774[a]
	90	0.23550	0.13429	0.15148	0.64322[a]
	100	0.14318	0.09131	0.10299	0.71935[a]

[a]indicates parameter is sensitive at this time (year) per this criteria

5.3 Predictive Results for Uranium

A contaminant transport model using MT3DMS, based on the calibrated steady state deterministic flow model, was used for predictive simulations. Simulation results were extracted for selected times up to 100 years into the future. Predicted uranium concentrations above the UMTRA Project maximum concentration level (MCL) of 0.044 milligrams per liter (mg/L) at 5, 10, 25, 50 and 100 years into the future are presented in Figures 18 through 22, respectively. The areas of the model in the figures that do not have color (are white) are below the MCL. For this scenario the maximum predicted concentration at 5, 10, 25, 50, and 100 years is 2.4266, 2.3683, 2.0257, 1.3047, and 0.23654 mg/L, respectively.

While these plots give a general aerial view of the remaining contamination area, they do not provide a clear picture of the contaminant change with time. The plots in Figures 23, 24, and 25 show the change in concentration versus time for monitor well locations MAU08, MAU07, and 548, respectively.

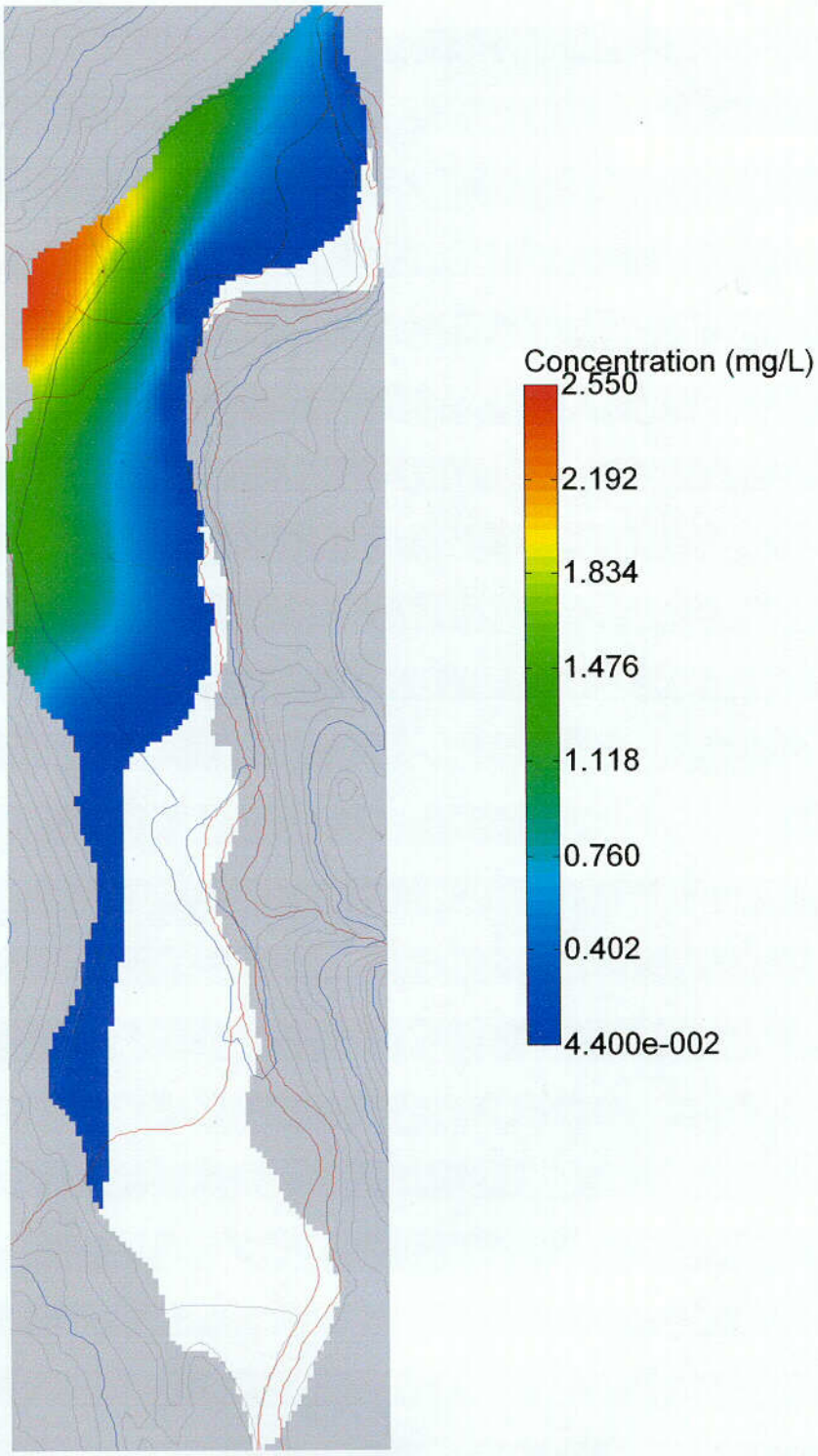

Figure 18. Predicted Steady State Uranium Concentration at 5 Years

C05

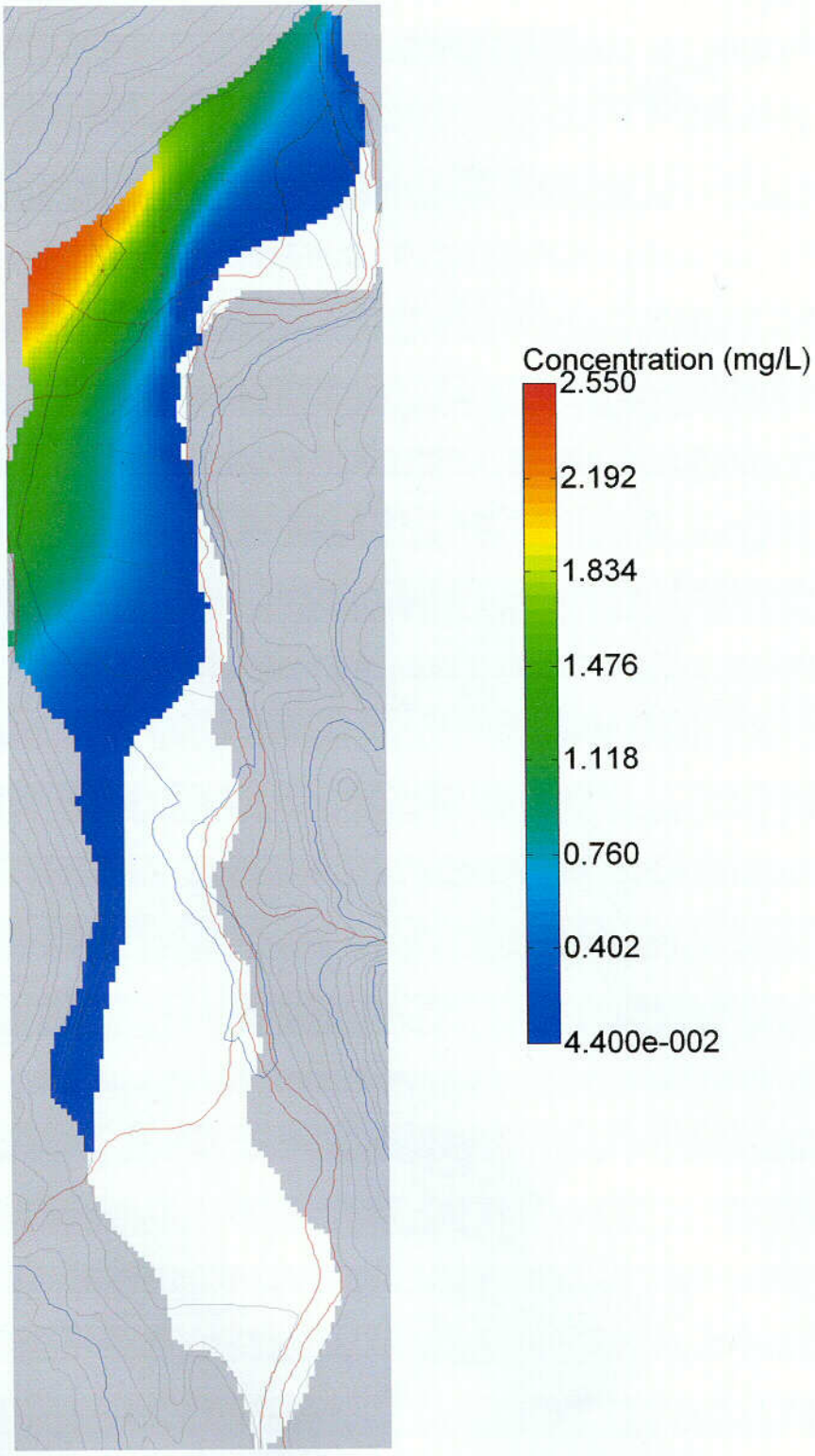

Figure 19. Predicted Steady State Uranium Concentration at 10 Years

C06

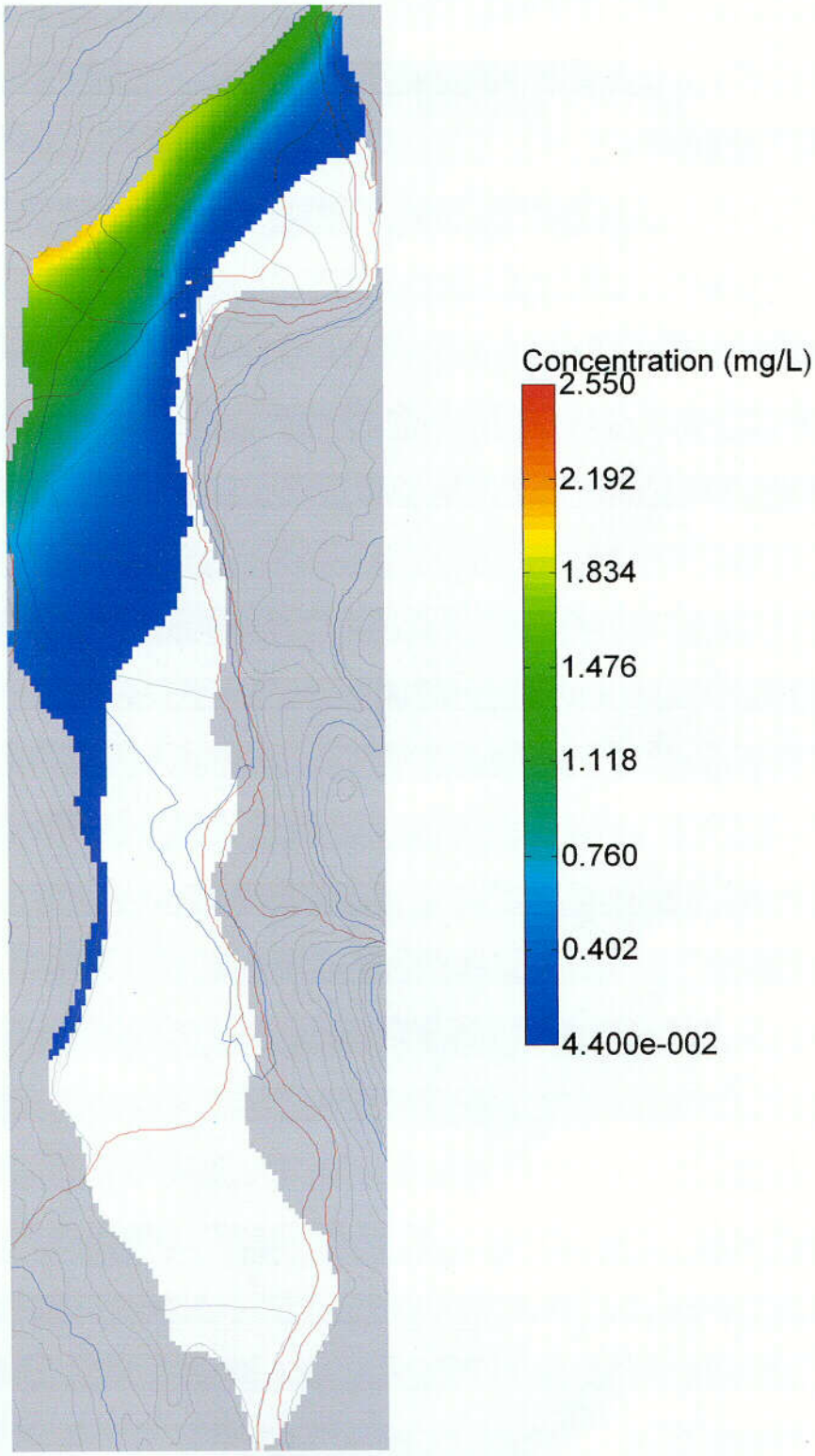

Figure 20. Predicted Steady State Uranium Concentration at 25 Years

C07

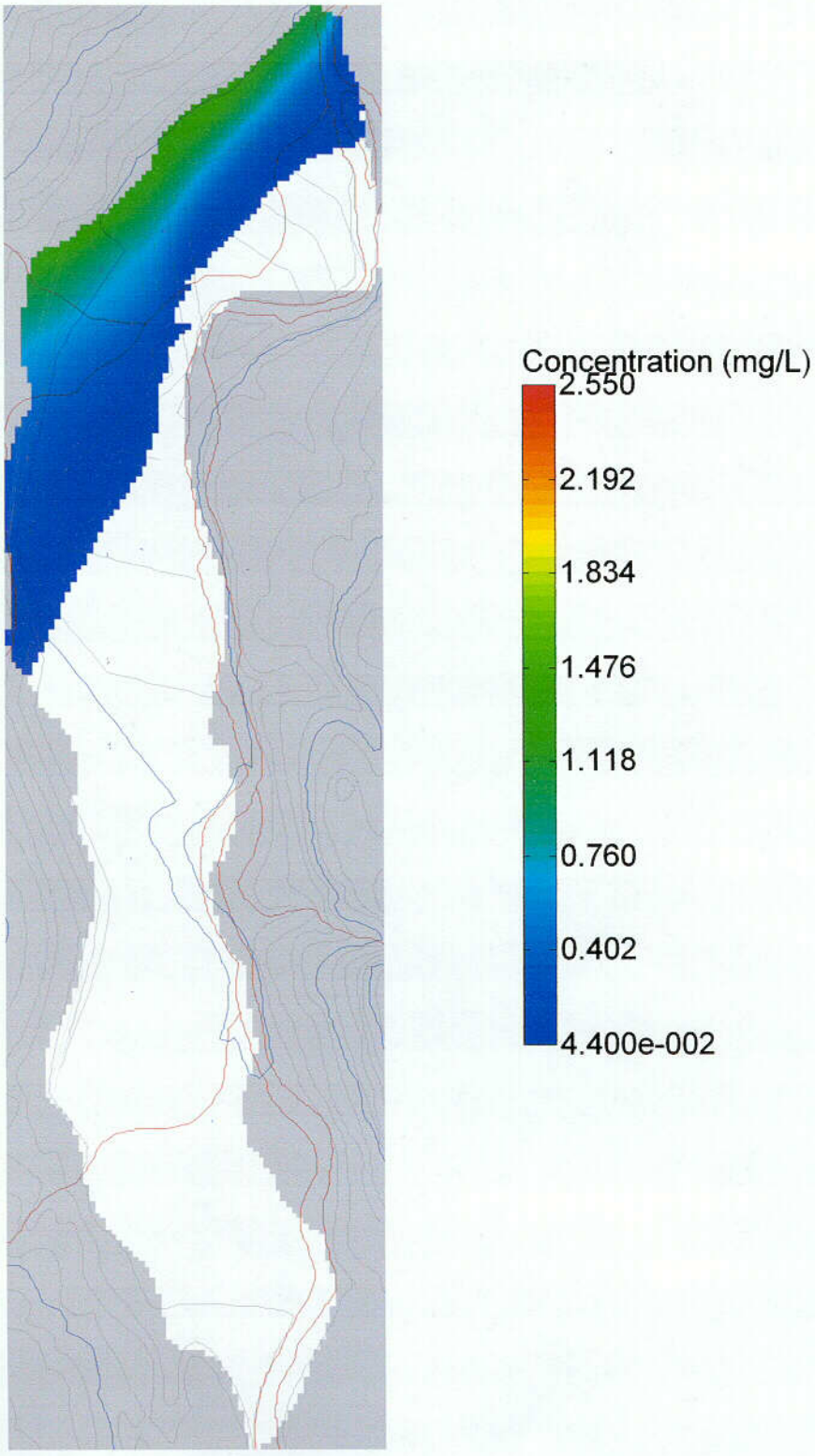

Figure 21. Predicted Steady State Uranium Concentration at 50 Years

C08

