Hydrogeologic Windows: Detection of Blind and Traditional Geothermal Play Fairways in Southwestern New Mexico Using Conservative Element Concentrations and Advective-Diffusive Solute Transport

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ABSTRACT

We combine trace element geochemistry and hydrologic tracer transport analysis to identify geothermal upflow zones within southwestern New Mexico. We analyzed about 1400-4000 wells with lithium and boron chemical analyses. Most of the geothermal waters had elevated lithium and boron concen-

trations (> 0.5 mg/l) that weakly correlate with reservoir temperatures. We used available water-table measurements to construct water-table maps and calculate groundwater flow directions. We used an "upwinding" approach to track mathematical particles through the flow field within the shallow aguifer system. Areas where particles with high tracer concentrations pass wells with low tracer concentrations may indicate the presence of a geothermal upflow zone. The approach was applied to the southern Albuquerque Basin near San Acacia and the southern Engle Basin near Truth or Consequences, NM. Although our approach revealed a potential geothermal upflow zone at Indian Wells spring near San Acacia NM, additional work is needed to refine the methodology. A multiple realization-based methodology for locating tracer sources was also developed. In this method, an advection-diffusion equation was solved for eighty realizations of different source locations in the Socorro-La Jencia Basin area. By comparing simulated tracer concentrations to measured values, a source-likelihood map was drawn, and the tentative source locations were identified. The region of high heat flow within the Socorro-La Jencia Basin at the base of Socorro Peak was found to have a local minimum of the root mean squared error of simulated minus observed normalized lithium concentrations. This suggests that our approach can identify geothermal up flow zones.

Introduction

We are assessing a risk analysis framework to locate and define potential blind geothermal resources in southwestern New Mexico (Figure 1). The presence or absence of a hydrogeologic window through Paleozoic, Mesozoic, and Paleogene confining units



Figure 1. Location map of study area within southwestern New Mexico showing basins, mountains, towns, major rivers and highways.



Figure 2. Conceptual model illustrating heat and solute transport through a hydrogeologic window. Advective-dispersive transport of a geochemical tracer (blue dashed lines) and heat (solid red contours) migrate through fractured crystalline basement (purple pattern) across a gap in a regional confining unit (gray unit). A shallow water-table aquifer is depicted by the yellow pattern. The contours along the top of this block model depict water-table elevations. The confining unit (gray pattern) blocks discharge of geothermal fluids in other locations. Trace element concentrations (in mg/l), such as boron or lithium, measured in shallow wells are depicted using the numbered black circles. Black arrows depict groundwater flow directions.

forms the basis of the play fairway framework (Figure 2). Hydrogeologic windows are zones where regional or local aquatards are breached by faulting, erosion, or fractured igneous intrusions, allowing relatively rapid vertical discharge flow from advective geothermal systems toward the surface. In many cases, the outflow plume associated with active hydrogeologic windows is hidden below shallow fine-grained facies in the basin fill or by deep static water tables, resulting in a blind system (Witcher, 1988; Barroll and Reiter, 1990; and Mailloux et al., 1999) (Figure 2). The conceptual model depicted in Figure 2 assumes that the crystalline basement is permeable and permits deep fluid circulation (Pepin et al., 2015). Geochemical tracers, such as lithium and boron, can be transported into shallow aquifers (yellow unit) and migrate down hydrologic gradient. These tracers are found at low concentrations in wells (black bullets) up gradient of the hydrogeologic window. We propose that the spatial distribution of geochemical tracers can be used in combination with shallow water-table gradient maps to identify geothermal upflow zones within blind geothermal systems.



Figure 3. (A) Water-table map and well locations for water samples having lithium (B) and boron (C) analyses across southern New Mexico. The water-table map is based on measurements of pre-development conditions. Sources: Laura Bexfield, USGS District Office, Albuquerque, NM; US DOE National Geothermal Data Base, Cron et al. 2011, Williams et al. 2013; Owens, 2013; US EPA.

