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SIMULATION OF GROUNDWATER FLOW AT THE LBNL SITE USING TOUGH2

Quanlin Zhou, Jens T. Birkholzer, Iraj Javandel, and Preston D. Jordan

Earth Sciences Division, Lawrence Berkeley National Laboratory
Berkeley, CA 94720, USA
e-mail: qlzhou@lbl.gov

ABSTRACT

In the late 1980s, groundwater contamination was detected at the site of the Lawrence Berkeley National Laboratory (LBNL). A detailed investigation was conducted to locate the source and the extent of the contamination. Interim corrective measures were initiated where appropriate and required, typically directed towards removing the source of contamination, excavating contaminated soil, and limiting further spreading of contaminants. As the first step for predicting the fate of remaining contaminants, a three-dimensional transient groundwater flow model was developed for the complex hydrogeological situation. This flow model captured strong variations in thickness, slope, and hydrogeological properties of geologic units, representative of a mountainous groundwater system with accentuated morphology. The flow model accounts for strong seasonal fluctuations in the groundwater table. Other significant factors are local recharge from leaking underground stormdrains and significant water recharge from steep hills located upstream. The strong heterogeneous rock properties were calibrated using the inverse simulator iTOUGH2. For validation purposes, the model was calibrated for a time period from 1994 to 1996, and then applied to a period from 1996 to 1998. Comparison of simulated and measured water levels demonstrated that the model accurately represents the complex flow situation, including the significant seasonal fluctuations in water table and flow rate. Paths of particles originating from contaminant plumes in the simulated transient flow fields were obtained to represent advective transport.

INTRODUCTION

In the late 1980s, groundwater contamination was detected at the “Old Town” area of the Lawrence Berkeley National Laboratory (LBNL) (Javandel, 2001). A detailed investigation was conducted to locate the source and extent of the contamination. The main plume originated from building 7, with maximum concentrations of 100,000 mg/kg measured in 2002. The principal contaminants originally released at this site were PCE, TCE, and carbon tetrachloride. Today, the contaminant sources have been removed, and several clean-up and/or containment measures have been initiated. Downstream, four groundwater collection trenches have been built (see Figure 1). The Building 7 trench system was installed in August 1996, and contaminated water has been pumped, treated, and re-injected in upstream wells to flush the contaminated soil. In terms of remediation expenses, it is important to predict how much longer the clean-up and hydraulic containment activities will have to last in the future. To that end, a numerical model was developed for the simulation of transient groundwater flow in the Old Town system, as the first step prior to development of a transport model. The following sections explain several stages of model development, including the geological framework, complex boundary conditions, model calibration, and predictive modeling results.

HYDROGEOLOGICAL MODEL

The morphological, hydrogeological and hydrological situation in the Old Town area is very complex. Morphology is accentuated with steep hills, deep ravines, and large gradients. Profiles demonstrate a complicated geologic structure with several units of vastly different hydrological properties. Permeability varies over several orders of magnitude. Landslides and artificial filling have changed and influenced the structural setting, as shown in Figure 2.

Geological data are available from 711 boreholes and wells, from cross section maps, and from an outcrop map. Where a borehole does not penetrate a geologic unit, interpolation was used and consistency analysis conducted to construct the unavailable information. Zero-thickness data points extracted from an outcrop map were used to better constrain the lateral extent of geologic units. Only the top five geological units, which contribute to groundwater flow, were considered in the hydrogeological model. These five geological units, starting from the ground surface, are the Artificial Fill unit, Colluvium unit, Moraga Formation unit, Mixed unit, and Orinda Formation unit. The Orinda Formation unit is thick and less conductive to groundwater, and only its top portion of about 50 feet was considered in numerical simulation.