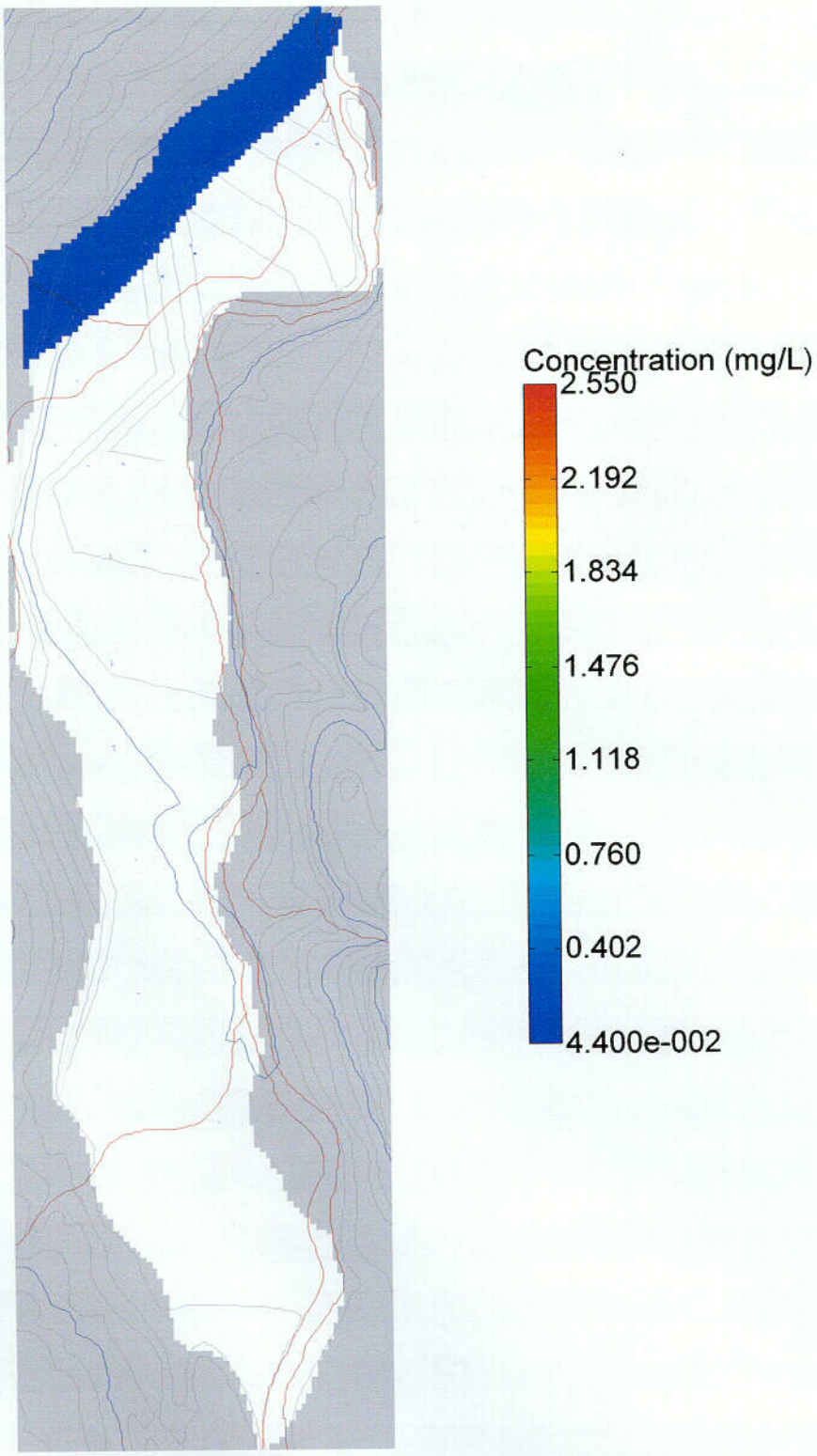

Figure 22. Predicted Steady State Uranium Concentration at 100 Years

C09

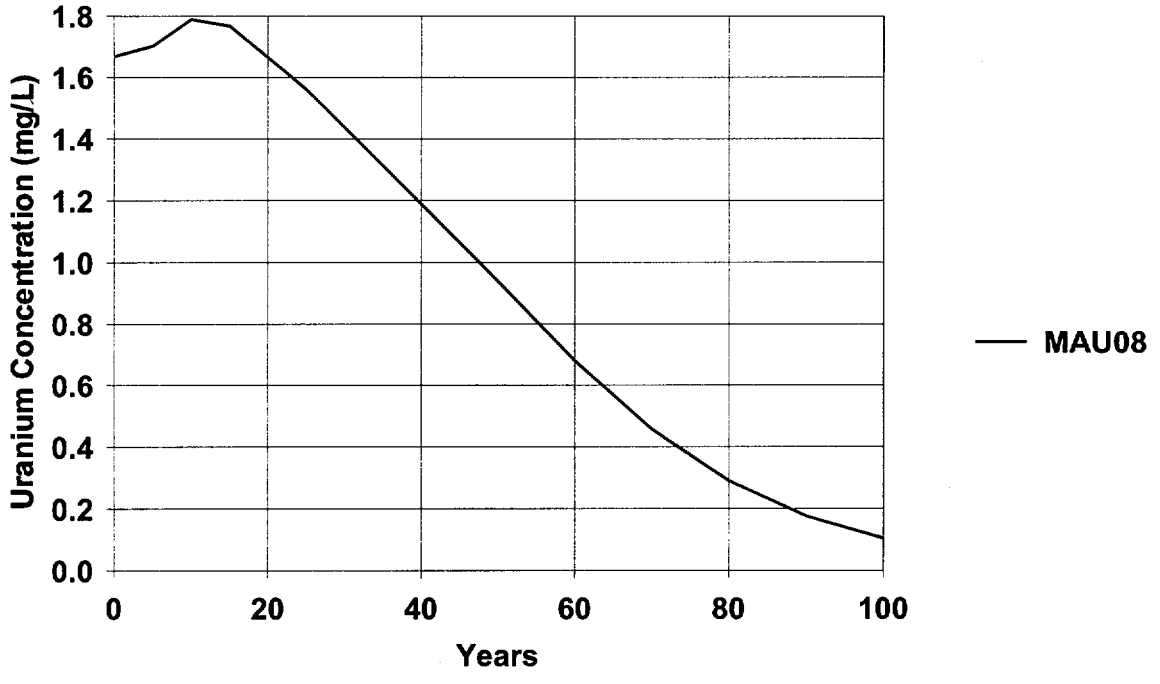

Figure 23. Uranium Concentration versus Time for Monitor Well MAU08

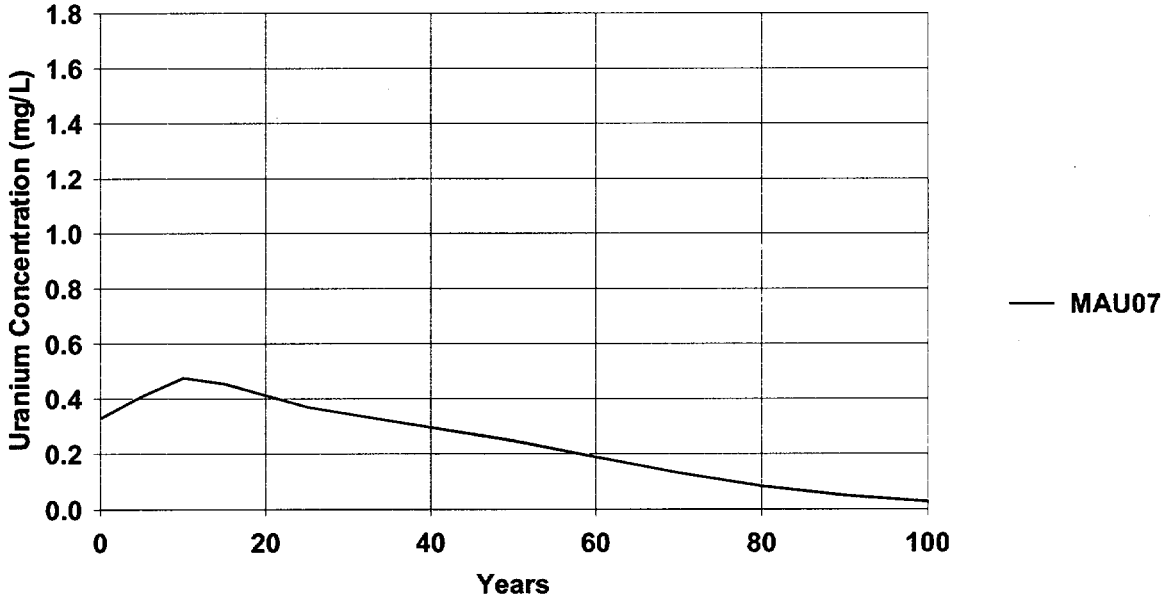

Figure 24. Uranium Concentration versus Time for Monitor Well MAU07

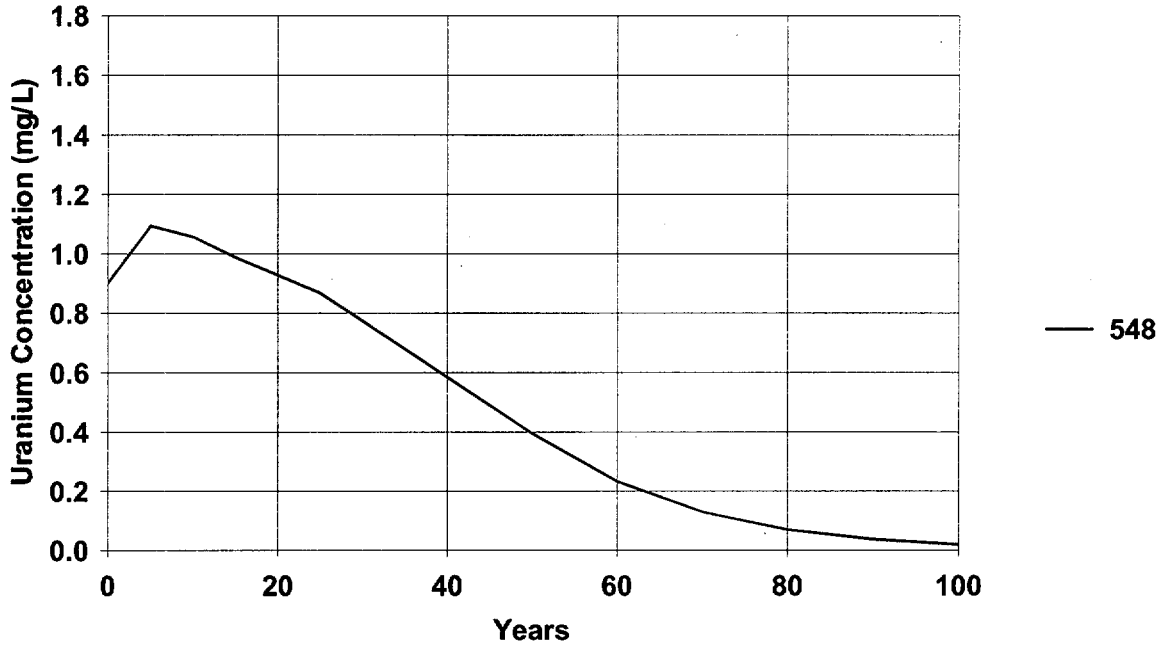

Figure 25. Uranium Concentration versus Time for Monitor Well 548

5.4 Predictive Results for Vanadium

Predicted vanadium concentrations above the risk-based concentration of 0.33 mg/L at 5, 10, 25, 50 and 100 years into the future are presented in Figures 26 through 30, respectively. The areas of the model in the figures that do not have color (are white) are below the risk-based concentration. For this scenario the maximum predicted concentration at 5, 10, 25, 50, and 100 years is 5.3589, 5.2583, 5.0065, 4.7099, and 4.3286 mg/L, respectively.

5.5 Predictive Results for Arsenic

Simulation results show that at 10 years the maximum remaining arsenic concentration is 0.045368 mg/L, which is below the UMTRA Project MCL of 0.05 mg/L. A concern regarding the arsenic plume was to ensure the maximum concentration does not exceed 0.05 mg/L as the plume migrates downgradient off site. The plots in Figures 31 and 32 show the concentration change with time at monitor wells MAU08 and MAU07, respectively. Both wells are off site and downgradient of the former millsite. Monitor well MAU08 is near the northern boundary of the site while MAU07 is close to where the alluvial aquifer discharges into the San Miguel River. Both plots indicate that the UMTRA Project MCL of 0.05 mg/L is not exceeded.

