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A Vadose Zone Flow and Transport Model for Los Alamos Canyon, Los Alamos, New Mexico

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ABSTRACT

A vadose zone flow and transport model for Los Alamos Canyon is presented that demonstrates that a comprehensive understanding of vadose zone hydrologic processes can be obtained by integrating data from geologic, hydrologic, and site characterization sources. The complex hydrostratigraphy of the canyon is captured using geologic characterization of extensive deep-well drilling samples, along with surface mapping. A water budget study for the surface and shallow subsurface hydrology is used to estimate spatially varying infiltration rates along the canyon. Three-dimensional flow model results show that mesa-top infiltration rates on the order of 1 mm yr^{-1}, and canyon-bottom rates several orders of magnitude higher, capture the water content profiles from available wells within the model domain. However, a range of a factor of three higher and lower than these mean values is also consistent with the data. Transient flow simulations show that episodic infiltration events can be effectively averaged in steady-state flow modeling, but transients that last on the order of a decade or more, such as climate related or anthropogenically induced transients, significantly change the predicted water content. Modeling of tritium transport through the vadose zone indicates that even for a nonsorbing contaminant, most, but not all, of the contaminant released since in the past 40 yr should still be present in the vadose zone. The mass predicted to reach the water table is primarily in locations in the canyon where the Bandelier Tuff is not present. Available groundwater surveillance data for regional aquifer water are consistent with this result.

Los Alamos National Laboratory (LANL or the Laboratory) is performing groundwater investigations as part of its Environmental Restoration and Groundwater Protection Programs to assess the impact of past contaminant discharges on the underlying groundwater system. One of the most important pathways from the points of discharge to the groundwater receptors is the vadose zone. In the semiarid environment in which the Laboratory exists, a deep vadose zone separates surface and alluvial groundwater from the regional aquifer used to supply the local population with domestic water. Birdsell et al. (2005) describe the elements of the conceptual model developed for vadose zone flow and transport at the site, and Robinson et al. (2005) and Stauffer and Stone (2005) further elaborate on the flow and transport mechanisms that are consistent with the observed field data.

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To gain an integrated understanding of flow and transport in the vadose zone and its role in transmitting contamination to the regional aquifer, conceptual flow and transport models must be combined with site-specific information on hydrostratigraphy, hydrologic conditions, and spatially distributed field measurements. In our study, we developed a large-scale numerical model of vadose zone flow and transport in Los Alamos Canyon with the objective of advancing our understanding of vadose zone processes and behavior. In addition to elaborating on the site-specific details of flow and transport at this site, the present study provides insights on the role of large-scale numerical simulation in the hydrologic behavior of vadose zones in semiarid systems.

Los Alamos Canyon, shown in Fig. 1, is one of the most complex sites at the Laboratory. A number of LANL facilities have been or are currently located in or adjacent to the canyon, resulting in multiple effluent and contaminant release locations along the canyon. Because the canyon serves as a collector of a wide range of contaminants and consists of a wide range of hydrologic conditions, it was decided that a numerical model at the scale of the canyon, rather than at the smaller scales typical of an instrumented field site, is appropriate. Through a synthesis of available data and the development of a numerical model we examined fluid flow and contaminant transport in the vadose zone beneath Los Alamos Canyon. Although we primarily restricted our attention to flow issues, tritium transport in the vadose zone was also modeled. Tritium, in the form of tritiated water, is an excellent tracer for groundwater, and hence it is included in this modeling study as a constraint on the flow model.

This paper is organized as follows. First, the model hydrostratigraphy and development of numerical grids are described, followed by hydrologic model assumptions and sources of information for property values and boundary conditions such as the infiltration rate. Then, numerical simulation results of water content measurements are presented, followed by sensitivity studies examining the degree to which uncertain parameters can be varied within the constraints provided by the data. Finally, tritium transport results are compared with available data on the distribution of tritium and other conservative contaminants to evaluate the ability of the model to describe the observed contaminant distributions.

MODEL DEVELOPMENT

Hydrostratigraphy

Accurate modeling of groundwater flow and transport in Los Alamos Canyon requires the integration of

Abbreviations: FEHM, Finite Element Heat and Mass; LANL, Los Alamos National Laboratory.

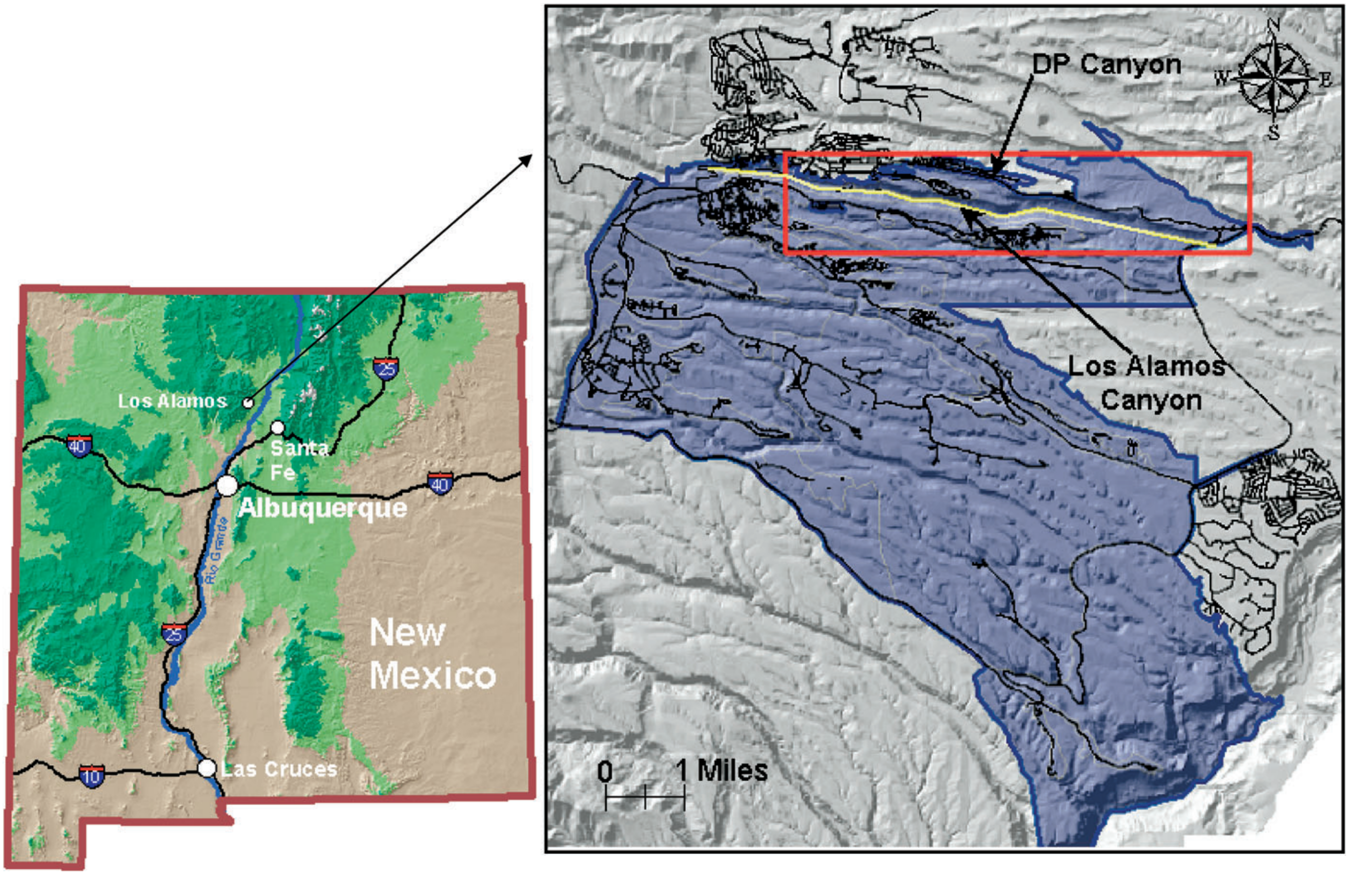

Fig. 1. (left) Location of Los Alamos, NM and (right) the Los Alamos Canyon study area and the flow and transport model domain. The shaded blue area is the LANL property, the red box indicates the areal extent of the three-dimensional model domain, and the yellow line is the trace of the two-dimensional model domain.

geologic model information with computational grids. In this study, a three-dimensional geologic framework model for Los Alamos Canyon was used for this purpose. The framework, consisting of 20 distinct geologic units, is the product of a continuous process of model development and improvement in support of continuing characterization-well drilling activities and numerical flow and transport model development. The record of model development and improvement is documented in Carey et al. (1999).

The stratigraphic units and their accepted designators are listed in Table 1; a detailed description of the geologic units themselves is presented in Broxton and Vaniman (2005, this issue). Figure 2 shows a two-dimensional cross section of the model, illustrating the complexity of the subsurface hydrostratigraphy. The subsurface environment in Los Alamos Canyon consists of an alluvial system containing groundwater perched on top of the underlying bedrock. Beneath this system, which in this model we treat as the source for vadose zone water, but do not simulate explicitly, are the porous and relatively permeable Bandelier Tuff units, as well as the Puye Formation, a highly heterogeneous fanglomerate deposit. Interwoven in the Puye Formation are basaltic rocks, which consist of a complex series of flow deposits of generally low matrix permeability and varying degrees of fracturing.

