Stochastic Model to Estimate Travel Times From the 52nd Street Facility in Phoenix, AZ

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Abstract: A stochastic approach, which consisted of varying hydraulic conductivity in a two-dimensional flow and advective transport model using the codes MODFLOW and MODPATH, was used to estimate travel times in the alluvial aquifer from the former Motorola 52nd Street facility in Phoenix, AZ. The model results demonstrate that contaminant sources other than the 52nd Street facility are required to explain the observed contamination at the Frazee Deer-O wells (and at wells further west) because a source at the 52nd Street facility could not have resulted in contaminant migration to this area by 1983-1986, when trichloroethene (TCE) concentrations were first observed. In addition, the model results demonstrate that contamination from a source at the former 52nd Street facility could not have migrated into the Operable Unit 3 (OU3) area before the start up of the Operable Unit 2 (OU2) remedy.

Key words: geostatistics, stochastic analysis, flow model, particle tracking, advective travel time

1. Introduction

Groundwater contamination by TCE was first discovered in the central Phoenix area in the early to mid-1980s. Numerous industrial facilities in the Central Phoenix Area have had documented releases into the environment [1]. Little investigation of the nature and extent of contamination that may have emanated from these facilities has been conducted to date. In 1983, extensive source area investigations were conducted at the former Motorola facility located at 52nd Street and McDowell Road (Figure 1). Pump-and-treat of contaminated groundwater on the former Motorola facility began in the source area in 1986 with pilot treatment plant operations. A full-scale Operable Unit 1 (OU1) remedy has captured contaminated groundwater east of approximately 46th Street (over 3600 feet down gradient of the source area) since its operation was initiated in 1992, discontinuing contaminant migration to the west of this hydraulic barrier. In 2001, the OU2 groundwater remedy was initiated. The OU2 remedy, located over 3 miles down gradient of the OU1 remedy, captures contaminated groundwater east of approximately 20th Street.

The objective of this advective particle tracking evaluation is to determine: (1) if volatile organic compound (VOC) concentrations observed at the Frazee Deer-O facility in the western portion of OU2 in 1986 could be explained by a source from the former Motorola 52nd Street facility; and (2) whether contamination originating at the former Motorola facility could have migrated into the OU3 area prior to the start of operations of the OU2 groundwater remedy. Motorola began limited operations at the former 52nd Street facility in 1957. In 1963, Motorola established a bulk chemical distribution center in the Courtyard and a dry well was installed that received releases of solvents. The dry well was abandoned in 1974. While knowledge of releases can be dated back to 1963, to be conservative in this particle tracking analysis, it was assumed that releases from the former 52nd Street facility began at the start of operations in 1957.

2. Model Description

The model uses the codes MODFLOW [2] to simulate flow and MODPATH [3] to simulate advective transport in the alluvium at the site. Flow in the bedrock was not simulated because of the low hydraulic conductivities measured in bedrock throughout the study area. The groundwater flow model is a steady-state, two-dimensional groundwater flow and advective transport model. It contains one layer, 60 rows, and 115 columns (Figure 1). The grid spacing is 200 feet and is uniform. The model grid is 23,000 feet by 12,000 feet in dimension. The model grid is oriented 23.75 degrees anticlockwise to be parallel to the regional flow direction. The western boundary of the model extends slightly beyond the OU2 extraction wells. The bottom of the model is the bedrock surface [4, 5], which agrees with the bedrock surface depicted by Arizona Department of Environmental Quality (ADEQ). The model is unconfined, thus, the top of the model is the water table. Within the model domain are bedrock ridges that have been buried by sediments. These buried bedrock ridges exert a local influence on groundwater flow and associated contaminant transport in the alluvium. The areas in the model where the bedrock ridges extend above the water table become dry cells, which are treated as no-flow cells.