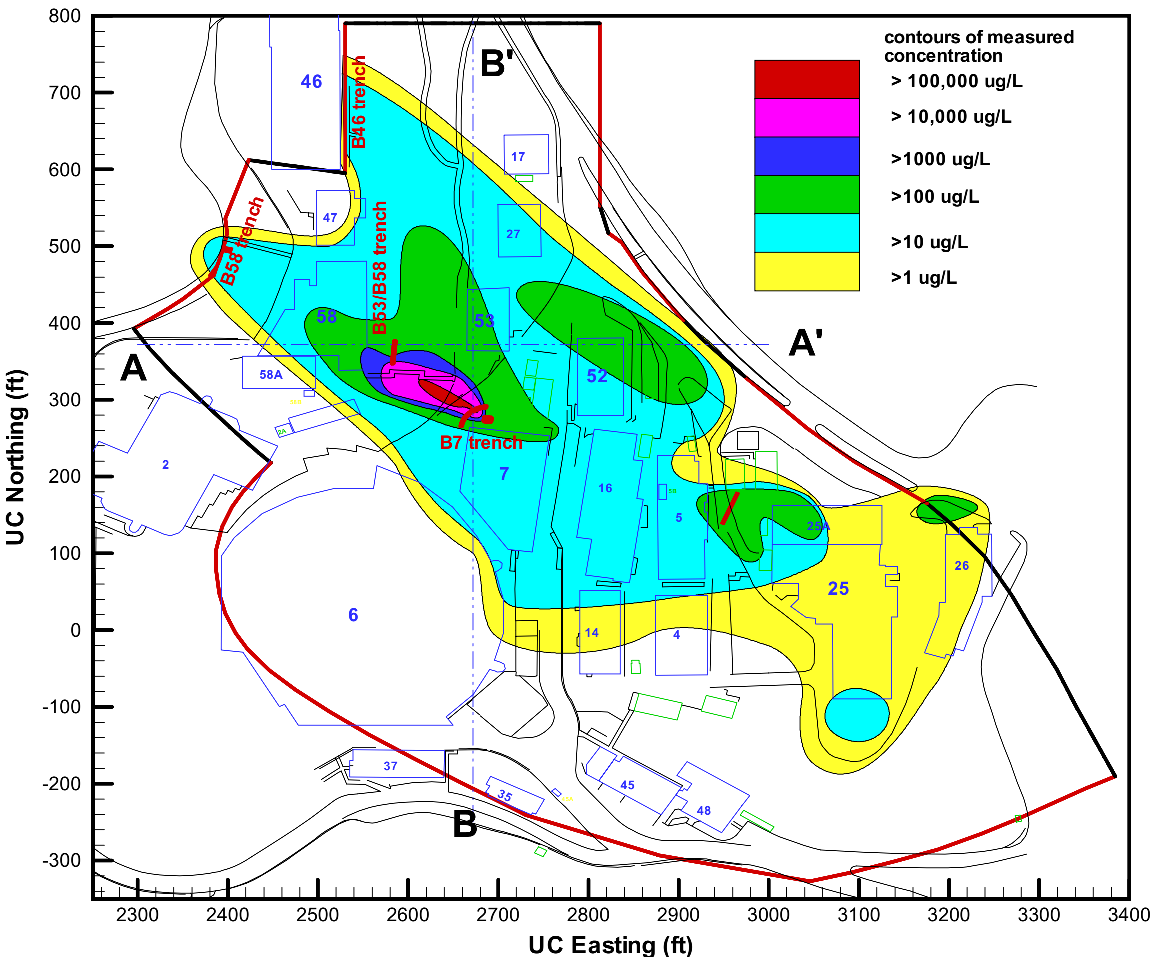

Figure 1. Contaminant plumes in the LBNL's Old Town area, with buildings in blue, roads in black, groundwater collection trenches in red, and model boundary in red line.

