Hydrochemical tracers in the middle Rio Grande Basin, USA: 2. Calibration of a groundwater-flow model

Ward E. Sanford · L. Niel Plummer ·
Douglas P. McAda · Laura M. Bexfield ·
Scott K. Anderholm

Abstract The calibration of a groundwater model with the aid of hydrochemical data has demonstrated that low recharge rates in the Middle Rio Grande Basin may be responsible for a groundwater trough in the center of the basin and for a substantial amount of Rio Grande water in the regional flow system. Earlier models of the basin had difficulty reproducing these features without any hydrochemical data to constrain the rates and distribution of recharge. The objective of this study was to use the large quantity of available hydrochemical data to help calibrate the model parameters, including the recharge rates. The model was constructed using the US Geological Survey's software MODFLOW, MODPATH, and UCODE, and calibrated using ^{14}C activities and the positions of certain flow zones defined by the hydrochemical data. Parameter estimation was performed using a combination of nonlinear regression techniques and a manual search for the minimum difference between field and simulated observations. The calibrated recharge values were substantially smaller than those used in previous models. Results from a 30,000-year transient simulation suggest that recharge was at a maximum about 20,000 years ago and at a minimum about 10,000 years ago.

Résumé Le calibrage d'un modèle hydrogéologique avec l'aide de données hydrochimiques a démontré que la recharge relativement faible dans le Grand Bassin du Middle Rio est vraisemblablement responsable d'une dépression des eaux souterraines dans le centre du bassin et de la présence d'une quantité substantielle d'eau du Rio Grande dans l'aquifère du Groupe de Santa Fe. Les modèles antérieurs avaient des difficultés à reproduire ses conclusions sans l'aide de données hydrochimiques pour contraindre les taux et la distribution de la recharge. L'objectif de cette étude était d'utiliser une grande quantité de données hydrochimiques permettant de calibrer les paramètres du modèle, et notamment les taux de recharge. Le modèle a été construit avec les logiciels MODFLOW, MODPATH et UCODE, et calibré en utilisant les concentrations en ^{14}C et la position de certaines zones définies par les données hydrochimiques. L'estimation de certains paramètres a été réalisée en utilisant une combinaison de techniques de régression non linéaire et une méthode de recherche exhaustive (Brute Force Search) de l'erreur minimum entre les résultats des observations et les simulations. Les valeurs de la recharge calibrée sont substantiellement plus basses que celles estimées dans les modèles antérieurs. Les résultats d'une simulation en régime transitoire sur 30.000 ans suggèrent que la recharge au maximum de la dernière glaciation (last glacial maximum, LGM) était 10 fois supérieure au taux actuel, mais que la recharge qui a suivit la LGM était plus bas que la recharge actuelle.

Resumen La calibración de un modelo de aguas subterráneas con el apoyo de datos hidroquímicos ha demostrado que la recarga relativamente baja en la cuenca media del Río Grande es probablemente responsable de una depresión de aguas subterráneas en el centro de la cuenca y de la presencia de una cantidad considerable de agua del Río Grande en el acuífero del Grupo Santa Fe. Los modelos propuestos con anterioridad para la cuenca tenían dificultades para reproducir estas características ya que no tenían datos hidroquímicos que permitieran delimitar los ritmos y distribución de recarga. El objetivo del presente estudio consistió en utilizar una gran cantidad de datos hidroquímicos disponibles para ayudar a calibrar los parámetros del modelo, incluyendo los ritmos de recarga. El modelo se construyó utilizando los modelos MODFLOW, MODPATH, y UCODE del USGS, mientras que la calibración se realizó en base a concentraciones de ^{14}C y a la posición de ciertas zonas definidas con los datos hidroquímicos. La estimación de parámetros se realizó en base a una combinación de técnicas de regresiones no lineares y a una búsqueda a viva fuerza del error mínimo entre los datos observados y los simulados. Los valores de recarga calibrados fueron significativamente más bajos que los estimados en los modelos anteriores. Los resul-

Received: 29 November 2002 / Accepted: 21 February 2004
Published online: 29 April 2004

W. E. Sanford (✉) · L. N. Plummer
US Geological Survey,
431 National Center,
Reston, VA 20192, USA
e-mail: wsanford@usgs.gov

D. P. McAda · L. M. Bexfield · S. K. Anderholm
US Geological Survey,
5338 Montgomery St., NE Suite 400, Albuquerque, NM 87109, USA

DOI 10.1007/s10040-004-0326-4

tados de una simulación transitoria de 30,000 años sugieren que la recarga durante la última glacial máxima (LGM) fue diez veces el ritmo moderno, pero que la recarga que ocurrió inmediatamente después de la LGM fue más baja que el ritmo moderno.

Keywords Groundwater age · Groundwater flow · Hydrochemistry · New Mexico · Numerical modeling

Introduction

In the Middle Rio Grande Basin (MRGB) of central New Mexico (Fig. 1) groundwater is the primary water source for all municipal, industrial, and domestic uses except agricultural irrigation. Groundwater withdrawals around the city of Albuquerque steadily increased from the 1940s through the 1990s, resulting in large declines in water levels. Investigations of geologic and hydrologic conditions in the MRGB began in the early 20th century, but began to increase in frequency during the 1960s. Three-dimensional groundwater models of the basin were developed in the 1980s (Kernodle and Scott 1986; Kernodle et al. 1987). Kernodle et al. (1995) constructed a new transient model of groundwater flow in the basin based on an updated synthesis of the knowledge of the basin hydrogeology (Hawley and Haase 1992; Thorn et al. 1993). This model was not rigorously calibrated because of the computational requirements of the model at the time, but it did predict more limited groundwater availability than had been previously estimated for the region. Comprehensive summaries of these investigations through the 1990s were compiled by Thorn et al. (1993) and McAda (1996).

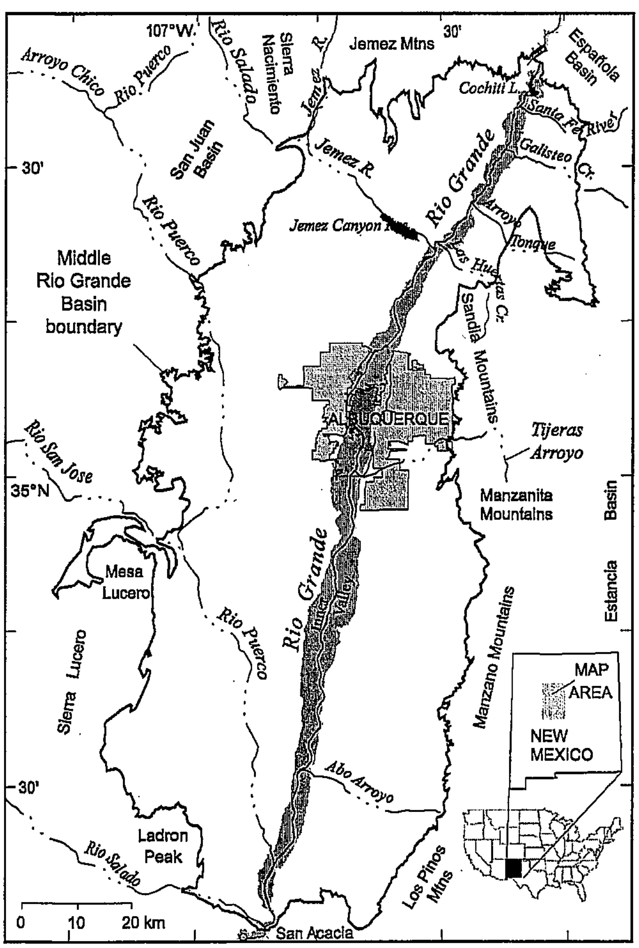


Fig. 1 Selected features and location of the Middle Rio Grande Basin

In 1995, the US Geological Survey, in cooperation with other Federal, State, and local agencies, began a multiyear study in the MRGB to improve the understanding of the water resources (Bartolino and Cole 2002). Geophysical studies under this program have included broad aeromagnetic and gravity surveys (Grauch et al. 2001). Geologic studies have included incorporating the stratigraphy (Stone et al. 2001) into a three-dimensional geologic model of the basin (Cole 2001). Field-based estimates of recharge were conducted for sections of the Rio Grande (Bartolino and Niswonger 1999), the eastern mountain front (Anderholm 2001), and sections of several prominent arroyos (Constantz 1998; Stonestrom and Atkins 1998). Geochemical studies focused on sampling the groundwater and surface water for major chemical constituents and environmental tracers (Plummer et al. 2004a), and using that information to estimate parameters for a groundwater-flow model (Sanford et al. 2004). These geological and hydrological findings have been incorporated into a new groundwater model of the basin (McAda and Barroll 2002).

As a part of the MRGB study, Tiedeman et al. (1998) used nonlinear regression methods to investigate the potential causes of a water-table trough discovered by Bjorklund and Maxwell (1961) and Titus (1963). Six different subsurface configurations were simulated assuming either (1) a high hydraulic conductivity zone, (2) a low-permeability north–south-trending fault, or (3) a greater total sediment thickness for the basin. The first two configurations resulted in a significantly better fit to the data, but the simulations could not offer proof of the cause of the trough. Field investigations have also failed to determine the cause.

The purpose of this paper is to describe the use of hydrochemical data to calibrate a groundwater flow model of the MRGB. The primary goal of this work was to improve estimates of model parameters, especially recharge values, as they are constrained by groundwater ages and other geochemical observations. Some of these estimates obtained in this model have been included in a new model of the basin (McAda and Barroll 2002). The model grids from Kernodle et al. (1995) and Tiedeman et al. (1998) were modified to give a more even resolution over the entire basin, and to extend the lower layers deeper into the aquifer system. The 3-D geologic model of Cole (2001) was used to define hydraulic conductivity zones within the groundwater model. Collection and analysis of the groundwater chemistry and age data were completed first and used to develop a conceptual model of groundwater

 DOI 10.1007/s10040-004-0326-4

flow (Plummer et al., 2004b). Novel methods were then developed to incorporate all of the hydrochemical data directly into the parameter-estimation process.

Hydrogeologic Setting

The MRGB occupies an area of ~7,900 km^2 in central New Mexico (Fig. 1). The climate is semiarid, with long-term average precipitation ranging from 21.8 cm/year near the Rio Grande to 48.3 cm/year at Sandia Park on the crest of the Sandia Mountains. Potential evapotranspiration ranges from less than 125 cm/year in the mountains to more than 150 cm/year near the Rio Grande (Thorn et al. 1993). The metropolitan area associated with the city of Albuquerque lies in the north-central part of the basin and had a population of greater than 700,000 in 2000.

The MRGB is defined as the extent of Cenozoic deposits bounded by several structural features including the Jemez Mountains, Sandia Mountains, Manzano Mountains, Los Pinos Mountains, the Sierra Lucero, and the San Juan Basin (Fig. 1). The Rio Grande flows into the basin through a northeastern constriction near Cochiti Lake and out of the basin through a southern constriction near San Acacia. Rock units in the MRGB include pre-Santa Fe deposits, Tertiary Santa Fe Group basin fill, Pleistocene volcanic rock, and Quaternary sediments. Geologic and geophysical studies have been conducted recently to characterize the location, extent, and properties of the depositional units in the basin (Bartolino and Cole 2002). Much of that work was compiled into a three-dimensional (3-D) geologic model of the basin (Cole 2001), upon which the hydraulic conductivity zonation of the groundwater-flow model in this study has been based.

The predominant deposit in the basin is the Santa Fe Group, the thickness of which ranges from about 1,000 m along the basin margins to greater than 4,000 m in the basin center. The axial-channel sands and gravels associated with the ancestral Rio Grande are especially coarse and well sorted. The sands of the middle and lower units of the Santa Fe Group tend to be finer and less well-sorted. The crustal extension that formed the Rio Grande Rift caused normal faults to develop throughout the MRGB during deposition of the Santa Fe Group. Some of these north–south-trending normal faults have been cemented and likely act as partial barriers to horizontal groundwater flow (Haneberg 1995a; Rawling et al. 2001; Plummer et al. 2004b).

Many aquifer tests have been performed and analyzed to estimate the transmissivity of deposits within the Santa Fe Group. Most tests were conducted in production wells with screens that are about 100 m long. Thorn et al. (1993) summarized the results of several of these aquifer tests and reported the hydraulic-conductivity estimate for each well as the transmissivity divided by the screen length. Hydraulic-conductivity estimates range from 0.1 m/day for silty-clay to 100 m/day for gravel deposits. In an earlier model, Kernodle et al. (1995) assigned horizontal hydraulic conductivities ranging from 1–20 m/day on the basis of field tests and on compiled unit descriptions from Hawley and Haase (1992). Tiedeman et al. (1998) obtained model-calibrated hydraulic conductivities from 1–30 m/day for the basin fill.