A characteristic of the stratigraphic model depicted in Fig. 2 that is different than other models developed for sites on the Pajarito Plateau such as Material Disposal Area G (Birdsell et al., 2000) and Mortandad Canyon (Dander, 1998) is the absence of significant thickness of the Tshirege member of the Bandelier Tuff. Los Alamos Canyon cuts deeply into the Bandelier Tuff; the Otowi member is the first unit encountered beneath the alluvium in the canyon bottom across much of the model domain. In the eastern portion of the model, even the Otowi member is not present, and instead the Cerros del Rio (Tb4) basalt is the first unit encountered. The hydrologic significance of this observation will be demonstrated in the numerical model results. Figure 3 depicts the full three-dimensional model stratigraphy, along with the locations of important wells and facilities referred to in our discussions below.

Numerical Grids

To provide flexibility in performing the numerical simulations, both two- and three-dimensional finite element grids were developed for the flow and transport model analyses. The principle advantage of the two-dimensional grid is the smaller number of nodes and elements. Model runs are computationally efficient, making the grid appropriate for scoping calculations and

Table 1. Stratigraphic units present in the vicinity of Los Alamos Canyon.

Group/formation	Unit name	Symbol
Tshirege member of the Bandelier Tuff	Unit 5	Qbt5
	Unit 4	Qbt4
	Unit 3	Qbt3
	Unit 2	Qbt2
	Vapor-phase altered member of unit 1	Qbt1v
	Glassy member of unit 1	Qbt1g
	Tsankawi Pumice	Qbtt
Cerro Toledo Interval of the Bandelier Tuff	Cerro Toledo	Qct
Otowi member of the Bandelier Tuff	Otowi member ash flow	Qbof
	Guaje Pumice bed	Qbog
Puye Formation	Puye fanglomerate	Tpf
	Totavi lentil	Tpt
Cerros del Rio basalt	Basalt 4	Tb4
	Basalt 3	Tb3
	Basalt 2	Tb2
	Basalt 1	Tb1
Tschicoma Formation	Tschicoma Latite	Tt2
	Tschicoma Dacite	Tt1
Santa Fe Group	Chaquehui (volcaniclastic) aquifer unit	Tsfuv
	Santa Fe Group undifferentiated	Tsfu

sensitivity studies. When very high vertical spatial resolution is required, two-dimensional grids are also more convenient. However, since the grid is two-dimensional, there are limitations as to what spatial variability of flow properties and infiltration rates can be simulated.

For the two-dimensional grid, the western boundary of the domain is located at New Mexico state plane coordinates, North American Datum 1983 (492 916.5, 541 257.7), in the northwest corner of the LANL property (coordinates expressed in meters). The model extends in a one-dimensional fashion from the western boundary to a coordinate location of (502 959.6, 539 688), at the northeastern boundary of the LANL property. The extent of Los Alamos Canyon in the two-dimensional model is represented by drawing a connected set of one-dimensional line segments as closely as possible

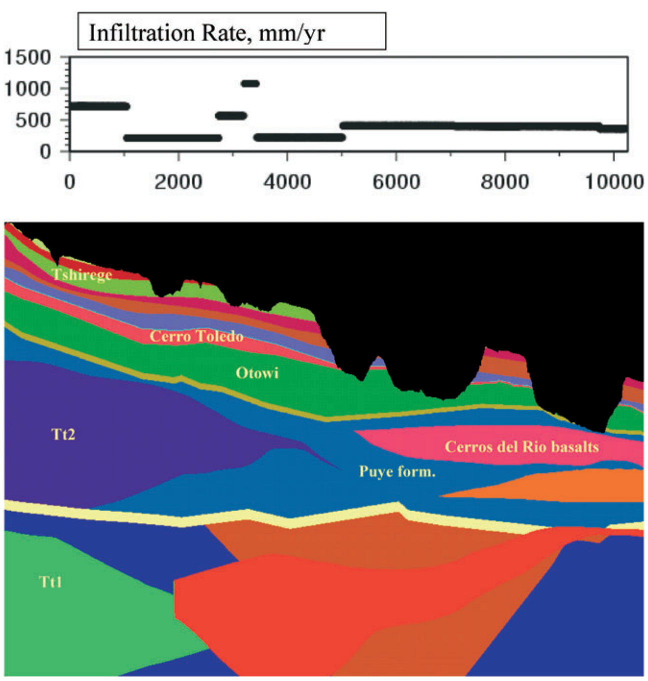

Fig. 2. Cross section of stratigraphy in the vicinity of Los Alamos Canyon. Also shown is the infiltration map used along the canyon bottom (derived from water budget study of Gray, 1997).

down the center of the canyon, thereby accounting for the bends in the canyon. The final version of the two-dimensional grid for Los Alamos Canyon consists of 57 004 nodes, 111 256 tetrahedral elements, and contains 11 materials.

In the process of selecting the simulation domain for the three-dimensional Los Alamos Canyon grid, we considered the historical information about contaminant releases and important sites along the canyon that may be relevant to contaminant transport issues. It was deemed necessary that DP Canyon, and Well R-9, along with facilities such as the Omega West reactor, should be within the domain of the three-dimensional grid. The three-dimensional model domain is rectangular and encompasses Los Alamos Canyon within the LANL property, DP Canyon, and some of the adjacent mesas to the north and south of Los Alamos Canyon. The model domain extends from the topographic surface to a depth of 1650 m. Within this grid, we capture both the mesas and the canyon, so that the wide range of infiltration rates as a function of location can be captured.

One of the most important constraints on the grid-building process is to keep the total number of nodes as low as possible but at the same time ensure that there is adequate resolution in the areas of interest. To achieve this objective, a high-resolution mesh is applied along the canyon. The final three-dimensional grid, shown in Fig. 4, consists of 301 436 nodes, 1 688 457 elements, and 14 stratigraphic units.

Conceptual Flow Model and Hydrologic Properties

The fundamental hydrologic assumption in this study is that the system can be characterized using an equivalent continuum model. For the Bandelier Tuff units, Robinson et al. (2005) demonstrated that this assumption is an acceptable approximation of the system, and that the matrix hydrologic properties measured in core samples provide a good estimate of the properties at larger scales, despite the abundance of fractures in some of the units. For the basaltic rocks, the hydrologic behavior under ponded conditions has been shown to be controlled by fractures (e.g., Stauffer and Stone. 2005). The

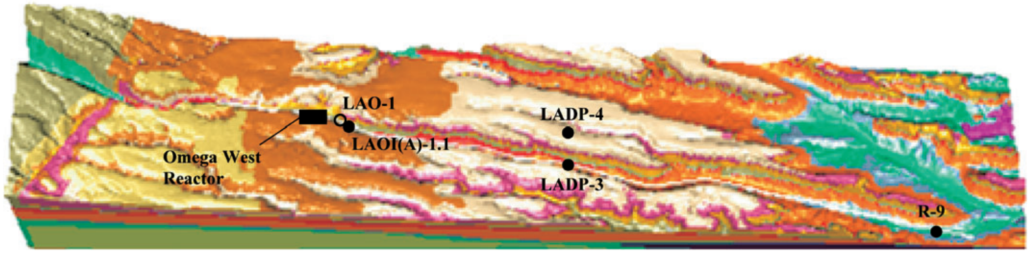

Fig. 3. Three-dimensional depiction of the stratigraphic framework model used to construct the flow and transport model for Los Alamos Canyon. Important wells and the site of a nuclear reactor are also shown.

present study deals with the fractured medium by assigning properties, particularly the porosity, representative of a fractured rock.

Table 2 lists the hydrologic properties used for the Los Alamos Canyon model. The table contains both the base-case permeability and porosity values used for each unit, as well as the unsaturated hydrologic parameters for the van Genuchten (1980) formulation used to model unsaturated flow. It is assumed that hydrologic properties are homogeneous within each individual unit, although it is undoubtedly true that variability in rock properties influences the measured moisture patterns. The properties for the Bandelier Tuff units and the Cerro Toledo interval are obtained from compilations of the properties measured on numerous core samples collected from boreholes across the site (Rogers and Gallaher, 1995). Basaltic and dacitic rocks units are given permeability and porosity values representing fractured rock. The Puye Formation, about which little is known, is assigned values indicative of a poorly consolidated, sandy porous medium.