The north and south edges of the model domain are approximate groundwater flow paths. Because groundwater cannot flow across a flow path, the north and south edges of the model were set as parallel no-flow boundaries. The east edge of the model domain is a constant head boundary set to 1200 feet above mean sea level, and the west edge of the model domain is a specified head boundary simulated with the drain package, which varied in elevation from 1022.5 to 1032.5 feet above mean sea level (Figure 1). These boundaries produced a maximum of 177.5 feet in hydraulic head relief across the model domain, yielding a hydraulic gradient across the grid of 0.008 feet per foot. The drain package was used for the west boundary because it only allows water to leave the model. The conductance factor for the drain cells was set high enough that it did not impede the flow of water out of the western model boundary.

The hydraulic heads used for these boundaries were based on the observed hydraulic gradient in the 1997 potentiometric surface. The 1997 potentiometric surface was used because of the extensive hydraulic head measurements available at that time. Hydraulic heads have dropped throughout the area during the time of interest (1950s to present), but the hydraulic gradient has remained relatively constant. Particle travel times are dependent on groundwater velocities, which are in turn dependent on hydraulic gradients rather than absolute head values; thus, the travel time results are independent of the uniform hydraulic head changes.

There are two Salt River Project (SRP) pumping wells within the model domain (Figure 1). Because the model is a steady-state groundwater flow model and does not consider variations with time, average pumping rates were used. The two SRP wells were set to pump at their 1965 through 1984 twenty-year average annual rates of 148,289 cubic feet per day (770 gpm) for Well SRP16.9E-6N and 51,013 cubic feet per day (265 gpm) for Well SRP18E-5N. These pumping wells have a local influence on the hydraulic gradients near these wells.

The contaminant source was simulated by four particles evenly distributed in the model cell containing the “Courtyard” source area. As shown in Figure 1, a row of well cells (artificial wells in the finite-difference grid used to capture the particles) was used as a particle capture zone extending 2000 feet north and south of the Frazee Deer-O wells near 24th Street, covering the majority of the width of the measured contaminant plume at that location. In the model runs, these well cells pumped at a low rate of one cubic foot per day (0.005 gpm), and thus did not significantly alter hydraulic gradients or groundwater flow. A second, similar row of capture wells (Figure 1), approximately 2,700 feet west of the row representing the Frazee Deer-O location, was used to represent the OU2 extraction wells (near 20th Street). Only one row of wells was used as a particle capture zone depending on whether the focus of the simulation was on the Frazee Deer-O location or the OU2/OU3 location.

Both sorption and biodegradation were not represented in the particle tracking analysis, which is a conservative assumption. The effect of sorption and resulting plume retardation is to lengthen travel times. Biodegradation would limit plume length as TCE would disappear as it migrated down gradient. Mechanical dispersion results from mixing that occurs largely due to heterogeneities in hydraulic conductivity [6] that generally are not accounted for in a mean advective calculation. In the stochastic analysis presented here, the effect of heterogeneities in hydraulic conductivity has been considered by the multiple realizations of hydraulic conductivity and by examining the distribution of travel times both above and below the mean travel time. Thus, significant aspects of mechanical dispersion have been accounted for in the analysis.