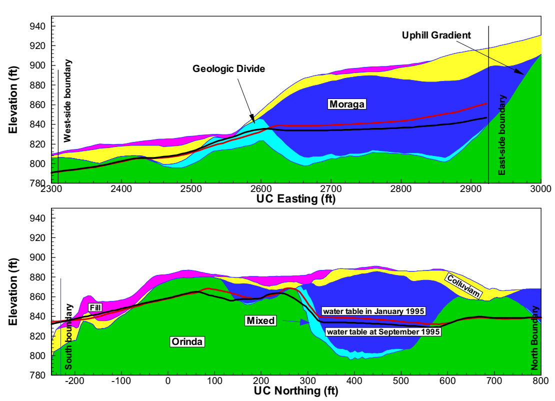

Figure 2. The west-east A-A' and south-north B-B' cross sections of geologic profiles, with seasonal fluctuations of the water table

The center of the Old Town area is located in a relatively flat part of the mountainous LBNL site. In the eastern direction of the Old Town area is a steep uphill gradient. Steep down gradients exist to the west and south (see Figure 2). Certain parts of the Old Town area have been artificially filled to create a flat ground surface. The maximum thickness (about 37 feet) of the Artificial Fill unit is located north of Building 6 and west of Building 7. Only this area is hydrogeologically important, since the groundwater table in all other areas is below this unit. A thin layer of the Colluviam unit, less than 10 feet thick, exists in most of the Old Town area. This soil layer does not conduct groundwater in most areas because the water table fluctuates within underlying units. The mixed unit, having a low permeability, is present in the area of the main contaminant plume, with maximum thickness of 30 feet in the northern edge of Building 7.

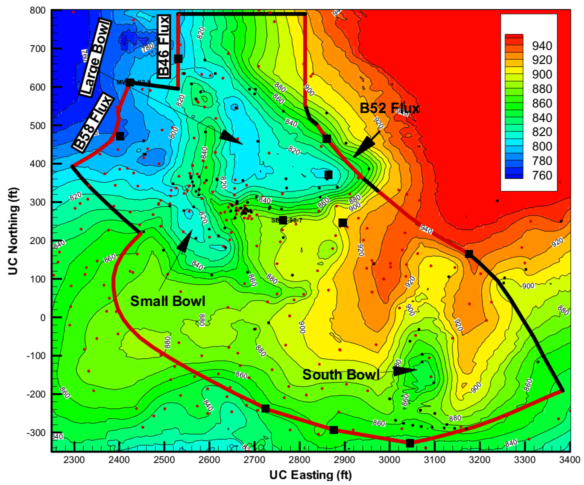

Figure 3. Contours of the bottom elevation of Moraga geologic unit with borehole data point, and model boundary with monitoring wells used to prescribe boundary conditions.

Compared with the four geological units mentioned above, the Moraga Formation is the most permeable and important unit for conducting saturated groundwater flow. Figure 3 gives the bottom elevation of the Moraga unit, and identifies the three Moraga bowls in the Old Town distinct areas, where the Moraga unit is thick as the bottom elevation forms a deep valley or bowl. These areas are defined to behave as Moraga bowls. The first one, referred to as Large Bowl, is located in the area of buildings 52, 53 and 27 in the north (see also Figure 2 for cross sections). The maximum thickness is about 85 feet, and saturated groundwater flows in the highly permeable zone from the upstream boundary downward to Building 46. The second Moraga bowl, referred to as Small Bowl, underlies Building 6, with a maximum thickness of about 35 feet. This bowl is smaller, but potentially important because contaminants may spread within this bowl, then flow toward Building 58 in the west. In the south, the third Moraga bowl, South Bowl, underlies Building 25. These Moraga bowls are important factors in the hydrogeological layers: flow may fill these bowls during the wet seasons, but water leaves these bowls only if a given water level is reached such that outflow is possible.

Note also that a geological divide exists between the Large Bowl and the area downstream of Building 58. Constructed by the less permeable mixed and Orinda units, this divide prevents groundwater flow in the east-west direction and forms the constrained channel for groundwater flow in the Large Bowl. It may explain the co-existence of two separate contaminant plumes originating in the north edge of Building 7. The main plume flows in the Small Bowl toward Building 58, and the small plume flows in the Large Bowl toward Building 46 (see Figure 1).

