

Development and Application of Numerical Models to Estimate Fluxes through the Regional Aquifer beneath the Pajarito Plateau

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ABSTRACT

Before recent drilling and characterization efforts in the vicinity of Los Alamos National Laboratory (LANL), conceptual models had been developed for recharge and discharge in the regional aquifer on the basis of sparse data. By integrating site-wide data into a numerical model of the aquifer beneath the plateau we provide new insight into large-scale aquifer properties and fluxes. This model is useful for understanding hydrologic mechanisms, assessing the magnitudes of different terms in the overall water budget, and, through sampling, for interpreting contaminant migration velocities in the overlying vadose zone. Modeling results suggest that the majority of water produced in well fields on the plateau, extracted at rates approaching 70% of total annual recharge, is derived from storage. This result is insensitive to assumptions about the percentage of total recharge that occurs in the near vicinity of water supply wells, because of strong anisotropy in the aquifer that prevents fast transport of local recharge to deeper units from which production occurs. Robust estimates of fluxes in the shallow portion of the aquifer immediately down gradient of LANL are important for contaminant transport simulations. Our model calculations show that these fluxes have decreased in the past 50 years by approximately 10% because of production in water supply wells. To explore the role of parameter uncertainty in flux prediction, a predictive analysis method was applied. Results showed that predicted flux through older basalts in the aquifer can vary by a factor of three because of uncertainty in aquifer properties and total recharge. We explored the impact of model parameter uncertainty on these results; however, the true uncertainty of our predictions, including the impact of possible conceptual model errors, is likely to be larger and is difficult to quantify.

GROUNDWATER beneath the Pajarito Plateau is part of a regional aquifer that extends throughout the Española Basin (an area roughly 6000 km²; Fig. 1). This aquifer is the primary source of water for the LANL; the communities of Santa Fe, Española, Los Alamos; and numerous pueblos. Four water supply well fields exist on the plateau (Fig. 2). One additional well field that supplies the City of Santa Fe (Buckman) sits just to the east of Rio Grande close to the plateau. As is the case for many aquifers in the semiarid southwest, there is concern that current withdrawal rates may not be sustainable for long periods of time, and current drought conditions might have significant impacts on both surface water and groundwater quantity and quality. Of particular concern is surface water flow in the Rio Grande, which is reduced both by direct diversions

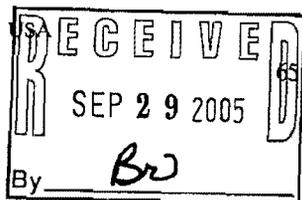
(primarily agricultural) and decreased baseflow because of groundwater production. For example, in 2002 the State of New Mexico was unable to honor interstate stream compacts for surface water delivery to Texas and incurred substantial penalties. There are also concerns about water quality at the regional scale because of a variety of contaminants, both nonanthropogenic and anthropogenic. Beneath the Pajarito Plateau, there is substantial contamination from various LANL sources in shallow groundwaters in some locations (primarily alluvial aquifers), and it is unclear what the ultimate impact of this contamination will be on the regional aquifer in the future. Some of the LANL-derived contamination has been observed in the regional aquifer at trace concentrations much below the EPA drinking water standards. To assess the future water quality and quantity issues, 21 deep characterization wells have been drilled since 1995, and flow and transport models have been developed both at the site- and basin-scale.

Historical liquid effluent discharges in canyons are the most likely sources of this deep groundwater contamination. These contaminants must migrate through the unsaturated rocks of the vadose zone before reaching the regional aquifer. Some of the most convenient sampling locations for groundwater contamination are the wells drilled to the regional aquifer, where samples can be obtained by pumping screened intervals. These samples provide important information on the rates of movement of water and contaminants in the vadose zone. However, to interpret the results, a basic understanding of the flow conditions in the regional aquifer is required. Therefore, studies of the regional aquifer serve the purpose of providing a stronger basis for evaluating the vadose zone travel times and contaminant transport behavior.

Beneath the Pajarito Plateau, the aquifer is very deep (up to 360 m below ground surface). The thick vadose zone is quite complex hydrologically (Birdsell et al., 2005) and includes perched aquifers in some locations. One emphasis of the recent groundwater characterization efforts has been to provide more quantitative estimates of recharge through the vadose zone (Birdsell et al., 2005; Kwicklis et al., 2005). The most obvious rationale for doing so has been to identify likely pathways and fluxes for contaminant transport through the vadose zone. A second, perhaps less obvious rationale, has been to determine fluxes through the regional aquifer, which in turn allow better estimation of aquifer properties, groundwater velocities, contaminant fate and transport, and water quantity issues. The importance of estimating recharge for water resource evaluation has been ques-

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Abbreviations: LANL, Los Alamos National Laboratory; PM, Pajarito Mesa.

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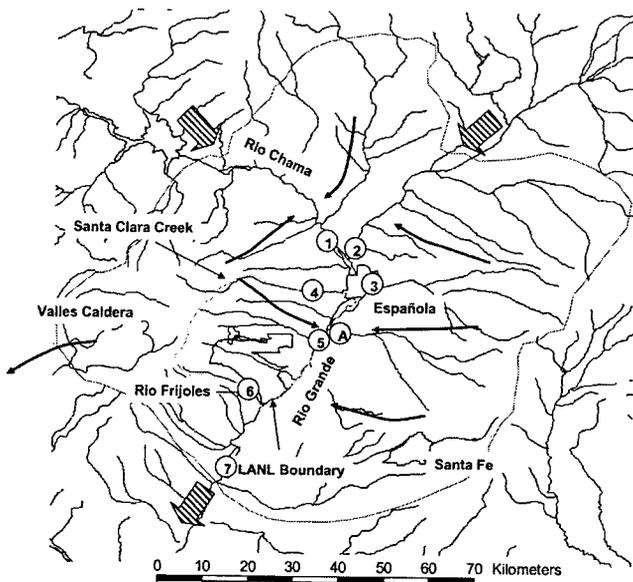


Fig. 1. The Española Basin and vicinity, with basin-scale numerical model outline shown in red, site-scale model outline shown in green. Black arrows are generalized groundwater flow directions, based on regional water level data (Keating et al., 2003). Striped arrows indicate groundwater flow between this basin and adjacent basins. Circled numbers refer to USGS stream gages: 1, Rio Chama at Chamita; 2, Rio Grande at San Juan; 3, Santa Cruz River; 4, Santa Clara Creek; 5, Rio Grande at Otowi; 6, Rio Frijoles; 7, Rio Grande at Cochiti. Circled "A" indicates the mouth of the Pojoaque Creek (see Table 4).

tioned by some (Bredhoeft, 1997). In this study we view recharge quantification as a critical component of assessing aquifer characteristics, groundwater velocities, and future water supplies.

Past studies of the regional aquifer beneath the plateau provided a conceptual model of groundwater recharge, discharge, flow directions, and velocities on the basis of very sparse data (Griggs and Hem, 1964; Purtymun, 1984; Purtymun and Johansen, 1974; Rogers et al., 1996). In many ways, this conceptual model has proven to be robust in light of more recent data collection and modeling analyses. However, providing quantitative predictions of future water quality and quantity in the regional aquifer requires a more detailed analysis than was previously possible. Here we describe the develop-

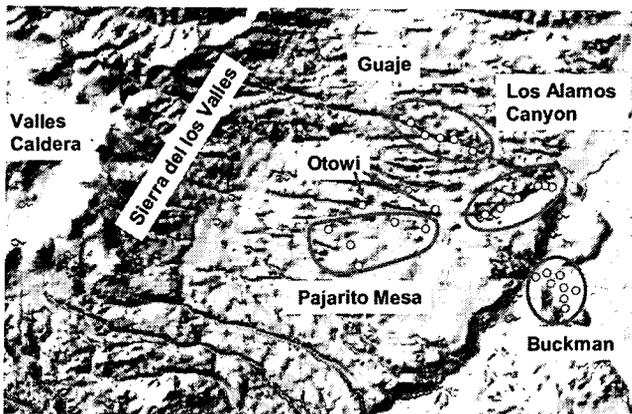


Fig. 2. The Pajarito Plateau, with major well fields indicated.

ment of a regional aquifer flow and transport model, coupled to a simple and flexible model of recharge for the plateau. We present model applications that address a key issue for both water resource and contaminant issues: the flux of groundwater off-site and the impact of production on this flux. We present simulations of the impact of groundwater production on the plateau on storage in the aquifer and baseflow gain in the Rio Grande and show the impact of uncertainty in the spatial distribution of recharge through the vadose zone. Using predictive analysis, we show the impact of uncertainty in aquifer properties and recharge on predicted flux downgradient from a contaminated site at LANL.

HYDROGEOLOGIC SETTING

This section provides a comprehensive literature review for the regional aquifer beneath the Pajarito Plateau. We also refer to studies conducted elsewhere in the Española basin. This is for two reasons. First, the hydrogeology of the plateau is certainly affected by regional flow. Second, the deepest aquifer unit beneath the plateau, the Santa Fe Group, is rarely exposed on the plateau and local studies have shed little light on its hydrogeologic character. However, this unit is ubiquitous elsewhere in the basin and has been studied extensively; it is insightful to examine these studies.

We supplement the previous literature with interpretations of new data collected by the LANL Groundwater Characterization program. These new data, combined with previous studies, provide the foundation for flow and transport model development presented in later sections.

Recharge

Recharge Distributions

Various theories have been proposed regarding the locations of recharge zones for this aquifer. Griggs and Hem (1964) suggested that most of the recharge occurred in the Sierra del los Valles and along stream channels in the western edge of the Pajarito Plateau (Fig. 2). Purtymun and Johansen (1974) proposed that the major portion of the recharge occurs in the Valles Caldera (Fig. 2), with smaller amounts recharging through stream channels in the Sierra del los Valles. Blake and others (1995) argued that recharge could not originate in the Valles Caldera, since the chemistry of geothermal waters in the western Valles Caldera is clearly distinct from the groundwaters on the Pajarito Plateau (Blake et al., 1995; Goff and Sayer, 1980). On the basis of stable isotope values in groundwaters beneath the plateau, these authors also proposed that recharge areas for the aquifer beneath the plateau were either to the north and/or to the east (Sangre de Cristo Mountains) and not to the west. They hypothesized that the two flow systems are separated by the Pajarito fault acting as a flow barrier (Blake et al., 1995).