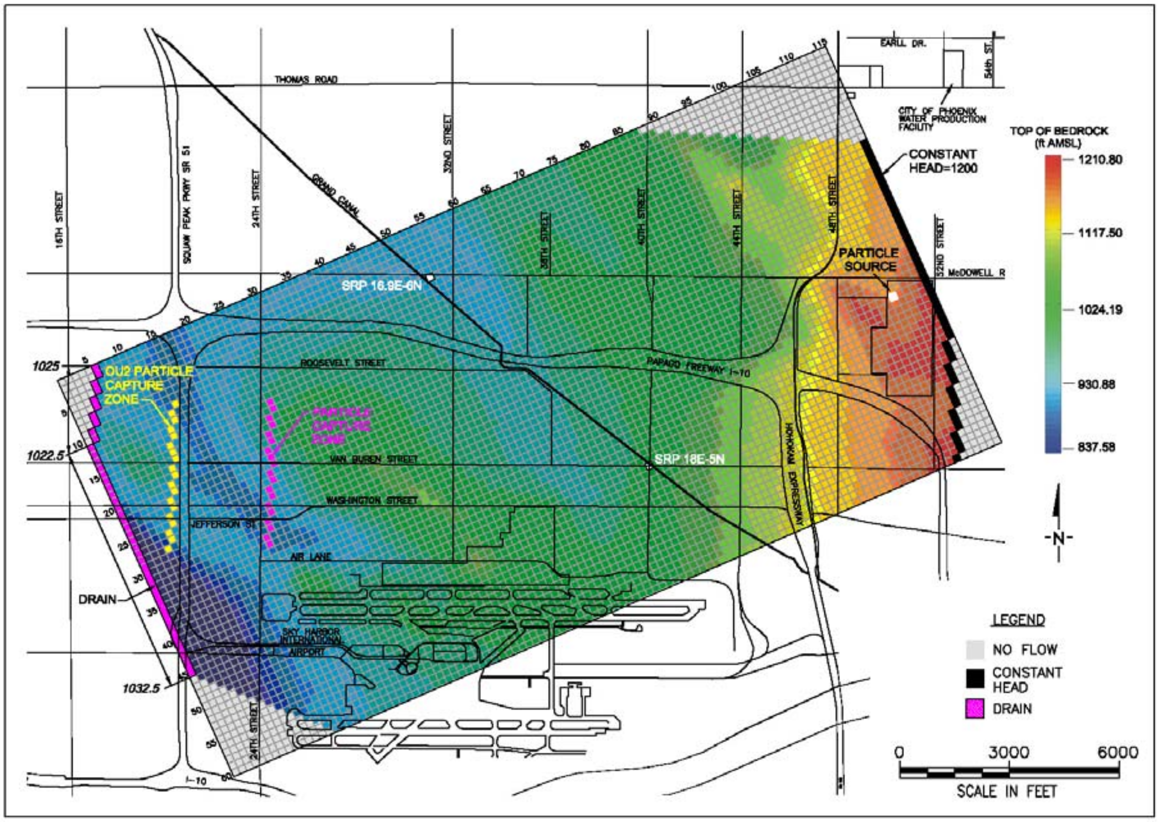

Figure 1. Model grid, boundary conditions, and bedrock surface.

3. Stochastic Analysis and Conditioning

This stochastic analysis focuses on the hydraulic conductivity field. A variogram (semivariogram) model analysis was performed to estimate the spatial correlation of hydraulic conductivity measurements within the Salt River Gravel and basin fill units. To perform the semivariogram analysis, a distribution of hydraulic conductivity is required. Hydraulic conductivity, which can vary over several orders of magnitude, can be assumed to have a log normal distribution [7]. For this semivariogram analysis, a log transformation was performed initially by taking the log (base 10) of the hydraulic conductivity data and a separate variogram analysis was performed for each unit (Salt River Gravels and basin fill). Because of its better statistical match to the log transformed data in each unit, an exponential variogram model was selected and used.

The code FIELDGEN [8] was used to generate multiple possible hydraulic conductivity distributions (realizations) using kriging of the measured data. The geostatistical fields of hydraulic conductivity values used in the model were generated by log normal kriging, using the log transformed measured hydraulic conductivity values as data points. Kriging was conducted independently for two zones representing the two geologic units. The Salt River Gravel (SRG) zone was primarily west of the Grand Canal; and the basin fill (BF) zone was primarily east of the Grand Canal. The same grid was used in kriging and in the flow model simulations. The means and variances for hydraulic conductivity in the two zones were calculated from all available measurements for the respective geologic unit in the zone, a total of 34 measurements. There were 14 data points in the SRG zone and 20 data points in the BF zone.

