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Comparison of Heat and Bromide as Ground Water Tracers Near Streams

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Abstract

Heat and bromide were compared as tracers for examining stream/ground water exchanges along the middle reaches of the Santa Clara River, California, during a 10-hour surface water sodium bromide injection test. Three cross sections that comprise six shallow (<1 m) piezometers were installed at the upper, middle, and lower sections of a 17 km long study reach, to monitor temperatures and bromide concentrations in the shallow ground water beneath the stream. A heat and ground water transport simulation model and a closely related solute and ground water transport simulation model were matched up for comparison of simulated and observed temperatures and bromide concentrations in the streambed. Vertical, one-dimensional simulations of sediment temperature were fitted to observed temperature results, to yield apparent streambed hydraulic conductivities in each cross section. The temperature-based hydraulic conductivities were assigned to a solute and ground water transport model to predict sediment bromide concentrations, during the sodium bromide injection test. Vertical, one-dimensional simulations of bromide concentrations in the sediments yielded a good match to the observed bromide concentrations, without adjustment of any model parameters except solute dispersivities. This indicates that, for the spatial and temporal scales examined on the Santa Clara River, the use of heat and bromide as tracers provide comparable information with respect to apparent hydraulic conductivities and fluxes for sediments near streams. In other settings, caution should be used due to differences in the nature of conservative (bromide) versus nonconservative (heat) tracers, particularly when preferential flowpaths are present.

Introduction

Surface water and ground water are a coupled resource, mandating examination as a continuum to fully characterize each resource. Hydrological tracers provide a tool for examining this continuum, because tracers move with flowing water across the surface water/ground water interface. Research hydrologists have demonstrated that chemical tracers are excellent indicators of spatial and temporal patterns of stream exchanges with shallow ground water (Bencala 1984; Harvey and Fuller 1998; Harvey and Wagner 2000). Often a surface water solute injection test is performed to change the solute concentration, rather than relying on natural changes in concentration over time. These injection tests are useful in facilitating estimates of surface water travel time velocities and dispersion, as well as exchanges with ground water (Nishikawa et al. 1999). There is growing interest in the use of heat as a tracer for examining stream/ground water interactions, through analysis of natural variation of stream temperature patterns and resulting exchange of heat with the subsurface (Lapham 1989; Silliman and Booth 1993; Constantz et al. 1994; Silliman et al. 1995; Constantz and Thomas 1996; Constantz et al. 2001; Constantz et al. 2002). Using heat as a tracer, Lapham (1989) analyzed deep temperature profiles at various times of the year to estimate hydraulic parameters below streams along the eastern United States. Silliman and Booth (1993) demonstrated that heat could be used as a tracer in a similar manner to a surface water solute tracer at streams in Indiana. Constantz (1998) analyzed diurnal changes in stream temperature to identify gaining and losing reaches, and examined the relative importance of evapotranspiration compared with seepage losses and discharge gains in different reaches of alpine streams in the western United States. He demonstrated that perturbations of the natural temperature patterns due to dam releases were useful in identifying the relative impact of bank storage in dif-

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ferent stream reaches. Lowney (2000) found that unique thermal patterns downstream of dams are useful in determining velocity regimes for great distance downstream of dams. Currently, a comparison of heat with more established chemical tracers is warranted, to determine the relative utility and accuracy of heat versus chemical tracers for predicting streambed hydraulic properties.

This study evaluates the relative attributes of heat versus bromide as tracers of shallow ground water movement. Two physically based simulation models designed to predict either heat or bromide transport during variably saturated ground water flow are presented. A previously published, highly relevant laboratory experiment is discussed at some length, because the experiment was designed to compare the transport of heat and bromide transport in a sand column. As an extension of this work, field experiments were performed in which temperature and bromide concentrations were monitored in shallow sediments during a surface water sodium bromide injection test. The simulation models were run to compare predicted temperature and bromide concentrations with field observations during the sodium bromide injection test. This comparison forms the basis for a discussion of the attributes and compatibility of each tracer for investigation of shallow ground water flow near streams.