Infiltration rates

The infiltration rate on the upper surface is one of the most important inputs in simulating flow and transport

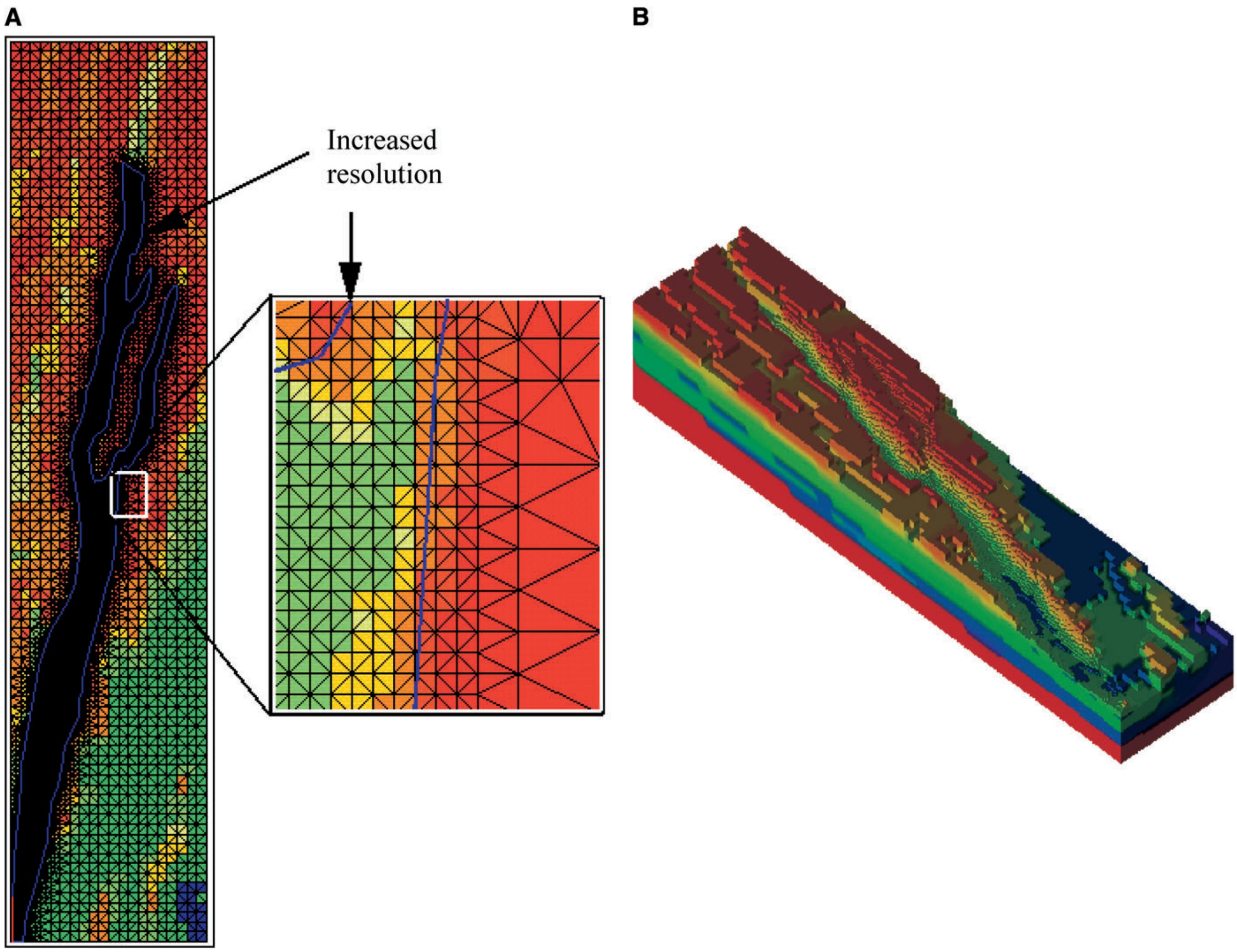

Fig. 4. Three-dimensional model grid. (a) Plan view showing the areas of enhanced grid resolution along Los Alamos and DP Canyons; (b) three-dimensional view of the numerical grid.

Table 2. Hydrologic property values in the Los Alamos Canyon model.

Hydrogeologic unit	Geologic designation	Permeability	Porosity	van Genuchten α parameter	Residual moisture content	van Genuchten n parameter
		m^2		m^{-1}		
Unit 3, Tshirege member	Qbt3	1.01e-13	0.469	0.29	0.045	1.884
Unit 2, Tshirege member	Qbt2	7.48e-13	0.479	0.66	0.032	2.09
Vitric unit, Tshirege member	Qbt1v	1.96e-13	0.528	0.44	0.009	1.66
Glassy unit, Tshirege member	Qbt1g	3.68e-13	0.509	2.22	0.018	1.592
Basal Pumice unit, Tshirege member	Qbtt	1.01e-12	0.473	1.52	0.01	1.506
Cerro Toledo Interval	Qct	8.82e-13	0.473	1.52	0.01	1.506
Otowi Member	Qbof	7.25e-13	0.469	0.66	0.026	1.711
Guaje Pumice Bed	Qbog	1.53e-13	0.667	0.081	0.01	4.026
Cerros del Rio basalt, Puye Formation	Tb4	2.47e-12	0.3	0.1	0.066	2.0
Tschicoma basalt	Tt2	2.96e-13	0.3	0.1	0.066	2.0
Cerros del Rio basalt, Santa Fe Group	Tb3	2.96e-13	0.3	0.1	0.066	2.0
Puye Formation	Tpf	4.73e-12	0.25	5.	0.01	2.68
Totavi Lentil	Tpt	4.73e-12	0.25	5.	0.01	2.68
Santa Fe Group	Tsfuv	2.65e-13	0.25	5.	0.01	2.68

through the vadose zone. Our treatment follows the conceptual model outlined by Birdsell et al. (2005), which discriminates between mesa and canyon settings in estimating infiltration. For the mesa areas, various hydrologic and chemical techniques have been employed to estimate infiltration rates across the Pajarito Plateau. Rogers et al. (1996) outlined a technique for estimating local infiltration rate based on measured hydrologic properties and water content values in samples collected from the vadose zone tuffs. They obtained infiltration rates on mesas as low as 0.06 mm yr^{-1} (essentially zero), with higher mesa values found where surface conditions such as ponds were present. In more recent analyses based on water-content profiles and chloride mass balance interpretations, Newman et al. (1997) and Birdsell et al. (1999) obtained a value on the order of 1 mm yr^{-1} for undisturbed mesa conditions at TA-49, and values estimated from 60 to 300 mm yr^{-1} beneath paved regions. In the Los Alamos Canyon model, an infiltration rate of 1 mm yr^{-1} is assumed at all locations except the canyon bottom.

To estimate the infiltration rate along Los Alamos Canyon, we used the study of Gray (1997), who performed a water budget for surface water stream and shallow alluvial aquifer in Los Alamos Canyon. The equation used to evaluate the water budget is:

$$I = P - R - \mathrm{ET} - \Delta S \quad [1]$$

where I is infiltration, P is precipitation, R is runoff, ET is the evapotranspiration term, and ΔS is the change in fluid storage. The Gray (1997) water budget calculations employed data from several sources, including streamflow data from three stream-flow gages that provide estimates of surface water flow rates, and meteorological data from five precipitation measurement stations. During the 3-yr period of that study, Gray estimated that 71 to 83% of the water introduced into Los Alamos Canyon was lost to evapotranspiration. Average infiltration rates applicable to the Los Alamos Canyon watershed were found to range from roughly 100 to 200 mm yr^{-1} for the period of study. These are average values for the watershed and might be expected to be higher locally directly beneath the stream channel.

In addition to the overall water budget, Gray (1997) conducted a detailed study using measured data and a calibrated numerical model of the alluvial groundwater system. This model divided the canyon alluvial aquifer model into nine zones that corresponded to locations of the monitoring wells used in the model calibration. The model calibration procedure involved adjusting the drain conductance term that controlled the water flux leaving the alluvial aquifer (and entering the underlying bedrock) to match the water level data. The water draining the alluvial aquifer provides a direct estimate of the spatially dependent infiltration rate along the canyon for the vadose zone model of our study.

Table 3 and Fig. 2 show the results of this detailed water budget analysis. The highest infiltration rate of 1076 mm yr^{-1} occurs in Gray's Zone 4, corresponding to Well LAO-0.8. This well falls in the Guaje Mountain Fault zone. This observation is consistent with a model of localized, high infiltration in this zone, perhaps due to enhanced permeability due to fracturing. Zones 1 and 3 also exhibit higher than average infiltration. Gray postulates that Zone 3 may be higher because of its proximity to the Guaje Mountain fault, and Zone 1 infiltration may be high due to a greater saturated thickness of the alluvial aquifer in this portion of the canyon. The rest of the Los Alamos Canyon study area exhibited lower infiltration rates than those just described.

Contaminant Sources

There are a host of possible contaminant source sites for Los Alamos and DP Canyons resulting from past and present Laboratory operations. The most important of these for our purposes is the Omega West reactor site, located in Los Alamos Canyon (Fig. 3), which was used from 1943 to 1994 to house and operate a series of research reactors. Early reactors were fueled by aqueous uranyl solutions, whereas other reactors were fueled by solid fuel elements. A variety of contaminants (mostly radionuclides) are suspected to have been released into the canyon, including tritium, which resulted from a leak in the primary cooling water system at the reactor. This leak was discovered in 1993, and tritium was detected within the Guaje Mountain Fault zone.

Typical tritium concentrations in the cooling water ranged from 15.7×10^6 to 20.2×10^6 pCi L^{-1}. The duration of the leak is not documented, but measurements of tritium concentrations in alluvial aquifer Well LAO-1 (located due east of the reactor) suggest that the

Table 3. Infiltration rates for various portions of the canyon.†

Zone	Location	Infiltration	ET	Down-gradient loss
		mm yr^{-1}		
1	LA Reservoir to 1100 ft east of bridge	714	464	56
2	end of Zone 1 to LAO-C	213	167	223
3	LAO-C to LAO-0.6	566	158	547
4	LAO-0.6 to LAO-0.8	1076	0	148
5	LAO-0.8 to LAO-1	222	195	93
6	LAO-1 to LAO-2	408	28	111
7	LAO-2 to LAO-6	399	93	46
8	State Rd. 4 to Lab boundary	362	139	19
9	East of Lab boundary	325	121	0

† Values from the analysis of Gray (1997).

leak may have begun between November 1969 and January 1970. This reactor was permanently shut down in 1994, and tritium concentrations in the alluvial groundwater in Los Alamos Canyon have subsequently declined to values at or near background levels (LANL, 2001).