Regional groundwater levels that represent predevelopment conditions have been compiled by Bexfield and Anderholm (2000) (Fig. 2). Some groundwater flows from the flanks of the basin inward toward the Rio Grande, but the predominant direction of flow is through the basin from north to south. The Rio Grande was losing water to the basin aquifer under predevelopment conditions in reaches just north of Albuquerque and 10–30 km south of Albuquerque. The water from the former moved into the aquifer system away from both sides of the Rio Grande and flowed southward parallel to the river until it discharged back into the Rio Grande along an extended reach in the southern part the basin. In one region west of Albuquerque and the Rio Grande, groundwater levels are lower than those at the adjacent Rio Grande. This area, known as the "groundwater trough", was originally described by Bjorklund and Maxwell (1961) and Titus (1963), and has been the subject of speculation ever since as to its cause. Tiedeman et al. (1998) performed numerical experiments to test different hypotheses by varying different aquifer properties, but the results were equivocal and no single hypothesis has been supported fully by field evidence. In the companion paper (Plummer et al. 2004b), it was shown that the trough contains water with radiocarbon ages of more than 20,000 years, representing recharge from the last glacial period, and is bounded on the west by younger water of Rio Puerco origin and on the east by younger water or Rio Grande origin.

The groundwater-flow system of the MRGB has several sources of recharge (Bartolino and Cole 2002). Precipitation in the mountains infiltrates along mountain fronts bordering the basin, and surface water infiltrates along streams and arroyos that are tributaries to the Rio Grande. Groundwater inflow from adjacent basins and mountains recharges as underflow to the northern and western parts of the basin. Recharge also occurs naturally as leakage from the Rio Grande in reaches in the center of the basin. Groundwater discharges under natural conditions from the MRGB by flow into the Rio Grande, by underflow at the southern end of the basin near San Acacia, and by evapotranspiration in the inner valley.

Geochemical data for groundwater in the MRGB has been compiled, collected, and analyzed by Anderholm (1988) and Logan (1990), and more recently and extensively by Bexfield and Anderholm (2002) and Plummer et al. (2004b) as part of the multiyear MRGB study. The data by Plummer et al. (2004a) include major and minor-element chemistry; ^{18}O and ^{2}H in water; ^{13}C and ^{14}C of dissolved inorganic carbon (DIC); ^{34}S of dissolved sulfate; ^{3}H; and selected dissolved gases including chlorofluorocarbons and sulfur hexafluoride. The chemical and isotopic composition of groundwater in the MRGB was mapped and used to identify 13 hydrochemical zones that have unique chemical and isotopic characteristics (Fig. 3). Twelve of the hydrochemical zones were inter-

DOI 10.1007/s10040-004-0326-4

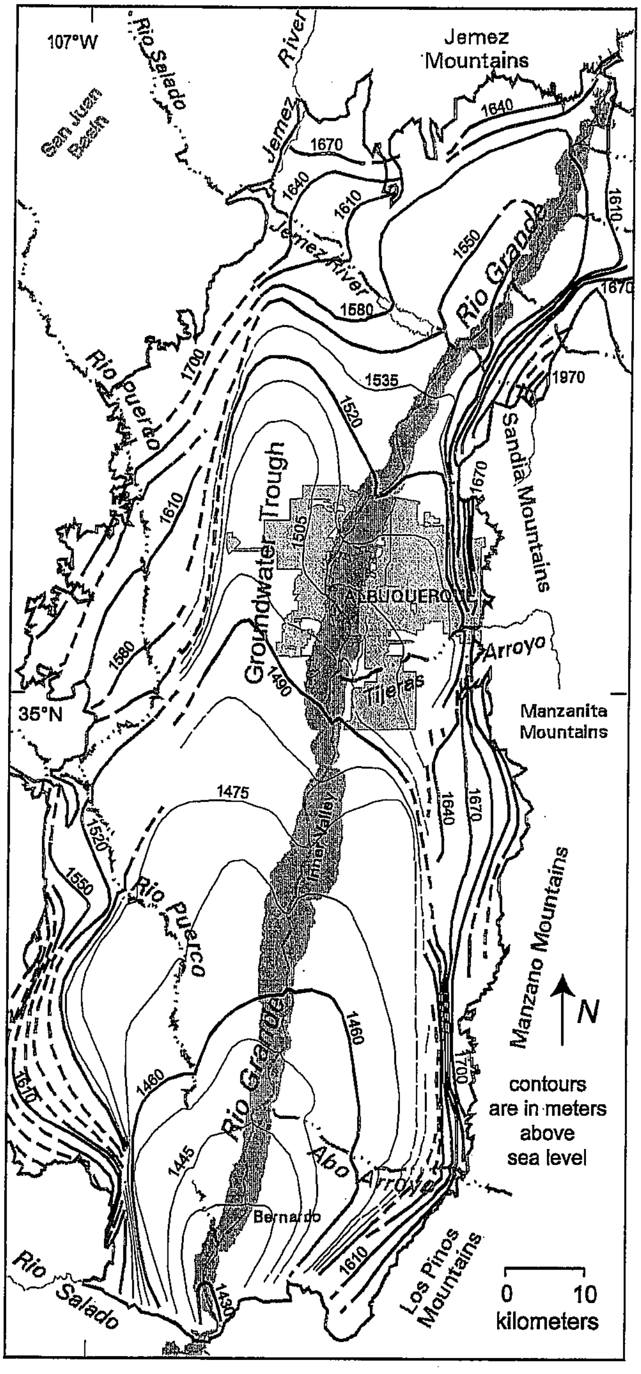


Fig. 2 Water table in its predevelopment configuration. After Bexfield and Anderholm (2000). Discontinuous contours indicate areas where water levels differ greatly over short distances, generally in close proximity to major faults

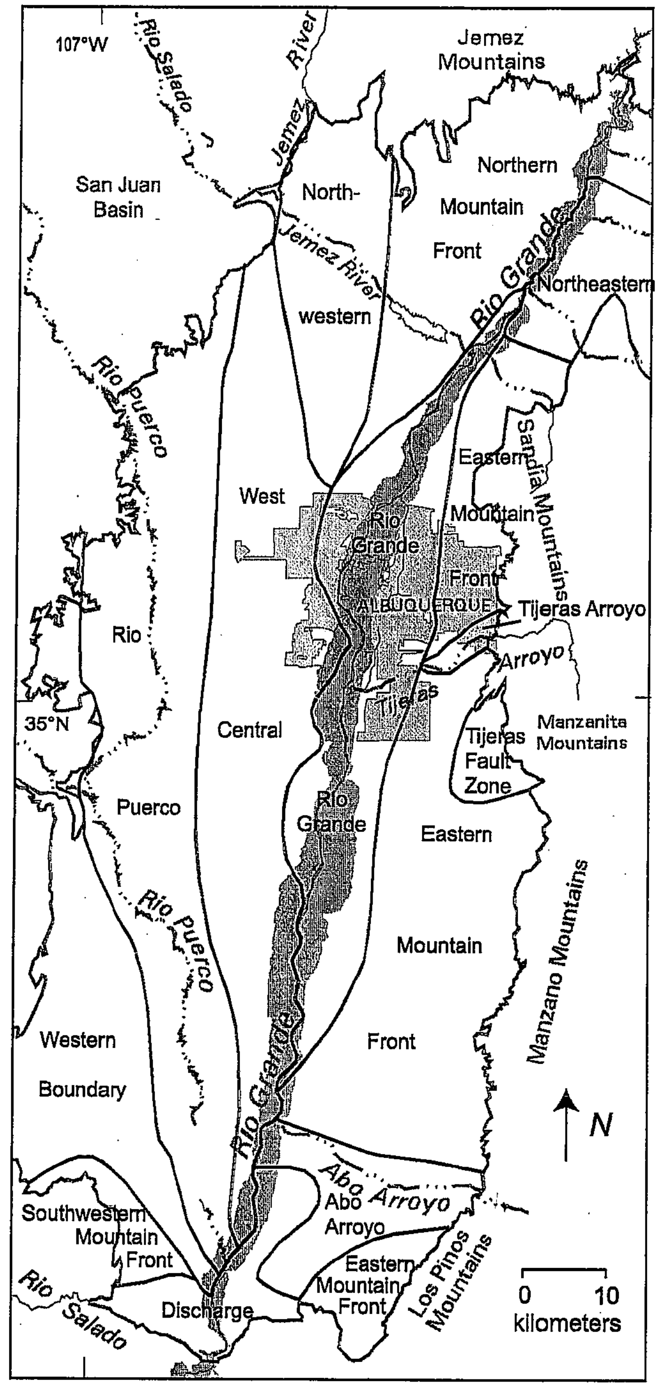


Fig. 3 Hydrochemical zones in the Middle Rio Grande Basin as defined by Plummer et al. (2004b)

preted as representing sources of recharge to the basin. The remaining zone was a discharge zone. The classification is based on water analyses from 288 wells, and is described in more detail in Plummer et al. (2004a).

Model Construction

The USGS software package MODFLOW (McDonald and Harbaugh 1988) was used to simulate groundwater flow in the MRGB. Travel times to observation wells were calculated using the USGS package MODPATH (Pollock 1994). The MODFLOW and MODPATH representations of the basin were calibrated in part using nonlinear regression methods implemented with UCODE

DOI 10.1007/s10040-004-0326-4

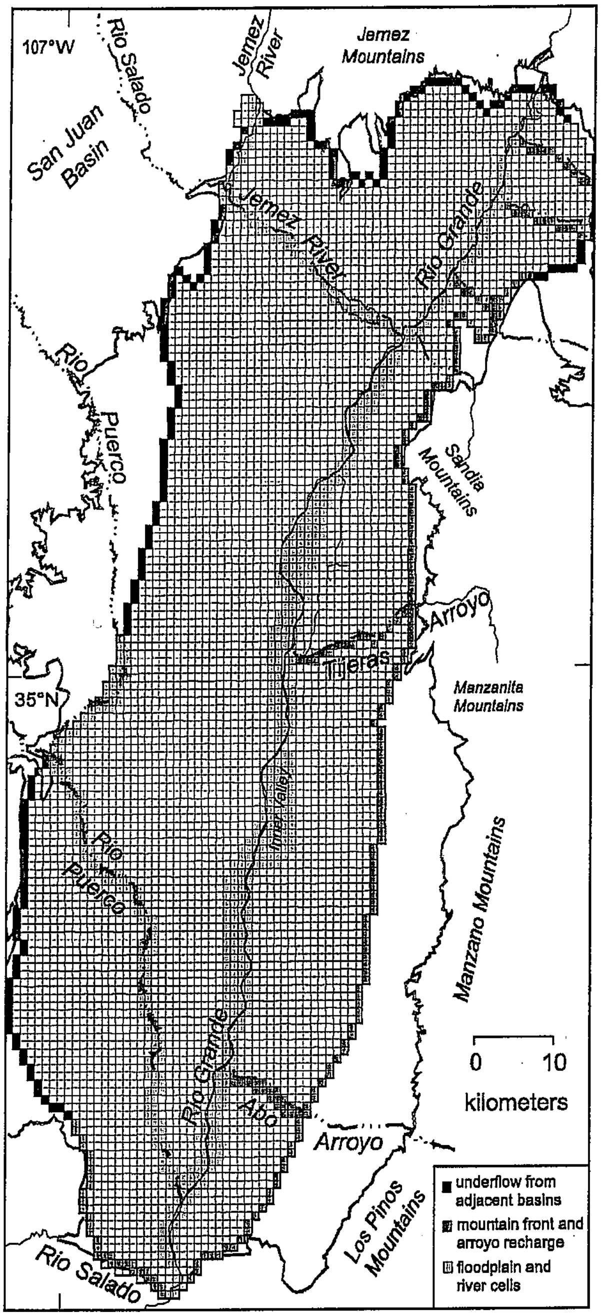


Fig. 4 Finite-difference grid for the groundwater flow model, with locations and types of boundary conditions

(Poeter and Hill 1998). The model domain covers an area somewhat smaller than the entire basin, and is divided into a rectilinear grid of equally spaced 1-km-square cells. The grid consists of 156 rows and 80 columns (Fig. 4). The eastern and western model boundaries are mostly coincident with faults thought to be partial to substantial barriers to horizontal groundwater movement. The vertical extent of the aquifer system is represented by nine model layers. The bottom of layer 1 is 6 m below the bed of the Rio Grande, and the altitude of the bottom of layer 1 is constant in an orthogonal direction away from the trend of the inner valley (Fig. 1). The upper seven layers

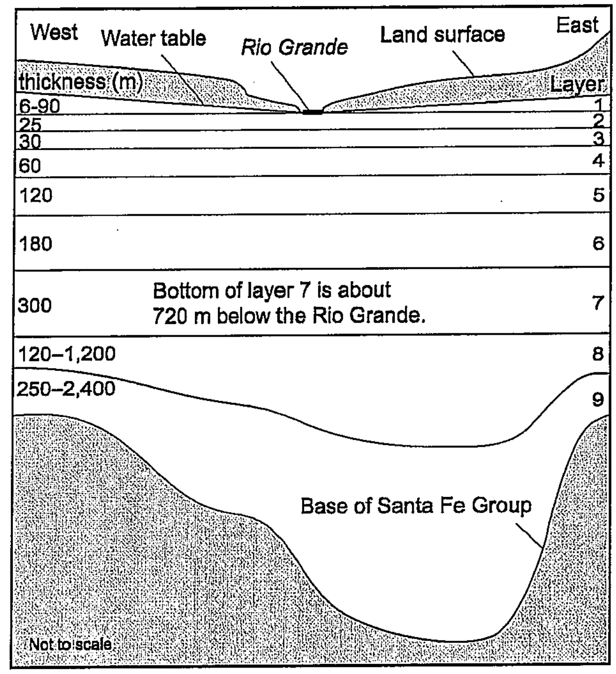


Fig. 5 Configuration of model layers

range in thickness from 6 to 300 m. Layers 8 and 9 are of variable thickness and represent the aquifer system from the bottom of model layer 7 to the base of the unconsolidated sediment (Fig. 5).