Qualitative Comparison of Heat and Bromide as Ground Water Tracers

The flow of heat and bromide along with ground water represent the transport of energy versus a chemical species, such that they possess both similar and dissimilar properties with respect to their ability to track the ground water movement. Operationally, the use of heat as a tracer requires the ability to measure temperature gradients, whereas the use of bromide as a tracer requires the ability to measure concentration gradients. Generally, temperature gradients occur naturally in response to cyclic upper-boundary conditions, on diurnal, annual, decadal, or geological time scales. In the stream environment, only the diurnal and annual time scales are of practical value. Thus, heat is "injected" naturally into the stream. Typically, gradients in bromide concentration are induced by introducing either a slug injection or constant-rate injection of bromide at the upstream boundary of the study reach (after appropriate permits are obtained).

Both heat and bromide are nonreactive in the sense that neither transforms into another form of energy or chemical species during transport through natural porous material; however, heat is not a conservative ground water tracer. Although heat does not decay into another form of energy, it dissipates during transport due to the large heat capacities of the solid matrix within the ground water system. In contrast, bromide remains in solution within the pore water domain and does not absorb onto or diffuse into the solid matrix participating in heat transfer. This is a significant difference between heat and bromide as tracers, and constrains the spatial scale in which heat can be practically used for a given time scale of interest. Generally, the spatial scale for which heat is useful depends on the time scale of periodicity at the boundary. For diurnal temperature variations, the spatial scale may be only 0.1 to 10 m, depending on the rate of water movement through the pore matrix, whereas for geological time-scale variations in boundary temperatures, the spatial scale may be measured at the basin-wide spatial scale (Reiter 2001). In contrast, the spatial scale for which bromide is useful is controlled by the total amount of bromide injected into the ground water system and its overall permeability.

From a practical perspective, heat is particularly well suited for investigations of stream/ground water exchanges for several reasons discussed in detail in the present work. Dynamic temperature patterns occur naturally in streams and underlying sediments, due to high rates of heat exchange between the atmosphere and stream. Because heat is a naturally occurring tracer, the use of heat as a tracer is free from (real or perceived) issues of contamination associated with use of chemical tracers in stream environments. (Injection of chemical tracers, such as bromide or Rhodamine WT, requires the granting of a use permit, with significant uncertainty of success.) Also, the use of heat as a tracer relies on the measurement of temperature gradients, and temperature is probably the most robust environmental parameter to continuously monitor. Finally, automated, instantaneous acquisition of temperature data has become trivial with electronic advances, while acquisition of bromide concentrations requires an elaborate, labor-intensive sampling protocol, followed by laboratory analysis. Consequently, if heat as a tracer of stream exchange with ground water proves to have similar utility compared with bromide, then the use of heat as a tracer may be preferred due to the natural input of heat and the rapid output of temperature data needed to estimate streambed hydraulic parameters.

Quantitative Comparison of Heat and Bromide as Ground Water Tracers

The transport of heat or solute in ground water systems may be described by the advective-dispersion equation. To solve this equation, analytical solutions have been successfully employed for steady-state conditions in homogeneous material, where the boundary conditions are represented by a constant value or simple function (Stallman 1965; Bredehoeft and Papadopulos 1965). Ground water systems near streams are often heterogeneous, influenced by rapid changes in stream stage, and have complex boundary conditions that are rarely approximated by a simple function (Constantz et al. 2001). Consequently, numerical modeling of heat and solute transport in the near-stream environment is generally required to represent ground water flow near the stream. VS2DH (Healy and Ronan 1996) and VS2DT (Healy 1990) are related numerical model simulation codes, which rely on the advective-dispersion equation to describe flow and transport through variably saturated ground water systems. VS2DH has been used to successfully predicted heat transport in variably saturated material at several sites (Ronan et al. 1998; Constantz et. al. 2002). VS2DT has been used to successfully predict solute transport through variably saturated material at several sites (Mills and Healy 1993; Halford 1997; McCord et al. 1997). These numerical models are used concurrently in the present study for com-

parisons of heat and bromide as ground water tracers near streams. Equations 1a, 2, 3, and 4 form the basis of VS2DH, whereas Equations 1b, 3, and 4 form the basis of VS2DT. Equation 1a represents transport of heat through variably water-saturated sediments (Healy and Ronan 1996), whereas Equation 1b represents simultaneous transport of a conservative solute through variably water-saturated sediments (Kipp 1987; Healy 1990).