Figure 2 shows the data points used for kriging and their hydraulic conductivity values as well as the Salt River Gravel and basin fill zones. Two control points, one in each zone, were used at the south edge of the model due to lack of data in this area. These control points constrained the kriging by using realistic hydraulic conductivity values for areas where no data exist. In the southwest corner of the model, a control point with a value of 250 feet per day was used in the SRG zone, representing a pump test result conducted nearby and west of this area near the 19th Avenue Landfill (Clear Creek Associates, written communication, October 2005 Figure showing measured hydraulic conductivity); [9, 10]. In the southeast corner of the model, a control point with a value of 30 ft/d was used in the BF zone, which represents approximately the mean hydraulic conductivity for the basin fill. Including these control points resulted in a total of 36 point hydraulic conductivity values for kriging, 15 in the SRG zone, and 21 in the BF zone.

Figure 2 also shows the geostatistically generated hydraulic conductivity distribution, which resulted in nearest-to- the-mean travel time. The kriging was performed separately for each zone (BF and SRG) with an exponential semivariogram having a sill equal to the variance of the log-transformed hydraulic conductivity values of each zone and a range of 8000 ft. The variance of the logs of the measured hydraulic conductivities for the geologic unit was used as the sill. For the hydraulic conductivity values in the BF and SRG zones, the mean and variance of the log transformed data were used as kriging parameters in FIELDGEN and are shown in Table 1.

The stochastic kriging process created statistically valid realizations of possible hydraulic conductivity distributions, but not all of these realizations were hydrogeologically plausible. The realizations had to be filtered by test criteria to determine which were plausible and which were not, in a process called conditioning. In order to eliminate hydraulic conductivity distributions that produced unrealistic flow fields, the geostatistical realizations were conditioned by discarding any realization in which one or more particles of the four particle set were not captured by the particle capture zone described above (i.e., particles that passed to the south or north of the observed plume location). In addition, any realization where a particle was obstructed by passing to the south of the bedrock ridge west of the Honeywell facility or was impacted by pumping at the SRP wells were also discarded. If all realizations been included, longer travel times would have resulted. Therefore, the conditioning process was conservative. As a result of conditioning, the hydraulic conductivity realizations in which the particles approximately followed the path of the measured contaminant plume remained. Of the total 220 hydraulic conductivity realizations that were tested, 20 were discarded and 200 were saved to produce 200 accepted travel time realizations.

4. Results

Figure 3 presents a log histogram of travel time using each of the 200 accepted realizations, which contained four particles with a total of 800 particle travel time values. As evident, none of the travel times reach the Frazee Deer-O well in the required time frame of 29 years (1957 to 1986). The distribution shows a tendency toward a central mean that is expected with a large number of samples. The geometric mean advective travel time from the Courtyard source area to the particle capture zone near 24th Street was 48.3 years, with a confidence interval (1σ) of +5.49/-4.93 years. The model calculated heads and particle paths for the realization with the nearest-to-the-mean travel time are shown in Figure 4. The minimum travel time to the Frazee Deer-O wells near 24th Street was 37.4 years and the maximum travel time was 71.1 years. Median travel time for the 800 particles was 48.5 years. The geometric mean travel time for the 159 particles that passed through saddles in the bedrock ridge was 52.0 years (+4.75/-4.36) to the Frazee Deer-O wells near 24th Street, as opposed to 47.5 years (+5.23/-4.71) for the 641 particles that passed north of the bedrock ridge. The difference in these mean travel times is 4.53 years.

The TCE source is assumed to start in 1957. Hence, whether the earliest travel time (37.4 years) or the geometric mean travel time (48.3 years with a confidence interval (1σ) of +5.49/-4.93 years) is used, particles reached the Frazee Deer-O wells for the first time by either 1994-95 (using the earliest travel time) or 2005-06 (using the mean travel time). As noted above, TCE was detected in 1986 in the Frazee Deer-O wells, and contamination at these locations likely occurred even earlier. The model results demonstrate that other contaminant sources are required to explain the observed contamination because a source at the former 52nd Street facility could not have resulted in contaminant migration to these areas by 1986.