Flow Model

Head-dependent boundaries are implemented in the inner valley of the MRGB to represent the interaction of the Rio Grande with the groundwater flow system. Likewise, head-dependent boundaries are implemented along the Jemez River and the Rio Puerco to represent the groundwater/surface-water interaction along those waterways. The head-dependent boundary is simulated using the river package of MODFLOW. The river cells in this study included all of the regions within the modern floodplains of the Rio Grande, Jemez River, and Rio Puerco (Fig. 4). This approach was used because rivers migrate across their floodplains over the course of several thousand years, and the objective was to simulate the long term average condition.

Mountain-front recharge and arroyo infiltration were simulated using the recharge package in MODFLOW. The recharge was divided into segments, each of which corresponds to a particular mountain region or arroyo. There were 12 recharge segments specified, and all of them were along the southern or eastern boundaries of the model (Fig. 4). Underflow along the basin boundaries was simulated as specified flow into layers 2, 3, and 4 of the model using the well package in MODFLOW. There were seven underflow segments specified, and most of them were along the northern or western boundaries of the model (Fig. 4).

DOI 10.1007/s10040-004-0326-4

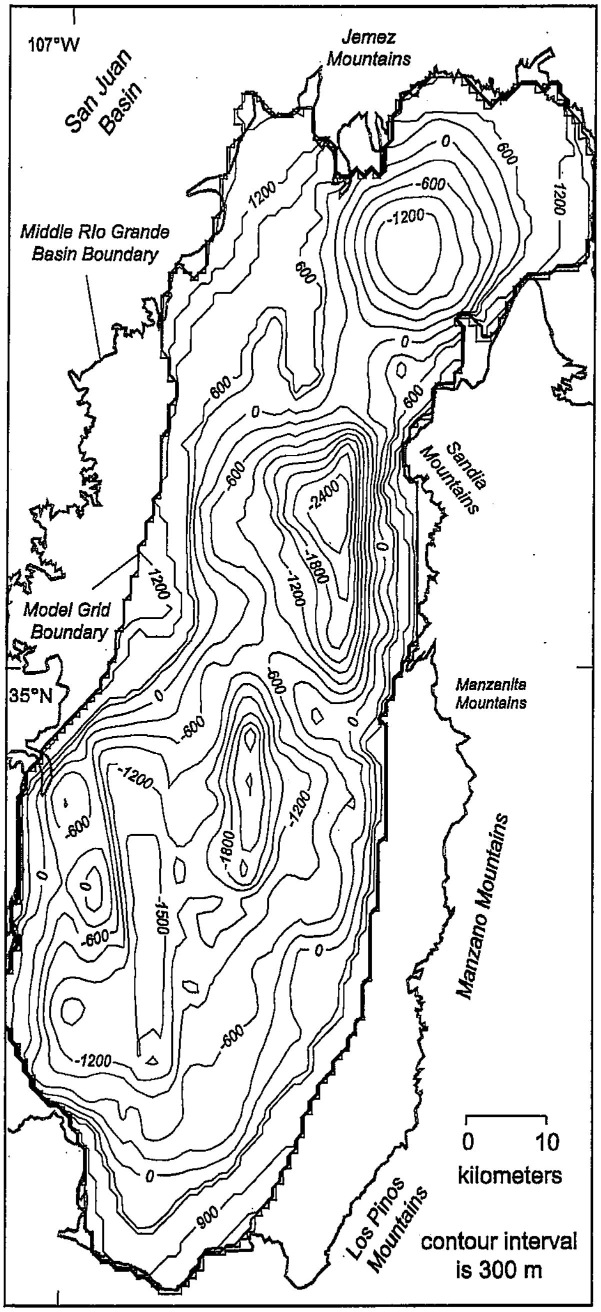


Fig. 6 Altitude of the base of the groundwater-flow model, in meters above or below sea level. Surface is based on compilation of data of Cole (2001) and Grauch et al. (2001)

The hydraulic-conductivity zones for the basin were based on the geologic model of Cole (2001). The 3-D distribution of geologic units within this model was based on recent geophysical investigations (Grauch et al. 2001) and reinterpretations of existing data. The revised geologic model was also based on stratigraphic and lithologic interpretations of the sediments penetrated by numerous wells in the basin. In general, delineation of hydrostratigraphic units was based on a conceptual understanding of overall rift history and the expected relationships between tectonic deformation and sedimentation (Stone et al. 2001). Because the pre-rift rocks are more dense than the basin sediments, the regional gravity data (Grauch et al. 2001) could be used to calculate the bottom of the unconsolidated sediments, which was used as the bottom of the groundwater-flow model (Fig. 6). A total of 21 hydraulic-conductivity zones were defined within the groundwater-flow model (Fig. 7). Vertical hydraulic conductances in the groundwater flow model were divided into 12 zones to represent vertical anisotropy. Two faults zones were added to the groundwater flow model as discrete (low) hydraulic-conductivity zones. These were added because a significant differential in water levels could be observed in these regions that could not be reproduced in the model without the implicit representation of the faults as low-conductivity barriers.

Advective Transport Model

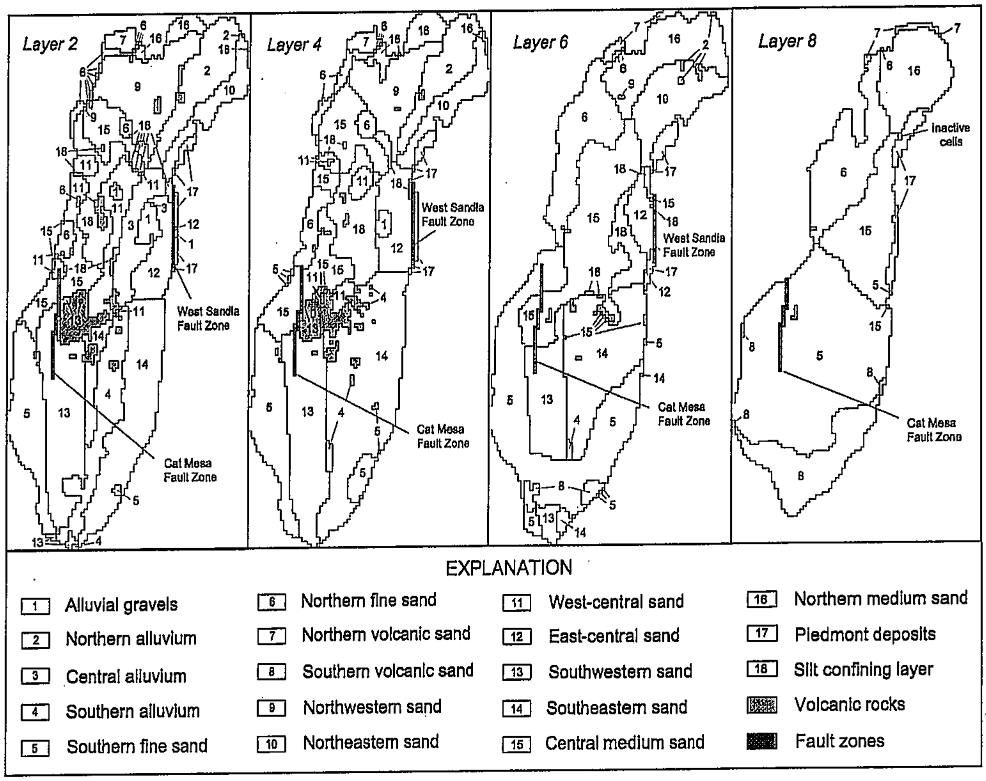
This study incorporates hydrochemical tracer data into the calibration of the groundwater flow-model. Groundwater ages obtained from ^{14}C activities are one set of these data. When the observed ages were compared with equivalent simulated ages, the residuals were used to directly improve the model calibration. The simulated ages were obtained by using MODPATH (Pollock 1994) to track the line of travel of a parcel of water from the observation well backward until it reached a recharge location. MODPATH is a post-processing program that is used in conjunction with the cell-by-cell flow rates calculated with MODFLOW. Time-of-travel is integrated backward along a path line to obtain a simulated groundwater age. Hydrodynamic dispersion in these calculations was neglected because the effect of dispersion on the activities from a nearly invariant source over a 100-km basin would be negligible for values of longitudinal dispersivity less than 1 km (Johnson and DePaolo 1996).

Another source of tracer information that was used for calibration is the delineation of the hydrochemical zones (Fig. 3). These zones represent waters with different source areas. A delineation of waters with different source areas was simulated using MODPATH. A map of the distribution of groundwater originating from different sources was constructed by backward tracking a parcel of water from every cell in layer 2 of the model, and then indicating the source area at every cell center. The simulated map was compared directly with the hydrochemical-zone map using a quantitative method in order to improve the calibration of the model.

The travel-time calculations required the seepage velocity, and thus effective porosity was a necessary parameter to specify or estimate in the calibration procedure. Groundwater ages provide inherent information on the groundwater flux, and therefore also on recharge rates. They do not, however, provide independent information on both the recharge rate and the effective porosity (Medina and Carrera 1996). Porosity for the unconsolidated sediment of the MRGB can be constrained from field measurements with a degree of certainty that is significantly greater than that for recharge rates. Stone

 DOI 10.1007/s10040-004-0326-4

Fig. 7 Hydraulic-conductivity zones based on geology (Cole 2001) as defined in layers 2, 4, 6, and 8 of the groundwater flow model. See Sanford et al. (2004) for details of remaining layers



and Allen (1998) report total porosity values between 30 and 40% from a 229-m-core from the Santa Fe Group. Haneberg (1995b) reports porosity values derived from geophysical logs that range from about 40% at the land surface to about 30% at 300 m depth. In addition, it is well established that porosity values decrease in an exponential manner with increasing depth in sedimentary basins (Athy 1930). Based on this information, porosities were assigned by layers beginning with 36% for layer 1 and decreasing 2% per layer down to 20% for layer 9. Given that each deeper layer increases in thickness, the assigned porosities decrease in an exponential fashion. For unconsolidated sediment such as in the MRGB basin, the total and effective porosities are likely to be nearly the same with respect to long-term regional transport of ^{14}C (Sanford 1997).

The relation between ^{14}C activity and groundwater age is one based on exponential decay, and is given by the equation (1):

pmC = Ao/(exp[time*ln(2)/5730])

where pmC is percent modern carbon; Ao is the ^{14}C activity at the recharge location; "time" is the simulated travel time from MODPATH; and 5,730 is the half-life of ^{14}C, in years. Most activities of ^{14}C were affected relatively little by geochemical reactions along their flow paths (Plummer et al. 2004b). ^{14}C activities in the atmosphere have varied over the past 24,000 years (Stuiver et al. 1998; Kalin 2000). Based on recent radiocarbon calibration data, Plummer et al. (2004b) related calendar years to ^{14}C years for the MRGB samples. For the groundwater-flow model, the geochemical reactions and the transient atmospheric effects were incorporated into a value of A_o assigned to each individual ^{14}C activity (Eq. 1). In MODPATH one parcel of water was tracked backward for each 30 m of observation well screen. All of the simulated travel times for a well were first converted to simulated ^{14}C activities using Eq. (1), then the average activity was calculated for the entire well. For long-screened production wells, as many as 12 parcels were used. In that little information was available on the vertical distribution of inflow to these wells, the parcels were distributed evenly along the well screen. In this manner a mixing effect was added to the final simulated ^{14}C age for long-screened wells.

The backward tracking in MODPATH brings the path lines to the location where that water would have entered the model of the basin. In many circumstances, the boundary of the model or basin does not coincide with a recharge location for the water where the ^{14}C activity would obtain its initial value. Underflow boundaries from bounding basins are the most common example of this, and along the eastern mountain front there are reaches where the water would actually have entered the subsurface many kilometers to the east of the model boundary. For these situations, an initial age was assigned for the water as it enters the basin. This initial age was added to the path-line age calculated by MODPATH. These initial ages were also treated as parameters in the model that were estimated during the inverse procedure.