Numerous lines of evidence indicate that the majority of recharge to the basin aquifer occurs in the mountains along the basin margin where precipitation rates are

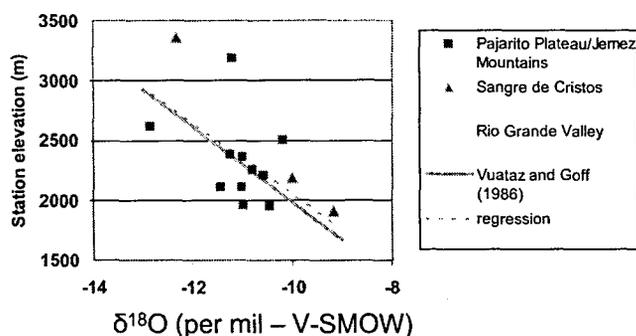


Fig. 3. Storm volume-weighted means in oxygen isotope values from 3 yr of precipitation, plotted as a function of precipitation station elevation, derived from Adams et al. (1995) and Anderholm (1994).

relatively high. This has been shown using water-budget and chloride-mass balance analyses in the eastern portion of the basin (Anderholm, 1994; Wasiolek, 1995) and by inverse modeling using head and streamflow data (Keating et al., 2003). Keating and others (2003) demonstrated that the elevation above which significant recharge occurs at the basin-scale is very well constrained (2195 ± 177 m). Using streamflow data from the Pajarito Plateau, Kwicklis (Nylander et al., 2003) calculated that if all streamflow loss becomes recharge on the plateau, this would contribute a maximum of 4 to 10% of the total recharge to the aquifer. A more recent estimate, by Kwicklis et al. (2005) using a combination of streamflow data and indirect estimations of streamflow, suggests a higher number, approximately 23% (14% total in streams that flow at least partly within LANL boundaries). At lower elevations, recharge occurs primarily along arroyos and canyons; very little or no recharge occurs on mesas except near the mountain front (Anderholm, 1994; Birdsell et al., 2005).

Although small volumetrically compared with mountain recharge to the west, there is no question that the aquifer recharge occurs locally on the plateau. Tritium data confirm that relatively young water is present in the aquifer (Rogers et al., 1996), indicating fast pathways through the vadose zone beneath LANL. Quantitative estimation of recharge using ^3H data is complicated by the sometimes confounding influences of bomb-pulse atmospheric ^3H and locally derived ^3H related to on-site LANL activities. Elevated ^3H in regional aquifer samples has been observed at O-1, TW-1, TW-3, TW-8, LA-1A and LA-2 (Rogers et al., 1996).

Blake et al. (1995) used $\delta^{18}\text{O}$ or δD values in local groundwater to predict elevations of recharge and location of recharge (Sangre de Cristos vs. Jemez Mountains) according to the regression proposed by Vuataz et al. (1986) based on spring data in the Valles Caldera. These inferences are based on the premise that $\delta^{18}\text{O}$ or δD values in precipitation, averaged over a sufficiently long time period, are correlated with recharge elevation. We show storm volume-weighted average $\delta^{18}\text{O}$ values in Fig. 3 from 3 yr of published data for local precipitation (Adams et al., 1995; Anderholm, 1994), along with a linear regression result. These data support the general trend proposed by Vuataz et al. (1986), but $\delta^{18}\text{O}$ and elevation are only weakly correlated ($r^2 = 0.29$) when

3 yr of precipitation data are considered. It is clear that variability in isotopic composition of precipitation at any given elevation is quite large; the standard error of the linear relationship is 370 m and the two largest errors exceed 700 m. These potential errors should be considered when evaluating uses of stable isotopes as tracers of recharge elevation or as a way to distinguish between recharge in the Sangre de Cristos and the Jemez Mountains based on differences in their maximum elevations. Although it is possible that collecting more data will improve the correlation, the variability evident in the available datasets at present suggests that inferences of precipitation or recharge elevation based on isotopic composition should be viewed with great caution. Another, perhaps more significant, problem with using isotopic trends in precipitation to predict recharge elevation is that in settings where streamflow losses are an important source of recharge, such as is the case in several locations on the plateau, the actual location of recharge may be much lower than the location of precipitation from which the recharge waters were derived.

Although there are problems with using stable isotope ratios to trace the *location* of recharge, they have been shown to be valuable in tracing the *timing* of recharge for very old waters (Phillips et al., 1986). Very low $\delta^{18}\text{O}$ values (less than -14), significantly lower than average modern precipitation signatures at all elevations in the basin (see Fig. 3), have been measured in groundwaters near the Rio Grande (Anderholm, 1994; Blake et al., 1995). These ratios are indicative of paleorecharge during a cooler climate (Phillips et al., 1986) and were interpreted by Anderholm (1994) and Newman (1996) to indicate recharge during the Pleistocene (with age in order of 8000–17 000 yr). These age estimates are consistent with ^{14}C dating of groundwaters in the same vicinity (Rogers et al., 1996). This is an alternative conceptual model to that proposed by Blake et al. (1995). Using the regression equation in Fig. 3, they interpreted very light isotopic values in wells just to the west of the Rio Grande to imply recharge from the Sangre de Cristos and underflow beneath the Rio Grande.

Total Recharge

Griggs and Hem (1964) estimated the total recharge to the aquifer beneath the Plateau to be between 168 and 216 kg s^{-1} . McLin et al. (1996) estimated an upper bound of 192 kg s^{-1} , based on recovery of water levels in supply wells rested for a period of several months to several years. Using a variety of methods and considering a larger area, Kwicklis and others (2005) estimated total recharge to the Pajarito Plateau of 336 kg s^{-1} . Baseflow gain to the Rio Grande has been used by a number of researchers to estimate total aquifer discharge, both from beneath the plateau and the eastern basin, which presumably approximated total aquifer recharge before significant pumping began. Long-term average aquifer discharge between Otowi Bridge gage and the now-submerged Cochiti gage, a reach which bounds the southern portion of the plateau, was esti-

mated by Spiegel and Baldwin (1963) to be 710 kg s^{-1} and more recently by the U.S. Department of Justice to be 400 kg s^{-1} . The former estimate is significantly higher because they ignored years of record that indicated the reach to be losing, which was attributed to measurement error. In Appendix A, we present an analysis of data from this reach as well as the reach immediately to the north (Española to Otowi), which bounds the northern portion of the plateau. This analysis estimates the total gain to the Rio Grande adjacent to the Pajarito Plateau (Santa Clara Creek to Rio Frijoles) to be approximately 911 kg s^{-1} ($\pm 30\%$). It is impossible to use streamflow data alone to determine the proportion of this gain that originates beneath the plateau. The modeling study of Hearne (1985) assumed 316 kg s^{-1} total recharge to the Pajarito Plateau; McAda and Wasiolek (1988) assumed 291 kg s^{-1} lateral inflow from the Jemez Mountains. Based on streamflow data and transient head data, basin-scale inverse modeling (Keating et al., 2003) indicated that approximately 253 kg s^{-1} of the gain to the river along this reach originated on the Pajarito Plateau and the Sierra de los Valles. This analysis probably underestimates total recharge on the plateau, in part, because the basin model was calibrated to a lower estimate of aquifer discharge north of Otowi Bridge than is indicated by the streamflow analysis presented in the Appendix. Part of the reason for the differences between these various estimates of total recharge is that several of the smaller estimates (McLin et al., 1996; Spiegel and Baldwin, 1963; Griggs and Hem, 1964) emphasized the southern portion of the plateau (including LANL), which according to our streamflow analysis in the Appendix, is discharging less water than the northern portion of the plateau. Although these various estimates are disparate and reflect real uncertainty, they are extremely valuable as bounding values for flow and transport modeling.

Discharge

Many authors have identified the Rio Grande as the discharge point for the regional aquifer (Cushman, 1965; Griggs and Hem, 1964; Hearne, 1985; McAda and Wasiolek, 1988; Purtymun and Johansen, 1974; Theis and Conover, 1962). Previous reports have cited a variety of evidence to support this, including streamflow gain along the Rio (Balleau Groundwater, 1995; Purtymun and Johansen, 1974; Spiegel and Baldwin, 1963), measured vertical upward gradients in the vicinity of the Rio Grande (Cushman, 1965; Griggs and Hem, 1964), the presence of flowing wells (McAda and Wasiolek, 1988; McLin et al., 1996; Spiegel and Baldwin, 1963), and springs along the river (McLin et al., 1996). Discharge to the river may occur as lateral flow, upward flow, or as flow from springs in White Rock Canyon. Purtymun (1966) suggested that all the springs, which collectively flow approximately 85 kg s^{-1} , discharge water from the upper surface of the main aquifer. Stone (1996) suggested that many of these springs may be discharging perched aquifers rather than the regional aquifer; unfortunately it is difficult to test these alternative hypothe-

ses. It has been emphasized that although discontinuous, low permeability beds produce confining conditions in the aquifer locally near the Rio Grande and elsewhere in the basin, flow is able to cross the low permeability beds in some locations as groundwater discharges to the river (Hearne, 1985; Spiegel and Baldwin, 1963).

The degree of connection between the aquifer and the Rio Grande has been investigated by Balleau Groundwater, Inc. (1995), who drilled 16 wells in the alluvial aquifer of the Rio Grande near the Buckman well field and conducted pumping tests. They found that head in the alluvium is generally 0.03 to 0.06 m higher than the Rio Grande, indicating discharge from the alluvium to the Rio Grande. Head in the regional aquifer below the alluvium, at a depth of 18 m, is about 0.8 m higher than the Rio Grande. From pumping tests, they concluded that the hydrogeologic system at the site behaves as a layered water table system in hydraulic contact with the river with delayed yield from pore-water storage and an adjacent river boundary source.

It is possible that virtually all the groundwater flowing beneath the Pajarito Plateau flows easterly/southeasterly and discharges to the Rio Grande. An alternative possibility, that deep flow discharges instead to the basins to the south, is difficult to confirm or refute because of the lack of hydraulic data collected at discrete intervals at great depths within the aquifer. The basin is separated from the Albuquerque and Santo Domingo basins to the south by a structural high, a prong of older sedimentary rocks, and several major fault zones (Golombek et al., 1983). The Santa Fe Group aquifer thins significantly at this boundary (Shomaker, 1974). If these structures do impede flow to the south, this might enhance both regional aquifer and interflow discharge to the surface. We have not evaluated the possible interflow component to streamflow gain in the southern portion of the basin; if it were significant our estimate of groundwater discharge would be erroneously high.

The Hearne (1985) model assumes no groundwater flow to the south; the McAda and Wasiolek (1988) and Keating et al. models (2003) predict much larger discharge within the basin (to the Rio Grande) than to basins to the south. Keating et al. (2003) estimated southerly flow from the Pajarito Plateau aquifer to the south to be approximately 9 kg s^{-1} . Uncertainty analysis showed a possible range of values $+34 \text{ kg s}^{-1}$ or -62 kg s^{-1} .

Aquifer Properties

The aquifer beneath the plateau consists of the fractured crystalline rocks of the Tschicoma formation, Cerros del Rio basalts and older basalt flows, as well as the sedimentary rocks of the Puye Formation and the Santa Fe group. These units were described in detail in Broxton and Vaniman (2005). Both the Santa Fe Group and the Puye Formation are alluvial fan deposits with alternating beds of high and low permeability, with north-south trending faults associated with basin-scale rifting (Kelley, 1978). Permeability estimates for the Santa Fe Group are primarily derived from pumping tests in water supply wells screened over large intervals;

estimates range from 10^{-11} to $10^{-12.8}$ m^2 (Griggs and Hem, 1964; Purtymun, 1995; Purtymun et al., 1995a; Theis and Conover, 1962). Testing of monitoring wells, with relatively short screens completed within the Puye Formation, has shown very large variability (10^{-11} to $10^{-13.5}$ m^2). The basalt flows beneath the plateau include massive, fractured lava units, breccia zones, and interflow zones with significant clay content. Permeability within the Cerros del Rio basalts ranges from $10^{-11.2}$ to $10^{-13.8}$ m^2 (Nylander et al., 2003).