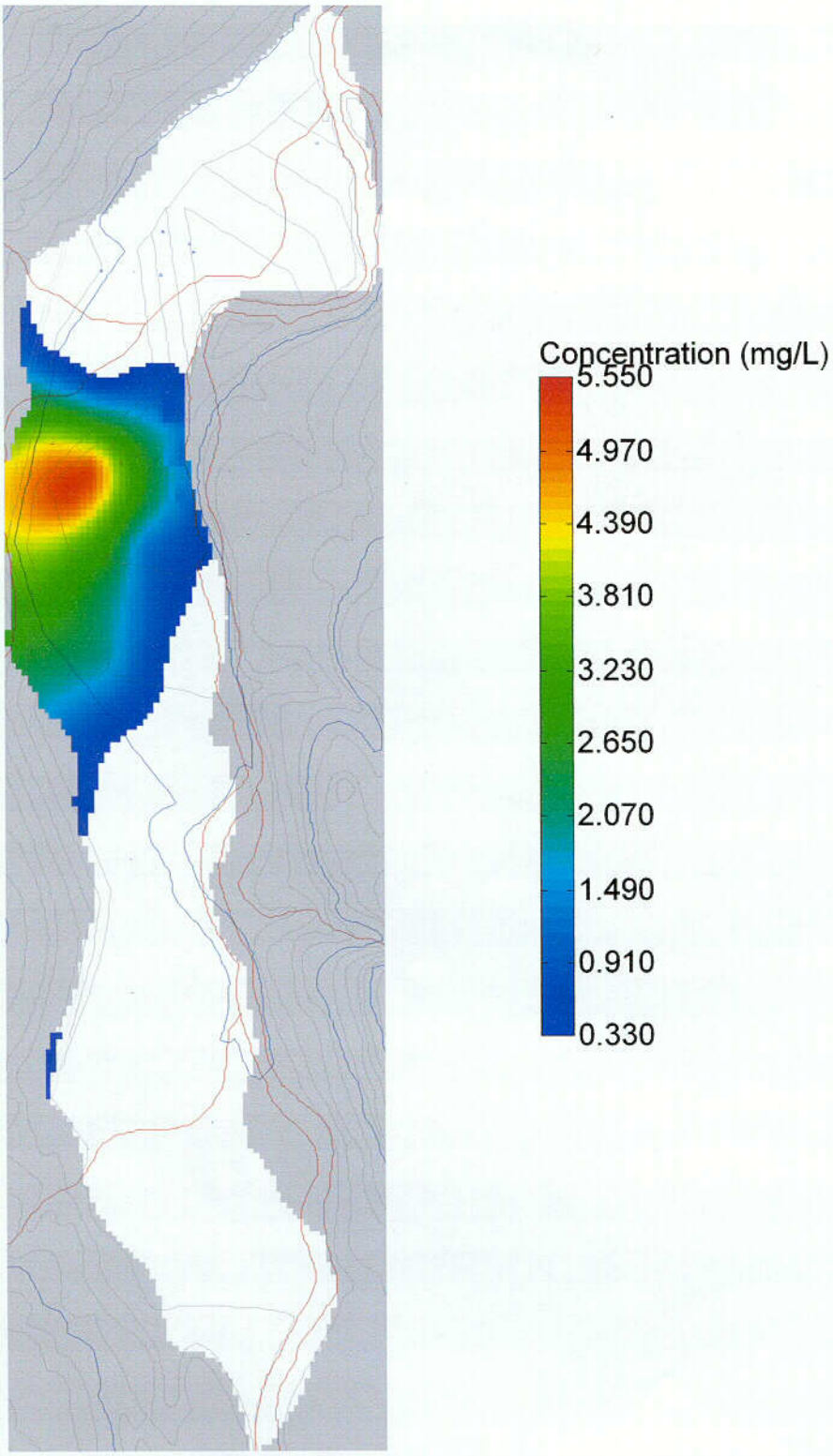

Figure 26. Predicted Steady State Vanadium Concentration at 5 Years

C10

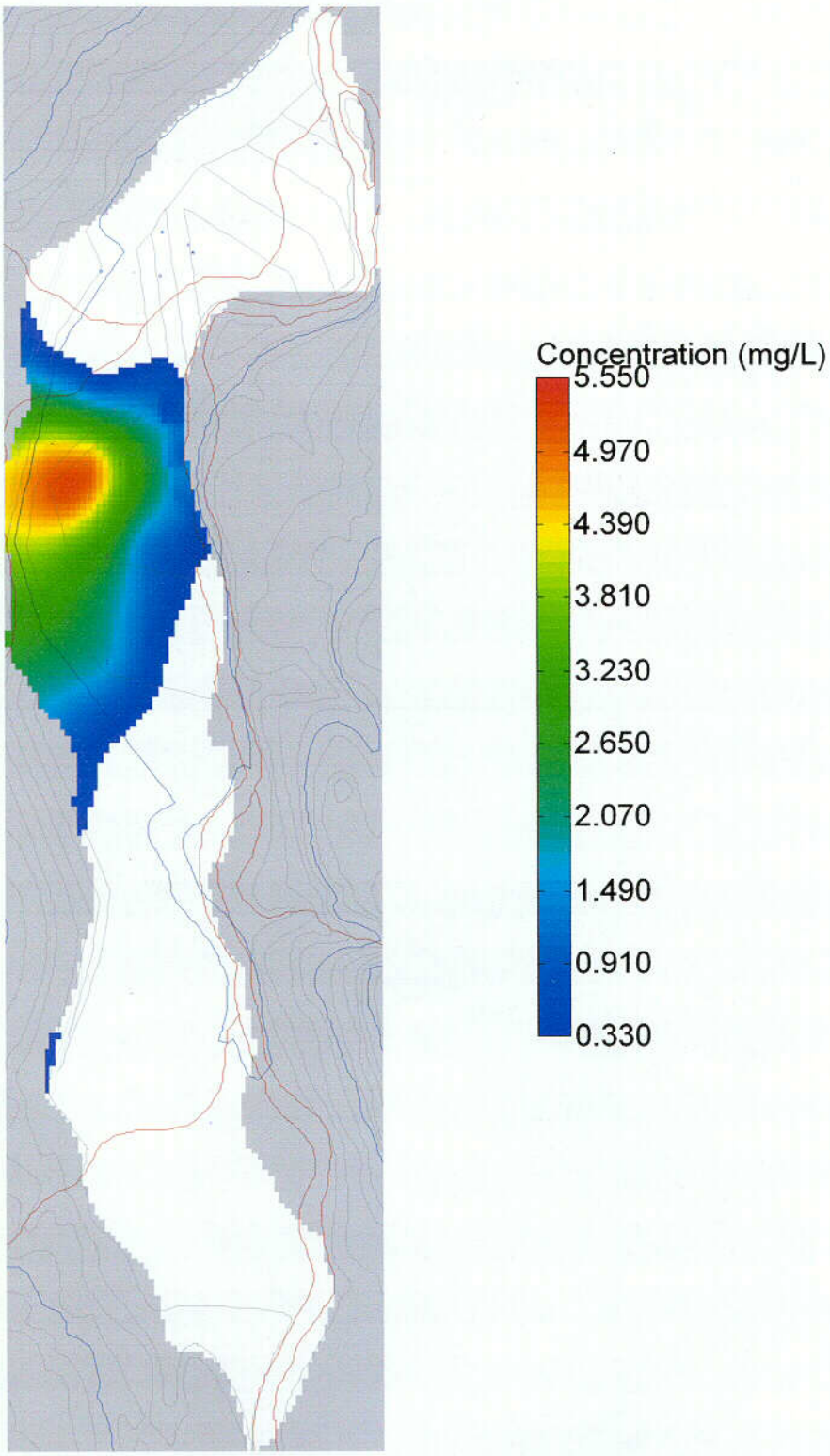

Figure 27. Predicted Steady State Vanadium Concentration at 10 Years

C11

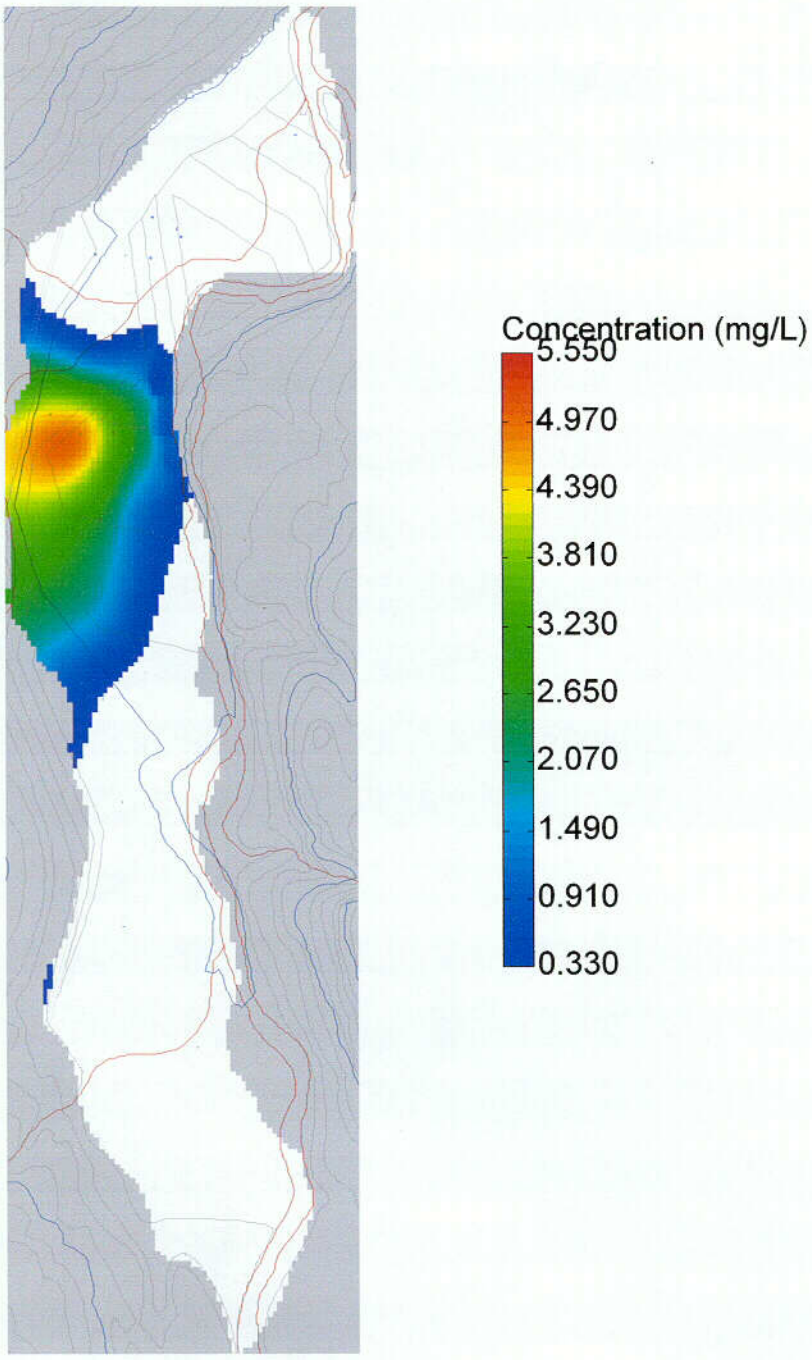

Figure 28. Predicted Steady State Vanadium Concentration at 25 Years

C12

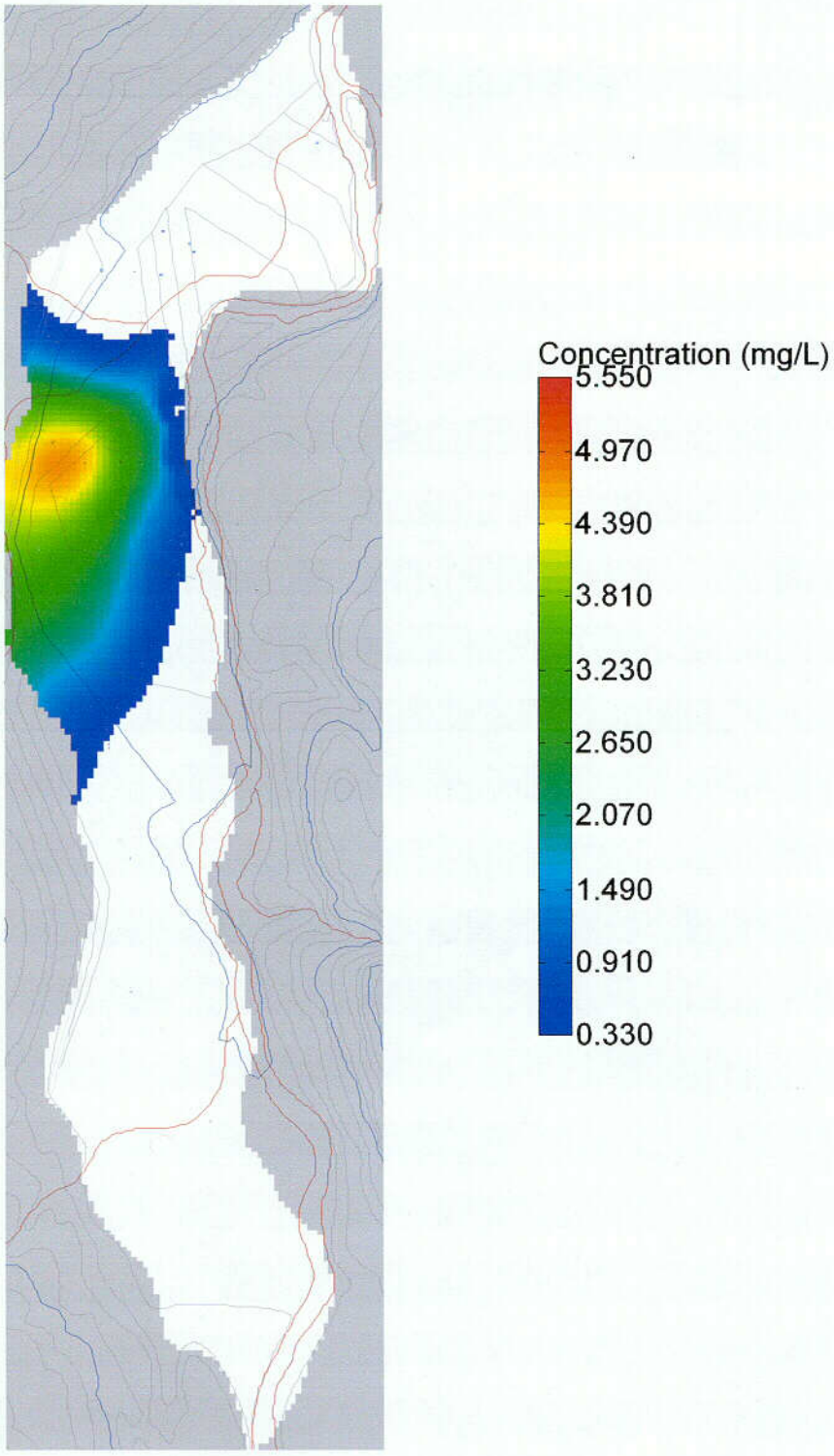

Figure 29. Predicted Steady State Vanadium Concentration at 50 Years

C13

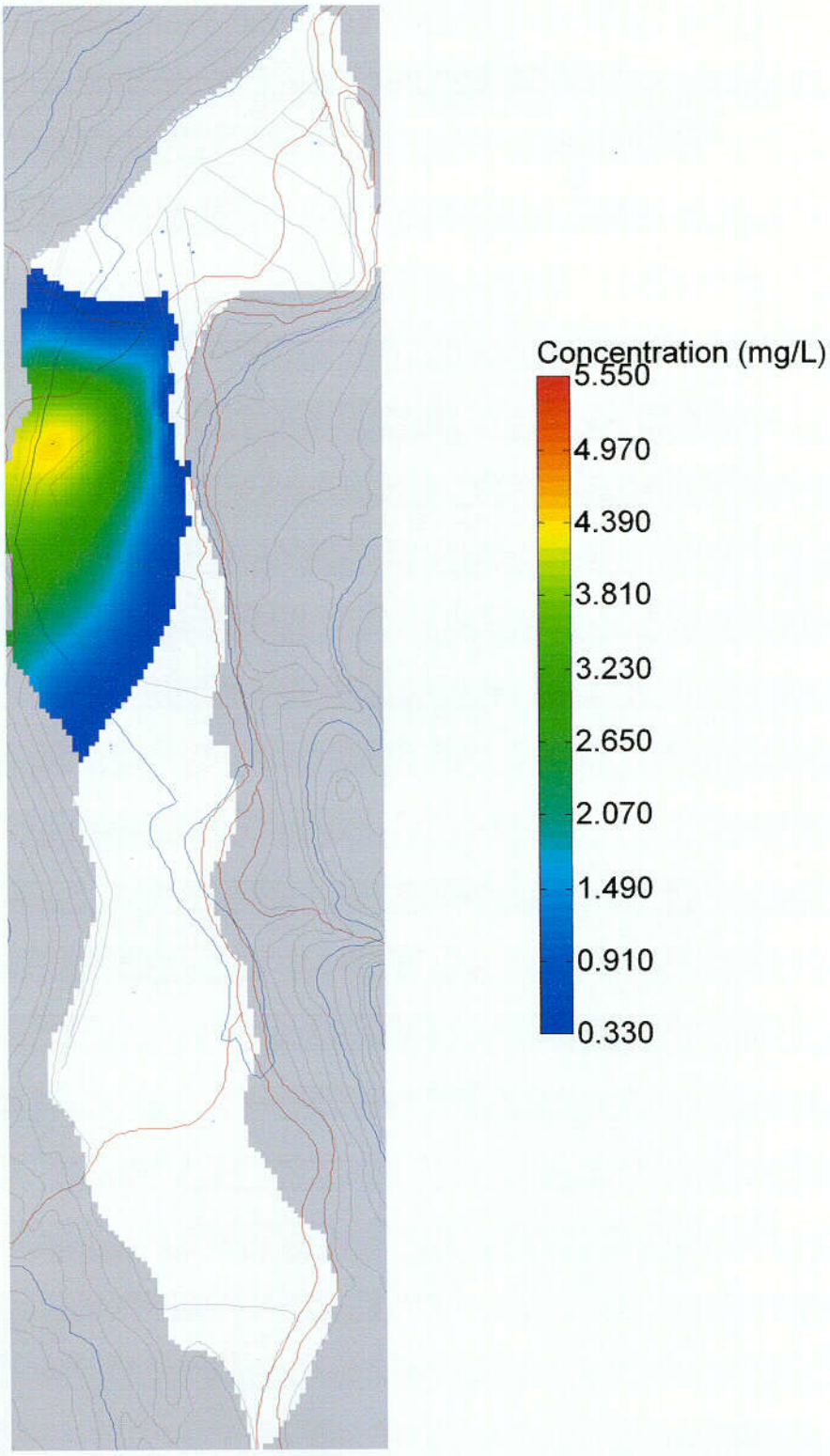

Figure 30. Predicted Steady State Vanadium Concentration at 100 Years

C14

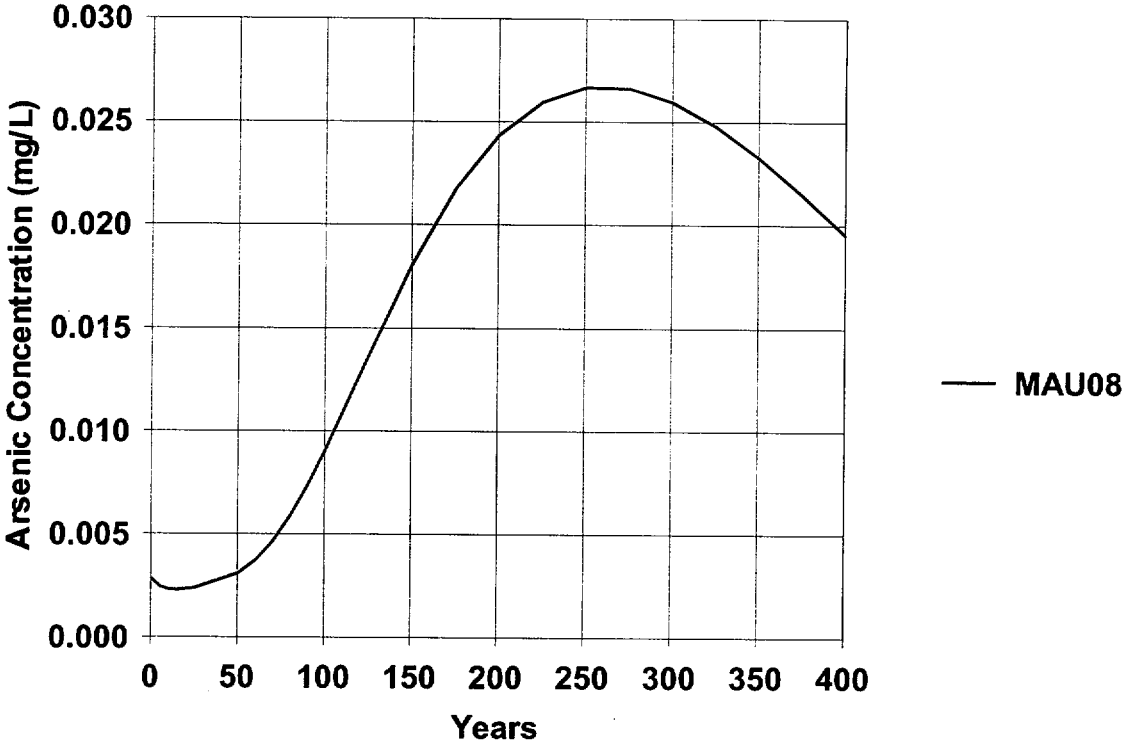

Figure 31. Arsenic Concentration versus Time for Monitor Well MAU08

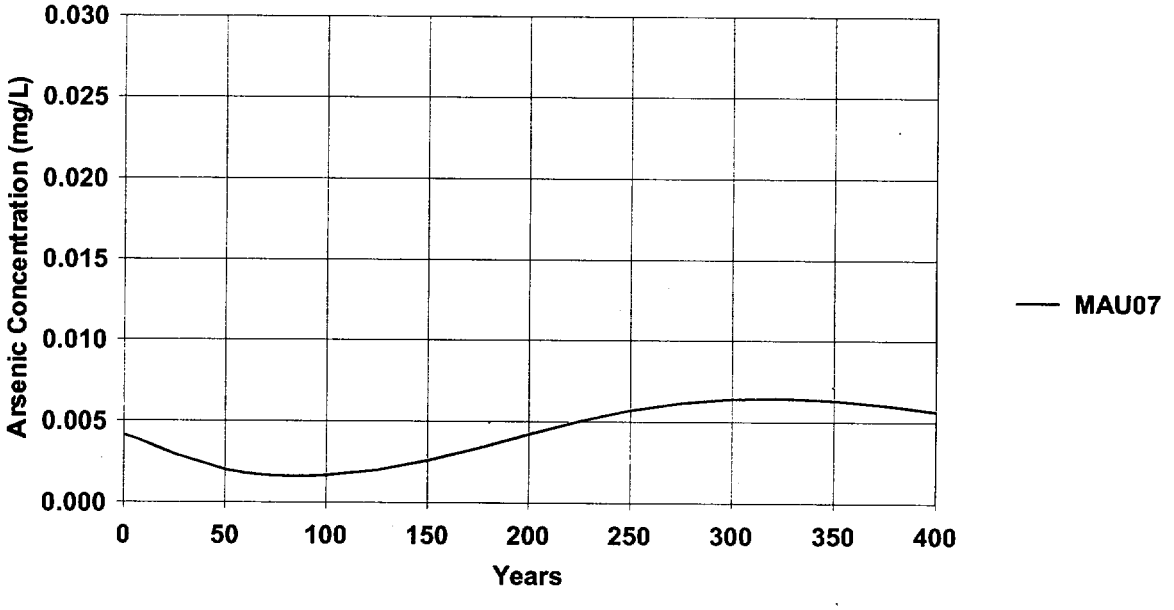

Figure 32. Arsenic Concentration versus Time for Monitor Well MAU07

6.0 Stochastic Simulations

6.1 Stochastic Parameters

Stochastic flow and transport simulations were run for only uranium. The flow and transport parameters that are treated as uncertain parameters are shown in Table 8. The distribution type and distribution parameters assigned to each of the stochastic parameters are specified.

Non-stochastic flow and transport parameters are listed in Table 9.

Table 8. Stochastic Flow and Transport Parameters

Parameter	Distribution			
	Type	Standard Deviation	Minimum	Maximum
Hydraulic Conductivity (ft/day)				
Longitudinal	Triangular	N/A	10	100
Transverse	Triangular	N/A	100% Longitudinal	
Dispersivity (ft)				
Longitudinal	Triangular	N/A	50	200
Transverse	Triangular	N/A	10% Longitudinal	
K_d				
Uranium (mL/g)	Triangular	N/A	0.3975	1.1225
(ft^3/lb)	Triangular	N/A	.006367	.01798
Recharge (ft/day)	Triangular	N/A	0	.00064
Recharge (in/yr)	Triangular	N/A	0	2.79
Porosity	Triangular	N/A	0.25	.40

Table 9. Non-Stochastic Flow and Transport Parameters

Parameter
River Stage (ft)
River Bed Conductance (ft^2/day)
River Concentration (mg/L)
GBH Head (ft)
GHB Conductance (ft^2/day)
GHB Concentration (mg/L)
Bulk Density (g/mL)

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

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 33 indicates that the cumulative average residual sum of squares becomes relatively stable at about 31.8 ft^2 after 160 realizations. Therefore, 200 realizations should be adequate to account for the uncertainty in the stochastic parameters.