In the transport simulations, among all possible contaminants, we choose tritium, which, in the form of tritiated water is among the simplest chemical constituents to model because its chemical state as a water molecule makes it a perfect tracer for water. Other contaminants may undergo sorption, precipitation, and complex speciation processes that complicate the transport simulation.

Model Implementation Issues

Issues described in this section include the method for assigning the flow boundary conditions, initial conditions for transient flow, and hydraulic parameters in the model. We will also discuss some assumptions employed in model implementation.

The infiltration values obtained from Gray (1997) for Los Alamos Canyon were applied directly to the two- and three-dimensional models. In the three-dimensional model, the estimated infiltration rate is applied on all grid nodes identified as representing the interface of the alluvium bottom and the bedrock. In the two-dimensional model, the flux input to the two-dimensional model is an areally averaged value across the canyon bottom. Figure 2 shows the infiltration map superimposed above the two-dimensional model domain. When the infiltration rates are varied within their uncertainty ranges in sensitivity analyses, it is assumed that the relative rates entering the subsurface at different locations along the canyon remain the same, but the absolute value of infiltration is uncertain.

The bottom boundary condition represents the water table. The water table elevation is estimated from results of measured water table elevations for deep characterization wells in the vicinity of the model. Any node falling below this surface is assigned a value of saturation equal to 0.999 to represent the regional aquifer. Therefore, the vadose zone model domain extends only down to this surface, and flow is not computed in the remainder of the model domain in the regional aquifer.

The steady-state, unsaturated flow equation is a difficult numerical problem to solve due to the nonlinear constitutive relationship between pressure and fluid saturation. In these simulations, steady-state flow model results are obtained by performing a long transient flow simulation in which the initial condition is developed based on an educated "guess" of the fluid saturation of the rock, or by using the final state from a previous model run. The model is run to very long times, and a check is performed to ensure that the global mass balance for water is satisfied; that is, flux in equals flux out at steady state. In transient flow simulations, the initial state is typically a steady-state model result, and the transient model run is performed at an equation tolerance sufficient to result in small mass balance errors.

The hydraulic properties at each grid node in the two- and three-dimensional models are determined by the properties of the unit in which the node falls. After a base-case set of hydraulic properties and boundary conditions is established as a reference, sensitivity analyses are used to evaluate the impact of uncertain hydrologic property values. In the base case, the values for the hydraulic properties are those shown in Table 2, and the infiltration rate for the canyon is taken from Table 3 (1 mm yr^{-1} for the mesas). The base case parameter set used the mean values of the hydrologic parameters for all units. This practice has been used in other modeling studies on the Plateau, including those by Dander (1998) and Birdsell et al. (2000), and has proven to be a useful starting point for numerical modeling of canyon systems.

The flow and transport equations are solved using the Finite Element Heat and Mass (FEHM) code (Zyvoloski et al., 1997). FEHM simulates heat conduction, heat and mass transfer for multiphase flow within porous and permeable media, and noncondensible gas flow within porous and permeable media. We used the physics package for an isothermal, two-phase solution of air and water flow. The code handles model geometries in two or three dimensions and has a variety of solute transport model options. Tritium transport simulations are performed using the continuum-based transport model option described in Viswanathan et al. (1998) and Robinson et al. (2000).

RESULTS

Flow Model

Base-Case Results

We begin by displaying graphically the base-case model results for the fluid saturation versus position. Figure 5 is a full three-dimensional view of fluid satura-

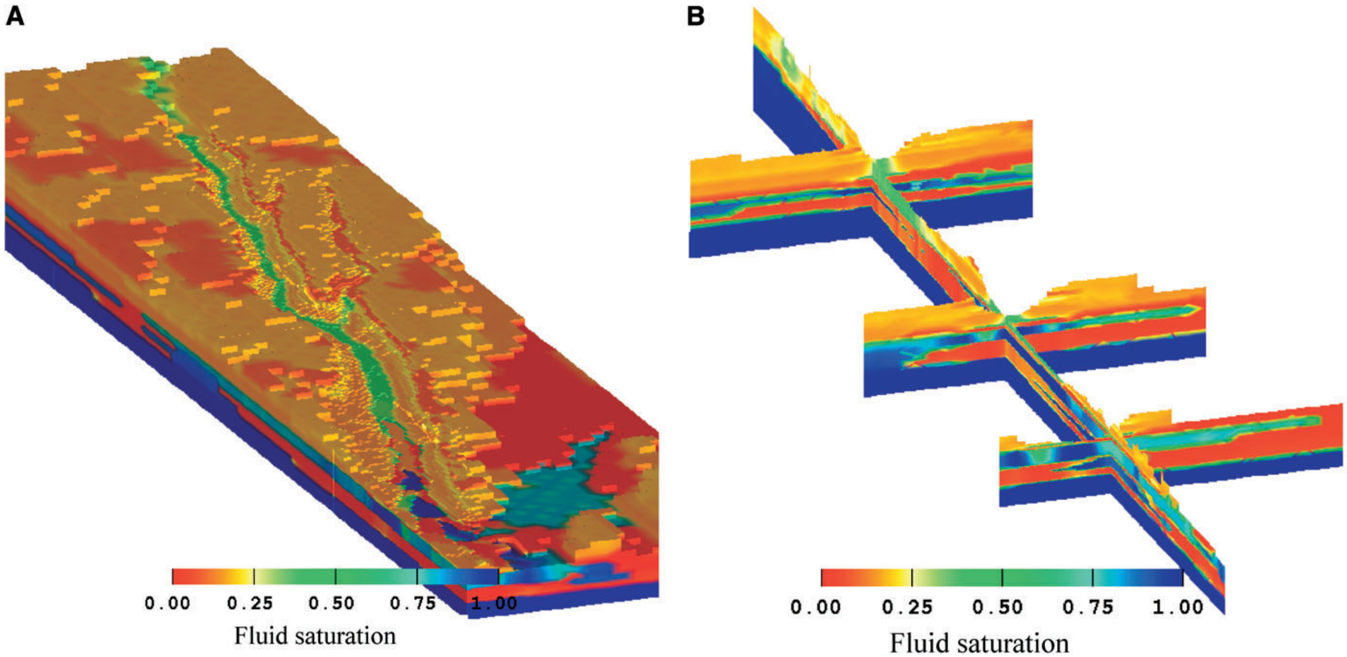

Fig. 5. Three-dimensional flow model results, showing fluid saturation predictions through the model domain. (a) Full model view and (b) fence diagram showing one north–south and three east–west cross sections.

tion (Fig. 5a) and a series of two-dimensional vertical slices through the three-dimensional model (Fig. 5b). The most obvious result is the overriding importance of stratigraphy on the computed fluid saturation. In addition, the local infiltration rate also exerts a strong control on the results. Directly beneath the canyon, fluid saturation is much higher within a given stratigraphic unit than in other parts of the model domain, a reflection of the high infiltration in the canyon.

To judge the adequacy of the base-case model results, the volumetric water content is the primary data set available. For the model, well data along the canyon bottom are used from three wells located in Los Alamos Canyon: LADP-3, LAOI(A)-1.1, and R-9 (Fig. 3). In addition, Well LADP-4, located on a mesa and representing flow from the mesa top to depth, is also represented. The fits to the data are presented for different infiltration rates, including the base-case infiltration map, a map with infiltration scaled down by a factor of three from the base map, and a map with infiltration scaled up by a factor of three.

The results in Fig. 6 through 8 show that the base infiltration map does an adequate job of jointly matching the water content profiles in the Bandelier Tuff in all wells, despite the different stratigraphy and position relative to the canyon bottom. For example, for LADP-3 (Fig. 6), the model captures the water content profile of the well, which consists of data points in the Otowi member, including the Guaje Pumice Bed, the unit that forms the base of the Bandelier Tuff. Both the profile within the majority of the Otowi member and the rise in water content values in the Guaje Pumice Bed are well matched by the simulations. In addition, the good fit for LADP-4 (Fig. 8) illustrates the ability of the three-dimensional model to capture adequately the water contents in the Tshirege member (not present in the canyon bottom wells), as well as in a region where mesa infiltration rates are taken to be significantly lower than in Los Alamos Canyon. The significantly wetter conditions in LADP-3 compared with the nearby mesa Well LADP-4 are simulated in the three-dimensional model through the setting of high infiltration in the canyon. It is evident from these comparisons that this difference in infiltration rate is required to match the data. The relatively poor fit to the data from LAOI(A)-1.1 is probably due to infiltration conditions in the vicinity of the well that are higher than suggested from the water budget study, or to local hydrologic properties that differ from the mean values used in the model.

Sensitivity to Infiltration Rates

As was discussed, there is significant uncertainty in the infiltration rates in Los Alamos Canyon. Therefore, it is important to investigate how the changes from the base case affect the model predictions. The comparison of observed water content and the prediction from the three-dimensional model using different magnitudes of the infiltration rate, depicted in Fig. 6 and 7, indicate that uncertainty in infiltration rate affects the estimates of water content within the Bandelier Tuff. Put differently, water content measurements in the porous tuff units may provide an indirect method of constraining the local infiltration rate in the canyon, by establishing bounds on the minimum and maximum rates that provide reasonable fits to the data. In this case, the model effectively brackets the data within a range of about a factor of three from the base-case value estimated from water budget information.