DOI 10.1007/s10040-004-0326-4

Model Calibration

The groundwater-flow model was calibrated using a combination of a nonlinear least-squares regression method, as it is implemented in the computer code UCODE (Poeter and Hill 1998), and manual adjustment of individual parameters. For this study, MODFLOW, MODPATH, and a small number of pre- and post-processing routines were called by UCODE during each iteration. In the regression procedure, optimal (best-fit) parameter values are estimated by minimizing the sum of the squared residuals (SSR) between observed and simulated values in an objective function (Hill 1998; Poeter and Hill 1998). In the process of minimizing the objective function, the regression procedure computes the sensitivity of a simulated observation at each observation location to each model parameter. Multiple types of data were used in this study to calibrate the groundwater-flow model. Hydraulic heads, ^{14}C activities, and the locations of the hydrochemical zones were all used as observations in the objective function. These values were each given weights in accordance with their perceived or estimated accuracy. A total of 200 hydraulic heads, 200 ^{14}C activities, and the fraction of river water in nine hydrochemical target regions (discussed below) were used as observations, making a total of 409 observations.

Although UCODE was run to improve the model fit, the discrete nature of the particle tracking prohibited the nonlinear regression method from obtaining the very best fit. After the UCODE run, individual parameters were adjusted further to obtain the best fit. Accuracy of the sensitivity calculations was limited by the discrete nature of the path-line calculations. Small changes in the parameters frequently caused sudden shifts in path lines from one source area to another, creating an associated jump in travel time. UCODE was also used during manual parameter adjustment to run multiple simulations varying only one parameter at a time over a finite range of values. These manual adjustments revealed the discrete jumps in the SSR associated with the nonconvergence in the nonlinear regression, and allowed the minimum SSR and associated parameter value to be identified. All of the individual parameters were adjusted manually one at a time to minimize the SSR. The entire set of parameters was adjusted consecutively in this manner three times, after which point the SSR converged to a new minimum.

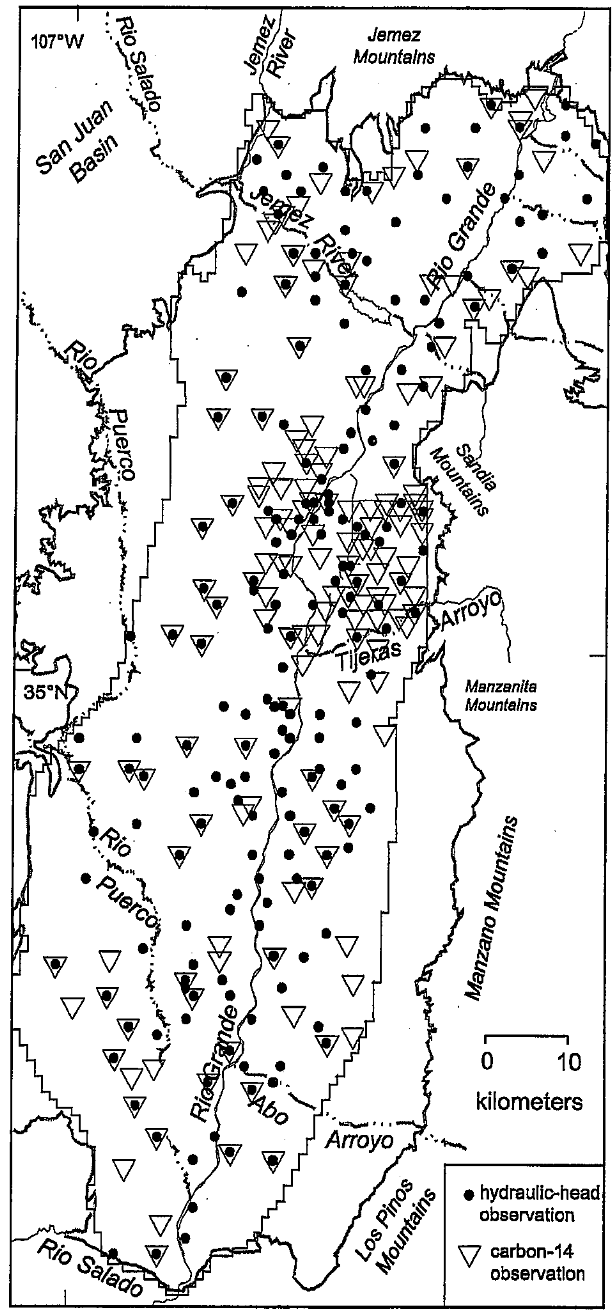


Fig. 8 Locations of wells from which hydraulic head and ^{14}C activity observations were taken

Water-Level Observations

The groundwater-flow model was set up to simulate steady-state groundwater flow prior to the development of groundwater as a resource within the basin. To calibrate the model, hydraulic-head data were needed that did not show the influence of any appreciable groundwater withdrawals within the basin over the last half century. The data were compiled from many sources by Bexfield and Anderholm (2000), who presented a map of the predevelopment water table (Fig. 2). The sources of the data include domestic wells, windmills, pueblo wells, and monitoring wells. Data from wells within the vicinity of the city of Albuquerque were only used if they were measured before 1960. Those that were measured during the 1950s were chosen carefully to exclude wells sited close to visible cones of depression. Wells in the basin away from the city were assumed to have water levels that contained negligible effects from anthropogenic stresses.

Two-hundred hydraulic-head values were used in total (Fig. 8). The screen depths from the wells were used to determine the layer in which the well would be located in the groundwater flow model. Well locations never fell exactly on cell-center coordinates, so to obtain the equiv-

DOI 10.1007/s10040-004-0326-4

alent, simulated value hydraulic heads were averaged from several cells. A trilinear interpolation scheme was used that interpolated the head value between the cells of the nearest two rows, columns, and layers. The expected measurement error for the hydraulic heads in the data set was estimated as an expected standard deviation, and was assigned values from 0.3 m for recently surveyed monitoring wells, to 3 m or more for domestic wells where the measuring-point altitude was estimated from a topographic map. These estimated measurement errors were used to assign weights to the head observations.

Groundwater-Age Observations

The activity of ^{14}C was measured in samples taken from over 200 wells and river locations throughout the basin (Fig. 8), as tabulated in Plummer et al. (2004b). Uncertainties were assigned that reflected the confidence that the ^{14}C measurement represents an appropriate age for water at that well location. This was difficult to assess on a well-by-well basis because it was unclear how the influx of water to a well varied vertically within the well screen. Thus, a simple scheme was adopted where uncertainties of 1 and 5 pmC were assigned to short- (<10 m) and long-screened wells (>10 m), respectively. Plummer et al. (2004a) estimated uncertainty for the long-screened wells might be up to ±20 pmC, but some of this uncertainty was already accounted for by tracking multiple path lines per well. The uncertainty values were assigned to the observations in the UCODE files, and so each ^{14}C observation was weighted based upon these values. The uncertainties in the ^{14}C activities were expressed in terms of the standard deviation for the activity. The weights for each of these observations were a function of the inverse of the standard deviation. Thus the ^{14}C observations for the short-screened wells were given five times more weight than those for the long-screened wells.

Hydrochemical-Zone Observations

In addition to water levels and ^{14}C activities, the location and extent of some of the hydrochemical zones (Fig. 3) were used as observations. Earlier idealized simulations of the basins indicated that the volume of Rio Grande and Rio Puerco water in the basin aquifer system would depend upon the recharge and hydraulic-conductivity parameters of the model. The less the recharge along the margins of the basin, or the higher the hydraulic conductivity of the aquifer, the broader the areal extent of the recharged river water adjacent to the river (Fig. 9). The end-member case is when there is no basin boundary recharge and river water will fill the entire basin (Fig. 9, center panel). In the case of the Rio Puerco and the Jemez River, the vertical hydraulic conductance for the riverbed also controls the extent of river water in the basin. These zones of river water can be observed with their hydrochemical signature. The hydrochemical zones described by Plummer et al. (2004b) include zones described as Rio Grande water and Rio Puerco water

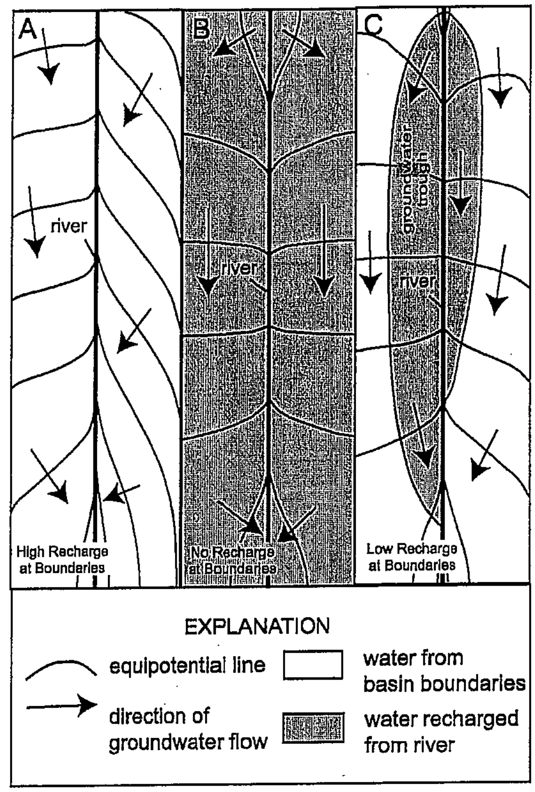


Fig. 9 Idealized simulations with **A** high, **B** no, and **C** low recharge from the basin boundaries, illustrating how low recharge can create a groundwater trough and a zone of river water in the center of a basin

(Fig. 10). The hydrochemical zone of the Jemez River water was substantially smaller and more difficult to distinguish. The exact positions of these boundaries were known to be a function of the recharge and hydraulic-conductivity parameters for the groundwater-flow model, and thus the positions of these boundaries could be used as observations in the model calibration using UCODE.

The nonlinear regression routine requires that simulated observations be continuous functions of the parameter values because small perturbations of the parameter values must produce a finite change in the simulated observations. The hydrochemical zones, however, represent discrete regions where water simulated to migrate to a certain point in the aquifer system either did, or did not, originate from a source location with a recognizable geochemical signature. A method was needed whereby path lines simulated using MODPATH would produce the source location of the water in such a way as to make a continuous or near-continuous function. To accomplish this, nine rectangular hydrochemical "target regions" were created that each included a fraction of a river-water zone defined by the hydrochemistry (Figs. 3 and 10). These nine hydrochemical target regions were used as observations. The observation value was the percentage of river water observed to be in any target region based on the hydrochemical zones. To simulate this, thousands of particles

DOI 10.1007/s10040-004-0326-4

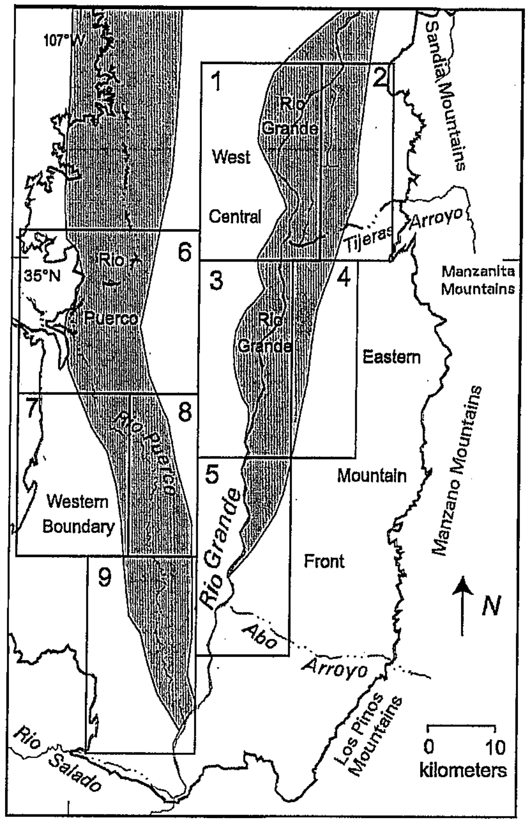


Fig. 10 Locations of the nine hydrochemical target regions in relation to the hydrochemical zones

were generated for each target region in layer 2 in a regular array pattern using MODPATH and tracked backward to the source (Table 1). Layer 2 was used because this represented an average depth of a large number of the wells in these regions. The number of paths originating from the river was then divided by the total number of paths for that target region. The very large number of particles allowed this simulated percentage to vary by finite, yet significant, amounts when each parameter was perturbed by only a few percent. Therefore, although the responses of the simulated observations were not continuous at an infinitesimally small parameter perturbation, they were continuous at the size of perturbations used in these simulations, and allowed for their use in the nonlinear regression methods.