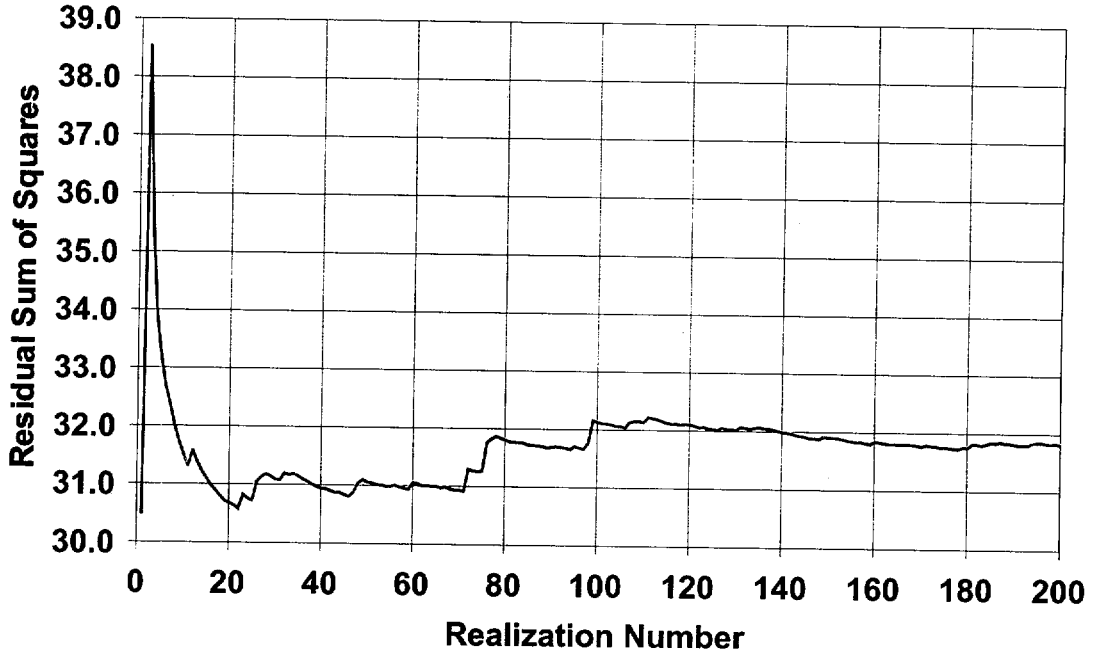

Figure 33. Cumulative Average Residual Sum of Squares versus Realization Number

Another useful evaluation tool is to look at how the individual realizations compare to the calibrated flow model results. The plot in Figure 34 shows the residual sum of squares for each of the 200 realizations. Few if any of the realizations are below the calibrated model residual sum of squares value of 28.878 ft^2, which is plotted on the figure. This indicates that the calibrated flow model is close to an optimum minimum. Note that at about realization 75 and 78 and again at about realization 99 the residual sum of squares is relatively high compared to the other realizations. These high values account for the jump at the same locations in Figure 33.

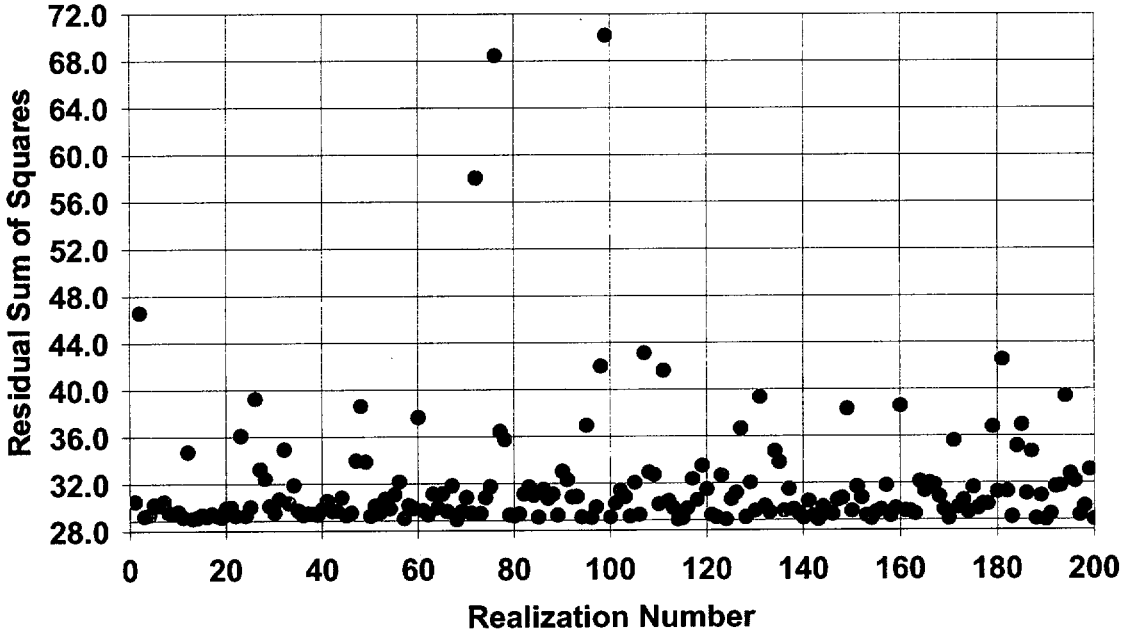

Figure 34. Residual Sum of Squares versus Realization Number

Based on the type of distribution associated with the uncertain parameters, the average remaining concentration from the results of the stochastic realizations will be lower than the deterministic results. Although this is not apparent, consider Table 10 which shows the mid-point of the triangular distributions used for each of the uncertain parameters (hydraulic conductivity, recharge, porosity, K_d, and longitudinal dispersivity). The mid-point stochastic values are higher than the deterministic values. For three of the five parameters (hydraulic conductivity, recharge, and longitudinal dispersivity) the mid-point stochastic value will result in a faster clean-up time. For the other two parameters (porosity and K_d) the higher mid-point stochastic value will result in a longer clean-up time. Table 5 indicates that both hydraulic conductivity and recharge are sensitive as early as 10 years while Table 7 indicates that porosity is not sensitive until 80 years and K_d is not sensitive until 50 years. While this is only a qualitative (subjective) analysis, it supports the notion that the remaining concentration at any time will be lower for the average stochastic results than for the deterministic results.

Table 10. Comparison of Deterministic vs. Mid-point Stochastic Parameter Values

Parameter	Deterministic Value	Mid-point Stochastic Value
Hydraulic Conductivity (ft/day)	30.	43.875
Recharge(ft/day)	0.	0.00019
Recharge (in/yr)	0.	0.7884
Porosity	0.25	0.29393
Kd (mL/g)	0.6078	0.69055
Longitudinal Dispersivity (ft)	100	113.397

If the mid-point stochastic parameter values are used in the deterministic model the maximum predicted concentration for uranium at 5, 10, 25, 50, and 100 years is 2.2380, 2.0111, 1.3038, 0.55829, and 0.030455 mg/L, respectively. These values are all lower than the deterministic

values reported in Section 5.3 and compare favorably with the average stochastic results in Section 6.2.

Figures 35 and 36 are plots of the average or mean head field of the 200 realizations. A visual comparison of Figures 35 and 36 with the steady state deterministic results in Figures 5 and 6 shows that they are almost identical. Figure 37, which presents the variability in head, represents the standard deviation in the heads of the 200 realizations. Although this plot is difficult to interpret, according to basic statistics about 68 percent of the heads in the simulation can be expected to fall within one standard deviation of the mean and about 95 percent can be expected to fall within two standard deviations. For these 200 realizations, the standard deviation in heads ranges from 0.0 to +0.3662. This indicates that there is very little variation in the results of the 200 realizations and essentially all of the results fall within one standard deviation of the mean.

6.2 Predictive Results for Uranium

Contaminant transport simulation results for uranium were extracted for selected times up to 100 years into the future. Average concentrations and the associated uncertainty at each time period of interest are based on 200 computer simulations. Figure 15 shows the initial concentration plume. Predicted uranium concentrations above the UMTRA Project MCL of 0.044 mg/L at 5, 10, 25, 50, and 100 years into the future are presented in Figures 38 through 42, respectively. The areas of the model in the figures that do not have color (are white) are below the MCL. The maximum average remaining concentration at 5, 10, 25, 50, and 100 years are 2.2156, 1.9671, 1.2854, 0.57426, and 0.12087 mg/L, respectively.

By varying the value of the uncertain or stochastic parameters during each of the 200 simulations, the variance associated with the mean predicted concentration was used to calculate the probability that the mean uranium concentration will exceed the uranium standard. Probability contour maps showing areas within the alluvial aquifer that exceed the uranium ground water standard at 5, 10, 25, 50 and 100 years into the future are illustrated in Figures 43 through 47, respectively. At 5, 10, and 25 years there is 100 percent probability that the standard will be exceeded over a significant part of the former millsite and downgradient. At 100 years there is still a 49 percent probability that the standard will be exceeded.

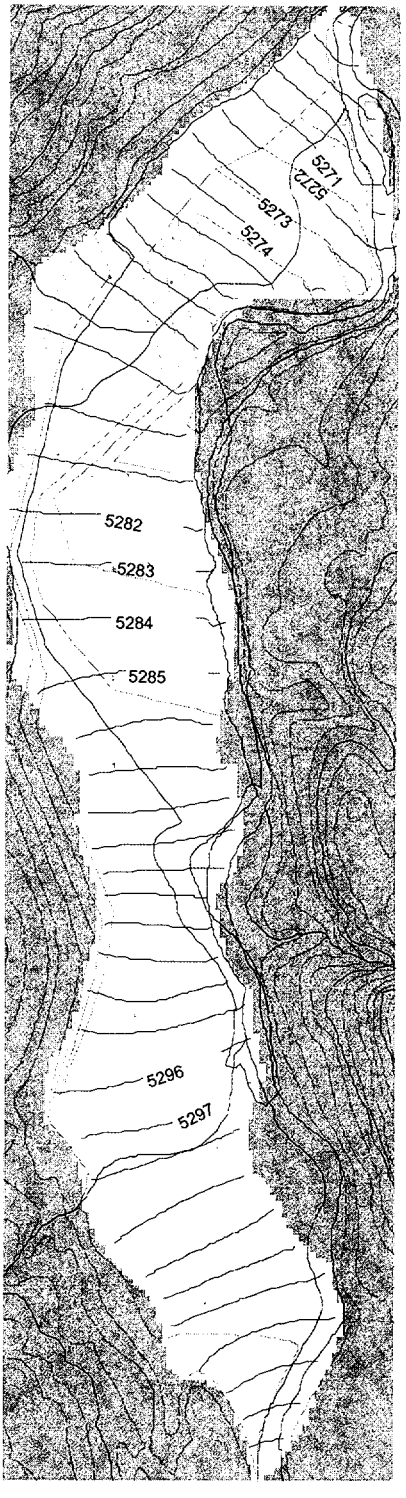

Figure 35. Average Simulated Steady State Stochastic Ground Water Elevations (in feet above MSL)

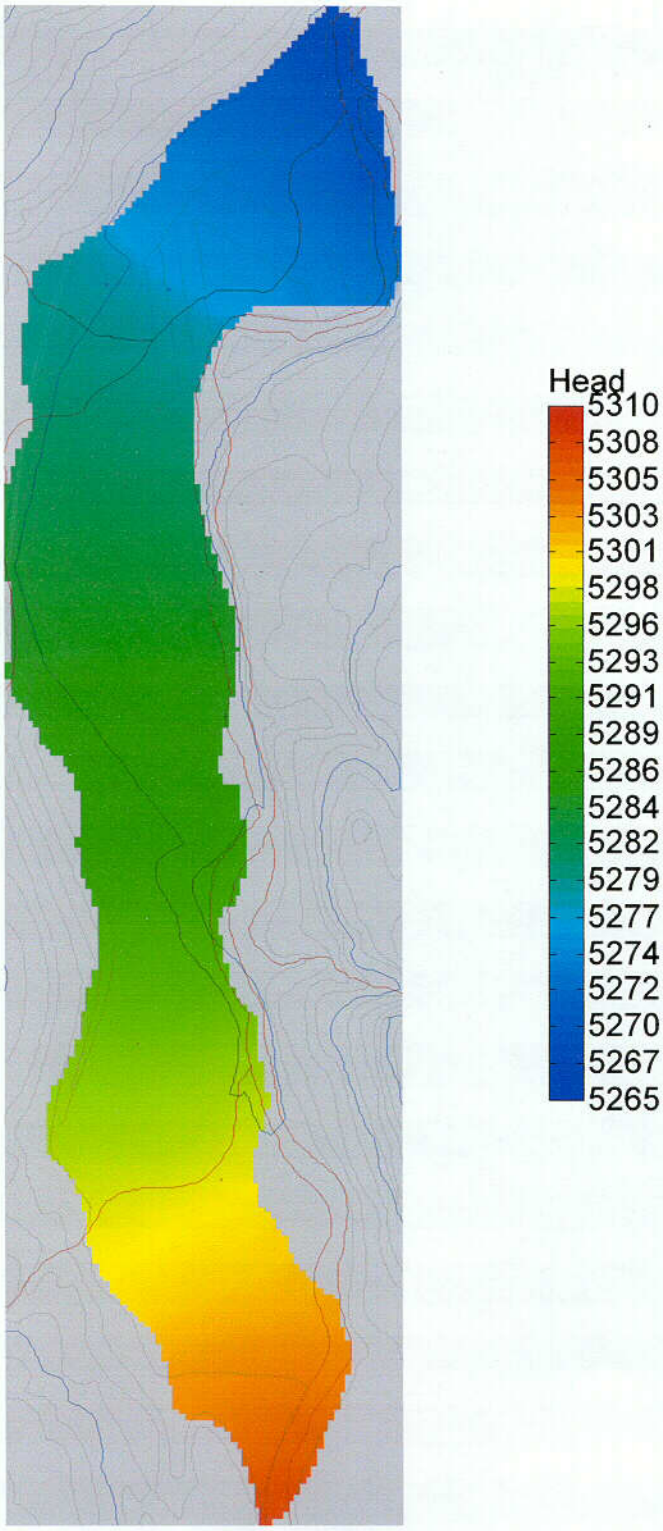

Figure 36. Average Simulated Steady State Stochastic Ground Water Elevations (in feet above MSL)