Both the Santa Fe Group and the Puye Formation are, at least locally, strongly anisotropic. Relatively short-term pumping tests have confirmed that permeability normal to bedding is much lower than permeability parallel to bedding, both on the Pajarito Plateau (McLin et al., 2003; Purtymun et al., 1990, 1995b; Stoker et al., 1989) and elsewhere in the basin (Hearne, 1980). Estimates of anisotropy vary from 0.00005 (Hearne, 1980, pumping test analysis) to 0.04 (Hearne, 1980, hydraulic gradient analysis), to 0.01 (McAda and Wasiolek, 1988). Effective permeability and anisotropy at large spatial scales is difficult to estimate. Many authors have noted the lack of spatial continuity of low or high permeability beds with the Santa Fe Group (Hearne, 1980; Spiegel and Baldwin, 1963; Theis and Conover, 1962) and the difficulty of correlating geophysical or lithologic logs between even closely spaced wells (Cushman, 1965; Shomaker, 1974). Hearne (1980) noted that because of limited spatial continuity in low or high permeability rocks, under a regional pressure gradient vertical flow will occur through circuitous routes; thus effective anisotropy may be less pronounced at large spatial scales compared with that measured at small scales during pumping tests. North-south trending faults, which are ubiquitous in the Santa Fe Group, contribute to the lack of spatial continuity in individual beds. These faults may also cause larger-scale permeability to be less than local-scale permeability, a factor proposed to explain relatively low permeability estimates for the Santa Fe Group in basic-scale model calibration (Keating et al., 2003).

There have been numerous theories in the literature on the degree and extent of confined conditions on the plateau. This is not too surprising considering the extremely complex geologic structure on the plateau and the inherent limitations of short-term pumping tests. On the basis of limited data, Cushman (1965) concluded that the aquifer is under water table conditions beneath the plateau, with the exception of the vicinity of the Rio Grande, where water table conditions exist in shallow layers and confined conditions exist at depth. Purtymun and Johansen (1974) suggested that water table conditions exist on the western margin of the plateau and artesian conditions exist along the eastern edge and along the Rio Grande. Recent drilling has confirmed existence of water table conditions at many locations beneath the plateau. Pumping tests from water supply wells drilled to a depth of 609.6 m (2000 ft) below the water table have suggested that the deeper portions of the aquifer behave as "leaky confined." Several estimates of specific storage (S_s) have been derived from various pumping tests: $10^{-4.8}$ m^{-1} in the Los Alamos

Canyon well field (Theis and Conover, 1962) and $10^{-5.5}$ and $10^{-3.8}$ m^{-1} in the Otowi well field (Purtymun et al., 1990, 1995b). In the Los Alamos Canyon well field, Theis and Conover (1962) expanded on the "leaky confined" interpretation by stating that there are, in fact, several aquifers and several semiconfining beds in this well field. Just to the southeast, along the Rio Grande, the aquifer has been called "partially confined" (Balleau Groundwater, Inc., 1995).

There are two possible alternative conceptual models for the observation of water table conditions at the top of the aquifer and leaky-confined conditions at depth. One is that the strongly anisotropic characteristic of the aquifer, which limits vertical movement of groundwater at all virtually all depths within the Puye Formation and Santa Fe Group, produces this trend. Cushman (1965) noted that this aquifer characteristic can cause an unconfined aquifer to appear confined in a short-term pumping test. This conceptual model is implemented in the numerical models of McAda and Wasiolek (1995) and Hearne (1980). The McAda and Wasiolek (1995) model place the majority of water supply wells in the basin within the upper 182.88-m (600 foot)-thick unconfined layer of the model. The other conceptual model is that a laterally extensive low permeability zone exists within the aquifer separating the shallow unconfined layer from a deeper confined aquifer. Such a zone has not yet been identified in boreholes on the Plateau, but further investigations may reveal one.

Hydraulic Heads, Flow Directions, and Travel Times

Easterly/southeasterly flow directions in the regional aquifer were suggested by water level data presented by Purtymun and Johansen (1974) and Rogers et al. (1996). This general trend is also supported by more recent data, which include a much larger number of wells than were available to earlier studies, particularly wells completed with short screens near the water table. Hydraulic head data from the top of the regional aquifer are shown in Fig. 4. The lateral component of gradients along the top of the aquifer beneath the plateau vary over one order of magnitude, from a low of 0.0026 (TW-3 to R-5) to a high of 0.04 (CDV-R-37 to CDV-R-15). Even higher gradients are evident west of R-25 (0.162; R-26 to R-25). A simple conceptual model for these trends is that gradients are high to the west where significant recharge is occurring and are low in the central plateau where lower recharge rates are occurring and higher permeability rocks are present (Purtymun, 1995). The general easterly/southeasterly flow direction these gradients suggest is consistent with radiocarbon ages of water from deep wells beneath the Pajarito Plateau, which increase from west to east. Age estimates for groundwaters beneath the plateau range from about 1000 to 6000 yr, increasing to several tens of thousands of years near the Rio Grande (Rogers et al., 1996). These datasets suggest that the general direction of flow has been consistent for the past several thousand years.

Head data along a vertical cross-section in the south-

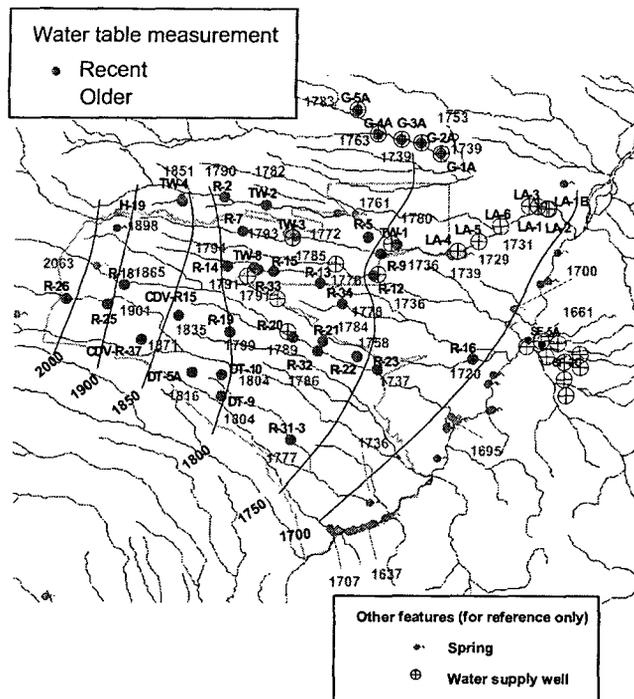


Fig. 4. Elevation of the potentiometric surface (meters) beneath the Pajarito Plateau. Elevations are derived principally from wells with short screens near the top of the aquifer, either indicated by a red circle (data collected post-2000) or a yellow circle (pre-2000). Further descriptions of the older measurements are discussed in Fig. 9 legend.

ern portion of the plateau, where there are several wells with multiple completions, are presented in Fig. 5. Pressures tend to decrease with depth in most wells with multiple completions in the regional aquifer and the vertical component of head gradients are larger than the horizontal components. More study is required to determine the mechanisms causing this trend. Locally, this type of trend could be caused by some combination of proximity to recharge zones (R-25) and pumping from deeper water supply wells (e.g., R-20 and R-16). The impact of pumping at Buckman is evident with head gradients at the far eastern edge of the transect.

The character of the measured head gradients suggests that flow in the shallow portion of the aquifer (<150 m) below the upper surface of the saturated zone is primarily easterly/southeasterly. The tendency for aquifer rocks to be strongly anisotropic will cause water to move preferentially horizontally, despite the strong driving force of vertical head gradients. Nevertheless, it is likely that both downward and upward movement of water and solutes does occur due to pumping of water supply wells at depth. Suggestions of pumping-induced upward movement of deeper water has been observed in the Los Alamos Canyon well field (Gallaher et al., 2004; Purtymun, 1977). In general, the direction of flow in deeper portions of the aquifer flow is unknown because of sparse data.

Fluxes between the regional aquifer beneath the plateau and the basin were estimated by Keating and others (2003) using basin-scale head and streamflow data and inverse modeling analysis. They estimated that flow into

the plateau from the north was very small or zero, with a relatively large degree of certainty. Inflow from the west (Valles Caldera) and outflow to the south are more uncertain, and could be as low as zero or as high as 94 or 34 kg s^{-1} , respectively. These fluxes are relatively small compared with estimates of total recharge for the plateau. Simulations suggest that flow beneath the Rio Grande (west to east) has been induced by production at the Buckman well field. Our calculations show that this flux may have increased from zero (pre-1980) to approximately 45 kg s^{-1} at present, or about 20% of the total annual production at Buckman.

Travel times through the regional aquifer are poorly understood because of the lack of tracer tests and in situ measurements of effective porosity. Data concerning the spatial distribution of anthropogenic contaminants in the regional aquifer has been inconclusive because of the exceptionally thick and complex vadose zone which makes it impossible to define the location and timing of contaminant entry to the regional aquifer. Isotopic data, described above, clearly demonstrate that some waters beneath the plateau and discharging to the Rio Grande are thousands of years old, similar to ages of groundwaters measured in the Albuquerque basin to the south (Plummer et al., 2004). Tritium data, described above, clearly demonstrate that young waters are present as well. These young and old waters may commingle at numerous locations within the aquifer, including the discharge zone at the Rio Grande.

Impact of Water Supply Production

The impact of water supply production on aquifer storage and discharge to the Rio Grande is also poorly understood. Production from major well fields on the plateau increased from near zero in 1945 to 183 kg s^{-1} in 1971 and has been relatively stable since then (171 kg s^{-1} in 2001) (Koch and Rogers, 2003), although year to year variability in pumping rates at individual wells has been large. In the Los Alamos Canyon well field, after substantial water level declines when pumping began in the 1940s, water levels rose and fell in response to interannual pumping variability. When the wells were retired during the late 1980s and early 1990s, water levels rapidly increased. Similarly, water levels in the Guaje well field decreased initially in response to pumping in the early 1950s and then stabilized until the 1970s. This was interpreted by Koch and Rogers (2003) to suggest that the aquifer had reached equilibrium. Water levels began to decline gradually again in the 1990s, perhaps due to pumping in nearby well fields. Water levels in the Pajarito Mesa (PM) well field have produced less water level decline than pumping in the Guaje or Los Alamos Canyon well fields, despite heavy usage. Nevertheless, water levels in PM-1 and PM-3, which have been pumped more consistently than other PM wells, have shown a long, steady decline. Test wells, which are much shallower than water supply wells, have also shown long, steady, declining water levels. Pre-1970 declines were very small (about 1 m); since 1970 declines have increased to a total of about 5 m.