Here, we focus on play fairway analysis of aqueous geochemistry data sets that have been compiled for southwestern New Mexico (Figure 3B, 3C). We use conservative element tracers that are commonly associated with geothermal systems (Arehart and Donelick, 2006; lithium, boron, bromide, chloride) to locate geothermal outflow plumes that might be leaking from hydrogeologic windows into shallow aquifers. We follow an approach first proposed by Neupauer and Wilson (1999) to identify the location of up-gradient contaminant sources using contaminant concentrations in down-gradient wells (Figure 2). This new exploration concept considers the dynamics of fluid flow and advective-dispersive geochemical tracer transport. The up-gradient path of conservative ions from each borehole in the southern Albuquerque Basin near San Acacia and the southern Engle Basin near Truth or Consequences was calculated using water-table contours (Figure 3A) and a simple particle-tracking algorithm. The particles are "upwinded" across the basins. For the Socorro Basin, we also consider forward models of advective-dispersive solute transport in order to identify the optimal source locations of geothermal up flow zones that also match observed well concentrations. In both approaches, the shallow groundwater flow vectors are calculated based on Darcy's law using available water-table data. The calculated particle trajectories and solute concentrations are then compared to Quaternary and older fault ArcGIS layers to try to identify geologic structures that might be the source of waters with elevated conservative ion concentrations.

Nature of Conservative Ions

Boron is an important component of tourmaline and can be present in biotite, amphibole, and other minerals in metamorphic rocks (Grew, 1996). Upon weathering, boron is sometimes incorporated into other compounds, but more commonly the uncharged ion dominates in water up to a pH of 9.24 (Hem, 1985). The uncharged or anionic boron does not absorb onto mineral surfaces and thus remains in solution. Boron measurements are essential to agricultural assessments because boron is toxic to certain plants (Hem, 1985). As a consequence, boron is commonly measured as part of routine water quality analysis. Lithium is found in spodumene and lepidotite in pegmatites and is found in rock-forming minerals like microcline and albite (Deer et al., 1992). Mica-rich granites, ash flow tuffs, and rhyolitic glass can also be sources of lithium (Witcher, 1988). Like boron, lithium does not absorb onto minerals once released into solution during weathering and it is toxic to certain plants. Both lithium and boron can be concentrated in playa deposits in closed basins. Bromine, a halogen, is an important component in seawater and evaporite minerals. Bromine has a large ionic radius, so it is uncommon in rock forming minerals. Bromide absorbs onto organic matter (Fuge, 1988).

Conservative Ions as an Exploration Tool

Conservative trace element analysis is commonly used in geothermal exploration (Arehart and Donelick, 2006) because rock-water geochemical reactions at temperatures above 100 °C liberate these elements. Lithium, arsenic, and boron are among the trace elements that are known to correlate with chloride-dominated geothermal waters within the Basin and Range of Nevada and the Rio Grande rift of New Mexico (Arehart, and Donelick, 2006; Owens, 2013). The approach assumes that the conservative ion tracers are retained in relatively high concentrations as they flow upwards from a geothermal reservoir into comparatively cool, water-table aquifers. For example, a plume of hydrothermal fluids in the Socorro Basin at the base of Socorro peak cools as it moves laterally toward the Rio Grande to the east and south, but lithium and boron are retained at relatively high concentrations ($\sim 0.1 \text{ mg/l}$) in non-thermal water supply

Figure 4. Contour map of lithium concentrations in wells across the Socorro and La Jencia Basins. A shallow plume of lithium-rich waters (> 0.1 mg/l)forms an outflow plume from the Socorro geothermal system near Woods Tunnel (0.97 mg/l) and flows toward the Rio Grande. Geochemical data from Owens (2013). The Socorro-La Jencia basin cross section location presented in Figure 7 is also shown.



wells (Owens, 2013; Figure 4). The highest lithium concentration in the Socorro system (0.97 mg/l; Owens 2013) is found within the Woods Tunnel geothermal well, drilled into the apex of highest heat flow anomaly (> 400 mW/m²; Barroll and Reiter, 1990).

Methods

Data Compilation

Laura Bexfield at the U.S. Geological Survey office in Albuquerque provided statewide water-quality files containing conservative ion (boron, lithium, and bromide) and chloride data and water-table elevations. Boron is more commonly analyzed (~ 4000 records; Figure 5) than lithium and bromide (~1500 records; Figure 5). In addition, we extracted data from University of New Mexico (Cron,

2011; Williams et al. 2013) and New Mexico Tech theses (Owens, 2013), the National Geothermal Database System (NGDS), the Environmental Protection Agency website, the New Mexico Environment Department, and the New Mexico Bureau of Geology and Mineral Resources Aquifer Mapping database. Boron, lithium, and bromide concentrations (mg/l), calculated Cl/Br ratios, and water-table elevations were plotted in ArcGIS. Isolated high values on these maps may be the result of errors in the database. Quality control for the large water quality data set involved removal of data with obvious typos and in some cases an evaluation of the original source of the data, looking for



Figure 5. Histogram showing concentrations of lithium and boron from the compiled NM geochemical database. The median concentrations for the entire compiled database and for geothermal waters (NGDS) are listed.

systematic trends in source data sets that might indicate differences in laboratory analysis procedures.