C15

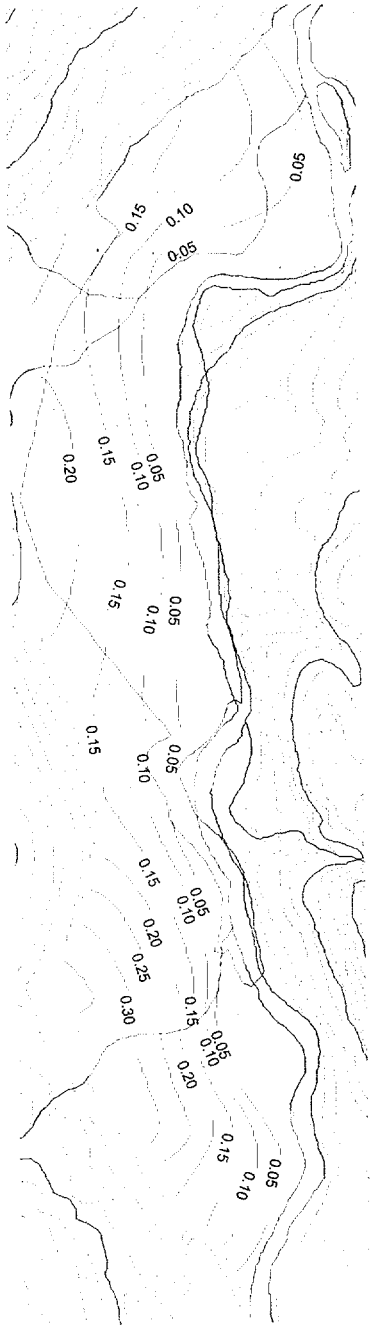

Figure 37. Standard Deviation of Head Field

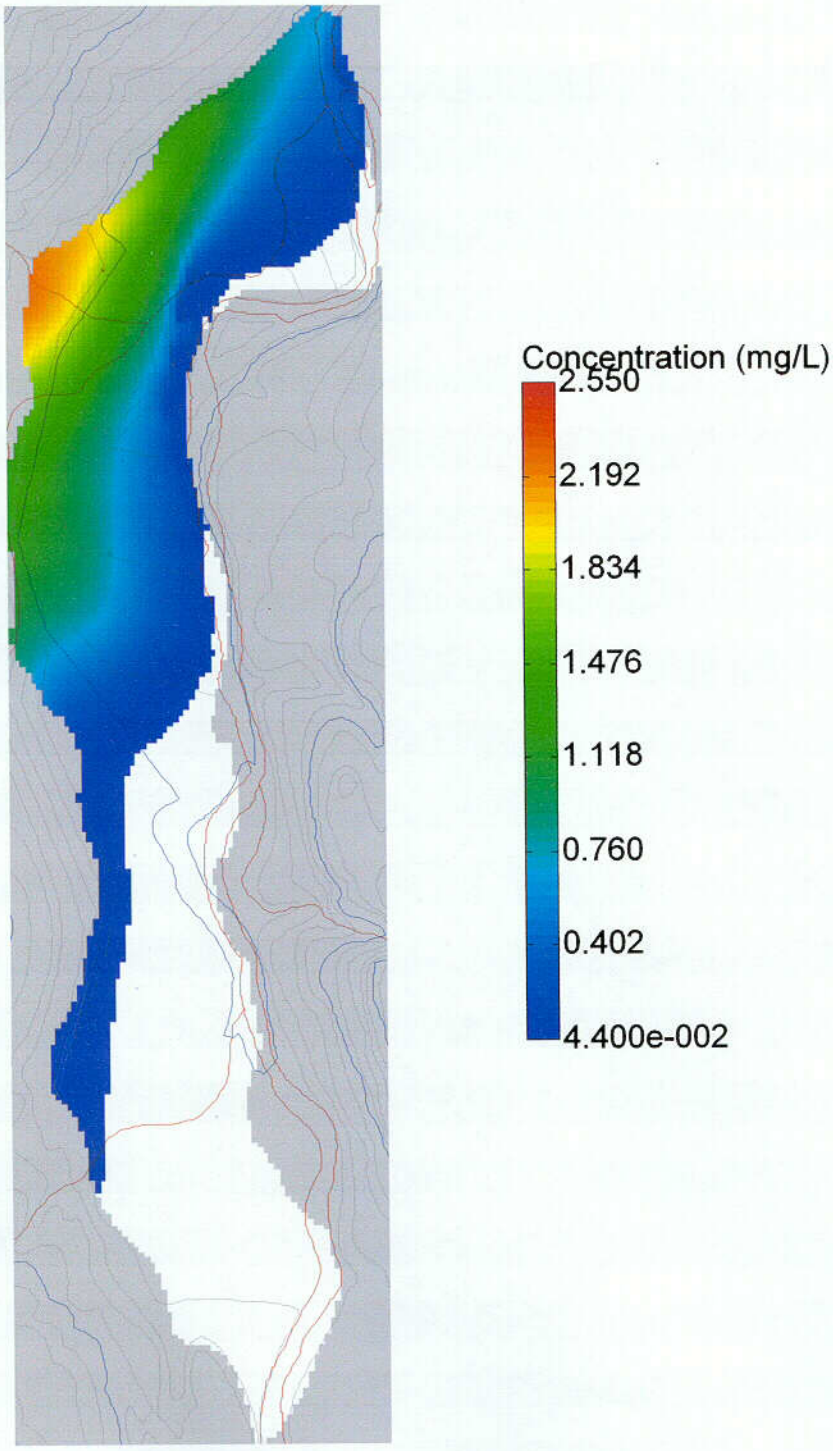

Figure 38. Predicted Steady State Stochastic Uranium Concentration at 5 Years

C16

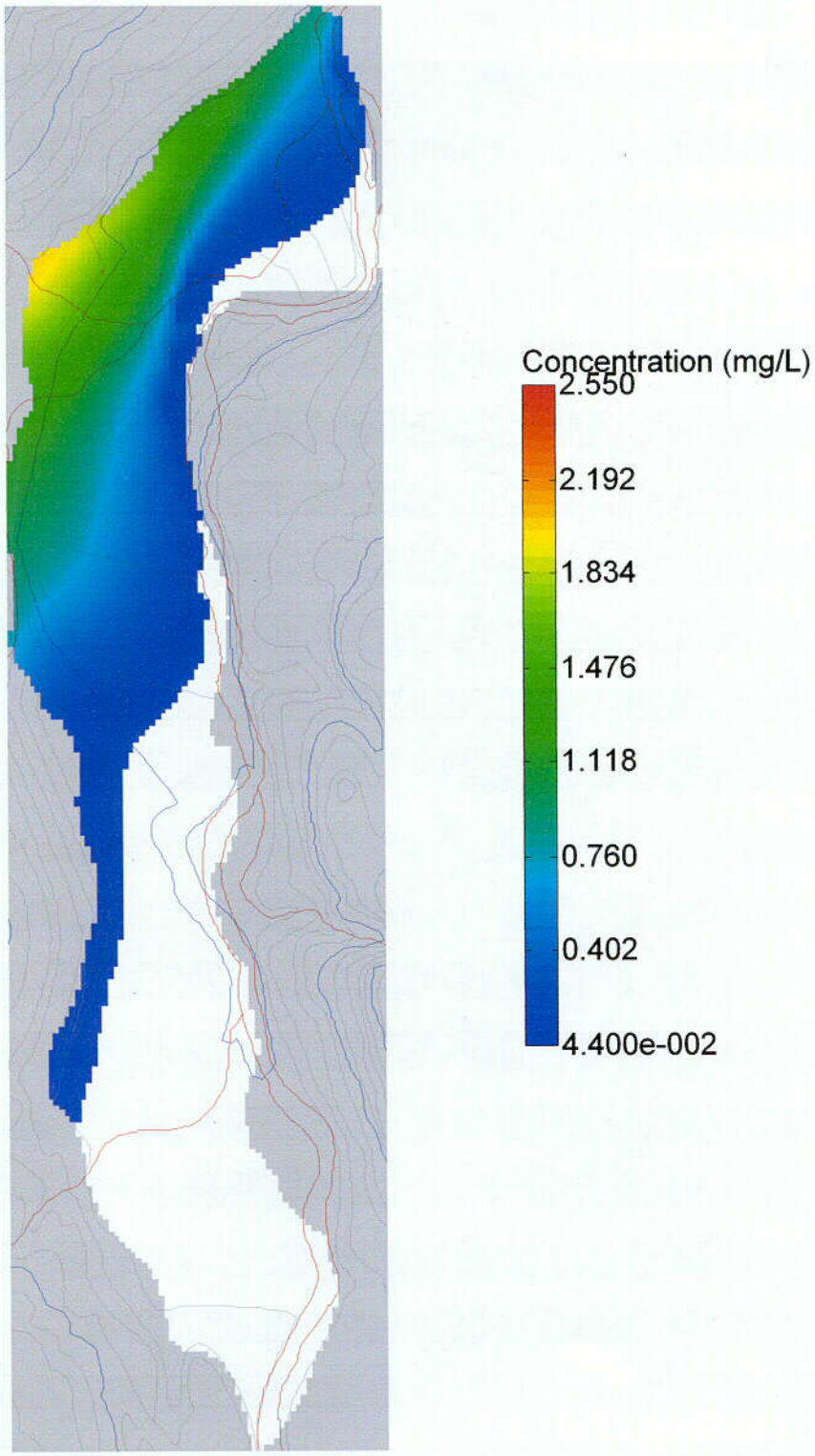

Figure 39. Predicted Steady State Stochastic Uranium Concentration at 10 Years

C17

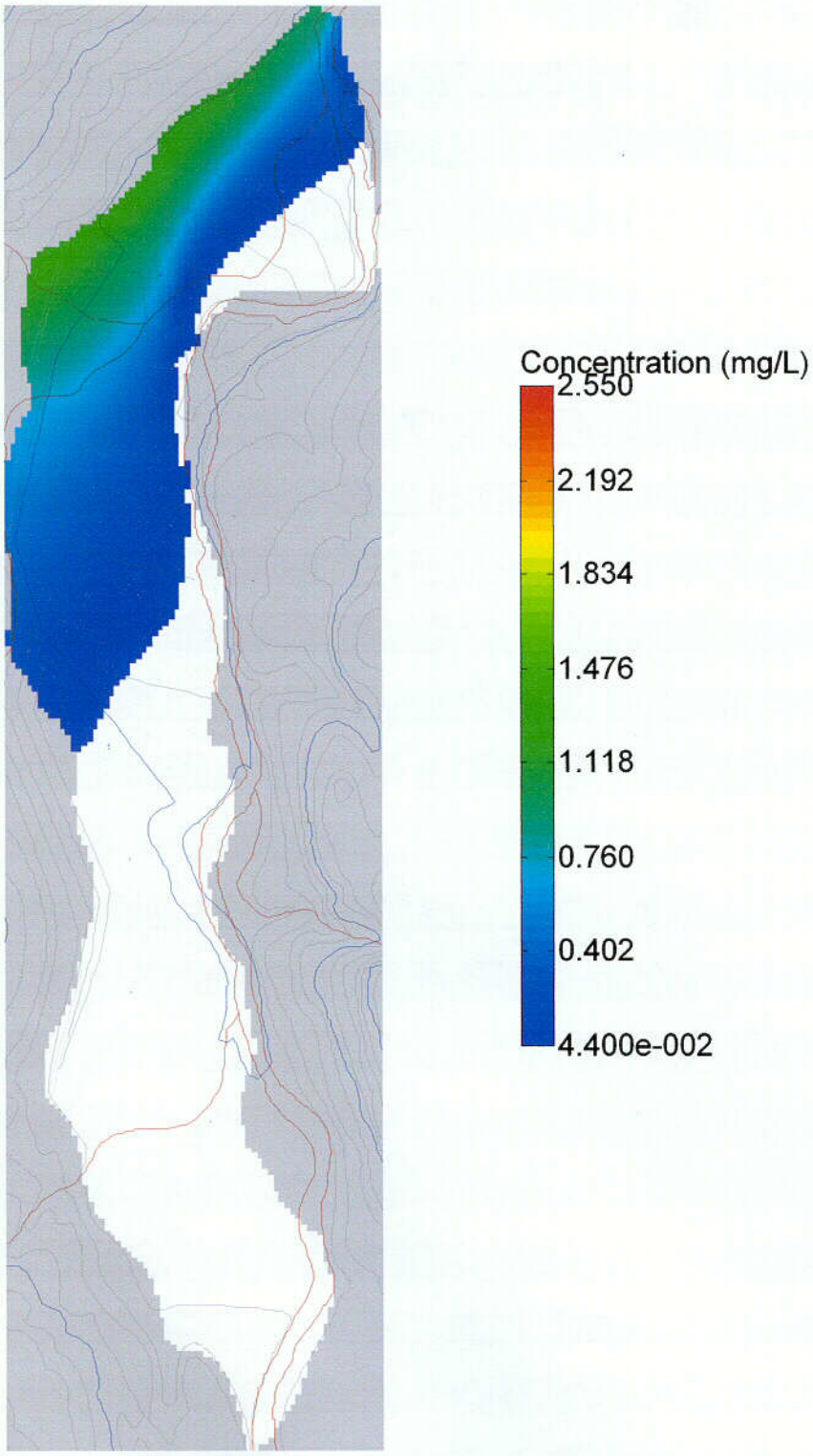

Figure 40. Predicted Steady State Stochastic Uranium Concentration at 25 Years

C18

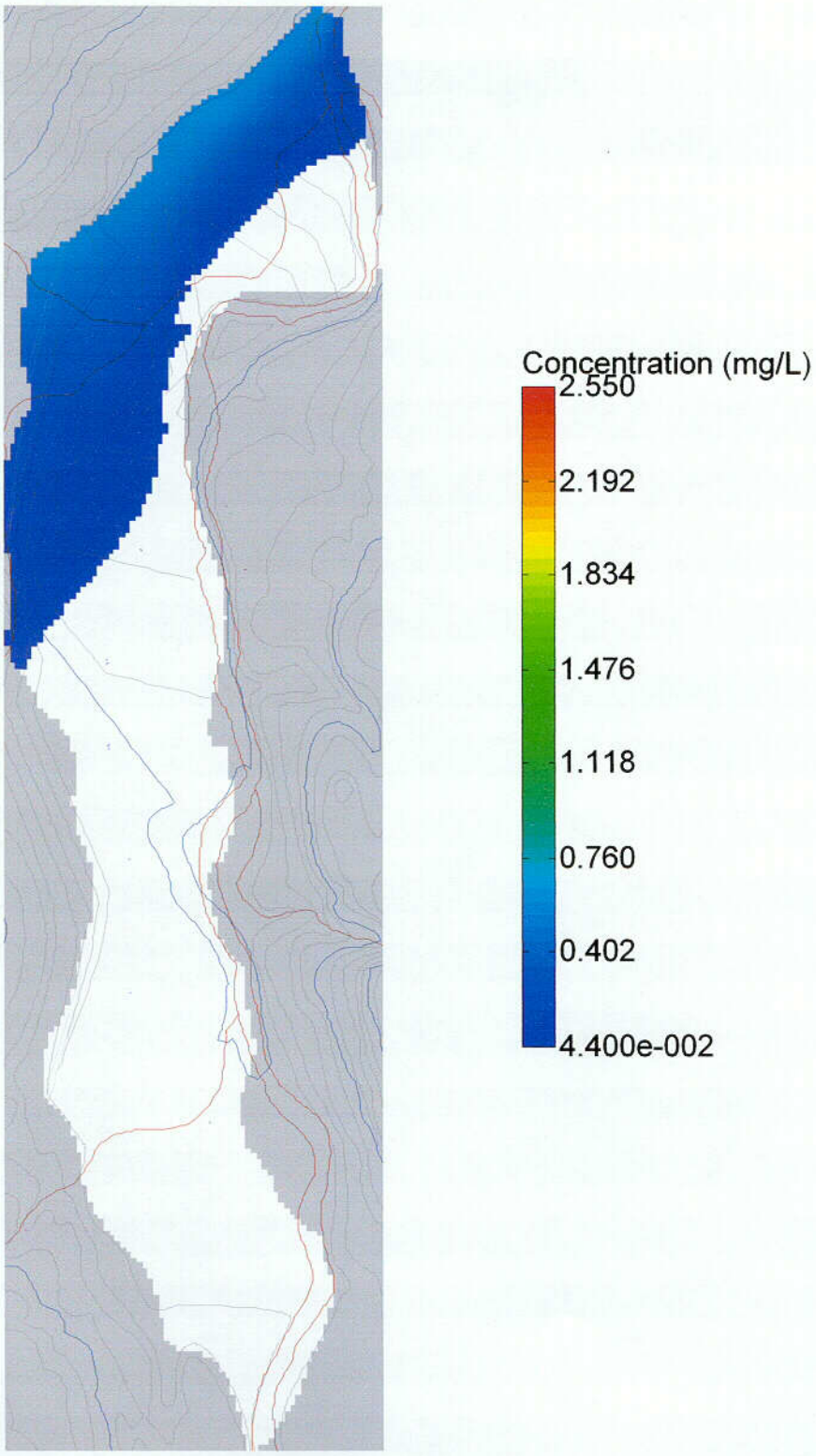

Figure 41. Predicted Steady State Stochastic Uranium Concentration at 50 Years

C19

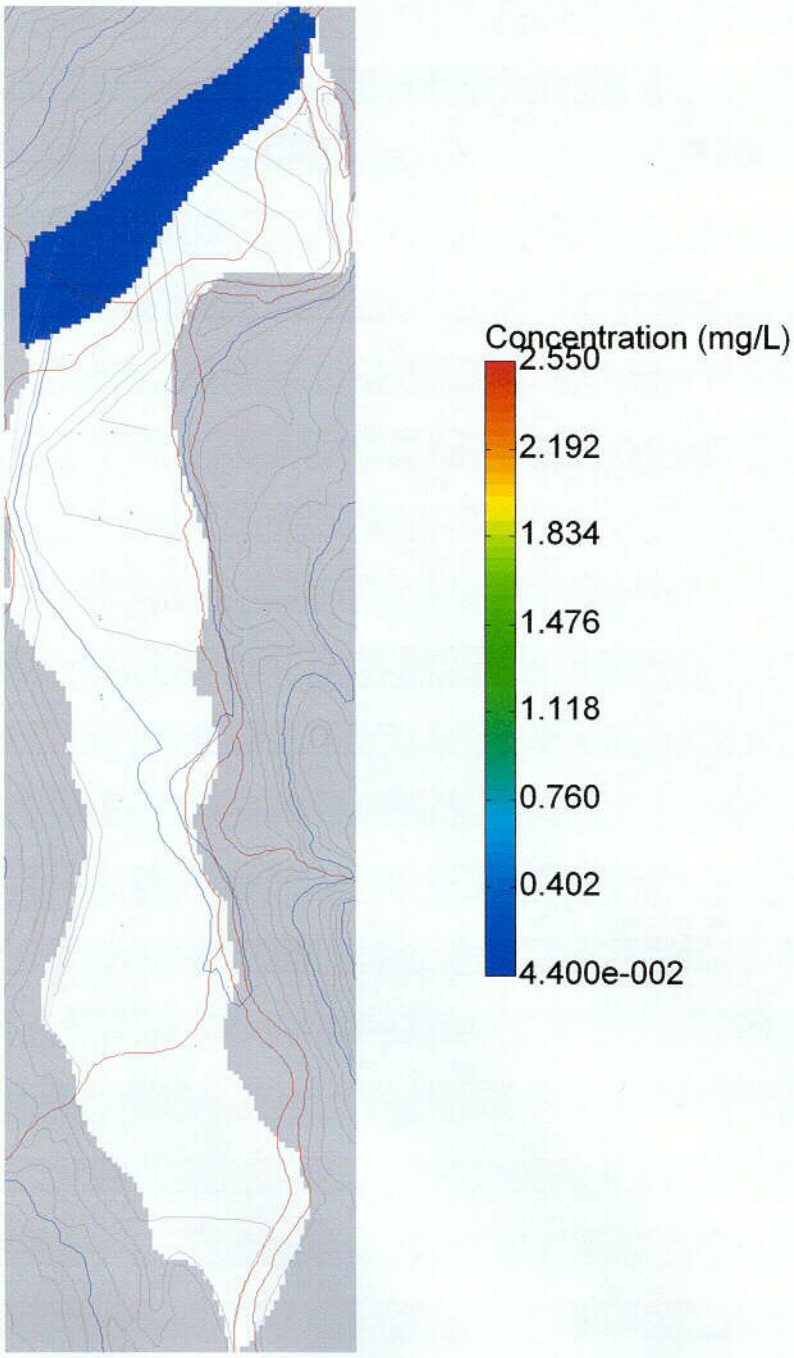

Figure 42. Predicted Steady State Stochastic Uranium Concentration at 100 Years

CZ0

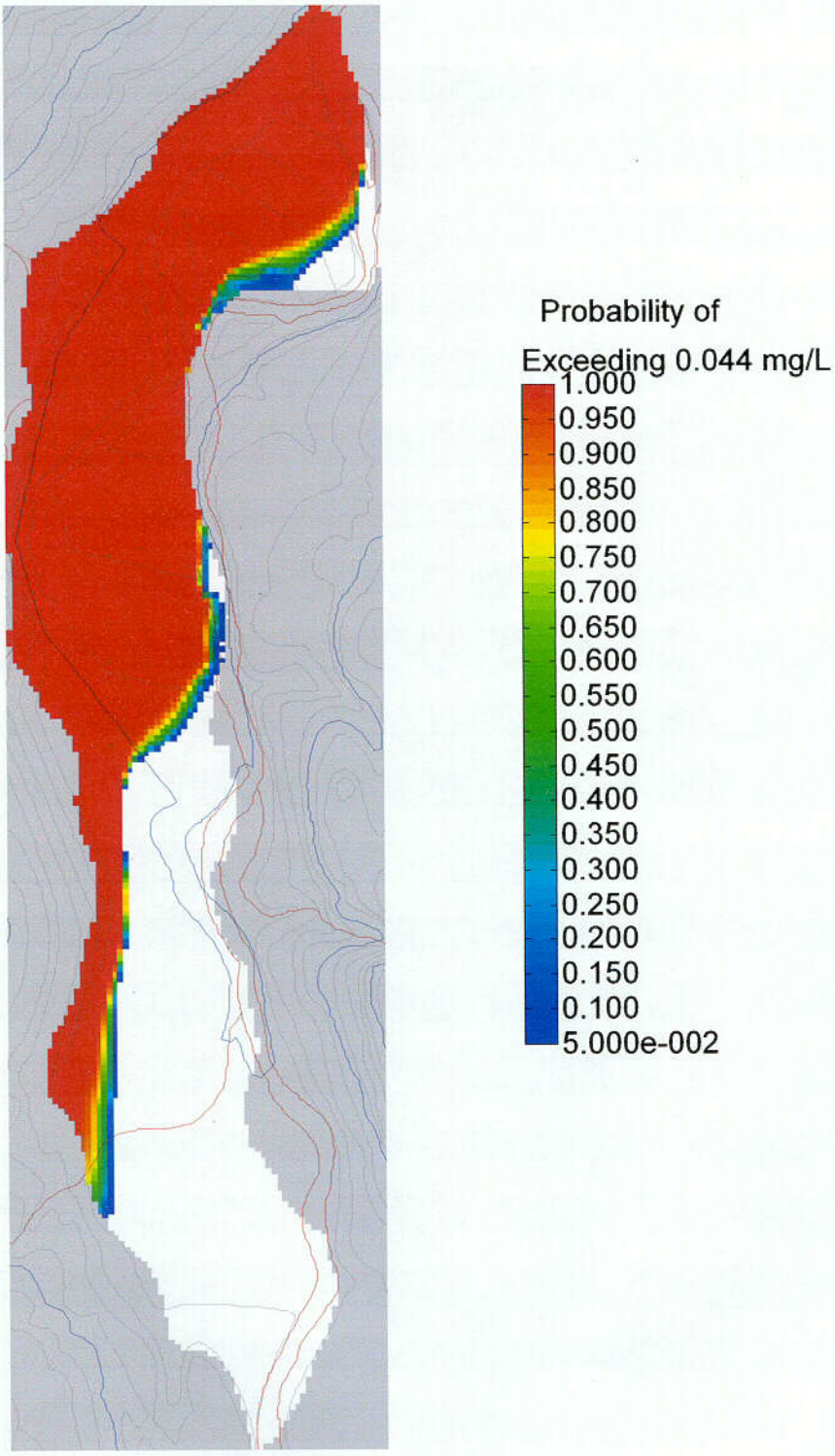

Figure 43. Probability of Uranium Concentration Exceeding the Standard at 5 Years