DEVELOPMENT OF NUMERICAL MODEL

One of the main modeling challenges in developing the numerical groundwater model for the LBNL Old Town area is the determination of the model boundary and the boundary conditions in the mountainous site. Another challenge is to accurately estimate infiltration by rainfall through unpaved areas in the urbanized site and infiltration through leaking storm drains in some particular areas.

Model Domain and Boundary Conditions

The model domain included the two major contaminant plumes (the Building 7 plume and the Building 25 plume) and all three water-bearing Moraga bowls. Because of the complexity of the system, defining appropriate boundary conditions is difficult: the water table in the Old Town area varies significantly in time and space. Therefore, model boundaries were placed along monitoring wells so that the measured water table could be used as a boundary condition (see Figure 3). Where monitoring wells were not available, information on flow paths was used to define no-flow boundaries or spatially uniform-head conditions. Vertically, the system extends from the ground surface to about 60 feet below the top of the Orinda Formation (bedrock).

The model boundary consists of four boundary-segment groups with water table prescribed and four no-flow boundary segments connecting these groups. In Figure 3, the no-flow segments are indicated in black line and the first-type segments are indicated in red line. Each of the segment groups consists of at least one boundary segment. Along a segment, when water table varies slightly in space, the time-dependent water table measured at one representative well was used as the first-type condition. Where the water table varies significantly, two representative wells and spatially linear interpolation were used to determine the first-type condition at each node/cell on the segment. Note that all the first-type conditions with either a uniform-head or a spatially varying head are time-dependent.

Groundwater flow from the uphill region into the model domain is a main water source for the Old Town groundwater system. Of the four upstream segments with the first-type condition, the segment along the Large Bowl is most important because the major fraction of the boundary inflow is through this segment. Significant amounts of water flow within the permeable Moraga Formation unit into the Large Bowl. This segment is referred to as "B52 influx" segment.

Of the downstream boundary segments, the B46 segment located at the east edge of Building 46 is most important for groundwater ouflow. A groundwater collection trench extends along this boundary, where contaminated water was collected for remediation. The small cross section of the Moraga Formation unit below the water table accounts for most of the system outflow. The B58 boundary segment located near Building 58 and the B58 trench accounts for a small fraction of the total outflow. Contaminated groundwater has been collected there since 1998.

Recharge and Storm Drains

Groundwater flow in the Old Town area is strongly affected by direct infiltration from rainfall, as well as from leakage out of storm drains. Careful estimate of infiltration from these water recharge sources is essential for the model. The areal net recharge through unpaved areas is calculated from rainfall intensity, the area of the unpaved areas, and a recharge factor (fraction of rainfall infiltrating into groundwater). Appropriate recharge factors were estimated from the slope of the topography and the properties of the surface soil. Some buildings with infiltration areas around them also contribute to direct infiltration, because the rainfall on their roofs directly drains into neighboring areas. In all paved areas, like parking lots or street, a very small recharge factor of 0.02 was used to represent unaccounted infiltration through small flower beds, which are too small to be included individually.

Leakage through storm drains is hard to estimate, because the amount of leaking water depends on many parameters, such as catchment area, type of damage, and soil type. However, this kind of recharge can be very important to the local groundwater system. Evidence of eroded metal pipes and rupturing of concrete pipes was observed in the field. The storm drain located in the north edge of Building 7 was believed to leak significantly. This storm drain consists of four pipe segments with different catchment areas. Each segment receives direct discharge from its catchment and discharge from the upstream pipe segment. The total flow rate into the segment depends on its catchment area, the flow rate coming from the upstream pipe, a recharge factor defining the relative amount of leakage into the underlying area, and the rainfall rate.

Calculation of Water Table

The TOUGH2 code with module EOS9 was used for the forward simulation of saturated-unsaturated groundwater flow (Pruess et. al., 1999). While TOUGH2-EOS9 is designed for the simulation of unsaturated and saturated flow, the main focus of our research was on the saturated flow region. Therefore, a simple linear model was used for the relative permeability and capillary pressure functions in the unsaturated flow region. The inverse version of this code, iTOUGH2, was used for model calibration (Finsterle, 1999). A preprocessor and postprocessor was developed in C++ to construct the input files for TOUGH2 and iTOUGH2, and to analyze simulation results.