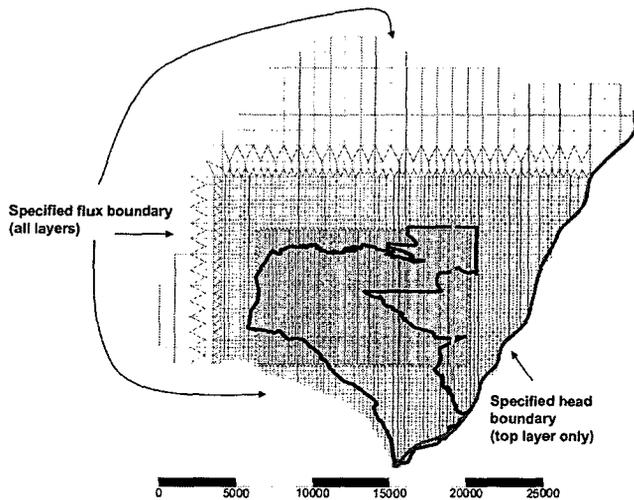


Fig. 6. Top view of the site-scale model grid. The LANL boundary is indicated, as well as trace of hypothetical vertical plane (green line) used for flux analysis.

three-dimensional hydrostratigraphic framework model (Carey et al., 1999), a three-dimensional numerical flow and transport model, and a model of recharge based on precipitation data. The flow and transport model is based on the Finite Element Heat and Mass Transfer (FEHM) code (Zyvoloski et al., 1997). Our general approach has been documented elsewhere. (Keating et al., 2000, 1999, 2003). The model grid is shown in Fig. 6. Horizontal grid resolution varies from 250 m near the margins to 125 m beneath LANL. Vertical resolution varies from 12.5 m in the upper portion of the aquifer to 500 m at depth.

Lateral boundaries for the model domain correspond to hydrologic and/or topographic boundaries: the Santa Clara River to the north, the Rio Frijoles to the south, the eastern topographic margin of the Valles Caldera to the west, and the Rio Grande to the east. Boundary conditions are assigned in accordance with basin-scale modeling results, which provide important constraints on groundwater fluxes and gradients at the site-scale (Keating et al., 2003). For some applications, fluxes are mapped explicitly on each boundary node. For the analyses presented here, we use a more simple approach: fluxes at the lateral boundaries are no-flow boundaries, which is within the uncertainty range of fluxes predicted by the basin model (Keating et al., 2003). To test the sensitivity of our results to this assumption, we applied transient fluxes as predicted by the basin model along the eastern site-scale boundary (outflow from the site-scale model due to pumping at the Buckman well field). Sensitivity results are discussed in the Model Sensitivity section below.

The upper boundary of model domain represents the top of the saturated zone. The total thickness of the saturated zone remains constant throughout the simulations (confined approximation). Along the upper boundary, the eastern edge of the model domain corresponds to the Rio Grande, where specified head boundary conditions are applied. Lateral flux across the boundary below the Rio is no-flow, except in the vicinity of the Buckman

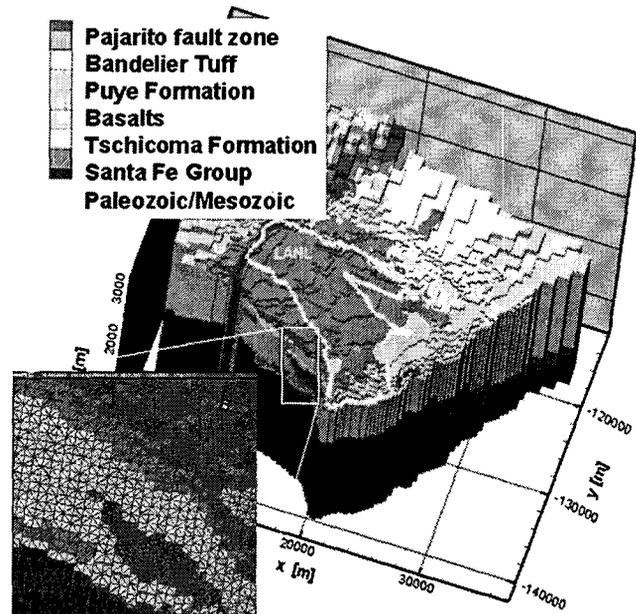


Fig. 7. Site-scale model grid, colored according to major hydrostratigraphic units.

well field. In this vicinity, transient fluxes (sinks) derived from basin-scale model results are applied to simulate the impact of production at Buckman.

For the analyses presented here, which evaluate large-scale aspects of the groundwater flow, aquifer heterogeneity within the aquifer is defined by relatively large-scale features in the three-dimensional hydrostratigraphic framework model. The heterogeneity defined by this model is shown in Fig. 7, with colors indicating 13 hydrostratigraphic units. Descriptions of the units appear in Table 1. The permeability and storage characteristics of the units are determined during model calibration, as described below.

Recharge

We represent recharge from the unsaturated zone as a specified flux boundary condition along the top of the model. Kwicklis and others (2005) proposed a detailed

Table 1. Hydrostratigraphic units in site-scale model

Unit	Subunit	Abbreviation	Volume	Fraction of total	
			km ³		
PreCambrian		pC	4.50	0.005	
Paleozoic/Mesozoic		P/M	273.53	0.292	
Santa Fe Group	deep	Tsf-deep	36.47	0.039	
	fanglomerate	Tsf-fang	23.62	0.025	
	sandy	Tsf-sandy	457.58	0.489	
Keres Group	deep	Tk (deep)	12.59	0.013	
	shallow	Tk (shallow)	1.15	0.001	
Basalts		Tb1	6.19	0.007	
		Tb2	5.61	0.006	
		Tb4	2.20	0.002	
		Tt	7.09	0.008	
Tschicoma		Tt	7.09	0.008	
	Puye Formation	Totavi Lentil	Tpt	2.02	0.002
		Pumiceous	Tpp	1.96	0.002
	fanglomerate	Tpf	5.45	0.006	
Uncertain (1)		Tb2s	14.02	0.015	
Uncertain (2)		Tb4f	0.45	0.000	
Pajarito Fault zone			82.04	0.088	
Total volume			936.51	1.000	

spatial distribution map of recharge for the plateau; here we use a more simple model that is sufficiently flexible to be able to simulate a wide variety of scenarios and thus can be used to explore model uncertainty (Keating et al., 2003). Vesselinov et al. (2002) used this approach to show that recharge uncertainty was the major factor contributing to uncertainty in PM-5 capture zone delineation.

The general trends in our simple recharge model are consistent with the trends described in the conceptual model above and with those proposed in the more detailed analysis by Kwicklis (2005). The primary data for this approach is a digital elevation model of the basin, with a resolution of 30 m off the plateau and 3 m on the plateau. It has four parameters that can be used to evaluate a wide range of scenarios for spatial distribution of recharge while maintaining consistency with total flux constraints provided by streamflow data and the basin model. The model distributes total recharge into three recharge zones: (1) low elevation, mesa-top recharge (where recharge is very low or zero), (2) high elevation, diffuse recharge (recharge is a constant fraction of precipitation, which is, in turn, an elevation-dependent model), and (3) focused recharge along stream channels in the vicinity of LANL. The flow of recharge through the unsaturated zone is assumed to be strictly vertical (no lateral redistribution) and constant in time. The four unknown parameters for this model are (i) R_T , total recharge; (ii) κ , the fraction of total recharge apportioned between Zones 2 and 3; (iii) Z_{\min} , the elevation separating Zones 1 and 2; and (iv) α , the fraction of precipitation that becomes recharge in Zone 2. α can be derived from Z_{\min} and R_T . For the simulations presented here we allow Z_{\min} and R_T to vary and calculate α accordingly. As described above, the range of total recharge (R_T) is fairly well-constrained by streamflow analysis and basin-scale modeling. To acknowledge its uncertainty, for some analyses (described below) we allow this parameter to vary freely. Kwicklis and others (2005) estimated that κ , while very uncertain, may be as large as 15%. Inverse analysis using head data and streamflow data shows Z_{\min} to be relatively well constrained at the basin-scale although we do allow this parameter to vary in the calibration process to allow for the possibility that local conditions differ from basin-scale averages.

Model Calibration

We calibrate the recharge and flow model simultaneously using flux estimates and head data. The calibration process includes sequential runs of a steady-state flow calculation followed by a transient simulation (1945–2004, in 1-yr time steps). Aquifer property parameters and recharge model parameters are adjusted using PEST (Doherty et al., 1994) to achieve the optimum agreement between measurements (45 steady-state head observations and 807 transient head observations in 26 wells) and model predictions. PEST determines the set of best-fit parameters and corresponding confidence limits. For the predevelopment head estimates (steady-

state simulation), we calculate a Nash–Sutcliffe (1970) model efficiency of 0.89. The constraints on total recharge are absolutely essential for estimation of permeability values. Unfortunately, previous work has shown that model calibration is insensitive to the parameter (κ), or the percentage of total recharge introduced along stream channels. Therefore, it cannot be estimated using the calibration process. It is quite possible that a parameter with little influence on model calibration will have great influence on model predictions. For the results described below, we initially set κ to zero, and then later raised it to 0.15 to investigate the sensitivity of the model predictions to κ .

Simulated and measured hydrographs for representative wells on the plateau are compared in Fig. 8. For water supply wells, long-term trends are represented reasonably well; interannual variability is represented less well. For the transient head observations we calculate Nash–Sutcliffe (1970) model efficiency of only 0.44. Most of these head data are measured in water supply wells (PM-2, PM-4, LA-6, and G-4); we compare simulated to “nonpumping” water levels because the grid size is too large to allow accurate representation of well hydraulics during pumping. Unfortunately, the length of time lapsed between cessation of pumping and the measurement of “nonpumping” water levels is unknown; this may explain some of the short-term discrepancies evident in Fig. 8 and the low model efficiency. The model simulates the recovery in LA-6 after cessation of significant pumping in 1975 reasonably well. As shown for TW-8, although the model overpredicts head here by 6 m, the temporal trends are very well represented. Water levels at TW-8 remained fairly constant until the 1970s when the nearby PM well field came on-line. Since then, water levels have declined approximately 9 m. Despite the limitations of the model in reproducing interannual variability of heads at water supply wells, the inclusion of transient data has substantially decreased uncertainty in model parameter estimates (Keating et al., 2000).

Simulated and measured heads at the top of the saturated zone along two east–west transects are shown in Fig. 9, emphasizing wells with short screens. The simulated heads represent the end of transient simulations (1945–2003). The measured heads are data collected since 2000, with the exception of a few wells that have not been accessible for recent measurements (see Fig. 9 legend). In both transects, the measured data show a flattening of the gradient in the center of the plateau. Along the northern transect (10a), the model underpredicts heads to the west, and overpredicts heads in the area of anomalously low heads (R-9 and R-12). The model also underpredicts the head at TW-1. Heads at this well have been steadily rising in the past several decades because of increased local recharge downstream of a sewage treatment plant (McLin et al., 1998); this transient recharge is not included in the model. Along the southern transect (9b), the model reproduces observed gradients fairly well, except for at CDV-R-37 and R-23.