$$\frac{\partial[\theta C_w + (1-\phi)C_s]T}{\partial t}$$

$$= \nabla \cdot K_t(\theta)\nabla T + \nabla \cdot \theta C_w D_h \nabla T - \nabla \cdot \theta C_w T q + Q C_w T \quad (1a)$$

$$\frac{\partial[q\,S]}{\partial t} = — \cdot \theta\, D_h\, \nabla S - \nabla \cdot \theta\, S q + QS \quad (1b)$$

where θ is percent volumetric water content, and ϕ is sediment porosity (both dimensionless). The concentration of a solute (i.e., chemical constituent) is S, in kg/m^3. Q is rate of fluid source in m/sec. K_t is the thermal conductivity, in w/m °C. C_w and C_s are the volumetric heat capacity of water and sediment, J/m^3 °C, respectively. The heat capacity of the sediments is based on the combined influence of C_w and the heat capacities of the mineral and organic solids, and for unsaturated conditions the air in the following manner:

$$C_s = f_w(C_w) + f_m(c_m\, p_m) + f_o(c_o p_o) + f_a\,(c_a\, p_a) \quad (2)$$

where f_m, f_o, f_w, and f_a are the volumetric fractions of the mineral solid, organic solid, water, and air, respectively; c_m, c_o, and c_a are the specific heat capacities in J/kg °C of the mineral solid, organic solid, and air, respectively; and p_m, p_o, and p_a are the densities in kg/m^3 of the mineral solid, organic solid, and air, respectively. D_h is the hydrodynamic dispersion tensor, in m^2/sec. The thermo-mechanical and hydrodynamic dispersion tensors are defined as

$$D_h = \alpha_T|v|\delta_{i,j} + \frac{(\alpha_l - \alpha_T)v_i v_j}{|v|} \quad (3)$$

respectively, where α_l and α_T are longitudinal and transverse dispersivities, respectively, in meters; $\delta_{i,j}$ is the Kronecker delta function; n_i, n_j are the ith and jth component of the velocity vector, respectively, in m/sec (Healy 1990). Freeze and Cherry (1979) stated that dispersivity is "the most elusive" parameter to identify in assigning values in transport models. They indicated that laboratory values for α_l range from 0.0001 to .02 m, but that these values have little relevance to field-scale values ranging from 10 to 100 m. In contrast, there is general agreement that values for α_T are only $0.01\alpha_l$ to $0.1\alpha_l$ regardless of spatial scale.

The magnitude of the solute dispersivity compared with the thermal dispersivity requires further discussion. Dispersion is defined as a scale-dependent mixing phenomenon related to the heterogeneity of microscopic pore velocities (de Marsily 1986), such that the magnitude increases with increasing heterogeneity and travel path. More recently, researchers argue that thermal dispersion is negligible relative to solute dispersion, due to the dominance of heat dissipation to the porous matrix over heat dispersion in the flowing pore water (Ingebritsen and Sanford 1998; Hopmans et al. 2002). In the present work, both dispersivity perspectives are explored through comparison of measurable versus negligible thermal dispersivities, during best-fit matches of simulated to observed bromide and temperature patterns in stream sediments.

Discussing the heat and solute transport equations in more detail, the left side of Equation 1a represents the change in energy stored in both the pore and solid volume over time. The first term on the right side describes the energy transport by heat conduction. The second term on the right side accounts for thermo-mechanical dispersion. The third term on the right represents advective heat transport, and the final term on the right represents heat sources and sinks to mass movement into or out of the volume. In comparison, the left side of Equation 1b represents the change in chemical concentration stored in the pore volume over time. The first term on the right side describes the chemical transport by hydrodynamic dispersion. The second term on the right side represents advective chemical transport during water flow through the sediments. The final term on the right side represents concentration sources or sinks due to mass movement into or out of the volume. Consequently, one difference between Equations 1a and 1b is that the former includes the capacity of porous material to absorb and conduct heat. Note that heat capacity retards the rate of heat transport during ground water flow, while the thermal conduction enhances heat transport. The relative importance of these processes to total heat transport is inversely proportional to the pore water velocity through a material. At low velocities, uncertainties in thermal parameters will lead to significant uncertainties in temperature-based estimates of K and q. As velocities increase, uncertainties in thermal parameters have a negligible effect on estimates in K and q, due to the increasing dominance of advective heat transport.

For both Equations 1a and 1b, the water velocity within variably saturated sediments is q, m/s, which is determined by the familiar water flow equation

$$C(\psi)\frac{\partial h}{\partial t} = \nabla[k(\psi)\cdot\nabla h + 1] \quad (4)$$

where C (ψ) = specific moisture capacity, which is the slope of the water retention curve; ψ is the water pressure in meters; h is the total head in meters; x is length in meters; t is time; and K is the hydraulic conductivity in m/sec (Buckingham 1907; Richards 1931).