The water table elevation can be directly obtained from the results of pressure and saturation in TOUGH2 simulations. A model element is considered saturated when its calculated pressure is larger than the reference air pressure and when saturation is close to or equals 1.0. Water table elevation was calculated from the elevation and calculated pressure of the first saturated element in a vertical column, as follows

$$Z_{wt} = Z + \frac{P - P_{air}}{\rho_w g}$$

where Z_{wt} is the elevation of water table (in meters), Z and P are the elevation and calculated pressure of the top saturated element, P_{air} is the reference pressure in Pa, ρ_w is the density of water, and g is the gravitational acceleration.

Heterogeneity Calibration

Strong hydraulic-conductivity variation between different geological units is exhibited in hydraulic conductivity measurements. About 108 measurements were obtained in the Old Town area using slug tests, pumping tests, and tracer tests. Each of the measured hydraulic conductivity values was assigned to one of the five geologic units, depending on the location of well screen. Most of the measurements in the model domain were conducted for the two most important geological units, the Moraga Formation and Orinda Formation. The geometric means of hydraulic conductivity for the Artificial Fill, Colluvium, Moraga, Mixed, and Orinda units are 2.75e-7, 1.12e-7, 2.81e-6, and 4.27e-8 m/s, respectively. However, the large standard deviation in measured hydraulic conductivity for each unit indicates that strong heterogeneity exists within each geological unit (as shown in Figure 4). For example, the most permeable Moraga zone is located in the Large Bowl with a maximum value of 3.98e-4 m/s, whereas the smallest conductivity is located in the north edge of Building 7, a value of 1.26e-9 m/s.

Capturing the strong heterogeneity within the Moraga Formation, Mixed, and Orinda Formation is particularly important, because these three units are either the most conductive or important for maintaining high water table measured in some specific areas. Rock zones having different rock properties in each unit were defined using clusters of hydraulic conductivity measurements. Rock properties within the Artificial Fill and Colluviam units were assumed homogeneous, because few measurements of hydraulic conductivities were available to define the heterogeneity of rock properties.

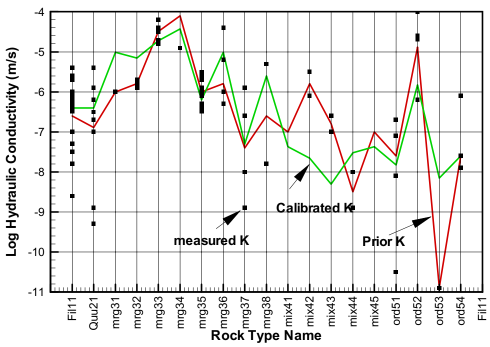

Figure 4. Calibrated hydraulic conductivity vs their prior values, and measured hydraulic conductivity for each defined rock zone.

The iTOUGH2 version 4.0 code (Finsterle, 1999) was used to calibrate hydraulic conductivity and "effective" porosity in the 19 rock zones defined within the five geological units. The geometric mean and standard deviation of hydraulic conductivity in each rock zone were calculated using available measurements. Calibration was conducted based on the measured water table in a number of monitoring wells and on the flow rate of water collected in the groundwater collection trenches at Buildings 46 and 58 during calibration (1994–1996).

To obtain realistic and accurate rock properties using the transient measured water table and collected flow rate, four separate but interconnected groundwater subsystems were defined, based on their flow characteristics (see Figure 5). The calibration was conducted in two steps. In the first step, rock properties specific to a subsystem were calibrated independently, using the measurements within the subsystem. In the second step, the rock properties for more than one subsystem were calibrated using all measurements in the entire groundwater system. This calibration method was used to avoid unphysical results obtained using the do-all-at-once method, which produced very small seasonal fluctuations around the mean water table at some wells. As shown in Figure 6, the match between measured and simulated water table in most monitoring wells was very good.