Accurate water-table maps were required for this analysis (Figure 3A). Repeat water-table elevations for many of the wells in the database were evaluated in several ways. First, the earliest measurements for all wells were plotted and contoured; this assumes pre-development water-level conditions (Figure 3A). Second, measurements collected during the winter, when irrigation rates are low, were used to construct a water-table surface. Finally, annual high, annual low, and annual average water-level values were incorporated in the water-table surfaces. These different approaches helped to quantify the potential uncertainty of groundwater flow directions.

Geochemical Tracer Analysis to Identify Blind Hydrogeologic Windows

Particle Tracking

Typically, geochemical geothermometers are used to estimate reservoir temperatures. Fluid flow and advectivedispersive solute transport are not taken into consideration. Our approach combines solute mass transport models of varying levels of complexity with tracer data to help identify hydrogeologic windows and geothermal up flow zones.

The average linear groundwater velocities are computed using the local water-table gradient:

$$v_x = -\frac{K}{\phi} \frac{\Delta h}{\Delta x} \qquad v_y = -\frac{K}{\phi} \frac{\Delta h}{\Delta y} \tag{1}$$

where K is hydraulic conductivity of the water-table aquifer, ϕ is porosity, h is hydraulic head, and v_x and v_y are the components of the groundwater velocities in the x- and y-directions.

The average linear velocities are used to track geochemical tracers up gradient through the flow field (Pollock, 1994). We placed a mathematical particle at each well location that had a boron or lithium analysis and tracked the particle up gradient from the wells through the shallow aquifer as follows:

$$x_{p}^{k+1} = x_{p}^{k} - \Delta t v_{x} \qquad \qquad y_{p}^{k+1} = y_{p}^{k} - \Delta t v_{y}$$
(2)

where x_p^{k+1}, x_p^k are the particle locations in the x-direction at the old (k) and new (k+1) time levels, and y_p^{k+1}, y_p^k are the particle locations in the y-direction at the old (k) and new (k+1) time levels. We hypothesize that a hydrogeologic window within a blind geothermal system should be some distance up hydrologic gradient of a high concentration well and down gradient of a low concentration well along the groundwater flow path.

We introduce mathematical particles into a triangulated grid at the well locations. The velocity was calculated at each triangle. Each particle is assigned its respective lithium or boron concentrations. We then use the flow vectors based on Darcy's law to upwind particles across the basin. In areas with sufficient well density, we can identify prospective geothermal up flow zones. Stratigraphic data can be used to estimate the hydraulic conductivity of each unit. We assumed that there was no lateral anisotropy in hydraulic conductivity.

Advective-Dispersive Transport

Particle-tracking analysis is limited in that it does not account for hydrodynamic dispersion, diffusion, and spreading of a trace element plume from an upflow zone. We solved the following two-dimensional advection-dispersion equation to simulate lithium tracer transport away from an upflow zone:

$$\frac{\partial}{\partial x} \left[D_{xx} \frac{\partial c}{\partial x} + D_{xy} \frac{\partial c}{\partial y} \right] + \frac{\partial}{\partial y} \left[D_{yx} \frac{\partial c}{\partial x} + D_{yy} \frac{\partial c}{\partial y} \right] = v_x \frac{\partial c}{\partial x} + v_y \frac{\partial c}{\partial y} + \frac{\partial c}{\partial t}$$
(3)

where x and y are the spatial coordinates, t is time, D_{xx} , D_{yy} , D_{yx} , and D_{yy} are the components of the hydrodynamic dispersion-diffusion tensor, v_x and v_y are the components of average linear groundwater velocities in the x- and y-directions, and c is trace element concentration. We systematically evaluated source locations within the basins, ranking locations based on how well relative magnitudes of simulated concentrations matched relative magnitudes of well concentrations in a model calibration exercise. The Rio Grande represented the sink for the solute tracers.