Approximately 2,700 feet down gradient of the Frazee Deer-O wells is a row of capture wells that represents the OU2 groundwater extraction wells.

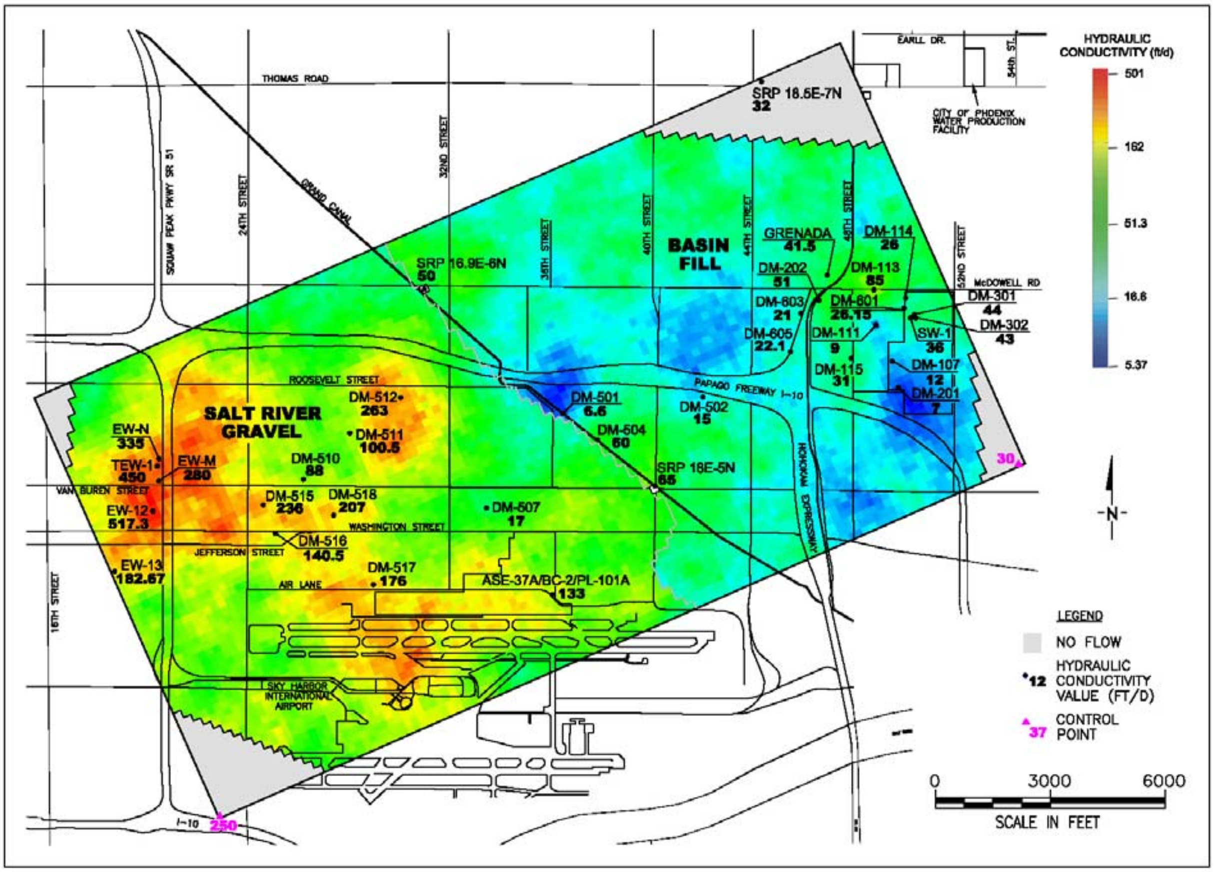

Figure 2. Example kriged hydraulic conductivity field and data points.