C21

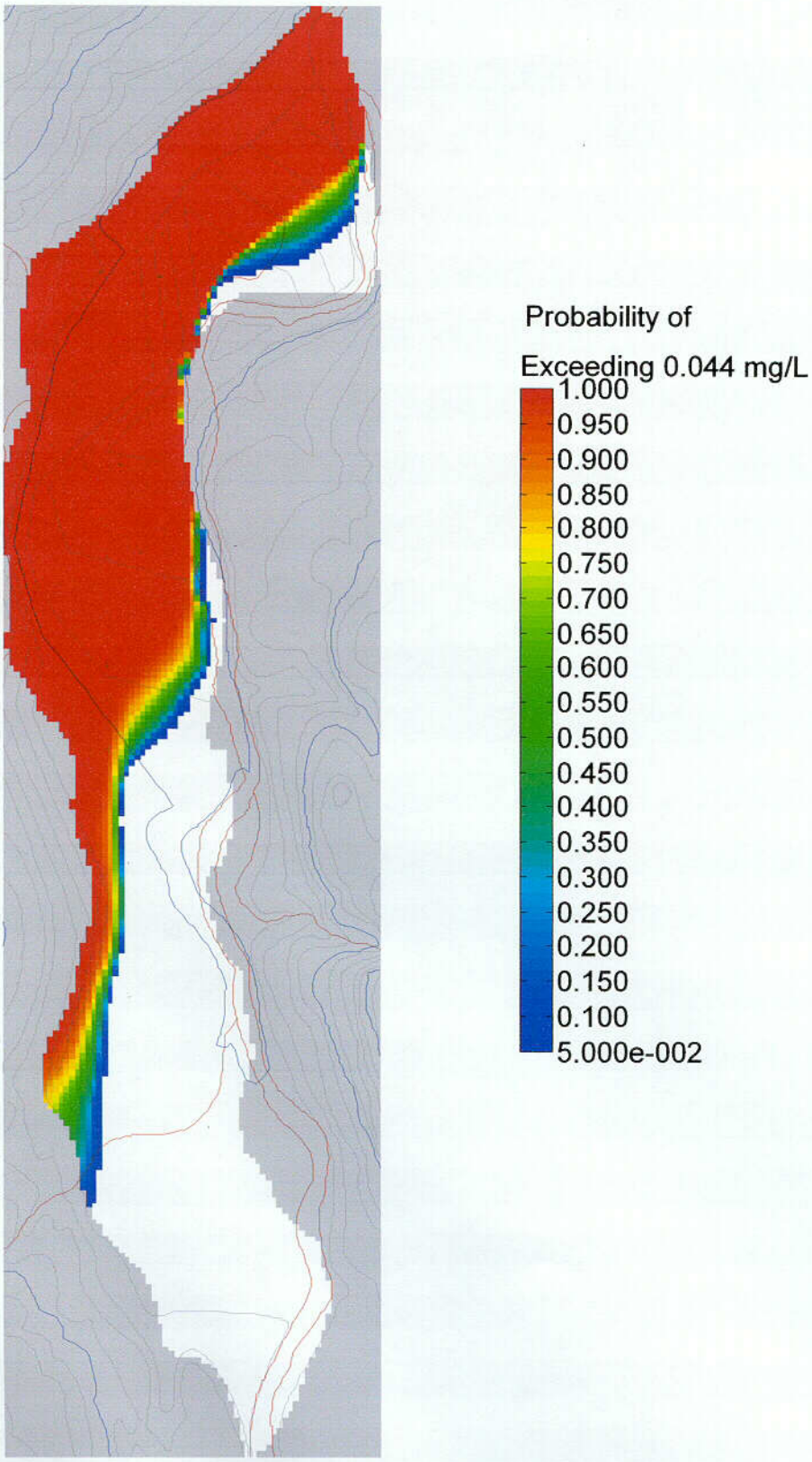

Figure 44. Probability of Uranium Concentration Exceeding the Standard at 10 Years

C22

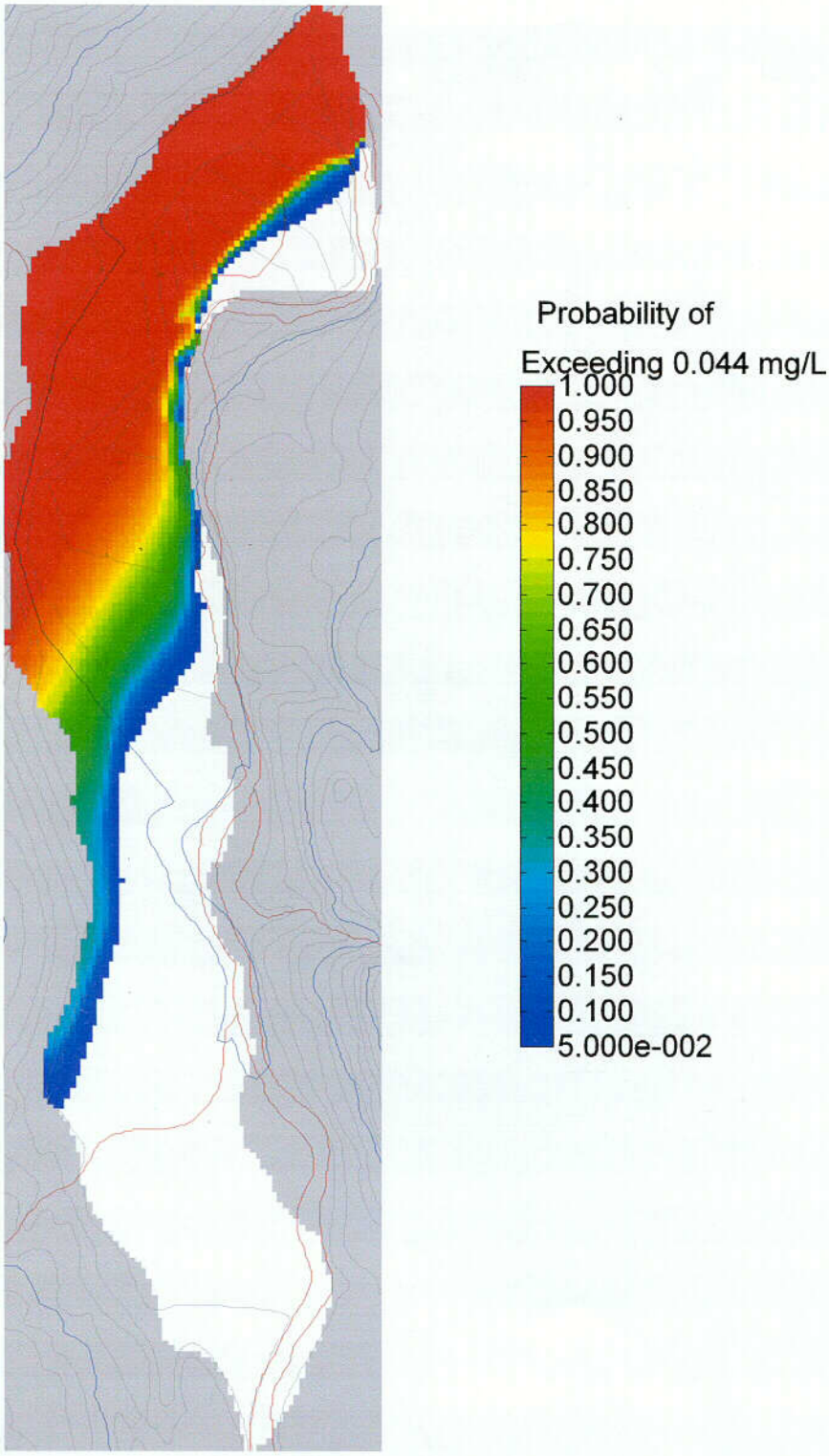

Figure 45. Probability of Uranium Concentration Exceeding the Standard at 25 Years

C23

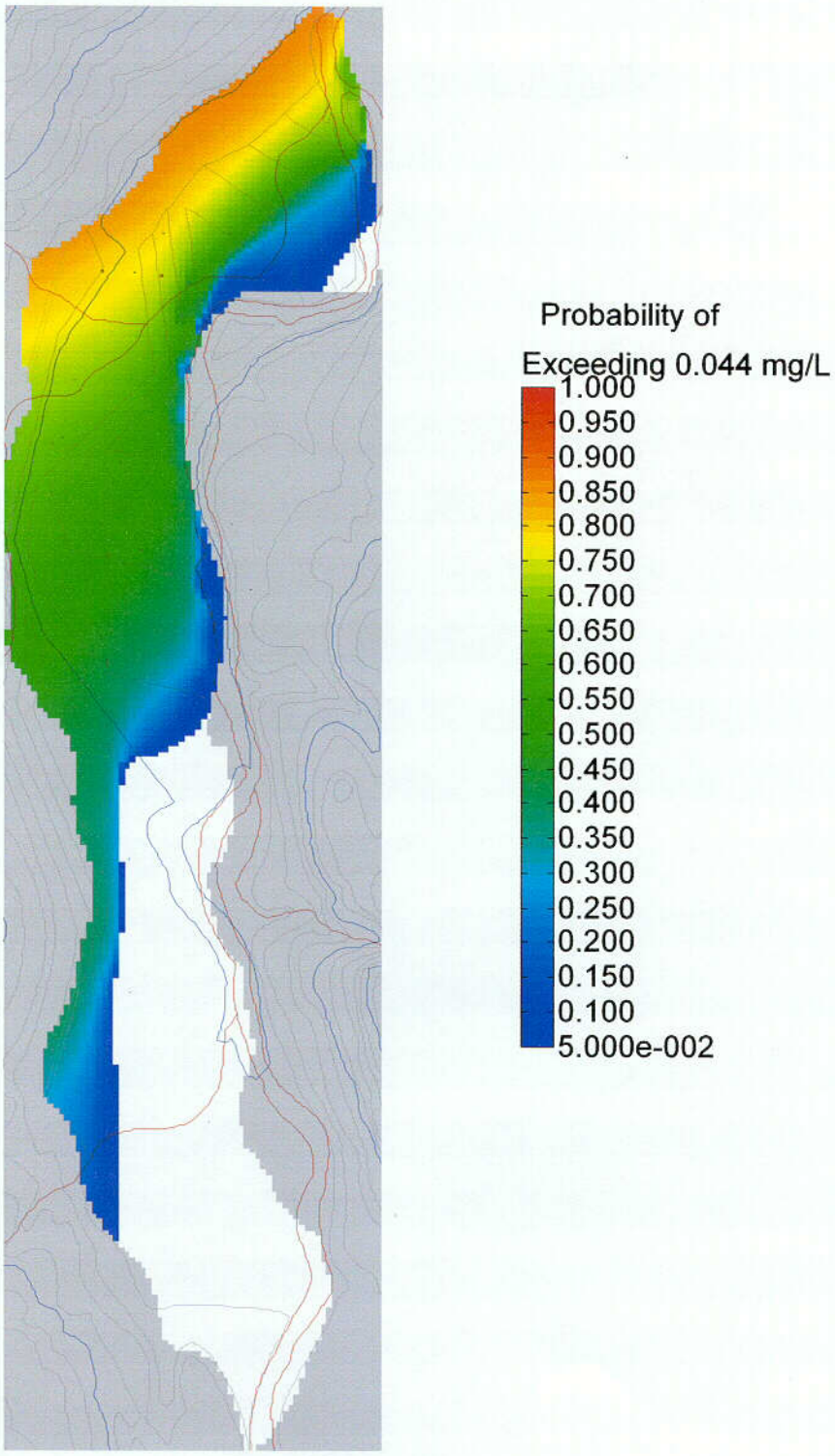

Figure 46. Probability of Uranium Concentration Exceeding the Standard at 50 Years

C24

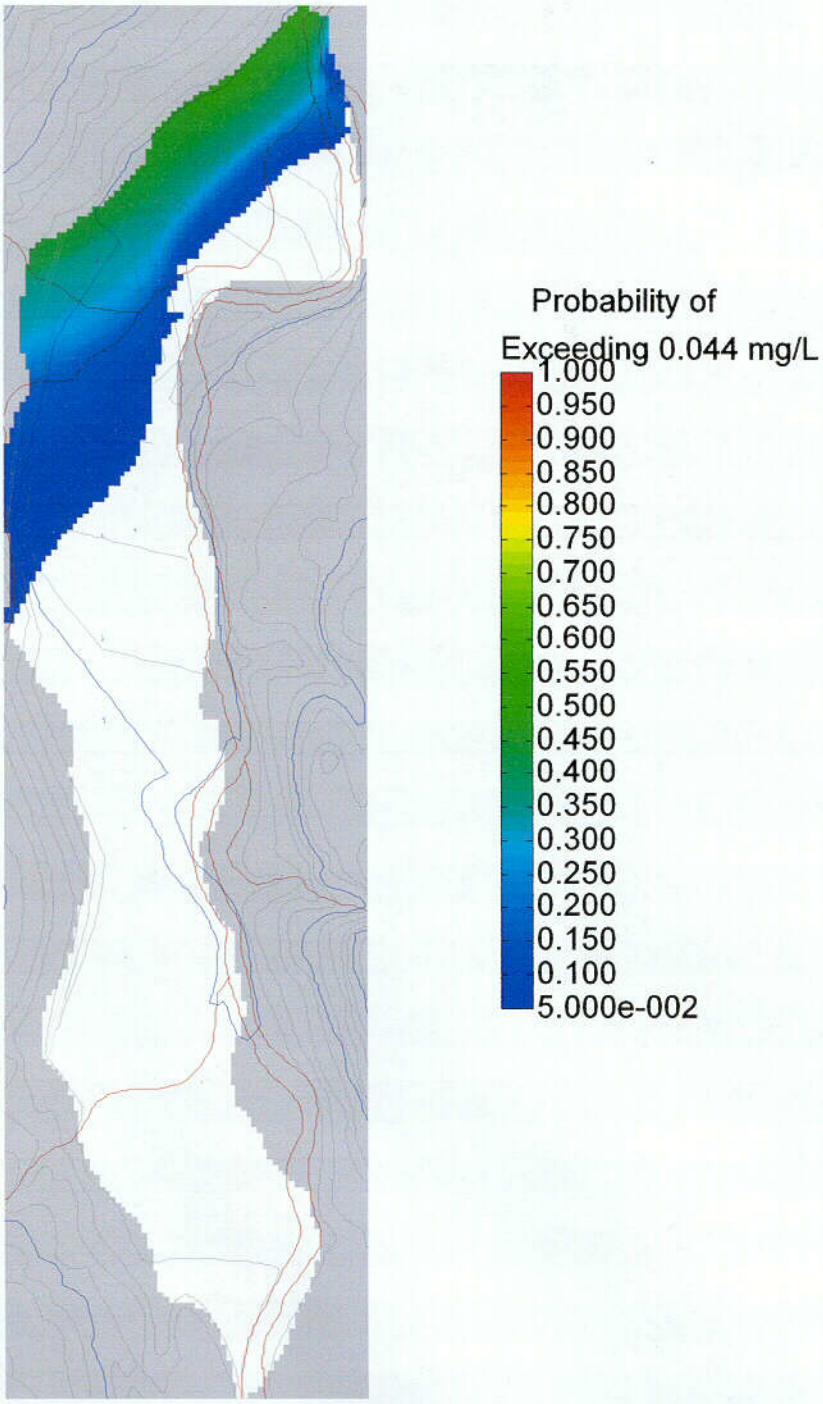

Figure 47. Probability of Uranium Concentration Exceeding the Standard at 100 Years

C25

7.0 Pumping Followed by Natural Flushing

This modeling task could be formulated as a classical optimization problem. Optimization modeling problems inherently require considerable time and effort. Therefore, before the time and effort were committed to developing an optimization model a much simpler approach was taken to determine if there was any reasonable possibility that this strategy would succeed.

7.1 Step/Task 1

The first task is to determine to what levels will uranium and vanadium need to be reduced, by pumping, such that each will meet the required standard within 100 years of naturally flushing? To do this it was determined how long it would take uranium and vanadium to naturally flush. Modeling indicates that it would take approximately 135 years for uranium to flush and more than 1000 years for vanadium to flush to the required standards. The maximum remaining concentration of vanadium at 1,000 years is approximately 2.31 mg/L. Vanadium is not considered further in this analysis because of the extreme time required to naturally flush.

This task can now be stated differently, i.e., what is the concentration of uranium at 35 years?

The maximum remaining concentration of uranium at 35 years is approximately 1.70 mg/L. Therefore, any pumping scenario would need to reduce the contamination level for uranium to this value in order for natural flushing to reduce contamination to the required standard within 100 years of natural flushing.