We solved for the average linear velocities (v_x and v_y) using PFLOTRAN (Lichtner et al., 2015). PFLOTRAN is a parallel subsurface flow and reactive transport simulator. This velocity field was prescribed as a steady-flux field for solving the advection-dispersion equation. In this work, we only assume diffusion without any dispersion. Geothermal up flow zones with elevated trace element concentrations are placed at different locations in the entire domain with a size of 5 km x 5 km. We selected 80 different locations within this particular domain size. An initial concentration of 0.001 mol/L was set at the source location for each realization and we ran each realization for 1 million years to approach steady-state conditions. The concentrations from each simulation were compared to measured data. The comparison was performed using the Python-based Model Analysis Toolkit (MATK) developed at Los Alamos National Laboratory. MATK allows for the simultaneous running of multiple realizations in parallel and provides tools for post-processing the data and calibration. We coupled MATK (MATK 2015) with PFLOTRAN (Karra and Kitay 2015), which is a Python-based toolkit to run PFLOTRAN, to run the eighty realizations and perform post-processing of the obtained data from those simulations. For this paper, we looked at a qualitative comparison to see if the regions of high and low concentrations were similar to those observed, and chose a fixed value for the source concentration. For our qualitative comparison, we scaled both the observed and simulated concentrations by their respective maximum and minimum concentrations to obtain a range between zero and one. Then, we evaluated the root mean squared error using these scaled values to get a quantitative comparison. We hypothesize that areas of high heat flow should coincide with regions of localized low root mean squared errors.

Results

Trace Element Data

The data shown in the maps (Figure 3B and 3C) are summarized in histogram form in Figure 5. Aqueous geochemistry data from the National Geothermal Data System (NGDS) represent waters from known thermal wells and springs in New Mexico; the medium boron and lithium concentrations are elevated in geothermal waters (Figure 5). The conservative ion NGDS data are plotted with similar data from low-temperature systems in Socorro (Owens, 2013) and in Truth or Consequences (Figure 6). The conservative ion data from the NGDS were broken out by county to account for differences in the geologic setting among the known systems. Gila River and Frisco hot springs are in Catron County. Doña Ana County includes wells drilled by New Mexico State University in the Las Alturas system in Las Cruces, deep oil wells, and Radium Springs. Cliff, Faywood, Gila, and Mimbres hot springs are located in Grant County. Most of the data from Hidalgo County is from Lightning Dock. The data from Socorro County overlaps with the data of Owens (2013) to some extent. The data from Sierra County overlaps with a few of the new Truth or Consequences data.

Plots of chloride versus boron, lithium, or bromide are useful in identifying dilution or evaporation trends (Figures 6A, 6C, and 6E). Thermal waters tend to cluster at similar chloride and conservative ion values, and linear arrays indicate mixing and dilution. The geothermal systems in the latest Eocene to Miocene volcanic terrains of Grant, Hildalgo, and Luna counties are characterized by low chloride and low conservative ion concentrations. The geothermal systems in the thick rift-fill sediments of the Mesilla Basin in Doña Ana County have higher chloride concentrations; the linear arrays indicate mixing of deeper saline waters with fresher water. The lithium signature of each of the geothermal systems in southwestern New Mexico is unique. Linear arrays on the lithium-chloride plot for the Catron and Doña Ana counties suggest dilution.

Figure 6. Correlation between boron, bromide, lithium and chloride for hot springs and wells in the six counties located in southwestern New Mexico. Geochemical data from the Socorro and Truth or Consequences systems are shown for comparison.

Ion-ratio versus ion plots (Figures 6B, 6D, 6F) are helpful in identifying the geologic provenance of water. For example, the Cl/Br ratio of seawater is 290, of meteoric water is 50-180, and of fluid interacting with igneous and metamorphic rocks is 100-500 (Davis et al., 1998). Many of the geothermal waters in southwestern New Mexico have Cl/Br ratios < 500 and most are <1000. One notable exception is water from Truth or Consequences, with several Cl/Br ratios are related to dissolution of evaporite minerals or to anthropogenic sources. The bromide-chloride plot reveals a wide range of bromide values for the Truth or Consequences system.

Most of the lithium, boron and bromide concentrations in geothermal waters in southwestern New Mexico vary between 0.5 and 4 mg/l, although they are as low as 0.01 in some regions (Grant County).

Particle Trajectory Maps

We developed particle trajectory maps for the southern Albuquerque Basin near San Acacia, NM. This area overlies the Socorro Magma Body. We also developed a particle trajectory map for the southern Engle Basin near Truth or Consequences, NM. Within the Truth or Consequences hot-springs





district, temperature profiles within shallow wells are nearly isothermal after about 10 m depth. Heat flow is estimated to be in the range of 500 to 1300 mW m⁻². A recent study of the Truth or Consequences geothermal system suggests that fluid circulation within the relatively permeable crystalline basement extends to 4-8 km below the Paleozoic sedimentary deposits (B-B', Figure 7).