Table 1: Geostatistical Model Properties

Zone Name	Salt River Gravel	Basin Fill
Log of Hydraulic Conductivity (ft/day)		
Mean	2.25	1.44
Variance	0.127	0.103
Kriging Parameters		
Data Points	15	21
Nugget	0	0
Semivariogram	0.127	0.103
Range	8000	
Anisotropy	0	
Type	Exponential	
Transform	log	

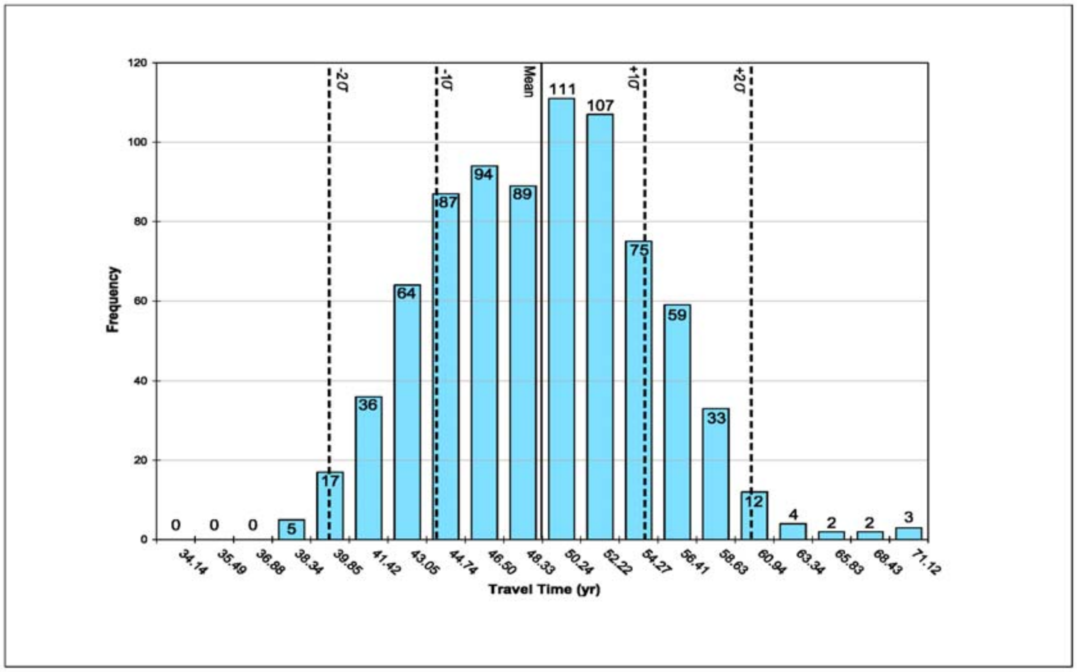

Figure 3. Histogram of advective travel times.