The "effective" porosity calibrated in the iTOUGH2 procedure is a model parameter that may be much smaller than the actual physical porosity. For example, thin layers of higher hydraulic conductivity and high porosity were found in the Mixed unit within bedrock of otherwise very low conductivity and porosity, leading to fast response to water table change with high seasonal fluctuations.

MODEL PREDICTION

The calibrated numerical model was used to predict groundwater flow in the Old Town system during the period of July 1, 1996, to June 30, 1998. In this period, the groundwater system was perturbed by pump-and-treat facilities established for the remediation of contaminated groundwater. Contaminated groundwater was extracted, treated, and finally reinjected into the groundwater system to flush the contaminated groundwater to downstream trenches. Because the objective of this investigation is to understand the general pattern of groundwater flow in the Old Town area, and since future investigation with a very fine numerical mesh will specifically focus on the contaminant transport plume in the north edge of Building 7, the effect of the remediation facilities on the local flow was neglected in this study.

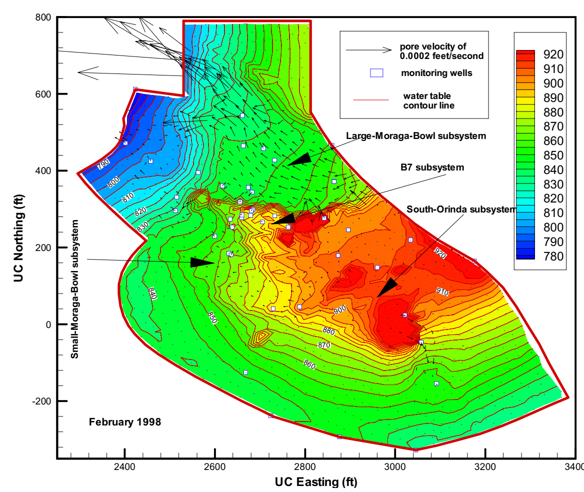

Figure 5. Simulated water table contour and velocity field at water table at February 1998.

Flow Results

Figure 5 shows water table contours and flow velocity vectors simulated at February 1998, representing the wet winter season. The velocity in the Large Bowl subsystem is large in comparison with that of the other three subsystems. The recharge to this bowl is from inflow through the upstream boundary, from the South-Orinda subsystem (due to steep hydraulic gradients), and from infiltration by rainfall and through leaking storm drains. Flow goes through a narrow channel of saturated Moraga unit from the southeast to the northwest. In comparison with the summer dry season, the water table is higher, and the total flow-bearing area of the channel is larger. This area varies from the southeast to the northwest. The smallest area occurs at the Building 46 boundary, resulting in the maximum velocity in the subsystem. In the summer dry season, groundwater flow results from the inflow through the upstream boundary and from the South-Orinda subsystem. The flow-bearing cross-sectional area of the saturated Moraga unit on the upstream boundary is much smaller than in the winter, and less inflow occurs through the B52 boundary segment. As a result, the water table returns to a lower level and produces less discharge through the channel due to its smaller flow-bearing cross-sectional area. Outflow rate through the Building 46 boundary is also much smaller.

In the Building 7 subsystem, the water table remains at a high level within the Moraga Formation and the Mixed unit. All geological units in this area are much less permeable than elsewhere. As a result, the velocity or flux is small. The subsystem receives recharge (1) from the South-Orinda subsystem, (2) from unpaved-area rainfall, and (3) from leaking storm drains. Groundwater flows into the Large Bowl subsystem because of steep hydraulic gradients. In the winter, the leakage of the storm drain in the north edge of Building 7 gives rise to significant flow into the Large Bowl subsystem. Groundwater flowing away from the Building 7 area goes to the northwest, and then is divided by the geological divide of Mixed and Orinda Formation (see Figure 3). This groundwater feature can explain the two co-existing contamination plumes, one toward Building 46 along the large Moraga bowl, and the other toward Building 58. The latter is of much higher concentration than the former plume because the velocity in the latter plume is much smaller (see Figure 7).