Our preliminary analysis of particle trajectories reveals some interesting patterns. Along the Rio Grande rift near the Sevilleta wildlife refuge, elevated boron concentrations (> 3 mg/l) occur in the vicinity of Indian Wells springs (dashed circles, Figure 8). Both up gradient and down gradient wells have lower boron concentrations, suggesting this may be an up flow zone associated with a hydrogeologic window or fault system overlying the Socorro magma body. Indian Wells spring also has elevated ³He/⁴He ratios, suggesting a potential deep

Figure 7. Schematic of fault-controlled hydrogeologic windows in the La Jencia – Socorro Basin (A-A') (Barroll and Reiter, 1990) and in the Truth or Consequences hot-springs district (B-B'; Pepin et al., 2015). Arrows indicate groundwater flow directions. Estimated shallow conductive heat flow for these two study areas is also shown. Cross-section locations are shown in Figures 4 and 9.

Figure 8. Boron concentrations (colored lines) upwinded along particle trajectories across the southern Albuquerque Basin near San Acacia, NM. Fault zones are also plotted (gray lines). Watertable gradients are plotted as a shaded-color relief map.

geothermal fluid source (Williams et al., 2013). Because this region is the southern terminus of the Albuquerque Basin, up flow of deep sedimentary basin fluids may also occur in this area (Hogan et al., 2007).

The Truth or Consequences hot-springs district has elevated lithium (up to 1.3 mg/l) and boron (up to 3.9 mg/l) concentrations in wells completed within a hydrogeologic window along the Rio Grande (dashed circle, Figure 9), where bedrock crops out near the land surface or is covered by a thin veneer of fluvial deposits (B-B', Figure 7). The lithium particle trajectories track up gradient to the northeast (Figure 9). Down gradient wells to the south of the hot-springs district and up hydrologic gradient near the Elephant Butte Reservoir have lower lithium concentrations.

Advection-Dispersion Modeling

Flow lines calculated by PFLOTRAN for the Socorro-La Jencia Basin are shown in Figure 10A. Our methodology for identifying geothermal up flow zones by varying tracer source locations gave interesting results. Simulated transient normalized lithium concentrations for two scenarios are shown in Figures 10B and 10C. The source regions are shown by the purple squares. Figure 10D shows the map of the root mean squared error using the scaled concentrations for 80 transient tracer simulations. At the base of Socorro





Figure 9. Lithium concentrations and particle trajectories within the Truth or Consequences hotsprings district region, NM. Light red line depicts the location of the southern end of the cross section (B-B') in Figure 7. Figure 10. (A) Streamlines obtained from solving Darcy's law in PFLOTRAN using the interpolated water-table map. Note that the low water table area is shown with the red line and is modeled as the Rio Grande. (B-C) Simulated transport of lithium for two cases assuming steady-state conditions assuming an arbitrary source lithium concentration of 0.001 mol/L. The location of the up flow zone is shown by the purple squares. (D) Root mean squared error of the scaled concentrations for 80 realizations of source locations. The error is obtained by comparing the simulated lithium concentrations with the observed well data from 43 locations. The higher value implies less likelihood of the location being a source location. The results suggest that the source location is more likely to be in the southern side of the domain and close to the Rio Grande. On the other hand, west and east regions of the river generally have medium likelihood with the northern side of the domain being the least likely.

Peak (white box, Figure 10A), the root mean squared error is a localized minimum. This is the region of the known geothermal upflow zone. However, lower values of root mean squared errors also occur in the southern region of the model domain, indicating the possibility of multiple upflow zones.



Discussion and Conclusions

The work presented here represents one of the first attempts to incorporate advective-dispersive transport into geothermal exploration. This concept is not new; a similar approach has been used in the ore deposits industry to locate diamond-rich kimberlite pipes within glaciated regions of the Canadian Shield (McClenaghan and Kjarsgaard, 2001). The particle-tracking algorithm shows promise for identifying geothermal upflow zones; however, more work is needed to consider multiple tracers and develop more formal concentration criteria for identifying upflow zones. Particle trajectories and groundwater velocities are only as good as the water-table map that they are based on. We found that particle trajectories changed when we modified the underlying assumptions on which the water-table map was constructed (e.g. whether or not to use perennial streams as observations points). Clearly, the method will only work if sufficient geochemical and water-level data are available. Multiple realizations based approach of varying the source region location and simulating tracer transport using advection-diffusion equation, and comparing with measured data at wells seems to be a good way of identifying blind windows, but the fact that multiple minima were produced indicates further work is required to refine this methodology. Future work will involve evaluating source strengths, dispersion parameters, and development of a methodology for combined lithium-boron transport analysis.

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