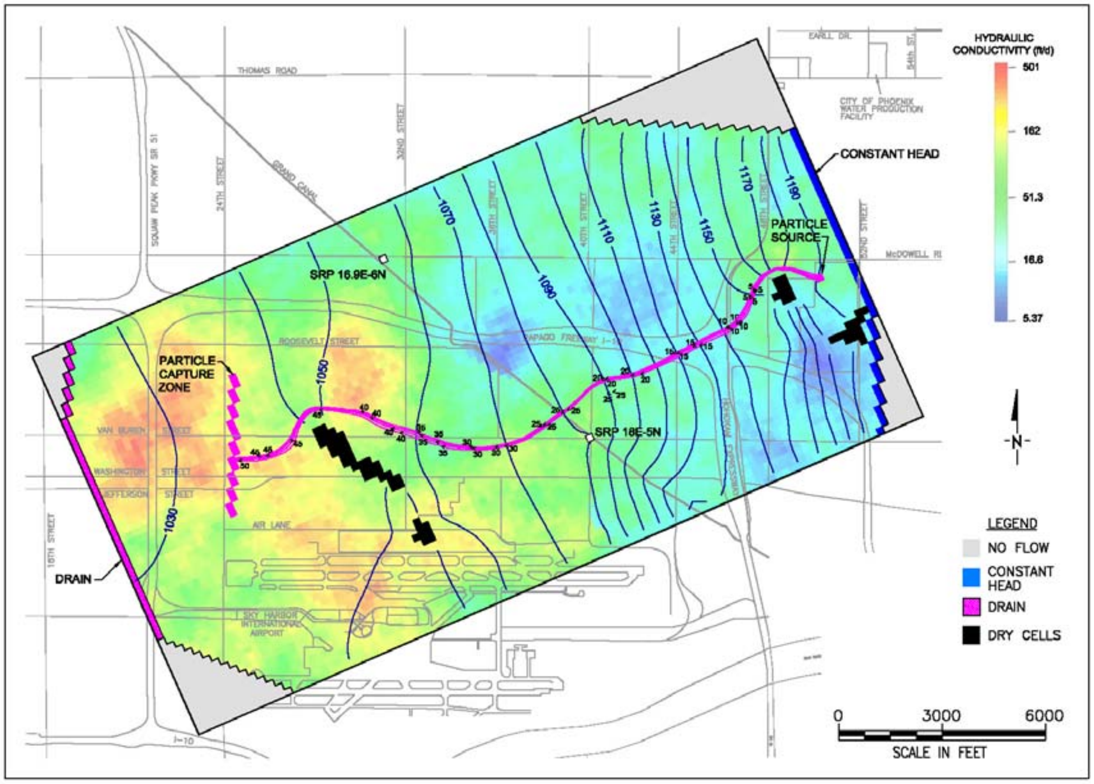

Figure 4. Model results for mean realization.

To approximate the travel time to the OU2 capture wells, five realizations with travel times nearest the mean travel time were used from the previous simulation. The average travel time to the OU2 capture wells for these five realizations was 54.1 years or by calendar year 2011. This date is significantly after the start of operations of the OU2 groundwater extraction wells in 2001. The model results demonstrate that contamination from a source at the former 52nd Street facility (assuming a Courtyard source as if it had occurred in 1957 instead of 1963) could not have migrated into the OU3 area before the OU2 remedy was put into place.

A sensitivity analysis was conducted for effective porosity and hydraulic gradient (Table 2). Instead of performing a sensitivity analysis on all 200 accepted realizations, the sensitivity was performed on the realization (1) with the minimum travel time (“minimum realization”), (2) with the maximum travel time (“maximum realization”), and (3) nearest to the mean travel time (“mean realization”). The sensitivity of effective porosity was examined using values of 20, 23, 27, and 30 percent, for comparison to the base case of 25 percent. Results of the effective porosity sensitivity analysis indicated that the travel time decreased approximately four percent for each one percent decrease in effective porosity. This consistency was due to the fact that effective porosity does not affect the flow solution, and therefore changes in the effective porosity only change the velocities of the particles not the paths.

The sensitivity of the hydraulic gradient was examined by changing the hydraulic head relief across the model domain to 170, 175, 180, and 185 feet, for comparison to the base case of 177.5 feet. Head relief was changed by modifying the value of the drain boundary on the west side of the model domain. The impact of changes in hydraulic gradient on travel times was more complex than that caused by changes in porosity because changing the hydraulic gradient altered the flow field, and thus the particle paths. In general, the mean and minimum realizations indicated a decrease in travel time of up to 1 percent per foot of increase in head relief. In the maximum realization, the correlation between changes in relief and travel times was reversed due to significant changes in the location and number of dry cells in the model, and thus the flow field and particle tracks. Because of this, the maximum realization showed on average a 0.3 percent increase in travel time per 1 foot increase in head relief.