Parameter Sensitivity

Composite-scaled sensitivities were calculated for each of the parameters from the MODFLOW and MODPATH model simulations. Based partially on the magnitude of the sensitivity, and partially on the availability of prior information, some parameters were assigned values, whereas other parameter values were estimated using nonlinear regression methods. After convergence was reached with the nonlinear regression, all parameters except porosity were adjusted manually in an attempt to further reduce the SSR. The parameters with the highest sensitivities were the hydraulic conductivities in the southern and east-central sections of the basin, the anisotropy of the Rio Grande alluvium near Albuquerque, recharge rates for the southern Sandia Mountain front, and underflow from the northern and northwestern boundaries. Based on low sensitivities, values were assigned to the vertical leakance of the northern and southern sections of the Rio Grande alluvium, and to the hydraulic conductivity of the Cat Mesa Fault Zone (Fig. 7). Porosity values were assigned because reasonable estimates could be made from field data.

Model Results

Simulations of groundwater levels and path-line tracks were completed in two stages. The goal was to obtain a set of parameters for the flow model that would yield a best fit with the observed data. The nonlinear regression methods in UCODE improved the fit of the model considerably relative to the fit based on the initial estimates. After a point of convergence was reached, individual parameters were adjusted manually to obtain a best fit. The results presented here are from the simulation with the final best fit of parameter values to the data.

Simulated Water Levels

The hydraulic heads from the final simulation are shown from layer 2 in Fig. 11. One of the features in the water

Table 1 Details of hydrochemical target regions defined for use in calibration against the hydrochemical zones

Region number	Hydrochemical target region name	Beginning row number	Ending row number	Beginning column number	Ending column number	Total number of path-lines in region	Fraction of region containing river water	Observed no. of path-lines that should end at the river
1	Rio Grande NW	47	76	26	45	5,400	0.40	2,160
2	Rio Grande NE	47	76	46	55	2,700	0.50	1,350
3	Rio Grande SW	77	106	26	40	4,050	0.47	1,890
4	Rio Grande SE	77	106	41	50	2,700	0.33	900
5	Rio Grande S	107	136	26	40	4,050	0.12	500
6	Rio Puerco N	72	96	1	25	5,625	0.32	1,800
7	Rio Puerco W	97	121	1	15	3,375	0.16	540
8	Rio Puerco E	97	121	16	25	2,250	0.80	1,800
9	Rio Puerco S	122	146	11	25	3,375	0.43	1,440

 DOI 10.1007/s10040-004-0326-4

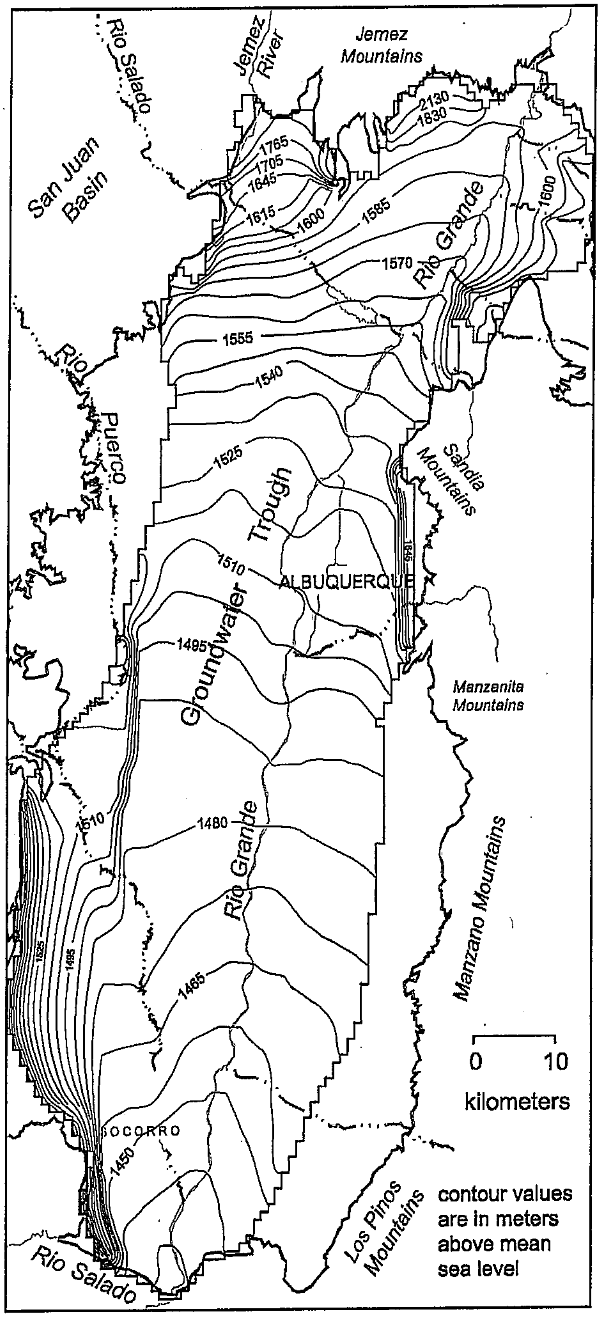


Fig. 11 Simulated hydraulic head in layer 2 of the groundwater-flow model

levels that has been an enigma for years is a region in the west-central section of the basin where the potentiometric surface is lower than the surrounding areas often referred to as the "groundwater trough" (see the observed predevelopment water table map, Fig. 2). The current model configuration reproduces this feature, although not as far north as some of the observed water levels indicate. Earlier models (Kernodle et al. 1995) did not reproduce any of this feature. Attempts were also made by Tiedeman et al. (1998) to investigate different conceptual models of what was creating this trough, including a high permeability zone or a north–south-trending fault. Earlier prototype models demonstrated that by lowering the mountain-front recharge in the model, the system changed from one dominated by the movement of water from the boundaries toward the Rio Grande to one dominated by water leaking from and back into the Rio Grande (see Fig. 9 and associated text). The latter conceptual system has heads to the west of the Rio Grande that are lower than the river, and is consistent with the presence of the trough and the lower recharge values estimated in this study.

Another main feature visible from the hydraulic head maps is the barrier specified at the Cat Mesa Fault Zone in the southwestern quadrant of the model (Fig. 7). The West Sandia Fault Zone (Fig. 7), just east of the city of Albuquerque, separates thick permeable basin fill from the less transmissive rocks to the east. Increases in water levels of over 60 m are observed east of the West Sandia Fault Zone. This feature can be reproduced readily in the model by an adjustment to the hydraulic conductivity east of the fault zone and the recharge along that section of the mountain front. Groundwater ages measured there give independent data upon which the inverse model can calibrate both hydraulic conductivity and recharge.

The model in this study also reproduces the losing section of the Rio Grande that occurs just north of Albuquerque (Fig. 12A). Groundwater moves away from the Rio Grande both to the west toward the trough and to the south beneath the city of Albuquerque, as is also shown in the predevelopment water table map (Fig. 2). This zone of Rio Grande water beneath the city is corroborated by the hydrochemical zone data (Fig. 3). The earlier version of the model by Kernodle et al. (1995) did not reproduce this losing section (Fig. 12B) because the higher mountain-front recharge amounts in that model overwhelmed any tendency for the Rio Grande to lose water to the aquifer system.

Simulated Hydrochemistry

Simulated ages were plotted by placing a 10×10 grid of particles in every model cell and tracking the path lines backward to the source location. For path lines that reached underflow boundaries, the basin-entrance ages were added to the MODPATH travel times. The basin-entrance ages were estimated in the inverse procedure, and although the values were not well constrained, they also did not greatly affect the SSR. All of the final ages were plotted as a function of their starting locations. Several patterns emerged. Young water (<3,000 years), represented by the dark blue areas in Fig. 13A, is present near the mountain fronts where recharge occurs at the land surface, and along the Rio Grande and Rio Puerco near areas where the rivers lose water to the aquifer system. Old water (>100,000 years), represented by the yellow and red areas in Fig. 13A, is present in the southern part of the basin farther down the flow paths. A cross section of the simulated ages is shown in Fig. 13. Although there is a general pattern of increasing simulated age with depth, the heterogeneity of the system in a

DOI 10.1007/s10040-004-0326-4

Fig. 12 Simulated hydraulic heads from **A** layer 2 of the model from this study, and **B** layer 1 of the model of Kernodle et al. (1995). *Arrows* indicate direction of groundwater flow

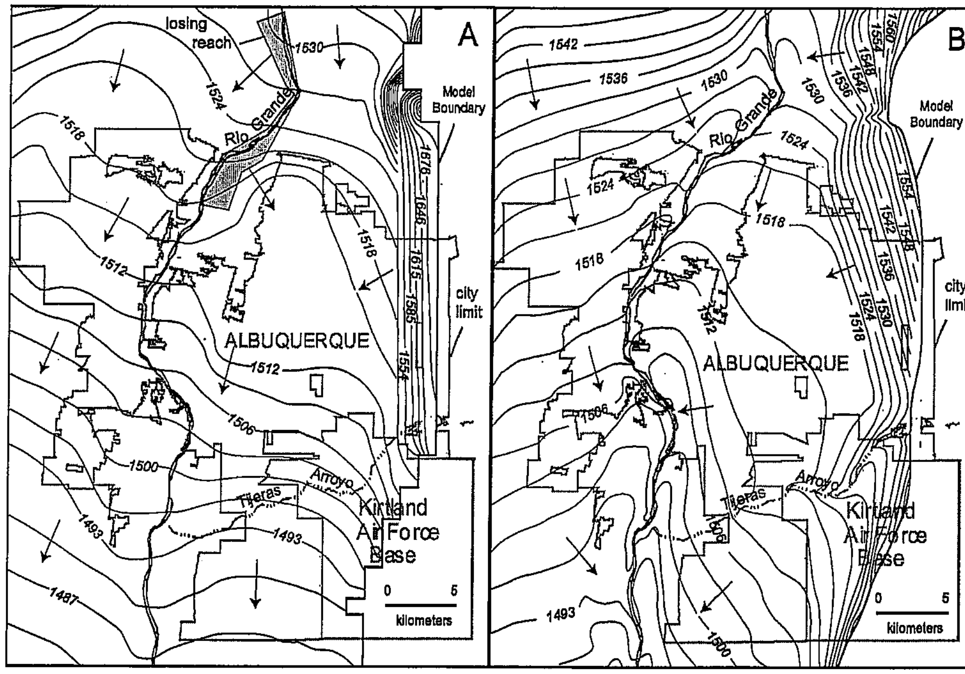
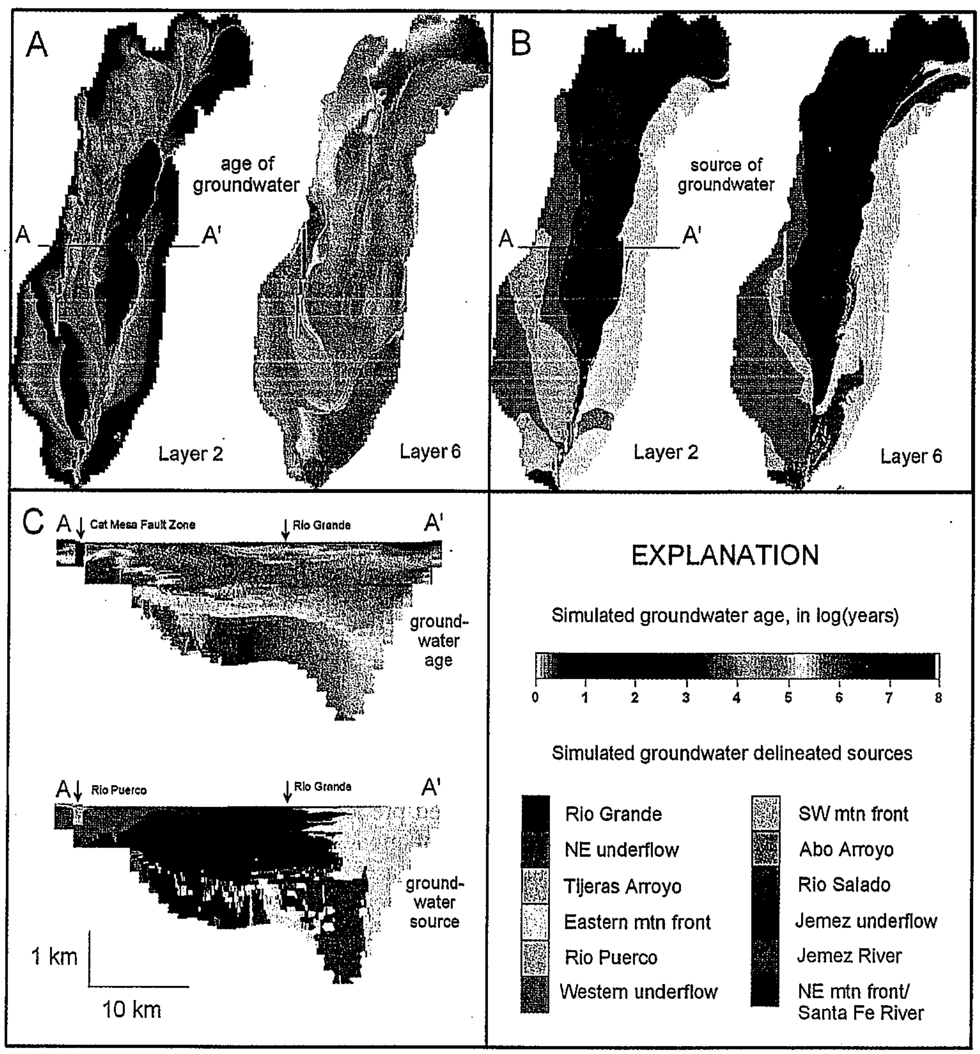


Fig. 13 Simulated **A** groundwater ages, and **B** groundwater source-area delineation in layers 2 and 6, and in **C** an east-west section A–A′



 DOI 10.1007/s10040-004-0326-4

few places creates local inversions where old water is predicted to occur above younger water that is moving through a more permeable zone. The age–depth relations are described in more detail in Plummer et al. (2004b).