7.2 Step/Task 2

The next task is to determine which wells or location should be used for pumping and what pump rates should be used? The rationale used, although obviously not optimal locations, was to select existing wells that show high concentration of either uranium or vanadium. These wells would be pumped at the highest possible rate such that the aquifer would not dry up. Four existing wells that show high concentration of either uranium or vanadium were selected as potential pumping locations. These wells are MAU08, NAT01-1, NAT03, and NAT06-1.

Initially it was decided to try pumping each well at 10 gallons per minute (gpm) or 1,925 ft^3/day. However, because of the limited saturated thickness (approximately 2 to 6 ft) and the low hydraulic conductivity, it is not possible to pump this amount of water from any of the wells.

Modeling determined the maximum pump rate that could be sustained at each of these wells, pumped individually, without drying up the area in the vicinity of the well. These values are shown in Table 11.

Table 11. Maximum Individual Pump Rates

Well	Pump Rate	
	gpm	ft^3/day
MAU08	1	192.5
NAT01-1	6	1,155.
NAT03	3	577.5
NAT06-1	3	577.5

Additional modeling determined the maximum pump rate that can be sustained, with all wells pumped simultaneously, without drying up the area in the vicinity of any of the wells. These values are shown in Table 12.

Table 12. Maximum Simultaneous Pump Rates

Well	Pump Rate	
	gpm	ft^3/day
MAU08	.5	96.25
NAT01-1	5	962.5
NAT03	2	385
NAT06-1	3	577.5

Three scenarios were modeled to determine if pumping could reduce the contamination to levels required for natural flushing to complete the cleanup. Pump scenarios were done only for uranium since the cleanup time for uranium is considerable less than for vanadium. Table 13 specifies the pump rates used in each scenario.

Table 13. Pump Rates for each Scenario

Well	Pump Rate (gpm)		
	Run 1	Run 2	Run 3
MAU08	1	1	0.5
NAT01-1	1	2	5
NAT03	1	1	2
NAT06-1	1	2	3
Total	4	6	10.5

Table 14 below shows the maximum remaining concentration at selected years for the natural flushing case (i.e., no pumping) and the three pumping scenarios.

Table 14. Maximum Remaining Concentration for each Scenario

Years	Maximum Remaining Concentration (mg/L)			
	Natural Flushing	Run 1	Run 2	Run3
0	2.5220	2.5220	2.5220	2.5220
5	2.4266	2.4358	2.4476	2.5043
10	2.3683	2.3797	2.3954	2.4873
15	2.2993	2.3285	2.3519	2.4594
25	2.0257	2.1147	2.1884	2.4077
50	1.3047	1.3527	1.4707	2.0998
60	1.0439	1.0400	1.1552	1.9028
70	0.78606	0.75038	0.85610	1.6842
80	0.55612	0.51044	0.60078	1.4563
90	0.37134	0.33101	0.40296	1.2332
100	0.23654	0.20698	0.26095	1.0258

The results, particularly for Runs 2 and 3, seem contradictory. Intuitively, it seems that if an aquifer is pumped the maximum remaining concentration at any time would be less than without

any pumping. However, the results show just the opposite. In fact, as more water is extracted from the aquifer, the higher the maximum remaining concentration. Why is this?

Two factors contribute to and cause the unexpected results. These are the saturated thickness and the low hydraulic conductivity. If the pump rate is such that the aquifer water level is drawn down to the point that the aquifer in the vicinity of a well is almost dry, there is no water moving through the soil matrix. All the water that flows toward the well is extracted from the well. The cone of depression that develops around each well will leave much of the soil matrix dry, i.e., no water flows through the soil. With no water moving through the soil, the contamination adsorbed (attached to) the soil does not dissolve into the water. Figure 50 which shows the maximum remaining concentration at 100 years for Run 3 does indeed indicate that some of the alluvial aquifer has begun to dry up.

If these results are accurate, and there appears to be a logical explanation, then pumping does not appear to be a viable alternative for reducing the concentration of uranium and vanadium to the required levels such that 100 years of natural flushing would complete the cleanup. These results indicate that it is highly unlikely that an optimization model would yield significantly different results. Therefore, the money, time, and effort to develop such a model were not expended.

Plots of the remaining uranium concentration above the MCL at 100 years for each of the three scenarios are shown in Figures 48, 49, and 50. The areas of the model in the figures that do not have color (are white) are below the MCL.

8.0 Summary and Conclusions

A ground water flow and transport model was developed to evaluate if natural processes will reduce site-related COPC concentrations to regulatory levels in the alluvial aquifer within 100 years. Several different versions of the model were developed and employed to address conditions in the vicinity of the site. A steady state deterministic flow and transport model was used as the basis for the stochastic model. 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 does not appear to be an acceptable compliance strategy that allows natural processes to reduce uranium and vanadium concentrations in the ground water below the standards within 100 years. Arsenic concentration level will be reduced below the standard within 10 years. A steady state deterministic flow and transport model with pumping well was used to evaluate the feasibility of pumping for a period of time followed by natural flushing. This option does not appear to be a viable alternative.

The gravel mining operation upgradient of the former site has recently expanded and it is likely that there will be future expansions. This operation was not considered in the USGS flow model and subsequently not considered in the transport modeling. The recent and future expansion of this operation could significantly impact the ground water flow and the transport of contaminants. Without modeling the impacts from the gravel mining operation, the predicted concentrations of the COPC in this report are most likely underestimated.

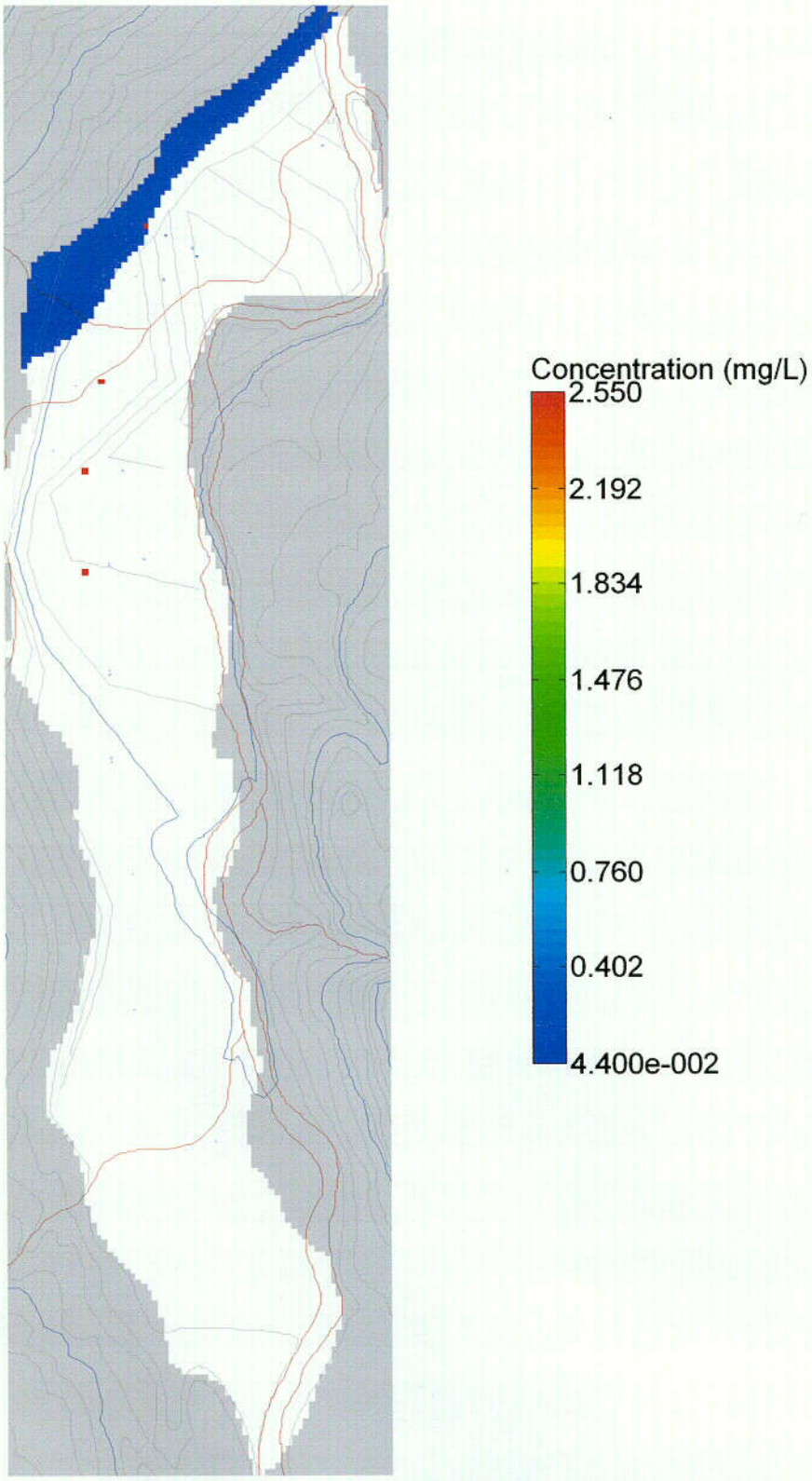

Figure 48. Uranium Concentration at 100 Years – Pump Scenario 1

C26

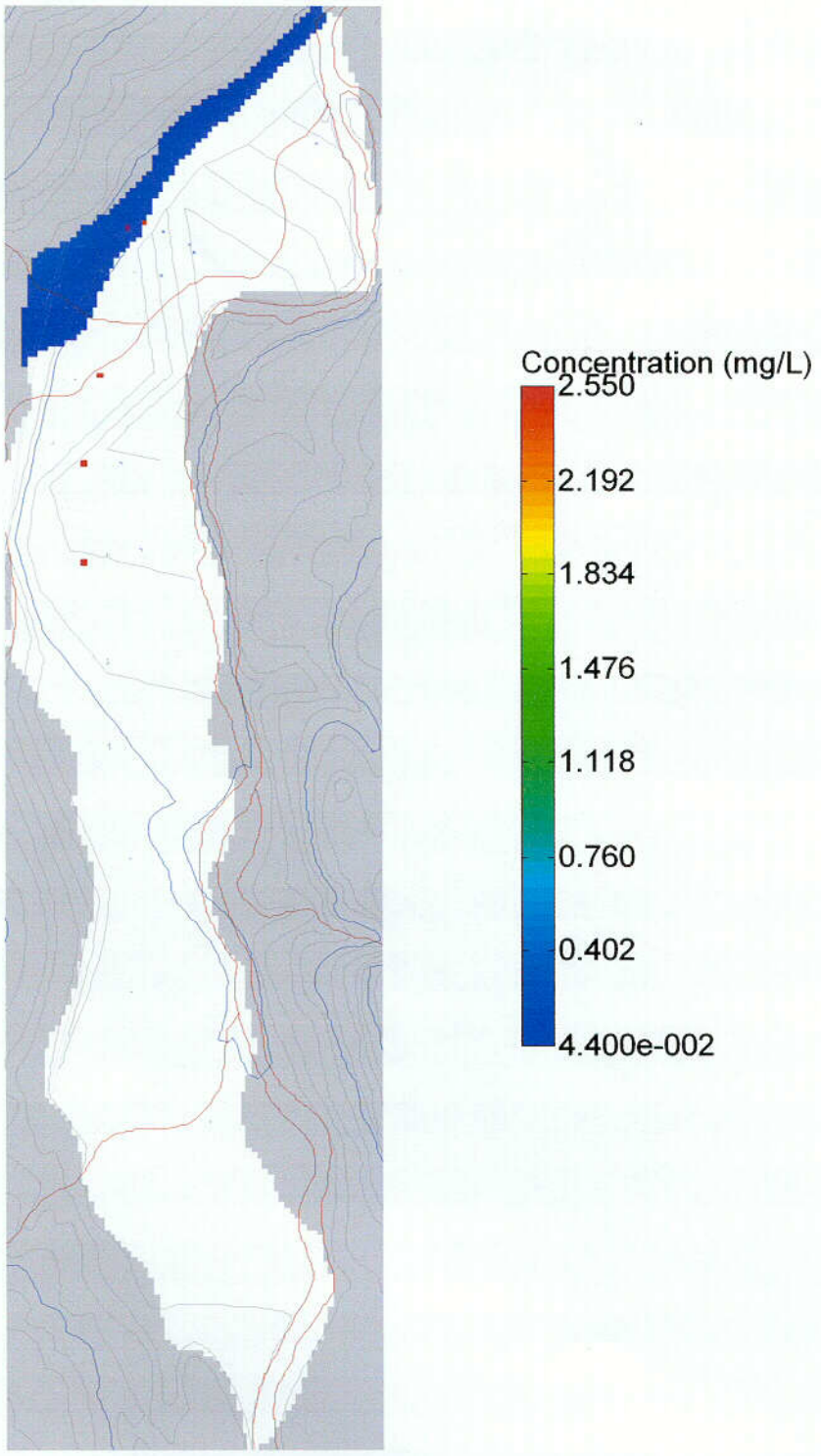

Figure 49. Uranium Concentration at 100 Years – Pump Scenario 2

C27

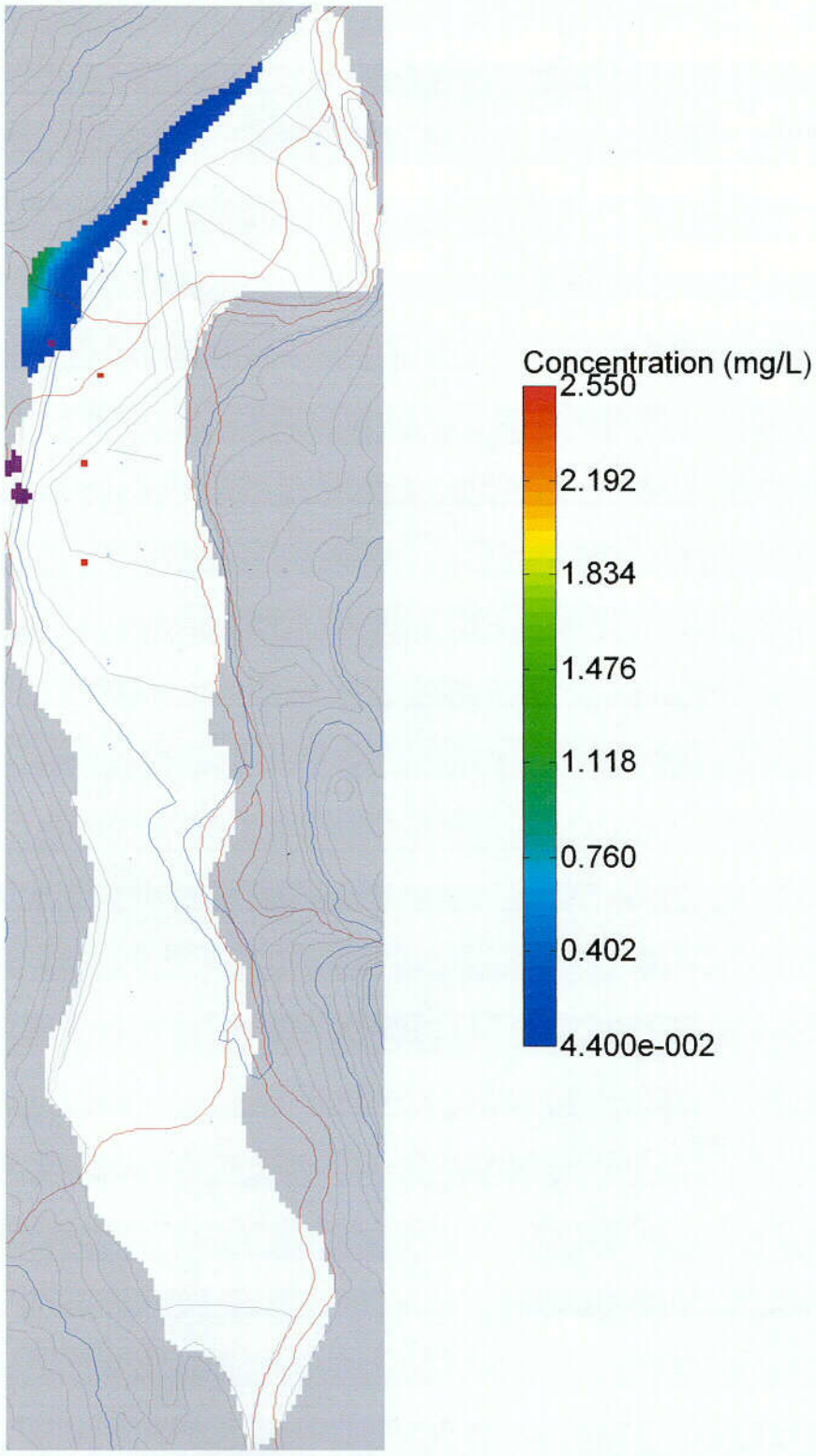

Figure 50. Uranium Concentration at 100 Years - Pump Scenario 3

C28

8.1 Qualitative Analysis

Ground water flow patterns predicted by the steady state deterministic flow model (Figures 5 and 6) and the steady state stochastic flow model (Figures 35 and 36) closely resemble the ground water gradient measured in February 2000. 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 1 and Figures 7 and 8 indicate that the calibrated steady state deterministic flow model satisfies the acceptance criteria and calibration objectives established before modeling. Calibration results presented in Figure 7 demonstrate that the flow model has a slight bias of underestimating water levels at the higher elevations. However, the target residuals are fairly evenly distributed, with 16 above and 25 below 0.0 ft, with a mean residual of –0.067 ft and an absolute mean residual of 0.737 ft. Results presented in Figure 8 demonstrate that the predicted hydraulic heads versus the observed heads fall on a straight line, as expected.

8.3 Model Predictions

Results of the steady state deterministic MT3DMS transport predictive simulations indicate that on average the maximum uranium concentration in the ground water at the Naturita site will not decrease to below the UMTRA Project MCL of 0.044 mg/L in 100 years (Figure 22).

The maximum predicted concentration after 100 years is 0.23654 mg/L. Results of the vanadium simulations show similar results. The maximum vanadium concentration in the ground water at the Naturita site will not decrease to below the risk-based concentration standard of 0.33 mg/L in 100 years (Figure 30). The maximum predicted concentration after 100 years is 4.3286 mg/L.

The maximum arsenic concentration in the ground water at the Naturita site will decrease to below the UMTRA Project MCL of 0.05 mg/L within 10 years. The maximum predicted concentration after 10 years is 0.045468 mg/L.