5. Conclusions

For this stochastic analysis, a source starting in 1957 at the Courtyard was assumed, and 220 geostatistically-determined hydraulic conductivity distributions (based on measured hydraulic conductivity) were generated in the code FIELDGEN that were used to create 200 model realizations with each realization containing four particles. Hydraulic conductivity distributions were accepted or rejected based on conditioning criteria to limit the results to scenarios where the particles passed through the plume location at 24th Street and were not obstructed, slowing the travel times. The resulting 800 particle travel times were analyzed. The geometric mean advective travel time from the former 52nd Street facility (Courtyard) to the vicinity of 24th Street (Frazee Deer-O) was 48.3 years (1σ confidence interval of +5.49/-4.93 years). The average travel time to the OU2 capture zone for the 5 realizations nearest the mean travel time was 54.1 years. Particle paths through saddles in the bedrock ridge west of Honeywell had an average of 4.53 years longer travel times than those passing north of this ridge.

The particles were started in 1957 corresponding to the earliest development at the 52nd Street facility. TCE was first detected in 1983-1986 in a number of wells located near the Frazee Deer-O facility. Hence, whether the earliest travel time (37.4 years) or the geometric mean travel time (48.3 years with a (1σ) confidence interval of +5.49/-4.93 years) is used, particles did not reach the Frazee Deer-O wells for the first time until either 1994-95 (using the earliest travel time) or 2005-06 (using the mean travel time), that is over 10 years after the elevated concentrations were first detected at this location. The model results demonstrate that other contaminant sources are required to explain the observed contamination at the Frazee Deer-O wells (and at wells further west) because a source at the former 52nd Street facility could not have resulted in contaminant migration to these areas by 1983-1986.

Approximately 2,700 feet down gradient of the Frazee Deer-O wells is a row of capture wells (in the model) that represents the OU2 groundwater extraction wells. To approximate the travel time to

Table 2: Sensitivity Testing

		Porosity					Per 1%	
Realization		30%	27%	25%	23%	20%	Mean	St.Dev
Mean	Travel Time (yr)	58.04	52.24	48.37	44.50	38.70		
	Difference (%)	20.00	8.00		-8.00	-20.00	4.00	0.00
Minimum	Travel Time (yr)	45.57	41.01	37.97	34.91	30.38		
	Difference (%)	20.00	8.00		-8.00	-20.00	4.00	0.00
Maximum	Travel Time (yr)	82.71	74.44	68.93	63.41	55.14		
	Difference (%)	20.00	8.00		-8.00	-20.00	4.00	0.00

		Head Relief					Per 1 ft	
Realization		170 ft	175 ft	177.5ft	180 ft	185 ft	Mean	St.Dev
Mean	Travel Time (yr)	52.81	49.62	48.37	47.19	44.24		
	Difference (%)	9.18	2.58		-2.44	-8.55	1.09	0.16
Minimum	Travel Time (yr)	39.49	38.64	37.97	37.55	36.70		
	Difference (%)	3.99	1.77		-1.11	-3.36	0.53	0.21
Maximum	Travel Time (yr)	66.89	68.31	68.93	69.34	72.05		
	Difference (%)	-2.96	-0.90		0.59	4.54	0.33	0.23

the OU2 extraction wells, five realizations with travel times nearest the mean travel time were used from the previous simulation that focused on the Frazee Deer-O location. The average travel time to the OU2 capture zone for these five realizations was 54.1 years or by calendar year 2011, significantly after the start of operations of the OU2 groundwater extraction system in 2001. The model results demonstrate that contamination from a source at the former 52nd Street facility (assuming a Courtyard source as if it had occurred in 1957 instead of 1963) could not have migrated into the OU3 area before the start up of the OU2 remedy.

Field data that account for advection, dispersion, sorption and degradation support these modeling results. Based on the 1992 measurements of the plume (Clear Creek Assoc., 2005, Figures 3.1 and 3.7), a concentration of 3,000 ug/L was observed about 3,600 feet down gradient of the Courtyard. Concentrations decline further down gradient toward the west. Thus, field data that account for advection, dispersion, sorption and degradation demonstrate that the 3,000 ug/L contour had only migrated about 3,600 feet from the former 52nd Street facility by 1992, and therefore, the Courtyard source can not explain the 3,300 ug/L TCE concentration detected in a well that was an additional 15,400 feet away from the Courtyard near the Frazee Deer-O facility in 1986.

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