Sensitivity to Hydrologic Properties

Because of spatial variability and scale effects, there is significant uncertainty in the hydrologic property values

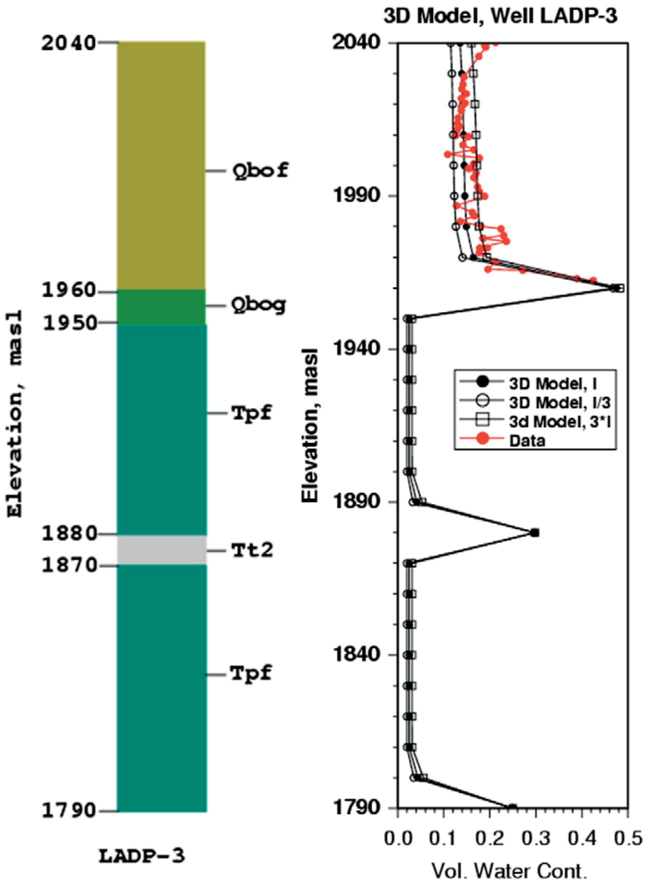

Fig. 6. Comparison of data and three-dimensional model predictions for water contents in Well LADP-3: (left) stratigraphy, (right) data–model comparison.

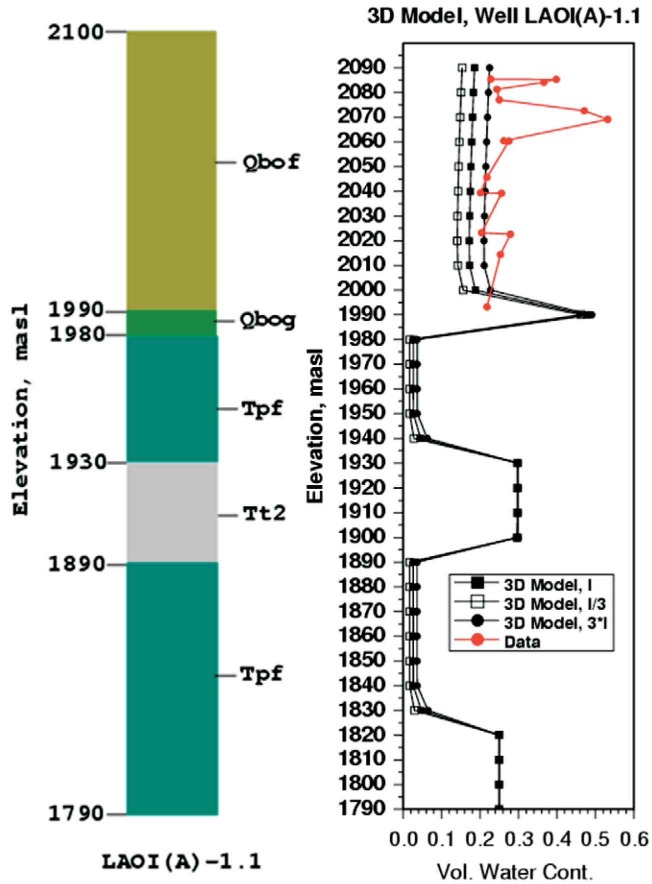

Fig. 7. Comparison of data and three-dimensional model predictions for water contents in Well LAOI(A)-1.1: (left) stratigraphy, (right) data–model comparison.

that are appropriate to use in a large-scale numerical model, which by necessity must employ simplifications. Furthermore, the difficulty of obtaining representative samples in deeply buried, heterogeneous deposits such as the Puye Formation has resulted in a lack of data on which to base the property values for some units. To explore the issue of the lack of information for the Puye Formation, the saturated hydraulic conductivity of the formation was lowered by an order of magnitude from the base-case value. This lower permeability case (labeled "Low k in Puye" in Fig. 9) results in a better fit to the data than the base-case parameter. Alternatively, the infiltration rate used in the simulation could be lower than the actual value at this well. For our purposes, we assume that the infiltration rate estimate is accurate, and take this permeability value to be a calibrated, field-scale value for the conductivity of the Puye Formation suitable for use in the model.

Note also that the water content values for the basaltic rocks are not well matched by the model. This result is a consequence of employing a fracture flow model for these units. No attempt was made to adjust matrix properties for these rocks to fit the data because this water is thought to be nonflowing pore water, and thus inconsequential for the purposes of representing the transport of water and contaminants through the vadose zone.

Another issue of property uncertainty arises in the Bandelier Tuff units from the assumption of mean hydrologic properties in the base-case simulations. Water-content measurements effectively constrain the infiltration rate by forcing the models to match the data for a given property set. It follows that, if different effective property values are used, infiltration estimates will change accordingly. To examine the potential for this uncertainty to corrupt our estimates of infiltration rate, two additional cases (not plotted) were performed using hydrologic properties from the Otowi member from two representative characteristic curve samples from Rogers and Gallaher (1995), rather than assuming the mean hydraulic properties. Our results indicate that, by this measure, the uncertainty of hydraulic properties could give rise to a difference in predicted water contents that is roughly equivalent to a factor of three to five difference in the infiltration rate. We believe that this is a worst-case estimate of uncertainty in infiltration, for the following reason. In the development of this model, additional constraints are effectively included via the incorporation of multiple, independent data sources. For example, water content measurements are augmented by water budget studies and observations of contaminant migration velocities, which, considered together, allow uncertainties to be reduced relative to estimates based on any one single data set.

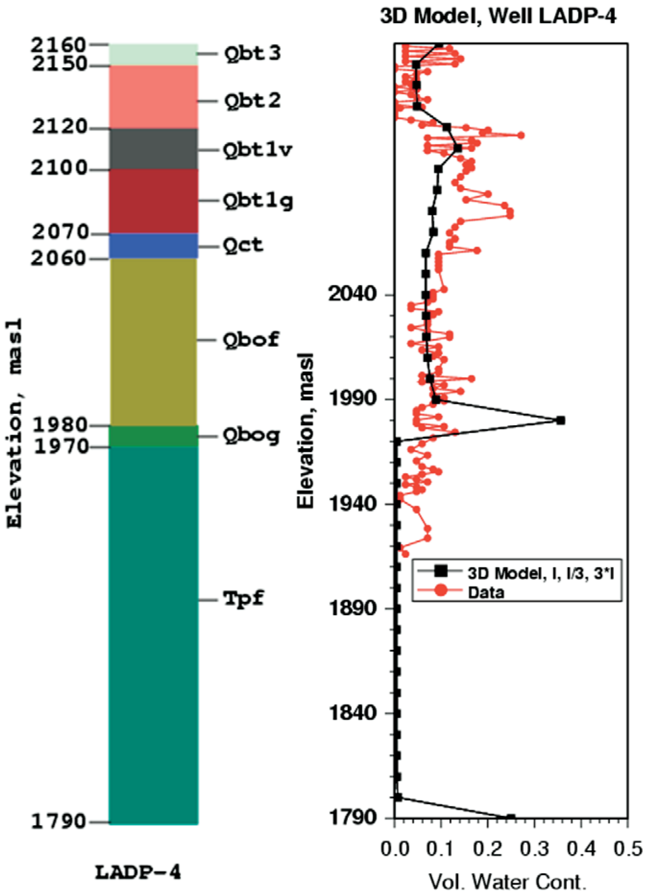

Fig. 8. Comparison of data and three-dimensional model predictions for water contents in Well LADP-4: (left) stratigraphy, (right) data–model comparison.

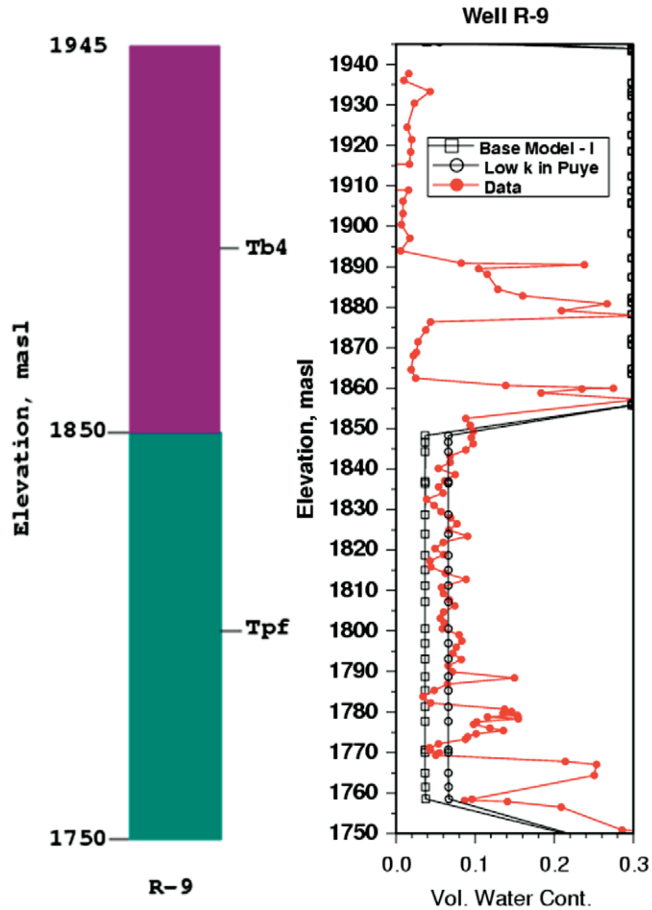

Fig. 9. Comparison of data and three-dimensional model predictions for water contents in Well R-9: (left) stratigraphy, (right) data–model comparison for different values of the permeability of the Puye Formation.