Some amount of flow goes through the Small Bowl in the Small Bowl subsystem. This system is recharged from (1) the upstream flow in the permeable Orinda area and (2) recharge from the unpaved areas and storm drain leakage. The flow rate is very stable in the downstream of the subsystem because seasonal fluctuations in the water table is very small. In addition, the effect of recharge resulting from the storm drain leakage can be seen in the winter season. Velocity fields also indicate some exchange flow rate with the Large Bowl subsystem. The exchange flow rate is larger in winter than in summer.

In most of the South-Orinda subsystem, the flow rate is very small owing to the small hydraulic conductivity of the Orinda Formation unit. In the area of Orinda zone with much higher hydraulic conductivity, noticeable flow rate from the upstream boundary can be seen. It is this flow rate that recharges the Small Bowl underlying Building 6. In the South Bowl, velocity is also noticeable because of the high hydraulic conductivity of the Moraga Formation.

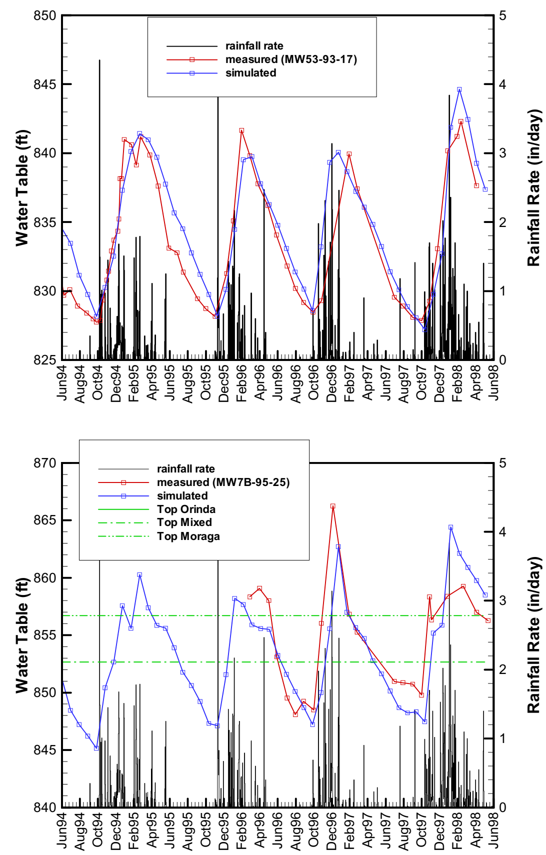

Figure 6. Comparison of the measured and predicted water table at two representative wells in the Large-Moraga-Bowl subsystem and the Building 7 subsystem.

In addition, local water mounts can be seen from water table contours in the winter season, as shown in Figure 5. All water mounts occur in the unpaved areas that have small hydraulic conductivity in underlying units. In the summer, the water table is smooth, and lower than in winter seasons.

Figure 6 shows a very good match between the predicted and measured water table at two monitoring wells in the Large Bowl subsystem and the Building 7 subsystem. This indicates that the groundwater flow model was validated against measurements.

Advective Transport Results

In this section, advective transport results were analyzed using a particle-tracking procedure. The groundwater flow is highly transient, with seasonal fluctuations in the water table and strong temporal variations in groundwater velocity. However, for simplicity, the streamlines of particles originating from the major Building 7 plume and other plumes in steady-state flow were calculated using Tecplot. Four particular transient flow fields (in a year) were used as steady-state flow, and the streamlines obtained on October 1997 were shown in Figure 7.

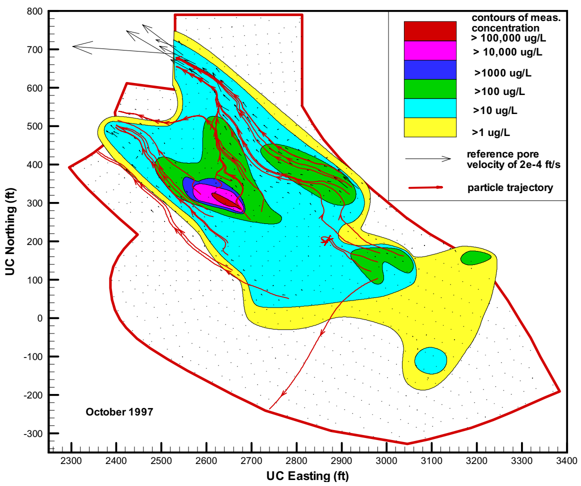

Figure 7. Trajectories of particles originating from contaminant plumes using steady-state flow.