Model parameters used for these simulations are listed in Table 2. Some parameters were held at fixed values

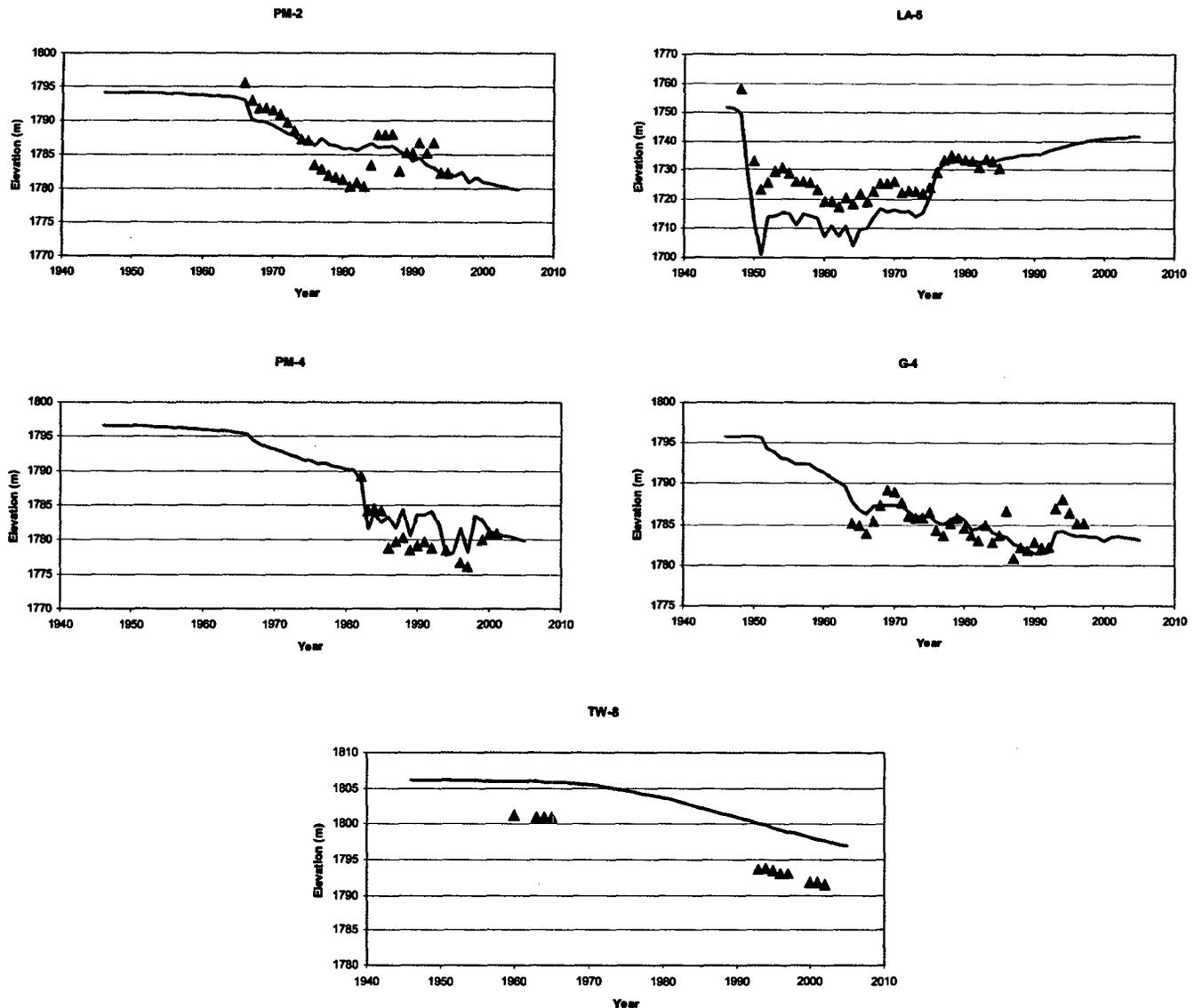


Fig. 8. Comparison of simulated and measured hydrographs for representative wells on the plateau. Model parameters shown in Table 2.

since previous calibrations demonstrated that the model has very low sensitivity to these values and therefore cannot be estimated using this inverse model. Of the parameters that were allowed to vary during calibration, six were estimated with fairly high degrees of confidence: Santa Fe Group (fanglomerate)_{xy}, Santa Fe Group (fanglomerate)_z, Santa Fe Group (sandy), Puye Formation, and specific storage. The high confidence in the Santa Fe Group permeabilities is probably a consequence of its relatively large volume. Since the horizontal gradients and total flux and through the aquifer is fairly well constrained, the large-scale effective permeability of this unit is correspondingly constrained. If independent geologic information were available to justify defining sub-units of the Santa Fe Group, their individual permeabilities might vary significantly from this large-scale average. As has been found in previous calibrations (Keating et al., 2003) the estimate for the Santa Fe Group (sandy) ($10^{-13.3} \text{ m}^2$) is significantly lower than most pumping tests. One possible explanation for this result is that

large-scale features exist in these rocks, such as north-south trending faults that are common in these rocks locally, which lower the large-scale effective permeability of the unit. The estimate of a relatively high permeability for the north-south trending Santa Fe Group (fanglomerate) ($10^{-11.1} \text{ m}^2$) is consistent with the conceptual model of Purtymun (1995), who hypothesized that this was a relatively permeable, coarse facies in the upper Santa Fe Group. Estimates for the Cerros del Rio basalt and the Puye (pumiceous unit) are unrealistically low. It is possible that good matches to heads and fluxes requires the introduction of a low permeability layer, separating deep and shallow flow. In this calibration, the model uses the relatively thin units Tpp and Tb4 to accomplish this. A more realistic model might be achieved by introducing very thin low permeability layers within hydrostratigraphic units or between units (at contacts). The estimated specific storage ($10^{-4.3} \text{ m}^{-1}$) is well within the range of measurements in wells on the plateau.

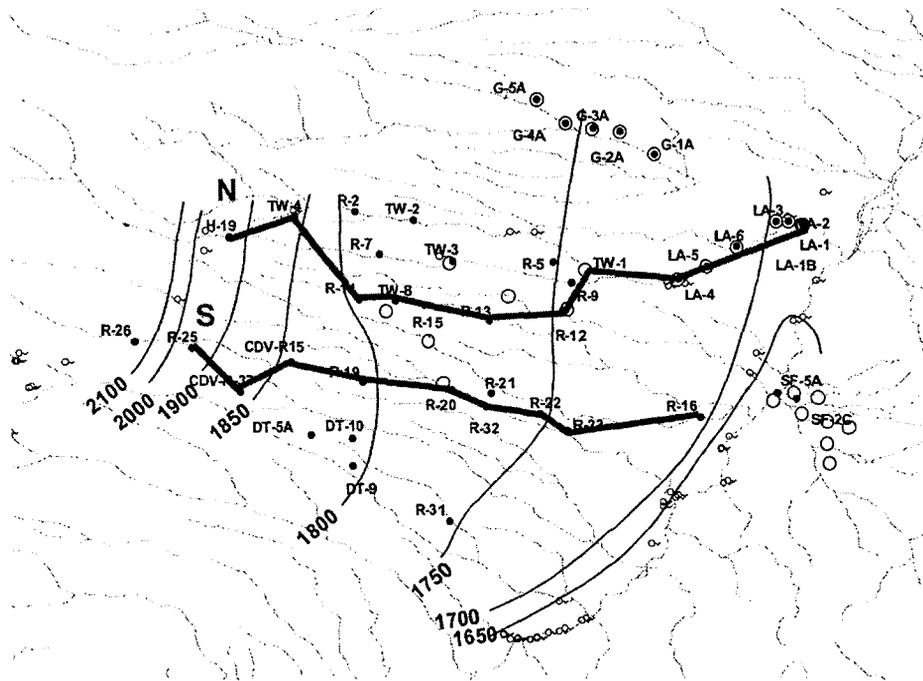
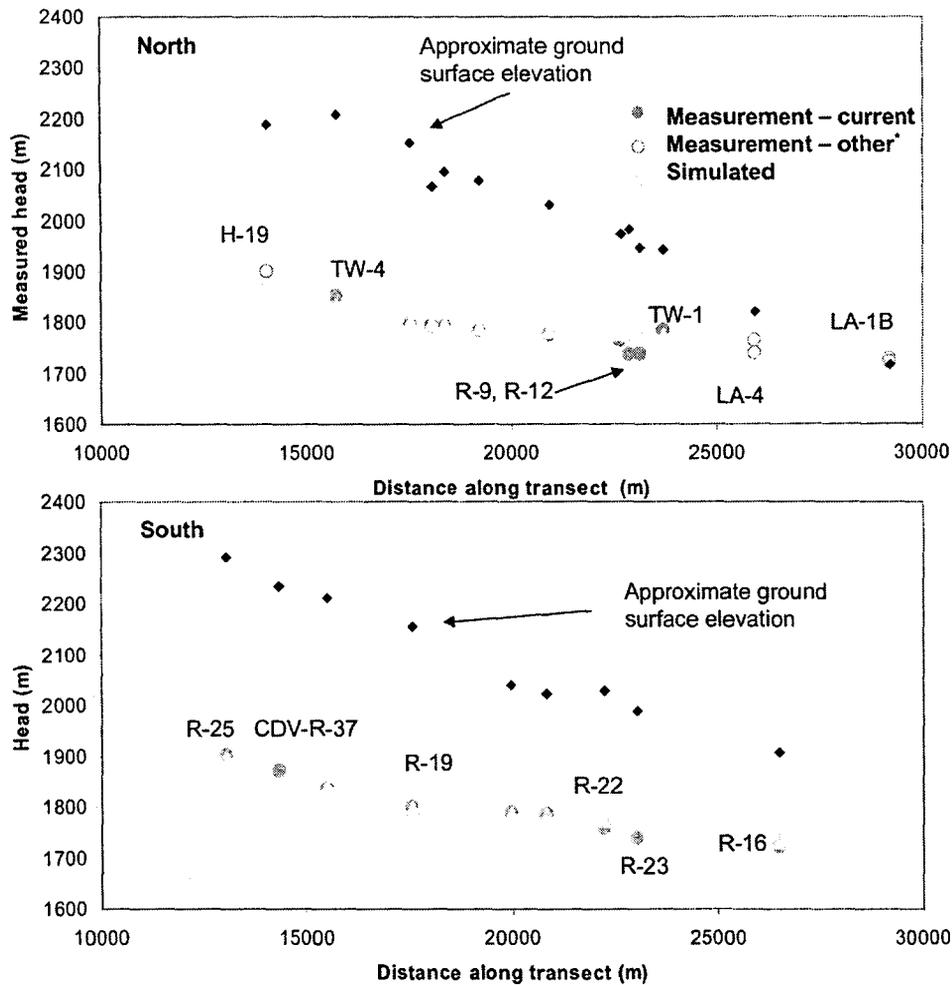


Fig. 9. Comparison of measured and simulated present-day heads at the top of the saturated zone along two east-west transects. *These data were collected in wells that are no longer accessible for measuring. LA4 and LA1B are in a well field that has been shut down since the early 1990s; all wells have shown significant recovery since they were shut down. The lower circle shows the most recent measurement available. The upper circle shows the water level measured during the initial drilling, which would approximate current water levels if the wells had fully recovered. H-19 has not been measured since 1949. Measured drawdowns in this portion of the aquifer have been very small. In 1997 the furthest western well (TW-4), closer to water supply wells than H-19, had declined <1 m since 1950.