Transient Flow Simulations

In all simulations presented so far, steady-state conditions are assumed, despite the fact that transients on a variety of time scales are likely. For example, Gray (1997) shows that in Los Alamos Canyon, water levels in alluvial aquifer wells fluctuate seasonally in response to summer storm events and spring snowmelt runoff. On decadal time scales, climate variability and changes to the surface hydrologic forcing conditions due to anthropogenic water sources and human-induced changes to the drainage conditions supplying water to the canyon must be considered.

To examine the influence of these transients on measured water content, the two-dimensional numerical model is used to provide insight into the likely effects. The two-dimensional approximation is suitable for this type of sensitivity calculation, and reduces computational burden. In the first simulation, seasonal variability is examined by introducing a very sharp impulse of water corresponding to the entire predicted infiltration volume of one-half year concentrated in a 1-wk time period. This bounding case is intended to model the situation in which all infiltration occurs in a single spring runoff event and a single summer storm event. Figure 10 shows the predicted water content profiles in LADP-3 and LAOI(A)-1.1 immediately after one such event of high infiltration. The influence of the transient is only felt in the uppermost 10 m or so of the vadose zone. The water input during the event, though intense, is insufficient to have a significant influence on the water content profile at depths greater than about 10 m. These events would then be followed by one-half year of no infiltration, which would cause the profile to bounce back to nearly its original state. Therefore, except for the rocks very close to the surface, directly beneath the alluvium–bedrock interface, the assumption of steady-state conditions appears to be an adequate approximation.

Longer-term variability in the infiltration rate is investigated in a simulation in which the steady state solution for a low-infiltration-rate scenario (infiltration of 1/5 the base case) is used as an initial condition, and the rate is increased to the base-case infiltration map at time zero. Figure 11 shows that in a time period of a few years, the water contents increase to significant depths. Within about a decade, the profile throughout the entire section of the Otowi member reflects the new, higher infiltration rate. At times of one or a few years, the transient water content profile shows curvature similar to that seen in several of the observation wells, including LADP-3 and LAOI(A)-1.1.

This simulation suggests that variability in infiltration

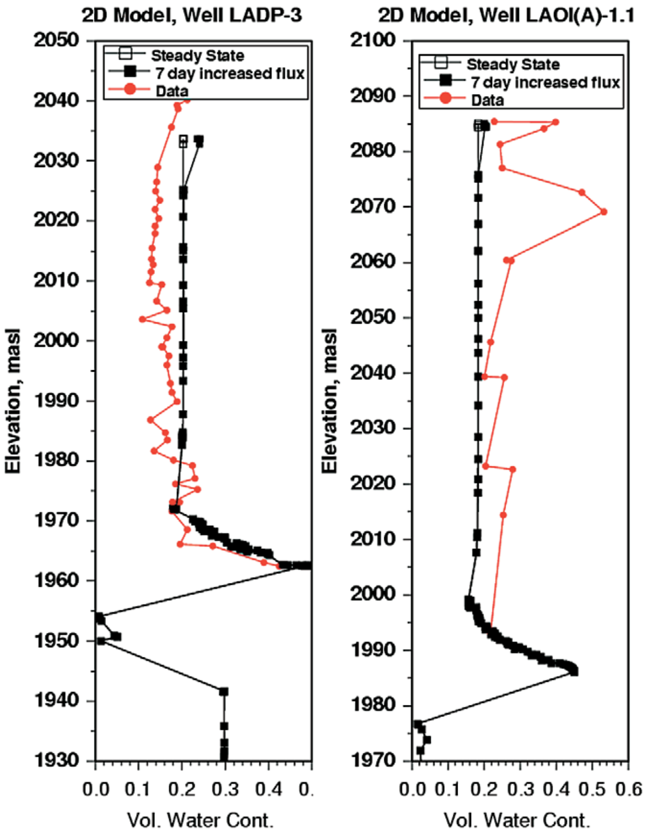

Fig. 10. Two-dimensional model predictions for the water content in response to a single 1-wk episode of enhanced infiltration: (left) Well LADP-3, (right) Well LAOI(A)-1.1.

rates over years to decades complicates the interpretation of the water content profiles, and must be considered. A canyon with effluent discharges that commenced since the Laboratory came into existence 60 yr ago will have significant perturbation to the natural surface and vadose zone hydrology. In addition to effluent discharges, drainages from the townsite or local paved areas can also alter the natural conditions. The simulations show that data in Los Alamos Canyon represent the fluid flow characteristics of the system within the previous 10 to 100 yr leading up to the collection of the water content data. Modeling interpretations of such data must consider these impacts either directly, using transient simulations, or indirectly, through parameter sensitivity studies that bracket the range of infiltration rates expected in the time period of interest.

This result for a wet canyon setting is in sharp contrast to the arid-system hydrodynamics present on the nearby dry mesas. In such systems on the Pajarito Plateau and elsewhere, long-term, climate change–induced transients in water flow and geochemistry are generally thought to take many thousands of years to propagate through a deep vadose zone (e.g., Walvoord et al., 2002; Birdsell et al., 2005). The critical difference is the infiltration rate, which is several orders of magnitude higher in a wet canyon setting than on a dry mesa top.

Tritium Transport

Tritium transport modeling, conducted using the base-case flow model, serves two main purposes. First, the

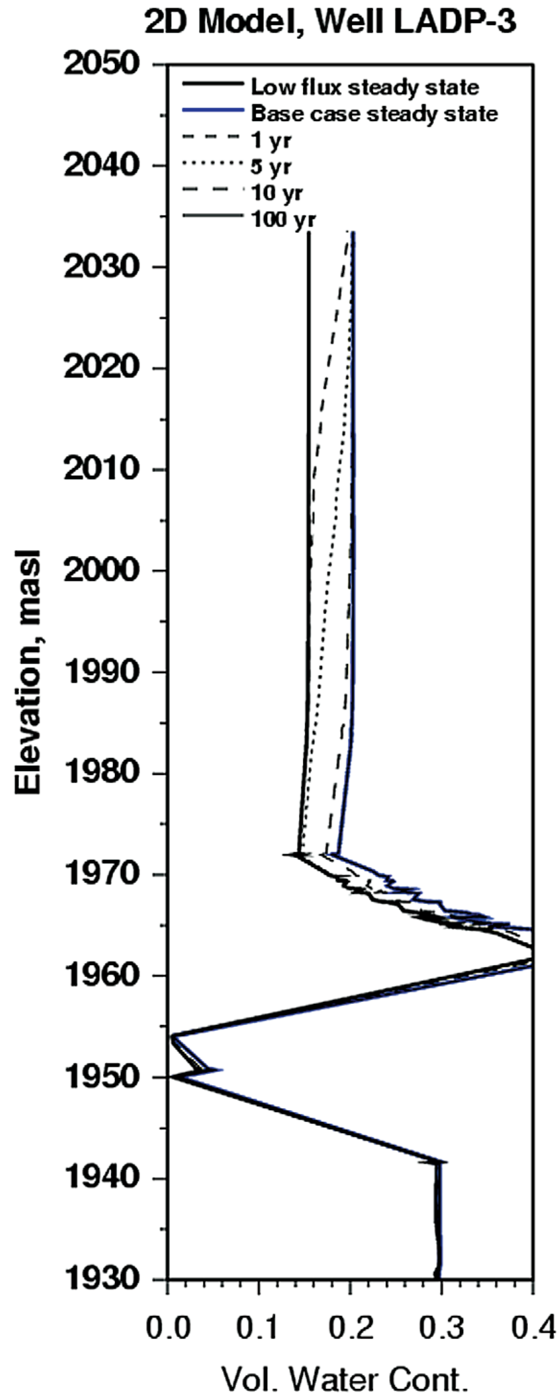

Fig. 11. Two-dimensional model predictions for the water content at Well LADP-3 in response to a prolonged period of enhanced infiltration. Infiltration is increased by a factor of five starting at time 0.

model is used to illustrate the likely behavior of conservative contaminants such as tritium, perchlorate, and nitrate in Los Alamos Canyon. The second, more research-oriented goal, is to demonstrate that the incorporation of contaminant transport information can provide confidence in and confirm aspects of the flow model that cannot be demonstrated with flow information alone. The analyses below address these two goals.