The hydrochemical zones (Fig. 3) were also simulated using MODPATH. The recharge regions were first divided into sections that roughly coincided with the areas identified as recharge sources by the hydrochemical zones. MODPATH was then run in the same manner as for the creation of the age maps except that the source location identification numbers were plotted according to the particle starting locations. The results for layer 2 are shown in Fig. 13B. The final estimated model parameters reproduce all of the major zones identified in the hydrochemical evaluation. The red area in the center represents water that was recharged from the Rio Grande. This area corresponds reasonably well to that in the hydrochemical zones (Fig. 3). One difference is that the model produces a central Rio Grande zone that extends farther to the southwest. This difference can be explained by the fact the model is steady-state. The hydrochemical zones would also reflect transient changes in recharge over tens of thousands of years. By contrast, earlier groundwater modeling efforts (Kernodle et al. 1995; Tiedeman et al. 1998) did not predict the presence of any Rio Grande water in the aquifer system beyond the shallow system in the inner valley. The region of groundwater that was simulated to come from the Rio Puerco also agrees with the hydrochemical evaluation, and the use of this area as an observation was important in the calibration of the amount of recharge estimated to be occurring from the Rio Puerco. Results of the hydrochemical-target-region observations are given in Table 1. A cross section of the simulated geochemical zones is shown in the lower part of Fig. 13C. In the simulation, the east and west basin boundary waters tend to remain along those boundaries, the Rio Grande water penetrates down to about 1 km, and the NE underflow waters occupy the central, deeper section of the basin.

Parameter Value Estimates

The combination of nonlinear regression runs and manual parameter adjustments led to a set of final best-fit hydraulic-conductivity and vertical anisotropy values. These values, along with their 95% linear confidence intervals, are shown in Fig. 14. It is clearly evident that some of the parameters values are relatively well constrained, while others values remain highly uncertain. Uncertainty in the model parameters is partially related to parameter correlation. UCODE evaluated the correlation matrix during the sensitivity analysis. High parameter correlations will result in a less well-constrained model. For this model, the inclusion of ^{14}C activities as additional observations substantially reduced parameter correlations from earlier models where mostly water-level observations were used. Out of 1,770 correlation values between parameters, only one value exceeded 0.8, and only two values were less than –0.8. Nearly 1,200 values were between –0.2 and 0.2, indicating relatively little correlation between parameters.

Values for the hydraulic conductivities fall mostly between 1×10^{-7} and 1×10^{-4} m/s, with a few exceptions (Fig. 14). These values are similar to estimates from

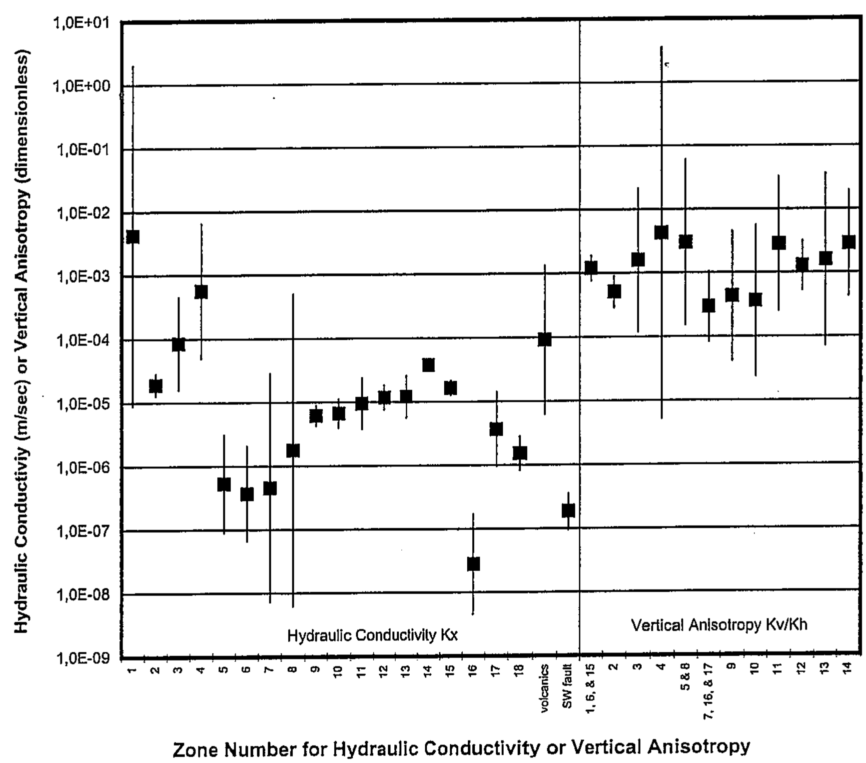


Fig. 14 Best-fit values of hydraulic conductivity and vertical anisotropy values for the groundwater-flow model, including 95% linear confidence intervals (see Fig. 7 for zone locations)

DOI 10.1007/s10040-004-0326-4

Table 2 Estimates of recharge (m^3/s) to the Middle Rio Grande Basin from recent studies

Region	Kernodle et al. (1995)	Tiedeman et al. (1998)	Anderholm (2001)	McAda and Barroll (2002)	This study
Jemez Mountains	0.56	0.27	N/A	0.58	0.08
Western boundary	0.18	0.18	N/A	0.07	0.06
Southwest boundary	0.30	0.09	N/A	0.03	0.17
San Juan Basin	0.05	0.05	N/A	0.04	0.27
Hagan/Espanola Basin	0.21	0.49	N/A	0.55	0.03
Northeast rivers	0.32	0.30	N/A	0.21	0.18
Tijeras Arroyo	0.41	0.41	0.07	0.03	0.00
Abo Arroyo	0.62	0.60	0.05	0.05	0.04
Rio Puerco	0.23	0.12	N/A	0.04	0.14
Jemez River	0.48	0.48	N/A	0.59	0.01
Rio Grande[a]	~0	~0	N/A	N/A	0.78
Rio Salado	0.28	0.28	N/A	0.08	0.06
Sandia Mtn front	0.74	0.41	0.16	0.21	0.16
Southeast Mtn front	1.06	1.16	0.19	0.16	0.17
Total	5.45	4.86	N/A	2.63	2.14

[a] This number represents flow from the inner valley to the regional aquifer system. The first two models calculated significant loss of water from the Rio Grande, but from their simulated head contours it seems likely that most if not all of this was immediately lost to evapotranspiration (ET) in the inner valley: very little if any of it reached the regional flow system outside the inner valley. McAda and Barroll (2002) also calculated a significant loss from the Rio Grande, but they did not quantify outflow from the valley to the regional flow system

previous models (Kernodle et al. 1995; Tiedeman et al. 1998) and to prior field measurements of the basin fill material (Thorn et al. 1993). Zones that have estimated values of hydraulic conductivity significantly less than 1×10^{-6} m/s are the silt layer (unit 18) in the central basin, the West Sandia Fault Zone, and many of the deeper zones (e.g., units 5, 6, 7, and 16). Zones that have estimated values significantly greater than 3×10^{-5} m/s are the volcanic rocks, the alluvial gravels (unit 1), and the river alluvium in the central and southern basin (units 3 and 4). The alluvial gravels (unit 1), most of the deep sediments (units 3–8), the central and southern river alluvium (units 3 and 4), and the riverbed conductances (not shown) had calibrated values with low sensitivities and high degrees of uncertainty. The anisotropy (K_v/K_h) was estimated individually for 12 zones within the basin, and the calibrated values ranged between 1×10^{-4} and 1×10^{-2} (Fig. 14). These values are consistent with what might be expected for a layered system where the individual layers are isotropic and have values that vary by 2 to 4 orders of magnitude. Zones that have silt, gravel, or volcanic layers incorporated within them would be expected to have anisotropy values that vary by more than this, but those units were accounted for explicitly as separate zones.

Recharge was not specified directly in the model for the Rio Puerco and the Jemez River, but model recharge estimates were calculated using the riverbed conductance parameters after they were adjusted during the regression. The final estimated recharge values were 0.14 m^3/s for the Rio Puerco, but only 0.01 m^3/s for the Jemez River (Table 2). The recharge for the Rio Puerco was similar to values used in earlier models, but the Jemez River recharge value was much lower. Recharge from the eastern mountain front (the Sandia and Southeastern Mtn fronts) is estimated at about 0.33 m^3/s, with another 0.04 m^3/s leaking through Abo Arroyo. These numbers are somewhat lower than previous estimates that were based on rainfall-runoff equations (Kernodle et al. 1995), but are close to recent estimates of recharge of 0.35 and 0.05 m^3/s along the eastern mountain front and Abo Arroyo, respectively, made using the chloride mass-balance method (Anderholm 2001), although the latter included some mountain front runoff adjacent to Abo Arroyo. Total recharge to the basin is estimated to be 2.15 m^3/s, with 0.78 m^3/s of the total leaking from the Rio Grande. Earlier models (Kernodle et al. 1995; Tiedeman et al. 1998) indicated there was recharge from the Rio Grande under predevelopment conditions, but virtually all of that water was lost to ET in the inner valley. The basin-margin recharge estimated from this model, 1.37 m^3/s, is one-fourth of the 5.43 m^3/s estimate used in the 1995 Kernodle model.

The overall low recharge can explain the presence of a groundwater trough and a zone of Rio Grande water in the central basin (Fig. 9). In the present modeling study, low recharge along basin boundaries induces the Rio Grande to lose water to the extent that it flows outward beyond the inner valley and into the regional flow system. The earlier models (Kernodle et al. 1995; Tiedeman et al. 1998; McAda and Barroll 2002) handled the Rio Grande boundary somewhat differently. The outflow from the Rio Grande to the regional system in those models must be inferred from water level contours. They simulated evapotranspiration directly in the inner valley, which directly accounted for water loss from the Rio Grande that quickly transpires within, but never leaves the valley. In this study no ET was simulated directly, but rather, the entire valley was treated as a river boundary, such that ET was lumped into the boundary condition at the valley-basin interface. Simulated water budgets from the earlier models quantify large losses from the Rio Grande, but do not distinguish between loss to the valley and to the regional flow system. Examination of water-level contours from those models within the basin, however, show all

DOI 10.1007/s10040-004-0326-4

water flow focused toward or parallel to the valley (e.g., Fig. 12b), suggesting that little to no regional water loss is occurring from the Rio Grande, and all simulated water loss is local. The value of 0.78 m^3/s (Table 2) represents a simulated predevelopment loss of water from the Rio Grande to the regional flow system. A value of regional loss to the basin in McAda and Barroll (2002) could not be determined or quantified because their water-level contours did not indicate clearly enough whether any substantial flow was directed out of the inner valley.

McAda and Barroll (2002) incorporated some of the new, lower recharge estimates (Table 2) into their revised model of the basin. The basin-margin recharge estimated from their model, 2.63 m^3/s, is roughly one half of the 5.45 m^3/s estimate used in the 1995 Kernodle model. The values McAda and Barroll (2002) used for recharge are in general agreement with this study for the western and southwestern boundaries, the eastern mountain front, and the eastern and northeastern rivers and arroyos. However, they used rates of underflow from the Española Basin and the Jemez Mountains and River that were consistent with the estimates used in the earlier models. Uncertainty analyses on the recharge values in this study (Sanford et al. 2004) indicated a high degree of uncertainty for inflow from the Española Basin, but 95% confidence intervals in this study for recharge from the Jemez Mountains and Jemez River give ranges of 0.04–0.16 and 0.00–0.03 m^3/s, respectively (Sanford et al. 2004). The estimate of recharge from the Jemez River was greatly reduced by the presence of old groundwater just south and downgradient of the river. It is shown in the next section that water levels in the northern basin were more difficult to fit, and residuals reveal a definite pattern with respect to the Jemez River. Therefore, more work is still needed in the Jemez region to improve confidence in groundwater-flow estimates for that region.