Table 2. Model parameters. Confidence limits are indicated for those parameters allowed to vary freely during calibration. They serve as only rough approximations to true (nonlinear) confidence limits.

Parameter	Value	95% confidence limits	
		Lower limit	Upper limit
Recharge model			
Z_{min} , m	2156.1	2142.1	2170.2
R_r , kg s ⁻¹	253.7		
α	.07		
κ	0		
Permeability, log₁₀(m²)			
pC	-18.0		
P/M	-13.7		
Tsf-deep	-16.0		
Tsf-fang	-11.1	-11.4	-10.9
Tsf-fang-z	-11.4		
Tsf-sandy	-13.3	-13.4	-13.2
Tsf-sandy-z	-14.2	-14.3	-14.1
Tk (shallow)	-12.7		
Tk (deep)	-13.7		
Tb1	-12.1		
Tb2	-12.2		
Tb4	-16.1	-22.6	-9.5
Tt	-15.3		
Tpt	-12.7		
Tpt-z	-12.7		
Tpp	-16.8	-17.9	-15.6
Tpf	-13.1	-13.3	-12.9
Tpf-z	-15.2		
Tb2s	-12.1		
Tb4f	-12.1		
Pajarito Fault zone	-15.0		
Specific storage, log ₁₀ (m ⁻¹)	-4.3	-4.4	-4.2

MODEL RESULTS

Shallow Fluxes Downgradient of LANL

Because of concerns about the impact of LANL-derived contamination on both surface water and groundwater downgradient from the site, we pay particular attention to model predictions of fluxes of relatively shallow groundwater immediately downgradient from LANL. We defined a hypothetical plane (shown in Fig. 6), extending vertically from the top of the aquifer (≈ 1800 m) to 1300 m (the approximate depth of water supply wells in this vicinity), and calculate fluxes through the plane. This rectangle comprises approximately 10% of the cross-sectional area of the submodel measured parallel to the Rio Grande at the location of the plane. The calibrated model described above predicts 49.5 kg s⁻¹ flows through this plane in 2003 (about 17% of the total recharge flowing through the aquifer). We did a simple test of sensitivity of this result to withdrawals at Buckman well field, just to the east of the model boundary. Basin model simulations suggest that pumping in this well field, which initiated in the 1980s, is now drawing approximately 20% of total water produced from the area within the site model, and this proportion is likely to increase in the future. We applied this transient boundary condition to the eastern boundary of the site-scale model and found that the predicted flux across the plane downgradient of LANL is not affected. This analysis is not comprehensive, but it does provide a preliminary indication of insensitivity to fluxes at this location to pumping outside model boundaries.

Because all our model parameters are uncertain, the prediction of 49.5 kg s⁻¹ through the plane downgradient

from LANL is also uncertain. We apply predictive analysis (Doherty et al., 1994), a tool to determine the range of possible predictions that at the same time satisfy our calibration criteria (matches to transient heads and predevelopment fluxes) within certain limits. This analysis will also allow us to determine which of the uncertain parameters most influence predictive uncertainty. The uncertainty in permeability of each unit will directly propagate into uncertainty of the respective flux through this unit because of the linear relationship between the flux and permeability through Darcy's Law. However, because of complex cross correlations between permeability, recharge, and specific storage, we can expect complex relationships between model parameters and uncertainty in the predicted fluxes.

The basis for the predictive analysis is as follows. First, we define an objective function:

$$\Phi = [\mathbf{c} - f(\mathbf{b})]^T \mathbf{W} [\mathbf{c} - f(\mathbf{b})] \quad [1]$$

where f' is our model, \mathbf{b} is a vector [$M \times 1$] of model parameters, and \mathbf{c} is a vector [$N \times 1$] of optimization targets, and \mathbf{W} is a diagonal cofactor matrix [$N \times M$]. Through model calibration we minimize Φ ; the corresponding parameters to Φ_{min} are the maximum-likelihood estimates \mathbf{b}_{ML} . Next, we define a prediction, p :

$$p = f'(\mathbf{b}) \quad [2]$$

where f' is our model under predictive conditions and we use predictive analysis to maximize or minimize p , subject to the constraint:

$$[\mathbf{c} - f(\mathbf{b})]^T \mathbf{W} [\mathbf{c} - f(\mathbf{b})] = \delta \Phi_{min} \quad [3]$$

For the maximum-likelihood case (Bard, 1974)

$$\delta = \frac{N}{N - M} F_{\alpha}(N, N - M) + 1 \quad [4]$$

where F is the F-distribution and α is the confidence level. The constrained optimization of \mathbf{b} is solved using PEST as an iterative nonlinear Lagrangian problem as proposed by Vecchia and Cooley (1987).

Because this is a computationally intensive procedure, we adjusted the model calibration procedure described above, implementing transients in 5-yr time steps rather than 1-yr time steps. The results for three models are shown in Table 3; the optimized model and the two models representing minimum and maximum fluxes through the plane. By comparing the best estimate parameters in Table 3 with Table 2, we see that the adjustment in calibration procedure results in changes in a few estimated model parameters that are quite significant in some cases. The two parameter sets can be considered equally well-calibrated models. The variations between parameters in Table 2 and Table 3 are another measure of parameter uncertainty. The calibrated model parameters shown in Table 3 predict a flux of 35.0 kg s⁻¹. The predictive analysis suggests that the flux can deviate from 31 to 54 kg s⁻¹ within the 95% confidence limits of our best objective function. These fluxes have declined 10 and 8%, respectively, since predevelopment conditions.

A portion of the variation in predicted flux results

Table 3. Model parameters and predicted fluxes through shallow plane east of LANL.

Parameter	Best estimate	95% confidence limits		Predictive analysis	
		Min.	Max.	Min.	Max.
Recharge model					
Z_{min}	2259.82	2182.28	2340.11	2264.71	2461.70
R_T	263.34	205.48	321.20	263.16	344.30
α	.089			.089	.171
κ	0.1			0.1	0.1
Permeability, $\log_{10}(m^2)$					
pC	-18.0			-18.0	-18.0
P/M	-13.7			-13.7	-13.7
Tsf-deep	-16.0			-16.0	-16.0
Tsf-fang	-19.00	-94.00	56.89	-19.00	-18.14
Tsf-fang-z	-18.36	-19.00	-17.71	-18.46	-18.37
Tsf-sandy	-13.38	-13.49	-13.27	-13.36	-13.29
Tsf-sandy-z	-13.49	-13.73	-13.24	-13.46	-13.31
Tk (deep)	-13.7			-13.7	-13.7
Tk (shallow)	-12.7			-12.7	-12.7
Tb1	-13.50	-13.86	-13.13	-13.63	-13.70
Tb2	-12.23	-12.59	-11.88	-12.48	-11.77
Tb4	-14.92	-16.65	-13.20	-14.93	-14.57
Tt	-14.55	-15.58	-13.51	-14.64	-14.36
Tpt	-11.94	-12.64	-11.24	-12.34	-11.74
Tpt-z	-17.46	-20.66	-14.27	-18.13	-18.13
Tpp	-11.91	-12.20	-11.62	-11.85	-11.83
Tpp-z	-11.00	-82.93	60.93	-11.07	-12.83
Tpf	-12.88	-13.59	-12.17	-13.13	-12.91
Tpf-z	-15.88	-16.38	-15.38	-15.99	-15.86
Pajarito fault zone	-13.89	-15.23	-12.56	-13.15	-14.01
Specific storage [$\log_{10}(m^{-1})$]					
Darcy fluxes, $kg\ s^{-1}$					
Total	34.96			31.44	53.70
Basalts (tb1, tb2)	5.05			5.04	15.40
Puye (tpf)	2.67			1.59	4.15
SF group (fang, west)	24.71			24.80	34.15
Totavi Lentil	1.17			0.66	1.94

from variation in total recharge that the analysis produced (263–344 $kg\ s^{-1}$). A comparison of the estimates of total recharge to the aquifer and flux through the plane for the four calibrated models is shown in Fig. 10. The variability in total recharge is greater than the variability across the plane east of LANL. This is an unexpected result because uncertainty in fluxes typically increases as the scale of interest decreases. This result is favorable for contaminant transport predictions, which are very vulnerable to flux uncertainty at small scales.

As shown in Table 3, a significant proportion of uncer-

tainty in fluxes downgradient of LANL results from uncertainty in the permeability of the basalts (factor of 3 difference between minimum and maximum predictions). The uncertainty is primarily a result of a one order of magnitude change in Tb2 permeability between the two model results. Basalt units are very important for potential contaminant transport because of their expected low effective porosity. Therefore, we can expect at least a factor of 3 uncertainty in the associated travel times resulting from uncertainty in the flow solution. Uncertainty in porosity will further increase the total uncertainty of

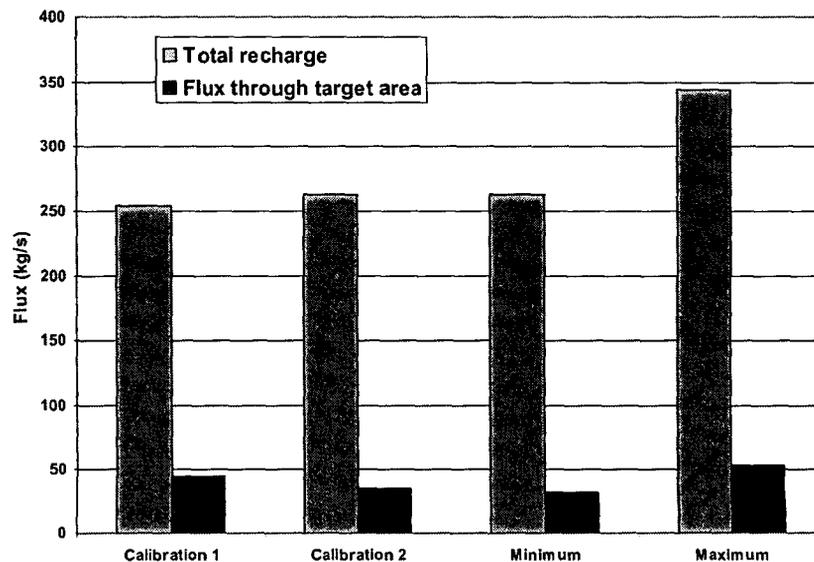


Fig. 10. Estimates of total recharge and flux through a vertical plane east of LANL, according to four sets of model parameters.