The most important conceptual model component for

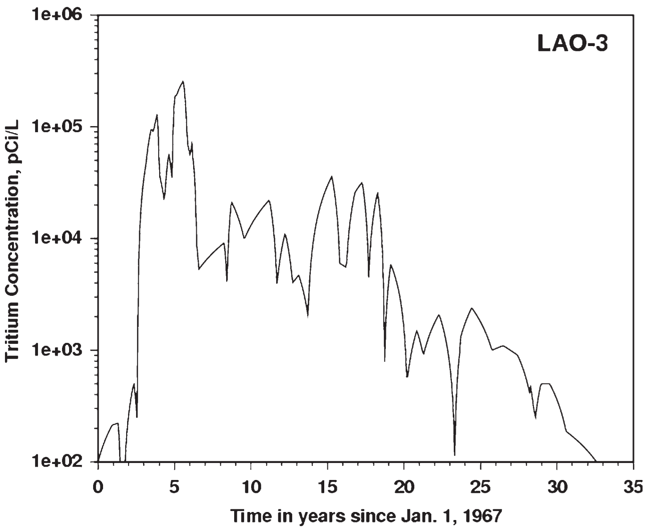

Fig. 12. Concentration and time history for tritium in alluvial Well LAO-3, located downstream of tritium release sources. Values less than about 1000 pCi L^{-1} are below the analytical detection limit for these data.

solute or contaminant transport is that an effective continuum model is valid. This model assumes that the medium can be represented with a continuum in which solute is displaced through rock with an effective porosity that is assigned for each hydrogeologic unit. For the Bandelier Tuff, we assume that flow is predominantly through the rock matrix, in keeping with the findings of Robinson et al. (2005) that flow through these rocks appears to be matrix dominated, so that the measured matrix porosity can be used for transport. For the basaltic rocks, flow is clearly controlled by complex fast paths, making a continuum model assumption more problematic. We treat this issue by assigning an effective transport porosity for these units that is small (0.05), to simulate rapid downward migration in these units. The use of a continuum model for the basaltic rocks is for convenience, and is not meant to imply that transport is uniform through these rocks. We capture preferential transport and fast pathways in an approximate way through the use of a low porosity in the basalts.

For the tritium source term, measured tritium concentrations versus time in the alluvial groundwater are used by introducing fluid with this time history of concentration into the model. Figure 12, a plot of tritium concentrations measured at alluvial Well LAO-3, located at the confluence of Los Alamos and DP Canyons, shows that in about 1970, high concentrations of tritium had migrated downstream of the Laboratory's nuclear research facilities. Similar data at three other wells upstream and downstream of this location were used to establish the time-varying and spatially varying input concentration along the canyon. The present-day concentrations in the alluvial groundwater have reverted back to low values (compared with their peak values), a consequence of source control efforts and the decommissioning of the Omega West reactor.

In all model runs, dispersivity values are set to low values to simulate advective movement of tritium through the vadose zone. Local dispersion is expected to play a relatively minor role in the behavior of the transport system compared with the wide range of travel times experienced as a function of infiltration and stratigraphic variability along the canyon. Tritium is taken to be a nonsorbing contaminant that undergoes radioactive decay only.

The initial condition (pre-1970) is established by assuming a constant, low concentration in the source fluid and running the model until a steady state is achieved. Because the concentrations during the remainder of the simulation are many orders of magnitude higher than these initial values, the details of this initial condition simulation do not affect the model results appreciably.

Tritium Model

To examine transport behavior through the vadose zone, we first present two-dimensional model results under base-case conditions. Figure 13 is a series of snapshots of concentration, plotted as log10 of the concentration in picocuries per liter on a range from 1 to 10 000 pCi L^{-1}. The tritium plume appears in the subsurface in 1970 when concentrations in the infiltrating fluid increased dramatically. Transport velocities predicted by the model are such that the majority of the released tritium stays within the vadose zone, where it undergoes natural attenuation by radioactive decay. However, the model does predict transport of a small fraction of the tritium to the regional aquifer. The regions where deepest transport occurred are those zones of highest infiltration, particularly the high-infiltration zone corresponding to the Guaje Mountain Fault. This result is consistent with observations of anthropogenic tritium detected in the regional aquifer, albeit at low concentrations.

The results also indicate preferential transport to the water table at locations downstream of the confluence of Los Alamos and DP canyons. This is depicted using tritium concentration results for fluid reaching the water table in the year 1999, predicted from the three-dimensional model (Fig. 14). The locations of important sampling locations for wells drawing fluid from the regional aquifer are also shown. Model predictions for Well O-4 indicate that most tritium entering the regional aquifer at that location is likely still present in the vadose zone; however, a small but non-zero concentration is predicted to have reached the regional aquifer. Well R-7, located downstream of tritium contaminants but even further upstream of the Los Alamos-DP canyon confluence, is predicted to have no tritium arriving at the water table. By contrast, the most rapid transport to the water table is predicted at R-9, where the peak concentrations of tritium are predicted to already have reached the water table.

The reason for this spatial dependence of transport velocity through the vadose zone is that the thickness of Bandelier Tuff is much greater at upstream locations in the canyon, whereas at downstream locations, no Bandelier Tuff is present. For example, in Fig. 3 the basalts are represented by the light bluish-green color, which is present at the surface in Los Alamos canyon

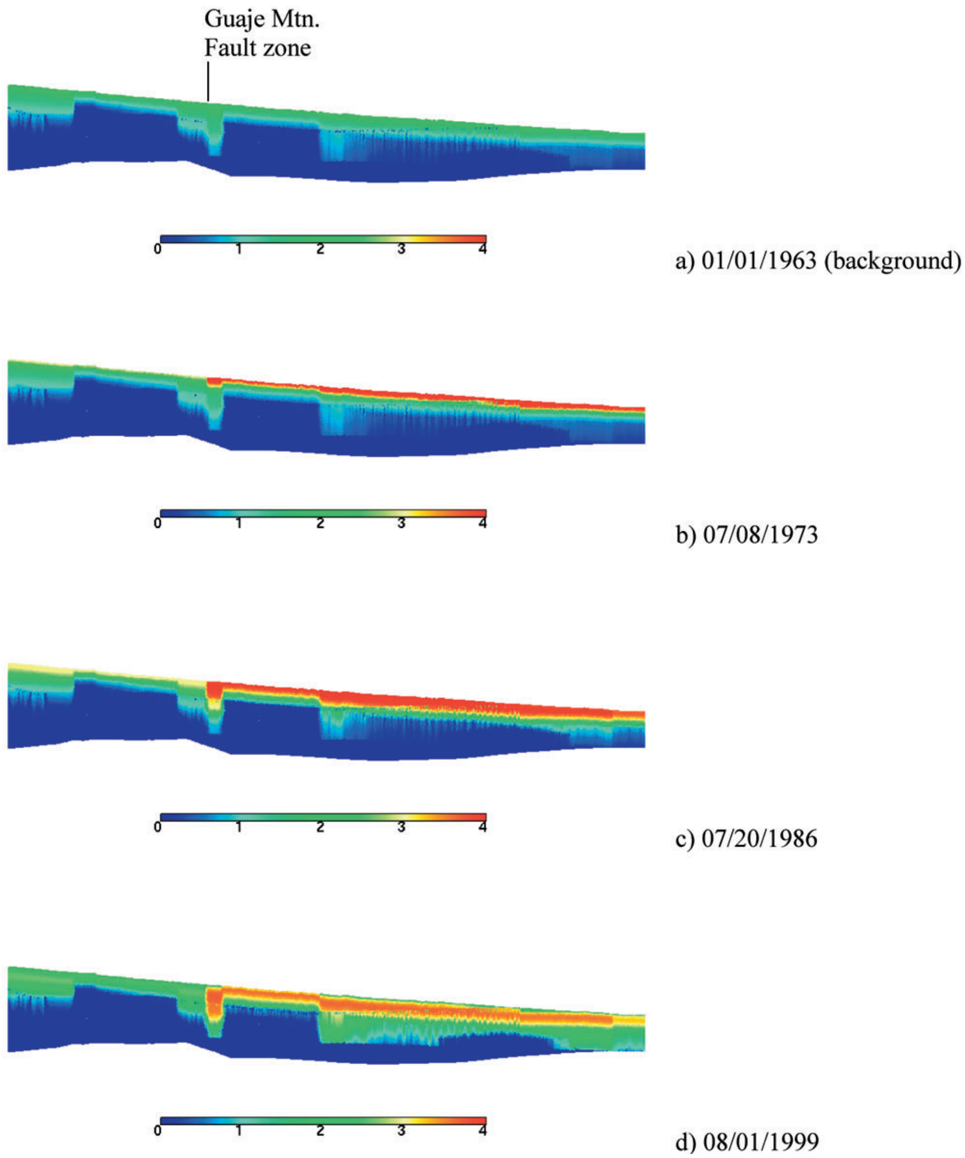

Fig. 13. Two-dimensional model predictions of the tritium concentration of fluid in the vadose zone at various times. Concentration units are log10 of concentration in picocuries per liter. (a) 1 Jan. 1963 (presumed to be background, before significant releases); (b) 8 July 1973; (c) 20 July 1986; (d) 1 Aug. 1999.

at Well R-9. The conceptual model for vadose zone flow, outlined in detail in Birdsell et al. (2005), consists of matrix flow and transport in the Bandelier Tuff, and preferential flow and transport in the basalt units. Rapid transport to the water table at the downstream locations is due to fracture flow in the basalts and fairly rapid transport through the Puye Formation. Therefore, concentration levels of fluid reaching the regional aquifer in these locations in the canyon are predicted to be significantly greater than zero (in the thousands of picocuries per liter) in this portion of the model domain.