Analysis of Fit

The observed hydraulic heads plotted against the simulated heads show a strong trend along the 1:1 line (Fig. 15). The observed ^{14}C values were also plotted against the simulated values, and show a substantially greater amount of scatter about the 1:1 line (Fig. 16) than the head observations. This poorer fit to the ^{14}C data was anticipated. Heads represent a smoothly varying potential field that can be fit without much difficulty to the solution of the flow equation. Groundwater ages are a function of velocities that are in turn a function of the first derivatives of the groundwater-potential field, and thus are more difficult to fit. This difficulty exists because although a travel time at a point in space is an integration of the upstream velocity field, errors in calculated velocities can accumulate down a flow path. In addition, multiple source areas in the MRGB (Fig. 3) create age patterns within the basin that are discontinuous (Fig. 13), increasing further the complexity and difficulty in fitting the age-related simulations to observations. The multiple sources of water in the MRGB create numerous flow divides. These divides often have very sharp gradients in age across them and are difficult to match exactly, increasing the scatter in simulated versus observed ages.

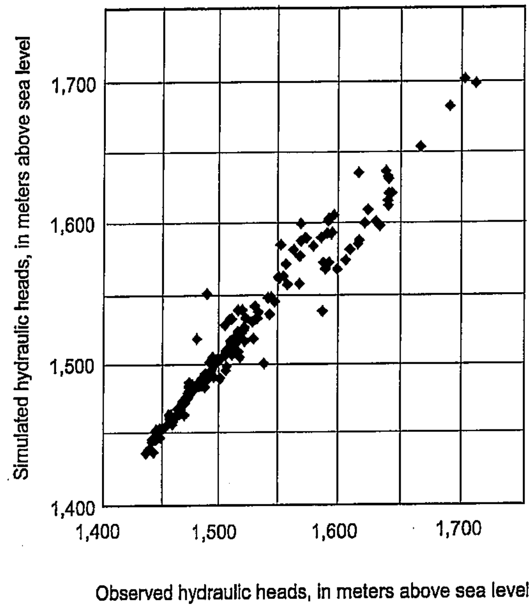


Fig. 15 Observed versus simulated hydraulic head data

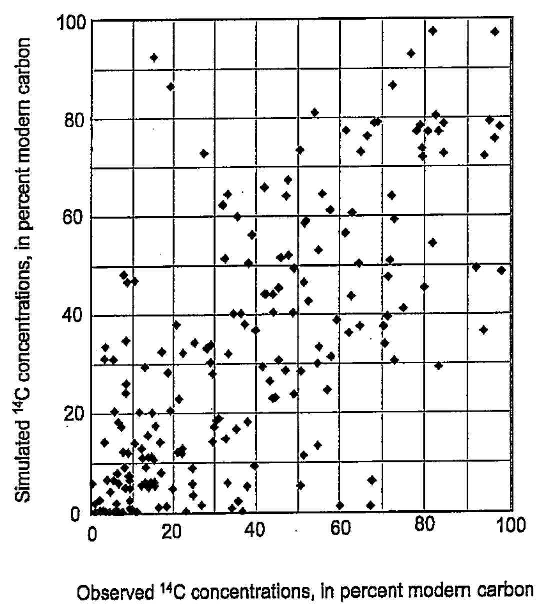


Fig. 16 Observed versus simulated ^{14}C activity data

The head residuals were plotted on a map of the MRGB to ascertain the regions of the basin where the model fit is good or poor (Fig. 17). It can be observed that better fits to the data exist in the center of the basin and along the Rio Grande. This is expected somewhat in that the Rio Grande acts as a line of constant head from which the head solution is not allowed to deviate substantially. The poorest matches to water levels occurred in the northern section of the basin. Heads were consistently simulated too low near the Jemez River and extreme

DOI 10.1007/s10040-004-0326-4

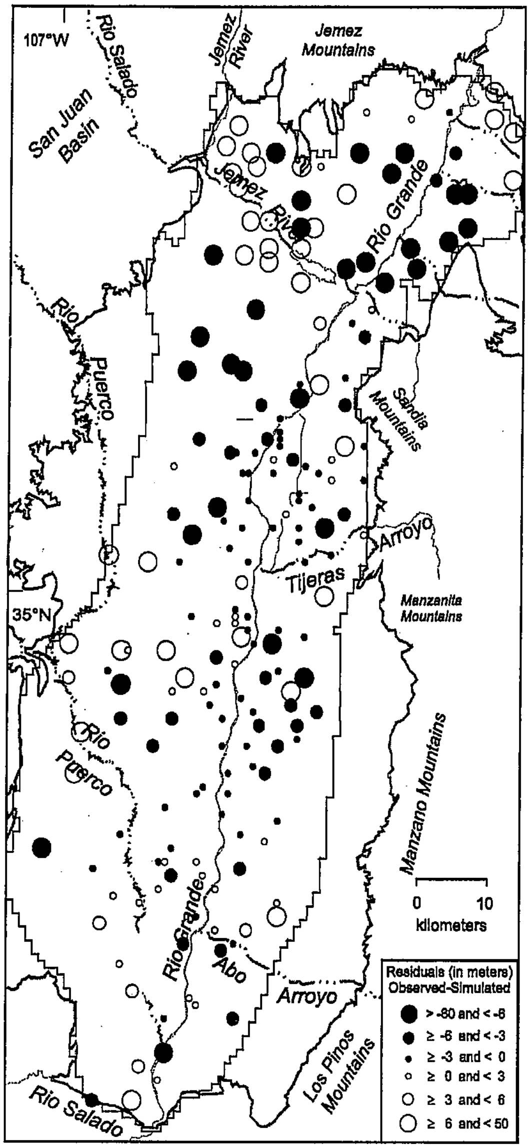


Fig. 17 Spatial distribution of the residuals between observed and simulated hydraulic heads

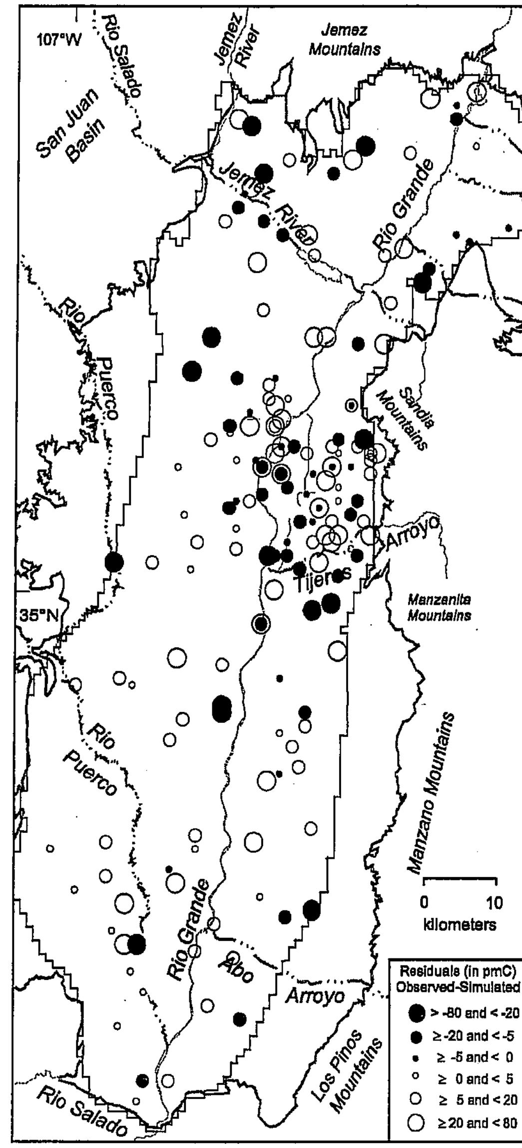


Fig. 18 Spatial distribution of the residuals between observed and simulated ^{14}C activities

northeast section of the basin, and too high in the Rio Rancho and northeast sections of the basin. These spatial patterns in the residuals suggest the calibrated recharge values in that region (Table 2) may also be somewhat in error. The groundwater trough appears to extend farther north (Fig. 2) than the current model simulates. To better simulate the northern section of the basin, a more local model may be required along with additional observation data.

The ^{14}C activity residuals also were plotted on a map of the Middle Rio Grande Basin (Fig. 18). The spatial distribution of residuals for the ^{14}C activities is more randomly distributed than for the water levels, even though substantially more scatter exists in the ^{14}C activities data (Fig. 16) than for water levels (Fig. 15).

Paleohydrologic Simulation

A transient ground-water-flow simulation was performed to investigate the effect of time-varying recharge rates over the past tens of thousands of years on simulated ^{14}C activities. A 30,000-year simulation was run using twelve 2,500-year time steps preceded by a near steady-state condition. During each of the time steps, all recharge and underflow boundary cells were multiplied by a single recharge multiplier. The multipliers were all given an initial value of 1.0 to reproduce the conditions in the steady-state simulation. The multipliers were then adjusted until a best fit was obtained between all the observed data and simulated observations. The nonlinear regression routine in UCODE was used initially to reduce the SSR, but eventually the individual recharge parameters were adjusted manually to obtain the best-fit recharge multiplier values.

DOI 10.1007/s10040-004-0326-4

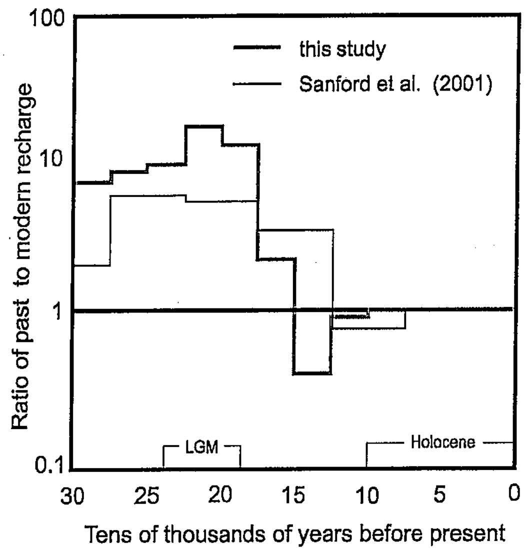


Fig. 19 Paleo-recharge estimates from groundwater-flow models based on ^{14}C activity data

Results from the transient simulation suggest that recharge rates were greater before 15,000 years ago than they are at present (Fig. 19). The optimal values for the recharge multipliers are greater than 10 for the period between 20,000 and 25,000 years ago. This corresponds to the last glacial maximum (LGM). The transient model also suggests lower recharge at or before 10,000 years ago. A previous transient simulation using unadjusted ^{14}C activities and 5,000-year time steps suggested an increase in recharge during the LGM of five to six times (Sanford et al. 2001). Evidence for a wetter climate during this period is also present in the Estancia Basin, just east of the Sandia Mountains, in the form of playa lake deposits (Bachhuber 1992; Allen and Anderson 2000). Although the exact values of these changes in recharge are rather uncertain, all of the results suggest substantially greater recharge during the last glacial maximum and slightly less recharge before the beginning of the Holocene 10,000 years ago.

Summary and Discussion

The question of the availability of groundwater as a long-term resource in the Middle Rio Grande Basin of central New Mexico has been addressed recently by the development of groundwater flow models by the US Geological Survey, in cooperation with Federal, State, and local agencies. Parameters in a model by Kernodle et al. (1995) were later calibrated using inverse methods and additional hydrologic observations (Tiedeman et al. 1998). In this study, ^{14}C activities and the location of hydrochemical zones were used as additional observations to estimate model parameters for the Middle Rio Grande Basin. The inverse modeling code UCODE was used to help estimate hydraulic conductivities of hydrogeologic units and current and past recharge to the basin along the basin margins and tributary rivers. The water levels in the basin were simulated using MODFLOW, and travel times to wells and source-area delineation were simulated using MODPATH.

A three-dimensional geologic model of the basin (Cole 2001) was discretized into a three-dimensional MODFLOW grid of the basin. Major hydrogeologic units in the geologic model included volcanic rocks, and several units that represent the Santa Fe Group sediments, including ancestral gravels from the Rio Grande and finer grained units that represent the middle and lower Santa Fe Group. The MODFLOW grid represented the hydrogeologic units with nine layers of variable thickness totaling more than 4,000 m in places, and a uniform horizontal grid resolution of one square kilometer. Observations that were used to calibrate a steady-state model and then a transient paleohydrologic model included 200 water levels, 200 ^{14}C activities, and nine hydrochemical-target regions. Observed water levels were compared with simulated water levels calculated with MODFLOW, ^{14}C activities were compared with simulated activities based on travel times to individual wells calculated with MODPATH, and the percentage of river water in the hydrochemical-target regions was compared with the simulated percentage of river water in these areas.