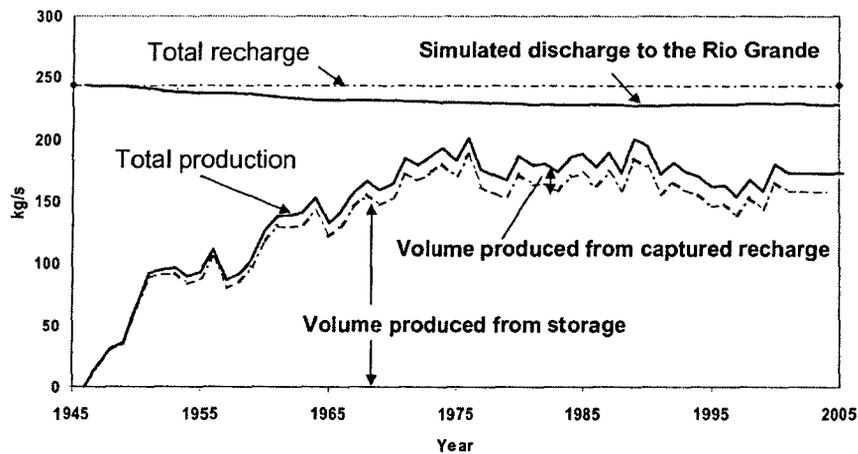


Fig. 11. Simulated discharge to the Rio Grande and estimated proportion of production in local well fields that originates as storage and as captured recharge.

travel times through this unit. Tb2 has not been observed below the top of the regional aquifer east of R-9 and R-12 and so uncertainty in these fluxes, while important for local contaminant transport issues, may not be an issue for contaminant transport in the regional aquifer from LANL to the Rio Grande.

It is evident from comparing Tables 2 and 3 that some parameter estimates (and confidence limits) are quite variable. In both inverse analyses, at least one of the shallow units has been assigned an unrealistically low permeability. This problem is presumably related to cross correlation between model parameters, where the inverse model can assign a low permeability to any of three units (Tsf-fang, Tpf, Tpp, or Tb4) as long as one of the others is relatively high in permeability. Some units have very large confidence limits (e.g., unit Tb4 in Table 2). For these units the calibration process cannot estimate a meaningful permeability because of a lack of data and/or correlation between other model parameters.

Impact of Production on Storage and Baseflow to the Rio Grande

Given that total production from well fields on the plateau in 2001 was 172 kg s^{-1} , which is a relatively large number compared with various estimates of total recharge on the plateau, it is very possible that production may be significantly impacting aquifer storage, discharge to the Rio Grande, or both. Theory suggests that during the early stages of pumping, the majority of the produced water will come from storage and there will be little (if any) impact on discharge to the Rio Grande. As production continues, however, the contribution of storage will decline and the contribution of captured recharge will increase until finally, at a new steady-state condition, baseflow to the Rio Grande will be decreased by an amount equal to groundwater production. As mentioned above, Rogers et al. (1996) calculated that most or all of the water produced between 1949 and 1993 was released from storage. Theirs was a very simple calculation that assumed water table conditions. Here, we provide a simulation based on transient flow model-

ing assuming confined conditions. The actual behavior of the aquifer, as described above, is a combination of confined and water table conditions resulting from local heterogeneities in the aquifer that are difficult to model because of lack of data.

The results of the production modeling are shown in Fig. 11, based on the parameters shown in Table 2. The results suggest that the majority of the water produced to date has come from storage (91%), and the impact to discharge along the entire reach of the Rio Grande downstream has been relatively small.

Model Sensitivity

The predicted impact of production on storage and discharge to the river will be affected by model assumptions including the confined approximation, aquifer properties, and boundary conditions. Specific storage (S_s) is of obvious importance, since lower values of S_s will cause less water supply production to come from storage and more to come from surface water (either directly or as captured recharge). Hearne (1985) reviewed hydraulic tests conducted within the basin and concluded that a possible range for S_s is $10^{-4.5}$ to $10^{-5.5} \text{ m}^{-1}$. Our estimates (Tables 2 and 3) show the range of calibrated values for this model to be $10^{-3.5}$ to $10^{-4.4} \text{ m}^{-1}$. The results presented above (parameter values shown in Table 2) are based on a value $S_s = 10^{-4.3} \text{ m}^{-1}$.

In this case, we use a simple sensitivity analysis to explore the uncertainty of our model predictions. Sensitivity analysis does not explore the full range of possibilities, since other parameters are held constant, and for the same reason it often forces a model well out of calibration. Nevertheless, it is a useful tool for illustrating uncertainties. We compared the storage vs. baseflow production results presented in Fig. 11 (parameter values shown in Table 2) with predictions based on another calibrated data set (Table 3, best estimate) and five other values of S_s , keeping all other aquifer parameters set to values specified in Table 2. The results of this analysis are shown in Fig. 12. For the two calibrated models, the percentage of produced water originating as storage ranges from 84 to 91%. By increasing and

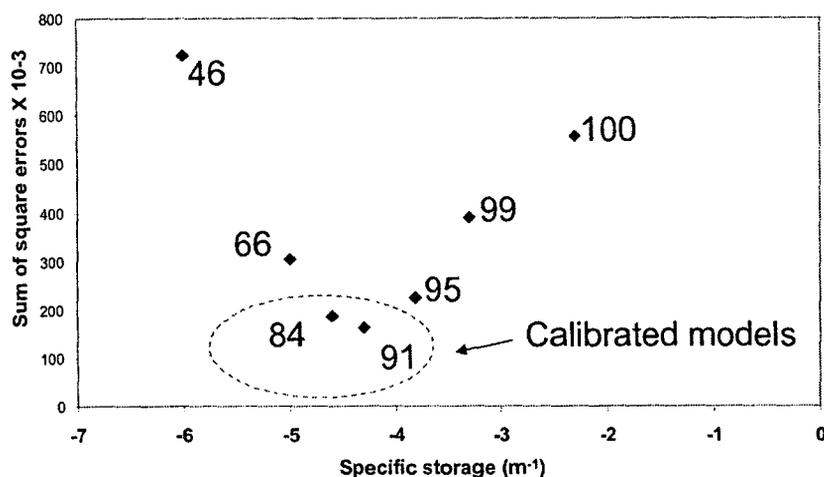


Fig. 12. Sensitivity of predicted percentages of production in 2004 coming from aquifer storage to values of S_s (in parentheses). The vertical axis is the sum of squared errors $\times 10^{-3}$, in meters $\times 10^{-3}$, for 929 water level measurements in 75 wells, from 1946 to 2004. Numbers indicate predicted percentages.

decreasing the value of S_s slightly, the model calibration is worse (by a factor of two, in the case of $S_s = 10^{-5} m^{-1}$) and the range of percentages increases from 66 to 95%. Very different percentages (100 and 46%) can be achieved by still larger and smaller S_s values, but these models are so far out of calibration that the predictions are unrealistic. This is confirmation that S_s is fairly well constrained in this model, and the percentage of water originating as storage is likely to be in the 84 to 91% range, not significantly less or greater.

We also varied κ , the percentage of recharge occurring locally along stream channels in the vicinity of LANL, to determine the influence of uncertainty in this parameter on the results. Interestingly, when we increased κ from 0 to 15%, the result did not change. This reflects the combined impact of anisotropy, which limits the degree to which local recharge can easily reach the deeper zones where production occurs, and the very large volume of the aquifer, which contains significant storage despite the relatively low values of specific storage assumed in these simulations ($10^{-5.5} m^{-1}$).

Comparison with Previous Models

Two previous basin-scale groundwater flow models have estimated the impacts of groundwater withdrawals in this region (McAda and Wasiolek, 1988; Hearne 1985). These models predicted the impact of pumping by the City of Santa Fe and by Los Alamos County on aquifer storage and on flow in the Rio Grande and its tributaries. They are not directly comparable with this study since they consider a larger area; however, with caveats this is a useful comparison. Hearne (1985) used a uniform hydraulic conductivity of $0.3 m d^{-1}$ and a specific storage of $10^{-5.2} m^{-1}$. His model estimates the total withdrawn from Buckman, Los Alamos County well fields ($318 kg s^{-1}$, based on late 1970s estimates) to be coming mostly from storage; by 2030 the proportions are predicted to be 78.1% plus 17.7% from Rio Grande stream capture and the rest from minor tributaries. Sensitivity analyses demonstrated that these esti-

mates were relatively insensitive to changes in specific storage and specific yield.

The model of McAda and Wasiolek (1995) has most of the pumping wells in the upper unconfined layer of the model ($S_y = 0.15$), except for the vicinity of the Guaje well field where a value of 0.05 was used. Lower layers were assumed to be confined ($S_s = 10^{-5.5} m^{-1}$). Hydraulic conductivity values vary spatially. At the end of transient simulations (1982) of the $340 kg s^{-1}$ produced that year, 85% of it was coming from storage. Future projections of the year 2020, show that from 78 to 83% of pumping comes from storage, depending on the pumping rates assumed. Sensitivity analysis showed that these results were relatively insensitive to variations in specific yield or specific storage.

Compared with our results, predictions by Hearne (1985) and McAda and Wasiolek (1995) for the larger basin are that a slightly lower proportion of produced water (basin wide) is coming from aquifer storage. The major reason for the discrepancy is likely to be differences in the spatial extent of the models. Since the basin-scale models include well fields close to rivers (such as the Buckman well field) these models will tend to predict more impact on river flow than our site-scale model, which only includes well fields relatively far from the river (Los Alamos County). In some respects, it is remarkable that this site-scale model, which approximates the entire thickness of the aquifer as confined, provides similar results to these other models, which have substantial unconfined layers that are able to provide a substantial percentage of produced water from storage.

CONCLUSIONS

We have presented new data and analyses pertinent to the regional aquifer beneath the Pajarito Plateau and compared the conceptual model that emerges with those published before recent drilling. In many aspects, the general picture of easterly/southeasterly flow toward the discharge point of the Rio Grande has not changed substantially. The current understanding of hydrostra-

tigraphy, as implemented in the numerical models, is sufficient to explain general trends in heads (spatial and temporal), but is lacking in a few key areas such as in the vicinity of R-9, R-12, R-22, and R-16 (see Fig. 4). Detailed transport calculations in the vicinity of these wells would benefit from a refinement of the hydrostratigraphic framework model. Furthermore, inverse estimates of permeability in several units are unrealistically low. This may result from the presence of a low permeability layer in the aquifer which separates shallow and deep flow and is necessary for the model to match heads and fluxes. Because this layer (or series of discontinuous layers) is not explicitly represented in the hydrostratigraphic framework model, larger units, such as Tb4 and Tpp are assigned a very low permeability.

Estimates of total recharge to the aquifer have not changed substantially since the early estimates of Griggs and Hem (1964). Quantitative analyses indicate that approximately 90% of the recharge occurs to the west of LANL; this result is in agreement with early qualitative estimates by Griggs and Hem (1964) and Purtymun and Johansen (1974). There is clear geochemical evidence that recharge does occur on the plateau and thus pathways for contaminant transport from LANL to the regional aquifer do exist.

Simulations of the regional aquifer suggest that most of the production from local well fields is coming from storage. Using a simple model of recharge, we demonstrated that this result is insensitive to assumptions about the percentage of recharge occurring on the plateau vs. to the west of LANL. This insensitivity reflects that degree to which the deeper zones in the aquifer (where most production occurs) are disconnected from more shallow zones that receive local recharge. As an example, inverse analysis results demonstrate that vertical permeability values in the Puye Formation and Santa Fe Group (sandy subunit) are more than 100 and 10 times lower than horizontal permeability, respectively.