These model results are consistent with the available field data. Regional aquifer fluid collected in Well R-7 has indetectable levels of tritium, as does the water supply Well O-4. In contrast, R-9 characterization sampling shows that tritium has reached the regional aquifer, and concentrations are among the highest observed in the aquifer. Determining more quantitatively the ability of the model to reproduce the field data is difficult because of mixing of the tritium percolating from the vadose zone with regional aquifer fluid, and the subsequent mixing of contaminated and clean fluid in the wellbore itself. This difficulty is especially acute for the water supply wells, which may draw water from a hundred of meters of screened length. In summary, though quantitative comparisons are not possible, the comparisons suggest that the conceptual model for transport is acceptable: transport occurs slowly through high-porosity rock in the Bandelier Tuff, but water and contaminants migrate much more rapidly to depth in the basaltic rocks. Parameters such as the effective porosity of the basalts are quite uncertain; the study of Stauffer and Stone (2005) suggests that lower values on the order of 0.01 to 0.001 may be in order. However, using even lower values would not change the basic conclusion or the modeling results of our study.

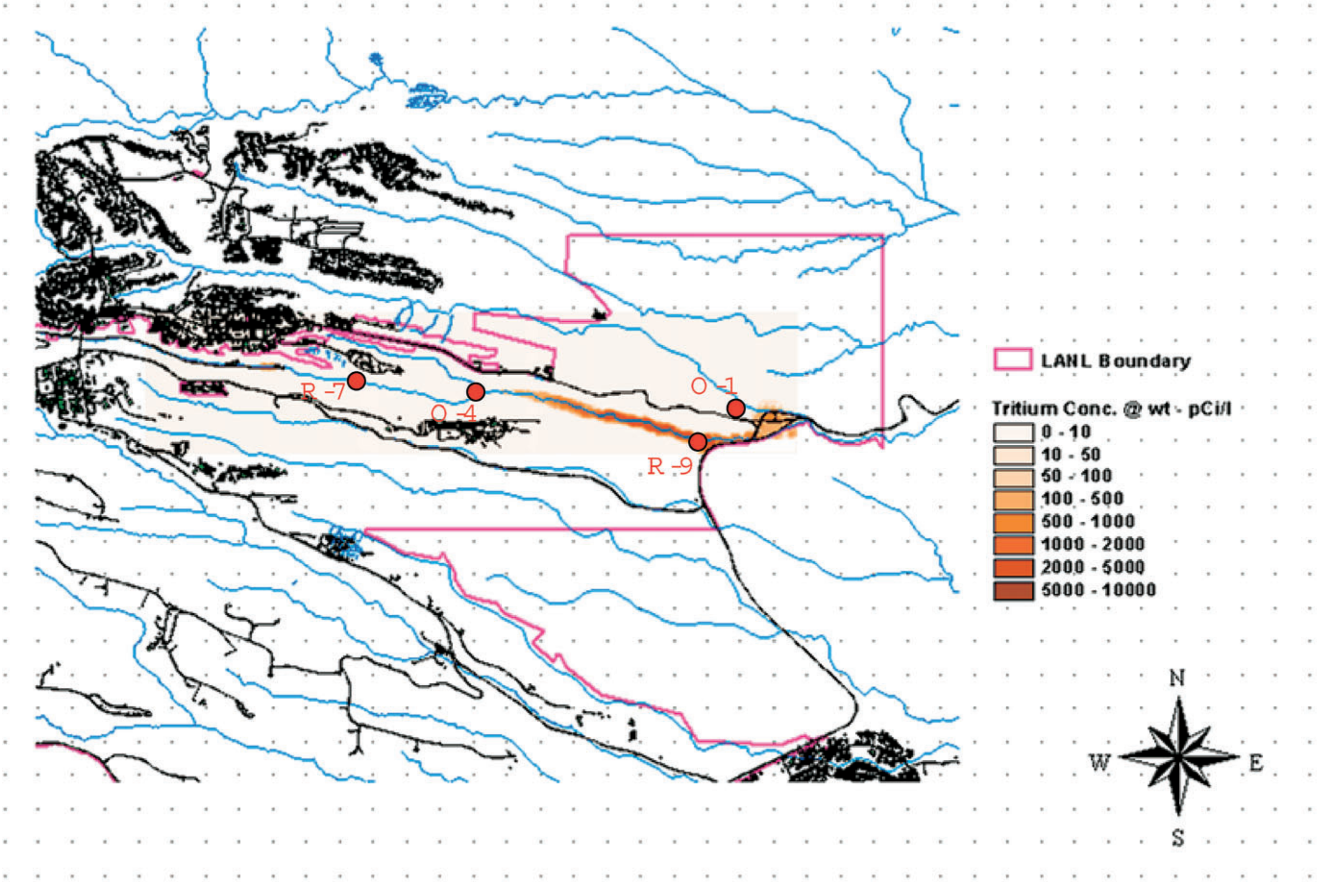

Fig. 14. Three-dimensional model predictions of the tritium concentration of fluid reaching the water table in 1999. Significant, above background concentrations are predicted along the canyon at locations downstream of where the Bandelier Tuff is not present in the canyon bottom.

As a final comparison to the available data, we contrast the model results with regional aquifer water supply Well O-1. However, because contaminant transport sources from Pueblo canyon (north of Los Alamos Canyon) were not included in this model, the conclusions related to O-1 are more qualitative. For this comparison, monitoring information published in LANL (2001) is used. Contaminants tritium, perchlorate, and nitrate are all thought to be nonsorbing in this system, and thus the combined results of all three contaminants are used in this interpretation. Well O-1 has been found to contain measurable levels of perchlorate at about a 5 ppb level, nitrate levels higher than at other regional aquifer wells in the area, and consistent, above-background levels of tritium in the 30 to 40 pCi L^{-1} range. All observations point to both Laboratory-derived contaminants and effluent discharges from Los Alamos County from past releases in Los Alamos and Pueblo Canyons having traversed the entire vadose zone. The present model explains these observations as a consequence of the hydrostratigraphy along the canyon, with rapid travel times at locations where the Bandelier Tuff is thin or nonexistent.

DISCUSSION AND CONCLUSIONS

In this paper we present a modeling study for the vadose zone beneath Los Alamos Canyon. This model demonstrates that a comprehensive understanding of vadose zone hydrologic processes can be obtained by integrating data from geologic, hydrologic, and site characterization sources. Insights gained from a numerical model of the vadose zone hydrology and tritium transport from the canyon bottom to the water table allow us to explain available observations, investigate the transient hydrologic behavior, and quantify uncertainties. These uncertainties are important if the model is to be used to predict future transport behavior for contaminants discharged to the canyon. More generally, the model demonstrates that extensive site characterization data focused on the surface, shallow subsurface, and deeper vadose zone are required to develop a model that has predictive value.

The complex hydrostratigraphy of the canyon was captured using geologic characterization of extensive deep-well drilling samples, along with surface mapping. The hydrologic conceptual model places a premium on capturing the thicknesses of the Bandelier Tuff units and the Cerros del Rio basalts. Slow percolation through the tuff, compared with rapid transport through the basaltic rocks, controls the rates of movement of contaminants to the water table. Using sophisticated grid-generation techniques, we were able to represent these rock layers quite accurately in the two- and three-dimensional models.

The water budget study used for the inlet flow boundary condition, though not a precise measure of infiltration rate, provides a reasonable constraint on the vadose zone model. Rates varying spatially from about 200 to 1000 mm yr^{-1} were estimated along the canyon. Uncertainties in these values were obtained principally from hand-calibration to water content profiles and sensitivity analyses. A range of a factor of three higher and lower than these mean values are consistent with the available data. More precise bounds do not appear to be possible without additional data, perhaps including detailed contaminant transport profiles in the vadose zone and joint calibration to these multiple data sources.

The flow model implements the conceptual model element of the large difference in infiltration rate from the canyon bottom to the mesa top. Mesa-top infiltration rates on the order of 1 mm yr^{-1}, along with canyon-bottom rates several orders of magnitude higher, capture the water content profiles measured in boreholes within the model domain. A three-dimensional model was required to demonstrate this facet of the system.

Transient flow simulations using the base-case model were used to assist in the interpretation of vadose zone water content profiles in this and similar canyons. Modeling results suggest the non- and partially welded Bandelier Tuff units, such as the Otowi member, have hydrologic properties that dampen episodic infiltration events. Thus, an average annual infiltration rate applied to a steady-state model yields a similar water content profile as one in which all water infiltrates in a single, yearly event. In contrast, transients that last on the order of a decade or more significantly change the predicted water content. This type of transient could be climate related or anthropogenic, the result of a facility discharging liquid effluents or drainage conditions altered from their natural state by human activities. This possibility must be considered during model development, and may limit the degree to which steady-state model calibrations can capture the available data.

Transport modeling of tritium provides an additional constraint on the vadose zone model. Modeling results indicate that even for a nonsorbing contaminant such as tritium, the majority of the released contaminant is present in the vadose zone, or, in the case of tritium, has decayed. A small fraction of the released mass has reached the water table, primarily in locations in the canyon of high infiltration rate, or where the Bandelier Tuff is not present. Water percolates through the matrix rock in the tuff units, whereas it travels rapidly through fast pathways in the basaltic rocks. This model therefore suggests that within this portion of the Pajarito Plateau, regional aquifer groundwater most at risk for contamination is at locations near or below the confluence of Los Alamos and Pueblo Canyons. Available groundwater surveillance data are consistent with this result, thereby providing an independent test of the validity of the model.

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