In any season, particles originating from the B7 lobe migrate in two different directions in any season. One is to the northwest, toward the B58 boundary, the other is to the north, toward the B46 boundary. Some particles may change their direction in different seasons, depending on the local flow field. In July 1997, the particles originating in the southwest side of the major plume move toward the B58 boundary, whereas the particles originating in the northeast side of the major plume move northward along the geological divide to the B46 boundary. Particles originating from the center of the major plume move downgradient northwest, until they reach an area where the flow is almost stagnant. The stagnant area is south of Building 53, where the regional flow in the Large Bowl encounters the flow going north from the geological barrier. no flow occurs at the saddle of the geological barrier, and no particles were found to cross the barrier toward the B58 boundary. In October 1997, recharge from the 9-inch rainfall elevates the water table, and some water flows through the saddle toward the B58 boundary. This flow results in some particles migrating through the saddle toward the B58 boundary. No stagnant area occurs around the major plume, and particles originating in the center of the plume migrate northward along the geological barrier. In January 1998, a heavy rainfall of 19 inches a month occurred. As a result, the velocity in the Moraga channel became larger, and water table became higher. On the other hand, the water table at the geological barrier was also higher, resulting from the large recharge through the overlying unpaved area. As a result, no flow occurred at the saddle, and no particles migrated westward to the B58 boundary through the saddle. In April 1998, while the velocity in the Moraga channel is still large, the high water table in the geological barrier area disappeared. A large amount of water flowed through the saddle to the B58 boundary, carrying many particles with it.

Although the contaminant transport is highly transient with seasonal fluctuations of velocity, most particle paths are stable or have small seasonal variations, except the significant variations around the saddle of the geological barrier mentioned above. Particle paths, as shown in Figure 6, are similar in the directions of the measured transport plume. This indicates that the groundwater flow model can produce reasonable flow fields.

CONCLUSIONS

A geological model of the LBNL Old Town area was developed based on borehole data, cross-sectional maps, and an outcrop map. The numerical model was developed to calibrate and simulate groundwater flow in the LBNL Old Town area. First, significant effort was needed to determine model boundaries, boundary conditions, initial conditions, and to estimate net areal recharge on unpaved areas and local recharge resulting from storm drain leakage. The strong heterogeneity of rock properties was taken into account by using rock zones of different rock properties in the Moraga Formation unit, the Mixed unit, and the Orinda Formation unit. These rock zones were defined using measured hydraulic conductivity and the hydrogeological model developed. The hydraulic conductivity and "effective" porosity of 19 rock zones were calibrated, using the measured transient water table at a large number of monitoring wells and transient flow rate collected in two groundwater collection trenches. Calibration results show that the match between measured water table and simulated water table, using the calibrated rock properties at most monitoring wells, are in good agreement. Also, good agreement was obtained between the measured flow rate at trenches and simulated boundary flux.

For validation purposes, a blind model prediction was conducted for the period between July 1996 and June 1998, using calibrated rock properties. Results were then compared to the measured data. The match between the measured and predicted water table with seasonal fluctuations at a large number monitoring wells was very good. Prediction results showed that the groundwater flow in the Large Bowl and the Small Bowl was significant, with some exchange between the two subsystems. Flow originating from the Building 7 area divides into the two subsystems, resulting in contaminant plumes in each of the subsystems.

Based on this groundwater flow model, a refined model will be developed for the localized area of the major contaminant plume. This refined model will be used as a tool to analyze and improve the current hydraulic measures conducted for contaminant remediation. The present model will provide the non-uniform, transient boundary conditions for the refined model.

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