There is sufficient parameter uncertainty, however, to significantly impact predictions of fluxes and velocities through individual hydrostratigraphic units downgradient of LANL. For example, predicted fluxes through deep basalt unit (Tb2) vary by a factor of two depending on parameter values. Some of this uncertainty is attributable to uncertainty in total recharge; other portions are attributable to uncertainty in permeability. By making simple assumptions about the porosity, we estimate that pore-water velocities through this unit could be as low as 1 m yr^{-1} or as high as 125 m yr^{-1} . This has important implications for predictions of contaminant transport off site in those portions of the aquifer where Tb2 is present: contaminants reaching the regional aquifer may have traveled a significant lateral distance in the regional aquifer.

In contrast, for rocks likely to possess higher porosity, such as those of the Puye Formation, transport velocities will be on the lower end of this range. The implication for understanding vadose zone transport is that these regional aquifer contaminant plumes are probably relatively stationary compared with, for example, an annual sampling schedule, unless the sample is located close to

a municipal water supply well. Therefore, a contaminant plume at the top of the regional aquifer reflects the behavior of these plumes as they migrated through the overlying vadose zone.

The implication of this work for water resources beneath the plateau is that groundwater production is mining an old aquifer that has not received significant recharge on the time scale of this study (decades). The implication of this work for contaminant transport issues is that because of parameter uncertainty, predicted fluxes and velocities are quite uncertain. Part of the reason for this is uncertainty in total recharge to the aquifer. Uncertainties in permeability and porosity values lead to additional model uncertainty. These uncertainties can be reduced meaningfully with more data collection, including multiwell pumping and tracer tests. Finally, local recharge does occur along canyons that cross the LANL property. From a large-scale water budget perspective, local recharge is relatively small. Nevertheless, this recharge has important water quality implications in locations where contaminated effluent discharges have been released.

APPENDIX

Estimating Aquifer Discharge Using Streamflow Data

The method we use for estimating baseflow gain along the Rio Grande is a simple one, also used by Spiegel and Baldwin (1963) and the U.S. Department of Justice and New Mexico State Engineer Office (1996). The strategy is to difference measured surface water flow at two gages during January, when other causes of streamflow loss or gain such as evapotranspiration and irrigation withdrawals are likely to be minimal. Because the calculated baseflow gain is generally small compared with total flow in the Rio Grande ($\approx 8\%$), small measurement errors in flow at the gages could have large influence on these calculations. Veenhuis (2004) reported that measurement errors at gages along the Rio Grande range from 2 to 25%, and for selected pairs of gages (such as Otowi and White Rock) calculated differences between daily flow are almost always less than the maximum measurement error. These facts clearly demonstrate the futility of using daily data to estimate daily baseflow gain in some cases. If measurement errors are not correlated in time, however, the mean difference of a large number of flow estimates can be calculated with greater confidence than a flow estimate for a single day. Our approach assumes that daily January flow departures from the long-term January mean flow are due to random measurement error. Using this assumption and applying the Student *t* test at 95% confidence level, we can detect statistically significant differences between mean January flow at the Otowi and Cochiti gages for most years on record. We have used time-series analysis to determine if nonrandom temporal trends are present in our baseflow estimates. We were not able to demonstrate influence of annual rainfall or production in local well fields. Although this does not prove that the interannual variation is due to random measurement error alone, it is consistent with that hypothesis. Veenhuis (2004) did not explicitly address the subject of correlation between measurement errors; this is a topic worthy of further examination. If significant bias is present in any flow dataset, this would impact our calculations.

We apply this approach to two reaches of the Rio Grande: (1) San Juan Pueblo to Otowi and (2) Otowi to Cochiti (see

Table 4. Estimates of long-term average flow at small tributaries.

Gage		Data source	Years of record	Period	Mean Jan. flow	
					kg s ⁻¹	
1	Pojoaque River, at mouth	Site 6	Reiland and Koopman, 1975	38	1935–1972	138.8
2	Santa Clara Creek	8 292 000	USGS, 2004	17	1936–1994	93.4
3	Santa Cruz River	8 291 500	USGS, 2004	10	1941–1950	167.1
4	Rio Frijoles	8 313 350	USGS, 2004	14	1983–1996	34.0

Fig. 1). Collectively, these two reaches span the entire length of the Rio Grande that comprise the eastern extent of the Pajarito Plateau, from Santa Clara Creek to Rio Frijoles. Using variations of this same method for one of these reaches, Otowi to Cochiti, Spiegel and Baldwin (1963) estimated a gain of 883.6 kg s⁻¹ (31.2 cfs) and U.S. Department of Justice estimated a gain of 397.6 kg s⁻¹ (14.04 cfs). We compare our results with theirs below.

San Juan Pueblo to Otowi

A major tributary to the Rio Grande, the Rio Chama, enters this reach just downstream from the gage on the Rio Chama at Chamita. There was a 23-yr period during which all three of these gages were operational (1963–1985). By comparing this period of record with a much longer period of record at the Otowi gage (1900–2004), flows were close to average during the 1963 to 1985 period, except for two unusually high flow years (1973 and 1975). The January flow at Otowi was highly correlated to, and slightly more than, the sum of flows at San Juan Pueblo and Rio Chama at Chamita, suggesting a consistent baseflow gain component along this reach. Three minor tributaries, the Santa Cruz River, the Pojoaque River, and the Santa Clara River, contribute to gain along this reach. Insufficient data during 1963 to 1985 prevented using measured flows for individual year; instead, we used a long-term average from other years, shown in Table 4.

For each year of the 23-yr period from 1963 to 1985, we calculated baseflow gain during January by the following relationship:

$$\begin{aligned} \text{Baseflow gain} = & \text{measured flow (RG Otowi -} \\ & \text{RG San Juan - Rio Chama, Chamita) -} \\ & \text{long-term average measured flow (Pojoaque +} \\ & \text{Santa Clara + Santa Cruz)} \end{aligned} \quad [A1]$$

The 23-yr average baseflow gain calculated using this approach is 1166.8 (± 362.5 at the 95% confidence interval). There is a strong trend evident for gain to be higher in years of higher flow; it is unclear whether this trend is real or is related to sources of error such as small unengaged tributaries, which may only be significant at high flow. If the trend is related to measurement error, our mean baseflow gain estimate may be too high. If baseflow gain was 1166.8 kg s⁻¹ and constant in time, calculated flow at Otowi (using Eq. [A1]) and measured flow would be identical. Departures from this ideal behavior are evident at high flows in Fig. 13a.

Otowi to Cochiti

These two gages were both operational during 74 yr (1926–1969), well before pumping began at the Buckman well field below Otowi. January flow at the two stations is highly correlated ($r^2 = 0.96$), for most years the data suggest that the reach is gaining; for some years the data suggest a losing reach (see Fig. 2). One tributary enters the Rio along this reach, Rio Frijoles, which was gaged from 1983 to 1996. We estimate average January flow to at the Rio Frijoles to be 34 kg s⁻¹. Accounting for the inflow from Rio Frijoles, the gain between

these reaches is 368.2 kg s⁻¹ (± 249.2 at the 95% confidence interval). The sum of the flow at Otowi and Rio Frijoles and this baseflow estimate, compared to the flow at Cochiti, is shown as a yellow line in Fig. 13b. This estimate is slightly lower than the U.S. Department of Justice estimate, presumably because of our consideration of surface water inflow at Rio Frijoles. We were able to reproduce the much lower estimate by removing from the analysis data from years that the reach appeared to be losing. Although we agree with Spiegel and Baldwin's (1963) assertion that data from these years are questionable, we have no independent information to confirm this.

Santa Clara to Rio Frijoles

This reach defines the eastern boundary of our flow model, so estimating baseflow gain of the Rio Grande along this reach is important. We extrapolate these estimates described above to this reach using stream length ratios. Santa Clara to the Otowi Bridge gage is approximately 6/10 the distance of Rio Grande San Juan Pueblo gage to Otowi Bridge; we estimate 699.5 \pm 218.1 kg s⁻¹ gain along this reach. Otowi to Rio Frijoles is approximately one-half the distance of Otowi to the Cochiti gage; for this reach we estimate 212.4 \pm 124.6 kg

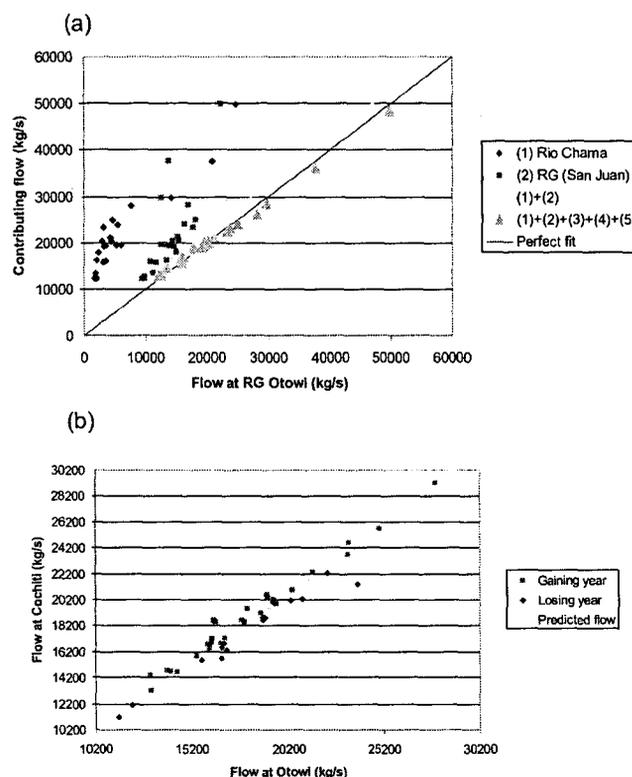


Fig. 13. Measured January flow at the Otowi Gage, compared with (a) contributing flow at Rio Chama, Rio Grande at San Juan, minor tributaries (Table 4), and estimated baseflow, and (b) measured January flow at the Cochiti gage. Numbers refer to reaches in Table 4.

s^{-1} . In total, our baseflow estimate for the Santa Clara to Rio Frijoles reach of the Rio Grande is $911.9 \pm 218.1 \text{ kg s}^{-1}$.

Sources of Error

Sources of errors in the method include systematic errors in stream flow measurements which both (i) affect one stream gage differently than other stream flow gages used in the differencing equations and (ii) are persistent for the entire period of overlapping record. Also, systematic departures of tributary flows (Pojoaque + Santa Clara + Santa Cruz) from the long-term averages shown in Table 1, and unmeasured surface water inflows and outflows will affect our results, although we expect this error to be small given the small flows at these tributaries. Significant long-term temporal trends, including those caused by pumping withdrawals, will impact our estimates. Time series analysis of the gage data by Kwicklis in Keating et al. (1999) suggested that temporal trends, if they exist, are very subtle and probably do not contribute significantly to errors in this analysis. Finally, using these discharge estimates to approximate long-term average recharge relies on an assumption that the aquifer was at steady state before significant pumping occurred. Significant departures of the aquifer system from steady state will impact the recharge estimates.

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