The steady state stochastic MT3DMS transport predictive simulations show similar results. Average uranium concentrations and the associated uncertainty at each time period of interest are based on 200 computer simulations. Figure 42 indicates that on average the maximum remaining concentration in the ground water (0.12087 mg/L) will not fall below the UMTRA Project MCL of 0.044 mg/L in 100 years. Furthermore, the stochastic simulations predict that at 100 years there is a 49 percent probability that the maximum concentration will be greater than the standard over a significant area of the alluvial aquifer (Figure 47). All these data suggest that there is a high probability that the remaining uranium concentration will exceed the standard, and natural flushing does not appear to be an acceptable compliance strategy.

The pumping followed by natural flushing modeling indicates that pumping water from the alluvial aquifer for a reasonable amount of time would not reduce the uranium and vanadium concentration to the required levels. Even after 25 years of pumping, the remaining uranium concentration is significantly higher than the concentration levels that would naturally flush within 100 years.

9.0 References

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

———, 1995. "Standard Guide for Documenting a Ground-Water Flow Model Application," ASTM D 5718-95, American Society for Testing and Materials.

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.

Freeze, R.A. and J.A Cherry, 1979. *Groundwater*, Prentice-Hall, Inc., Englewood Cliffs, New Jersey.

Fetter, C.W., Jr., 1980. *Applied Hydrology*, Charles E. Merrill Publishing Co., Columbus, Ohio.

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

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.

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, *Baseline Risk Assessment of Ground Water Contamination at the Uranium Mill Tailings Site Near Naturita, Colorado*, DOE/AL/62350-195, Rev. 1, U.S. Department of Energy, Grand Junction Office, Grand Junction, Colorado, November.

———, 2000a. *Contaminants in Subpile Soils, UMTRA Ground Water Project, Gunnison, Colorado, Site*, ESL-RPT-2000-09, prepared by MACTEC Environmental Restoration Services, LLC for the U.S. Department of Energy, Grand Junction Office, Grand Junction, Colorado.

———, 2000b. *Determination of Distribution Ratios, UMTRA Ground Water Project, Gunnison, Colorado, Site*, ESL-RPT-2000-04, prepared by MACTEC Environmental Restoration Services, LLC for the U.S. Department of Energy, Grand Junction Office, Grand Junction, Colorado.

Zheng, C., 1990. *MT3D, A Modular Three-Dimensional Transport Model, Documentation and User's Guide*, First Edition, S.S. Papadopulos and Associates, Inc., Bethesda, Maryland.

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 Groundwater Systems, Documentation and User's Guide*, Department of Geological Sciences, University of Alabama, Tuscaloosa, Alabama.

Appendix G

Data Set Used in Pattern Recognition Modeling

Table 1. Chemical, physical, and isotopic data used in pattern recognition modeling at the Naturita study site. Data were collected and analyzed by the U.S. Geological Survey during June 2000.

[Al, aluminum; Alk, alkalinity as calcium carbonate; B, boron, Br, bromide; Ca, calcium; Cl, chloride; DO, dissolved oxygen; Fe, iron; K, potassium; Mg, magnesium; Na, sodium; ORP, oxidation reduction potential; Si, silicon; SO4, sulfate; SC, specific conductance; Sr, strontium; T, water temperature; U, uranium; V, vanadium; $\delta^{18}O$, delta oxygen-18; δD, delta deuterium; mg/L, milligrams per liter; µg/L, micrograms per liter; µS/cm, microsiemens per centimeter; mV, millivolts; deg. C, degrees Celsius; permil, parts per thousand]

Sample site	Al, mg/L	Alk, mg/L	B, mg/L	Br, mg/L	Ca, mg/L	Cl, mg/L	DO, mg/L	Fe, mg/L	K, mg/L	Mg, mg/L	Mn, mg/L	Na, mg/L	ORP, mV	pH, units	Si, mg/L	SO_4, mg/L	SC, µS/cm	Sr, mg/L	T, deg. C	U, µg/L	V, µg/L	$\delta^{18}O$, permil	δD, permil
DM1	0.29	227	0.04	0.1	54.1	4.7	0.35	0.29	1.85	20.3	0.32	18.2	-67	7.12	4.64	131	589	0.83	14.2	4.32	0.04	-105.58	-14.71
DOE547	0.28	160	0.04	0.1	64	11.5	0.33	0.07	1.65	28.1	0.26	32.8	120	7.1	4.5	308	864	1.11	15.3	4.66	0.04	-83.36	-9.2
DOE548	0.39	326	0.1	0.24	157	39	0.3	0.18	9.38	47.3	1.57	134	-23	7.21	6.93	566	1660	1.95	13.2	907	0.13	-99.78	-13.71
MAU01	0.41	502	0.12	25.4	224	148	0.6	0.03	21.9	106	0.89	259	221	6.8	8.46	950	2890	4.8	14	710	0.04	-97.46#	-12.82#
MAU02-2	0.32	359	0.08	1.49	180	49	0.27	0.36	8.47	52.6	3.07	127	44	6.9	6.74	597	1820	2.34	13.7	646	0.04	-100.22	-13.52
MAU02-3	0.32	365	0.08	1.57	179	53	0.32	0.44	8.91	56.6	3.93	128	69	6.95	7.09	611	1880	2.48	12.1	535	0.04	-99.8	-13.52
MAU03	0.28	229	0.04	0.07	60.2	8	0.73	0.12	2.15	26.8	1.12	27.3	116	7.12	6.31	210	818	1.1	14.6	106	0.04	-105.0	-14.39
MAU04	0.29	269	0.06	0.14	61.8	15	0.25	1.32	2.62	33.1	1.35	38.4	-76	6.95	7.01	233	945	1.18	15.1	172	0.04	-102.62#	-14.11#
MAU05	0.37	369	0.09	0.55	193	57	0.4	0.75	6.81	55.2	4.84	141	-8	6.99	7.22	639	1900	2.52	*12.9	331	0.04	-100.5	-13.48
MAU06	0.29	221	0.04	0.15	60.7	8.2	1.05	0.25	2.95	29.4	0.42	20.8	95	7.17	6.43	219	807	1.18	11.9	62.3	0.04	-104.96	-14.28
MAUO7	0.36	397	0.1	0.36	193	70	0.32	1.88	5.5	65.6	1.59	136	-64	6.83	7.56	614	1910	2.64	14.7	525	0.04	-96.98	-13.26
MAU08	0.41	464	0.11	15.4	273	262	1.64	1.52	40.2	93.8	1.35	374	1	6.9	6.99	1200	3550	4.69	13.1	1660	0.04	-94.4	-12.71
NAT01-1	0.37	359	0.14	0.58	214	80	0.26	1.53	11.4	64.1	2.1	231	-68	7.1	6.93	904	2380	2.59	13.1	1230	0.04	-99.3#	-12.87#
NAT01-2	0.38	346	0.14	0.42	222	82	0.21	2.46	12.2	66.3	2	230	-68	7.11	7.11	924	2400	2.92	19.6	1200	0.04	-99.3#	-12.87#
NAT02	0.28	314	0.08	9.15	131	17	0.86	0.09	36.9	36.6	0.33	63.8	-23	7.25	5.14	376	1290	1.59	15	439	2.25	-100.38	-13.49
NATO3	0.36	365	0.12	11.8	194	50	0.34	0.04	20.7	59.3	0.94	178	-18	7.17	7.92	734	2060	2.29	14.9	1030	4.88	-99.33	-13.43
NAT04-1	0.39	389	0.11	0.4	195	40	0.43	0.03	13.2	55.1	0.81	159	171	7.02	7.36	686	1900	2.2	12.8	697	2.78	-96.57	-13.02
NAT04-2	0.35	361	0.1	0.58	195	40	0.29	0.03	12.1	54.6	0.78	156	143	7.01	7.33	686	1900	2.2	13.3	684	2.9	-96.57#	-13.02#
NAT04-3	0.41	371	0.1	0.4	194	40	0.29	0.03	12.1	54.6	0.78	155	137	7.01	7.35	688	1890	2.18	13.5	678	2.93	-96.57#	-13.02#
NAT05	0.38	405	0.15	0.4	184	140	0.64	0.05	13.4	82.3	1.25	366	22	7.12	8.42	1110	3040	3.3	14.5	1540	4.54	-99.23	-13.17
NAT06-1	0.39	401	0.14	0.46	224	68	0.3	0.14	20.1	66.8	1.03	247	-29	6.95	7.83	970	2510	2.62	13.4	1170	2.57	-100.7#	-13.59#
NAT06-2	0.34	401	0.13	0.46	225	64	0.27	0.03	20.2	65.8	1.1	243	23	6.92	7.81	962	2510	2.61	13.5	1160	3.17	-99.37#	-13.45#
NAT07-1	0.29	330	0.07	1.3	150	22	0.28	0.06	11.2	36.2	0.56	78.8	46	7.11	6.17	403	1330	1.33	13.9	509	1.87	-101.81#	-13.76#
NAT07-2	0.32	326	0.07	0.9	151	21.5	0.28	0.05	10.6	36.1	0.52	77.9	75	7.09	6.12	402	1330	1.33	14.4	493	2.07	-100.65#	-13.69#

NAT07-3	0.31	324	0.08	0.79	152	21.5	0.34	0.03	9.8	36.7	0.48	77	98	7.1	6.2	404	1370	1.36	14.6	493	2.23	101.23#	-13.72#
NAT08	0.29	379	0.11	0.4	189	50	0.26	0.05	16.4	58.7	1	176	-50	7.16	7.75	724	2030	2.24	13.3	1010	5.65	-101.97	-13.57
NAT09	0.33	379	0.11	1.36	195	54	0.54	0.03	16.1	61.3	0.81	182	54	7.13	8.09	750	2080	2.47	14.3	1050	4.54	-100.98	-13.53
NAT10	0.32	389	0.12	1.62	217	60	0.32	0.05	19.9	63.1	0.91	208	-37	7.1	7.77	862	2300	2.49	13.3	1080	5.51	-101.18	-13.44
NAT11	0.37	389	0.14	4.8	227	66	0.31	0.05	17.2	69.5	1.99	248	19	6.96	8.16	992	2560	3.2	13.4	994	1.64	-102.17#	-13.34#
NAT12-1	0.31	407	0.17	1.98	204	126	0.82	0.05	7.72	75.2	2.56	331	115	7.06	6.93	1100	2980	3.32	14.2	1120	0.04	-95.74#	-12.56#
NAT13-1	0.36	415	0.12	0.42	217	62	0.31	0.3	16.4	64.8	1.97	235	-35	7.07	7.93	922	2390	2.91	13.3	983	1.85	-97.3	-13.08
NAT13-2	0.32	409	0.12	0.58	213	58	0.27	0.75	14.9	68	1.92	233	-76	7.06	8.35	934	2400	3.15	13.8	955	1.59	-96.86	-12.95
NAT13-3	0.38	415	0.15	0.64	221	60	0.2	1.15	12.9	71.6	1.88	233	-59	7.07	8.59	958	2410	3.55	14.3	918	1.47	-96.01	-12.89
NAT14-1	0.38	413	0.12	0.44	219	56	0.24	0.27	14.8	67.7	1.93	229	-49	7.05	8.24	930	2390	3.12	13.7	949	2.5	-97.07	-12.86
NAT14-2	0.32	415	0.13	0.54	220	56	0.23	0.34	14	69.4	1.91	228	-52	7.05	8.42	934	2430	3.26	13.9	933	2.36	-96.42	-12.84
NAT14-3	0.28	413	0.15	0.52	223	58	0.23	0.32	13.5	73	1.93	230	-64	7.07	8.73	972	2470	3.37	14.5	908	2.11	-97.22	-12.87
NAT15-1	0.29	452	0.15	0.42	184	132	0.37	0.38	14	81.8	1.32	352	-37	7.12	8.49	1100	3010	3.27	13.8	1510	4.48	-98.48#	-12.97#
NAT15-2	0.31	425	0.14	0.52	183	138	0.3	0.07	14.2	82.2	1.25	362	-88	7.14	8.49	1120	3090	3.32	13.7	1550	5.23	-98.48#	-12.97#
NAT15-3	0.28	407	0.14	0.52	183	136	0.28	0.11	14.2	82	1.25	359	-58	7.14	8.51	1110	3110	3.28	14.4	1560	5.16	-98.48#	-12.97#
NAT16-1	0.3	361	0.09	0.36	191	39	0.27	0.29	12.7	54.7	0.79	152	41	6.98	7.32	686	1900	2.15	13.5	669	3.1	-101.17#	-13.35#
NAT16-2	0.31	365	0.09	0.43	190	38	0.25	0.22	12.5	54.5	0.78	152	-20	6.99	7.34	684	1900	2.17	13.9	675	3.19	-101.17#	-13.35#
NAT16-3	0.28	361	0.09	0.48	195	38	0.27	1.22	12.7	55	0.77	153	-97	6.98	7.35	684	1900	2.18	14.1	685	2.41	-101.17#	-13.35#
NAT17-1	0.3	373	0.05	0.29	210	35	0.25	0.28	5.16	59.1	1.31	146	-15	6.9	6.05	726	1920	2.36	13.6	90.8	0.33	-94.5	-12.67
NAT17-2	0.28	381	0.06	0.45	207	35	0.24	0.64	5.46	58.9	1.27	146	-57	6.92	6.13	723	1910	2.33	13.4	91.9	0.21	-93.16	-12.66
NAT17-3	0.36	369	0.07	0.7	205	41	0.29	0.33	6.6	61.2	1.1	153	-13	6.92	6.25	735	1950	2.55	14.3	102	0.29	-94.98	-12.68
NAT18-1	0.36	385	0.06	0.25	209	41	0.33	0.06	5.8	60.7	1.16	152	85	6.86	6.18	735	1960	2.49	14.6	90.9	0.55	-94.27	-12.63
NAT18-2	0.36	369	0.05	0.3	209	36	0.28	0.17	5.08	59.5	1.28	147	21	6.89	6.05	730	1930	2.38	13.4	86.6	0.37	-95.38	-12.69
NAT18-3	0.36	365	0.06	0.27	211	34	0.26	0.31	4.97	59.1	1.31	147	-14	6.86	6.06	722	1920	2.37	13.4	91	0.3	-94.62	-12.65
NAT19	0.32	353	0.07	0.2	207	36	0.69	0.24	4.72	59.4	1.26	145	20	6.91	6.01	722	1960	2.35	14.1	85.4	0.31	-93.54	-12.63
NAT20	0.28	231	0.05	0.12	64.1	11	0.43	0.17	2.55	30.9	0.04	40.7	79	7.1	5.17	324	963	1.19	14.4	12.9	0.04	-85.4	-9.9
NAT21-1	0.3	274	0.05	0.1	65.6	10.5	0.32	0.43	2.71	31.6	0.04	42.2	-14	6.97	5.32	320	1020	1.23	14.4	13.7	0.04	-90.52	-10.93
NAT21-2	0.28	239	0.05	0.1	64.2	10.5	0.3	0.03	2.65	31.5	0.04	42.1	-34	6.99	5.33	319	1020	1.22	15.5	12.9	0.04	-89.09	-10.72
NAT22-1	0.28	261	0.05	0.1	64.9	10.5	0.28	0.5	3.34	31.5	0.04	42.5	68	6.94	5.43	319	1020	1.22	14.9	14.9	0.04	-90.89	-11.1
NAT22-2	0.28	253	0.05	0.11	64.6	10.5	0.25	0.03	2.7	31.2	0.04	42.8	67	6.96	5.36	318	1020	1.22	15.4	14.6	0.04	-89.57	-11.03
NAT23	0.33	332	0.1	0.34	168	43	0.52	0.11	9.99	45.7	0.12	135	57	6.76	7.26	577	1730	2.03	15.4	710	0.04	-100.99	-13.69
NAT24	0.29	340	0.11	0.48	170	54	0.37	0.33	11.9	51.1	1.47	170	23	6.94	6.94	658	1910	2.04	12.4	945	0.04	-98.51#	-13.28#
NAT25	0.42	515	0.14	0.98	228	292	0.37	0.66	12	73.1	0.34	532	-28	6.88	6.99	1250	3870	3.7	12.5	1840	0.04	-94.03	-12.47
NAT26	0.35	549	0.43	4.8	195	632	0.68	0.03	23.1	91.4	0.35	912	146	7.05	6.02	1690	5720	4.54	13.8	2410	0.04	-91.25#	-11.94#
NAT27-1	0.28	312	0.09	24	137	71	0.23	0.04	9.61	53.1	0.97	74.9	65	7.28	6.38	435	1750	2.57	15.2	237	0.26	-99.27	-13.31
NAT27-2	0.29	300	0.11	26	148	73	2.76	0.03	12.4	59.9	0.62	84.4	122	7.32	6.76	440	1620	3.21	18.3	218	0.13	-99.16	-13.18

NAT28-1	0.3	304	0.08	47	111	47	0.24	0.04	26.8	47.7	1.24	65.9	66	7.3	6.37	446	1570	2.58	15.1	248	0.12	-99.96	-13.38
NAT28-2	0.28	302	0.1	41	128	39	1.57	0.03	26.2	55.5	1.36	70.3	112	7.32	6.86	425	1570	3.27	18.4	245	0.05	-100.39	-13.34
NAT29	0.37	300	0.15	11.5	183	42	4	0.04	8.9	68.5	0.85	81.4	176	7.17	8.38	580	1650	5.22	*16.75	258	0.04	-98.46	-13.35
NAT30-1	0.3	292	0.05	0.1	116	11	0.36	0.19	2.85	32.7	0.87	45	28	6.97	6.36	324	1080	1.4	15.3	15	0.04	-89.41	-12.11
NAT30-2	0.28	308	0.05	0.1	120	11	0.6	0.17	2.94	33	0.83	45.2	26	6.94	6.46	327	1110	1.4	15.7	16.2	0.04	-90.13	-12.02
SM1	0.29	71	0.04	0.08	35.6	1.72	7.64	0.03	0.93	6.77	0.04	4.96	78	8.54	2.66	64.8	241	0.4	16.6	0.84	0.04	-106.89#	-14.29#

* Actual data missing, value estimated from adjacent wells during June 2000 sampling period.
# Actual data missing, value substituted from March 2000 data or set equal to value at the adjacent sample point in each multi-completion well cluster.

THIS PAGE IS AN OVERSIZED DRAWING OR FIGURE,

THAT CAN BE VIEWED AT THE RECORD TITLED:

PLATE 1
Naturita Base Map w/Aerial Photo
April 15, 2001

WITHIN THIS PACKAGE

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