Hydraulic conductivities estimated for the model were not dissimilar to values that had been estimated in the previous models of Kernodle et al. (1995) and Tiedeman et al. (1998). The estimates for the hydraulic conductivity of the Rio Grande alluvium ranged from 1 m/day in the north to 30 m/day in the south, with estimated values substantially higher for the gravels beneath Albuquerque. In addition, the hydraulic conductivity of the volcanic rock unit was estimated to be 8m/day, and the hydraulic conductivity of a silty layer identified in the geologic model was estimated to be 0.13 m/day. Estimates of vertical anisotropy for the various units ranged from 0.0001 to 0.01.

Basin-margin and tributary recharges estimated for the model were lower than values used in previous models. The model also indicated a substantial amount of flux from the Rio Grande into the Santa Fe Group aquifer system. The earlier models of Kernodle et al. (1995) and of Tiedeman et al. (1998) indicated recharge from the Rio Grande, but virtually none of that recharge reached the regional aquifer system outside the inner valley. Although the latter model was calibrated, the great majority of observations were water-level measurements, with few flux-based observations to constrain flow or recharge rates. The current model has 200 groundwater ages to constrain fluxes, which should increase the accuracy of estimated recharge values. The rainfall-runoff methods used to estimate recharge in the earlier models did not account for runoff that enters the Rio Grande, or evapotranspiration of runoff once it enters the subsurface. In addition, recharge estimates for the eastern mountain fronts have been made independently using the chloride mass-balance method (Anderholm 2001). Estimates by the chloride method were very close to the estimates from this modeling study. McAda and Barroll (2002) have in-

 DOI 10.1007/s10040-004-0326-4

corporated some of the results from this study into their more recent groundwater-flow model.

In the current study, a groundwater trough was simulated west of the Rio Grande with an associated partial zone of groundwater east of the trough axis that is derived from the Rio Grande. The trough and the presence of Rio-Grande-derived groundwater are observed in the predevelopment water-table map and hydrochemical zones. The earlier models with greater recharge could not reproduce these features without invoking unrealistically high values of hydraulic conductivity. The steady-state simulation overestimates the amount of Rio Grande water in the trough based on the hydrochemical zone delineation. One likely explanation for this is the different response times for the water levels that define the trough and the dissolved chemical constituents within the trough. The low head values of the trough may reflect current low recharge conditions in the basin. If so, the trough was less likely to exist during the higher recharge conditions of the past (Fig. 9), and yet hydrochemical conditions require tens of thousands of years to reach steady state, as indicated by the radiocarbon ages (Plummer et al. 2004b). Thus, the hydrochemical-zone delineations probably represent groundwater flow over tens of thousands of years, and could easily be out of equilibrium with modern water levels and flow conditions.

A transient paleohydrologic model was run to determine if the ^{14}C data as a whole contained information indicating that recharge rates had changed for any time during the past 30,000 years. The transient simulation was for a period of 30,000 years, with an independent value of recharge estimated every 2,500 years. The model suggests that recharge to the basin during the last glacial maximum was considerably higher than at present, and somewhat lower just before the beginning of the Holocene period. The results are consistent with an earlier transient model calibrated with the unadjusted ^{14}C ages and 5,000-year recharge intervals (Sanford et al. 2001).

References

Allen BD, Anderson RY (2000) A continuous, high-resolution record of late Pleistocene climate variability from the Estancia basin, New Mexico. Geol Soc Am Bull 112:1444–1458

Anderholm SK (1988) Groundwater geochemistry of the Albuquerque–Belen Basin, central New Mexico. US Geol Surv Water-Resour Invest Rep 86-4174

Anderholm SK (2001) Mountain-front recharge along the eastern side of the Middle Rio Grande Basin, central New Mexico. US Geol Surv Water-Resour Invest Rep 00-4010

Athy LF (1930) Density, porosity, and compaction of sedimentary rocks: Bull Am Assoc Petrol Geol 14:1–24

Bachhuber FW (1992) A pre-late Wisconsin paleolimnologic record from the Estancia Valley, central New Mexico. In: Clark PU, Lea PD (eds) The last interglacial–glacial transition in North America. Geol Soc Am Spec Pap 270:289–307

Bartolino JR, Cole JC (2002) Groundwater resources of the Middle Rio Grande Basin. US Geol Surv Circular 1222

Bartolino JR, Niswonger RG (1999) Numerical simulation of vertical ground-water flux of the Rio Grande from ground-water temperature profiles, central New Mexico. US Geol Surv Water Resour Investig Rep 99-4212

Bexfield LM, Anderholm SK (2000) Predevelopment water-level map of the Santa Fe Group aquifer system in the Middle Rio Grande Basin between Cochiti and San Acacia, New Mexico. US Geol Surv Water-Resour Invest Rep 00-4249

Bexfield LM, Anderholm SK (2002) Spatial patterns and temporal variability in water quality from City of Albuquerque supply wells and piezometer nests, with implications for the groundwater flow system. US Geol Surv Water-Resour Investigat Rep 01-4244

Bjorklund LJ, Maxwell BW (1961) Availability of ground water in the Albuquerque area, Bernalillo and Sandoval Counties, New Mexico. New Mexico State Eng Tech Rep 21

Cole JC (2001) 3-D geologic modeling of regional hydrostratigraphic units in the Albuquerque segment of the Rio Grande rift. In: Cole JC (ed) US Geological Survey Middle Rio Grande Basin Study: Proceedings of the Fourth Annual Workshop, Albuquerque, New Mexico, 15–16 February 2000. US Geol Surv Open-File Rep 00-488, pp 26–28

Constantz J (1998) Measurements of tributary, inter-arroyo, and mountain-front recharge on the Santa Fe River, Bear Canyon, and Abo Arroyo, New Mexico. In: Slate JL (ed) US Geological Survey Middle Rio Grande Basin Study: Proceedings of the Second Annual Workshop, Albuquerque, New Mexico, 10–11 February 1998. US Geol Surv Open-File Rep 98-337, pp 55–56

Grauch VJS, Sawyer DA, Keller GR, Gillespie CL (2001) Contributions of gravity and aeromagnetic studies to improving the understanding of the subsurface hydrogeology, Middle Rio Grande Basin, New Mexico. In: Cole JC (ed) US Geological Survey Middle Rio Grande Basin Study: Proceedings of the Fourth Annual Workshop, Albuquerque, New Mexico, 15–16 February 2000. US Geol Surv Open-File Rep 00-488, pp 3–4

Haneberg WC (1995a) Steady-state groundwater flow across idealized faults. Water Resour Res 31:1815–1820

Haneberg WC (1995b) Depth-porosity relationships and virgin specific storage estimates for the upper Santa Fe Group aquifer system, central Albuquerque Basin, New Mexico. New Mex Geol 17:62–71

Hawley JW, Haase CS (1992) Hydrogeologic framework of the northern Albuquerque Basin: Socorro. New Mex Bureau of Mines and Mineral Resources Open-File Rep 387

Hill MC (1998) Methods and guidelines for effective model calibration. US Geol Surv Water-Resources Investig Rep 98-4005

Johnson TM, DePaolo DJ (1996) Reaction-transport models for radiocarbon in groundwater: the effects of longitudinal dispersion and the use of Sr isotope ratios to correct for water-rock interaction. Water Resour Res 32:2203–2212

Kalin RM (2000) Radiocarbon dating of groundwater systems. In: Cook PG, Herczeg AL (eds) Environmental tracers in subsurface hydrology. Kluwer Academic Publishers, Amsterdam, pp 111–144

Kernodle JM, Scott WB (1986) Three-dimensional model simulation of steady-state groundwater flow in the Albuquerque–Belen Basin, New Mexico. US Geol Survey Water-Resour Investig Rep 84-4353

Kernodle JM, Miller RS, Scott WB (1987) Three-dimensional model simulation of transient groundwater flow in the Albuquerque–Belen Basin, New Mexico. US Geol Surv Water-Resour Invest Rep 86-4194

Kernodle JM, McAda DP, Thorn CR (1995) Simulation of groundwater flow in the Albuquerque Basin, Central New Mexico 1901–1994, with projections to 2020. US Geol Surv Water-Resour Invest Rep 94-4251

Logan LM (1990) Geochemistry of the Albuquerque municipal area, Albuquerque, New Mexico. MSc Thesis, New Mexico Institute of Mining and Technology

McAda DP (1996) Plan of study to quantify the hydrologic relations between the Rio Grande and the Santa Fe aquifer system near Albuqueruque, central New Mexico. US Geol Surv Water Resour Investig Rep 96-4006

McAda DP, Barroll P (2002) Simulation of ground-water flow in the Middle Rio Grande Basin between Cochiti and San Acacia,

 DOI 10.1007/s10040-004-0326-4

New Mexico. US Geol Surv Water Resour Investig Rep 02-4200

McDonald MG, Harbaugh AW (1988) A modular three-dimensional finite-difference groundwater flow model. US Geol Surv Tech Water-Resour Invest, vol 6, ch A1

Medina A, Carrera J (1996) Coupled estimation of flow and solute transport parameters. Water Resour Res 32:3063–3076

Plummer LN, Bexfield LM, Anderholm SK, Sanford WE, Busenberg E (2004a) Geochemical characterization of groundwater flow in the Santa Fe Group aquifer system, Middle Rio Grande Basin, New Mexico. US Geol Surv Water Resources Investig Rep 03-4131

Plummer LN, Bexfield LM, Anderholm SK, Sanford WE, Busenberg E (2004b) Hydrochemical tracers in the Middle Rio Grande Basin, USA: 1. conceptualization of groundwater flow. Hydrogeol J DOI 10.1007/s10040-004-324-6 (this issue)

Poeter EP, Hill MC (1998) Documentation of UCODE, a computer code for universal inverse modeling. US Geol Surv Water-Resour Investig Rep 98-4080

Pollock DW (1994) User's guide for MODPATH/MODPATH-PLOT, version 3: a particle tracking post-processing package for MODFLOW, the US Geological Survey finite-difference groundwater flow model. US Geol Surv Open-File Rep 94-464

Rawling GC, Goodwin LB, Wilson JL (2001) Internal architecture, permeability structure, and hydrologic significance of contrasting fault-zone types. Geology 29:43–46

Sanford WE (1997) Correcting for diffusion in Carbon-14 dating of ground water. Ground Water 35:357–361

Sanford WE, Plummer LN, McAda DP, Bexfield LM, Anderholm SK (2001) Estimation of hydrologic parameters for the groundwater model of the Middle Rio Grande Basin using carbon-14 and water-level data. In: Cole JC (ed) US Geological Survey Middle Rio Grande Basin Study: Proceedings of the Fourth Annual Workshop, Albuquerque, New Mexico, 15–16 February 2000. US Geol Surv Open-File Rep 00-488, pp 4–6

Sanford WE, Plummer LN, McAda DP, Bexfield LM, Anderholm SK (2004) Use of environmental tracers to estimate parameters for a predevelopment ground-water-flow model of the Middle Rio Grande Basin, New Mexico. US Geol Surv Water Resources Investig Rep 03-4286

Stone BD, Allen BD (1998) The 98th Street core: key to analysis of Santa Fe Group stratigraphy and hydrogeology in the central Middle Rio Grande Basin. In: Slate JL (ed) US Geological Survey Middle Rio Grande Basin Study: Proceedings of the Second Annual Workshop, Albuquerque, New Mexico, 10–11 February 1998. US Geol Surv Open-File Rep 98-337, pp 41–46

Stone BD, Cole JC, Sawyer DA (2001) Regional stratigraphic framework of the three-dimensional geologic model of the Rio Grande rift. In: Cole JC (ed) US Geological Survey Middle Rio Grande Basin Study: Proceedings of the Fourth Annual Workshop, Albuquerque, New Mexico, 15–16 February 2000. US Geol Surv Open-File Rep 00-488, pp 11–13

Stonestrom DA, Akstin KC (1998) Environmental tracers of recharge at Abo Arroyo, Bear Canyon, and the Santa Fe River, Middle Rio Grande Basin, New Mexico. In Slate JL (ed) US Geological Survey Middle Rio Grande Basin Study: Proceedings of the Second Annual Workshop, Albuquerque, New Mexico, 10–11 February 1998. US Geol Survey Open-File Rep 98-337, pp 57–59

Stuiver M., Reimer PJ, Bard E, Beck JW, Burr G, Hughen KA, Kromer B, McCormac FG, van der Plicht J, Spurk M (1998) INTCAL98 Radiocarbon age calibration, 24,000–0 cal B.P. Radiocarbon 40:1041

Thorn CR, McAda DP, Kernodle JM (1993) Geohydrologic framework and hydrologic conditions in the Albuquerque Basin, central New Mexico. US Geol Surv Water-Resour Investig Rep 93-4149

Tiedeman CR, Kernodle JM, McAda DP (1998) Application of nonlinear-regression methods to a groundwater flow model of the Albuquerque Basin, New Mexico. US Geol Surv Water-Resour Investig Rep 98-4172

Titus FB (1963) Geology and groundwater conditions in eastern Valencia County, New Mexico. New Mex Bureau Mines Mineral Resour Groundwater Rep 7

DOI 10.1007/s10040-004-0326-4