A fortuitous, uniquely relevant laboratory experiment provides an example comparison of bromide and heat as tracers. This experiment was designed to compare heat and bromide as tracers of water flow through a sand column (Taniguchi and Sharma 1990), and affords the opportunity to examine expected relative travel times and rates of dispersion for heat versus bromide. The experimental setup was as follows. A 1.0 m long, 0.1 m diameter column was

filled with Bassendean Sand, then demineralized water was applied to the top of the column at 2.25×10^{-5} m/sec, and the saturated K was determined to be 2.0×10^{-5} m/sec. A solute of 0.5 M KBr was applied as a 0.42 L pulse at a temperature of 35°C. Note that the laboratory was maintained at 20°C, resulting in at least some loss of heat in the radial direction during pore water flow down the sand column. Several plots of temperature and bromide concentration patterns observed in the column were provided in the original citation. Figure 1 gives a summary of results, with temperature and bromide normalized by their input values. Inspection of the figure reveals an increasing disparity between the peak bromide concentration and the peak temperature as pore water continues to flow through the sand column. As shown in the figure, the conservative nature of bromide is clearly seen as the concentration peak is well in advance of the temperature peak, and the magnitude in the concentration peak remains relatively large during flow through the sand column. Although the disparity may be sharpened by the radial loss of heat, this column experiment gives a general expectation leading up to a field analysis of bromide versus temperature arrival times at shallow depths (i.e., <1 m) in the streambed of similar texture, as the result of a surface water bromide injection into a stream with a measurable (i.e., 15°C) temperature variation. The Santa Clara River possesses similar thermal and hydraulic properties in the middle reaches west of the Valencia Water Reclamation Plant (WRP).

Site Description and Experimental Procedure

As depicted in Figure 2, the Santa Clara River is in the northwest portion of Los Angeles County, California. The river flows from the San Gabriel Mountains ~200 km to the Pacific Ocean. In the upper reaches, the gradient is steep and the stream generally flows over bedrock, with a steady gain of ground water. In the middle reaches, the stream flows over a wide sandy channel, resulting in large diurnal stream-temperature fluctuations, as well as significant potential for stream/ground water interaction. The streambed consists of unconsolidated, interbedded medium and fine sand layers, with no visible clogging layer at the streambed surface. Clogging layers are common in streambed and often result in a low K value for the streambed, which can create hydraulic disconnection between the stream and the water table for losing reaches. However, for this reach of the Santa Clara River, the lack

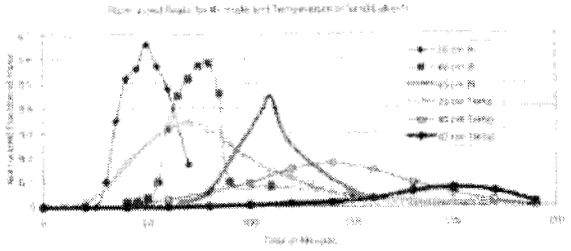

Figure 1. Normalized bromide concentrations and temperatures at specified times within a laboratory sand column (Taniguchi and Sharma 1990).

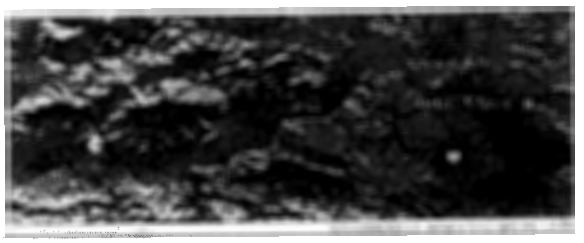

Figure 2. Site map for the study reach on the Santa Clara River (California) flowing east to west from Los Angeles County into Ventura County. Sodium bromide was injected at the discharge point at the Valencia Water Reclamation Plant.

of a clogging layer resulted in relatively high K values, allowing hydraulic connection between the stream and the water table.

During May 2000, a 17 km study reach was instrumented with piezometers at the five sites indicated in Figure 2. Along the study reach, the water table was located above the stream-surface elevation (i.e., stream stage) in the upper end of the reach, and located at increasingly lower elevations relative to the stream stage downstream. Cross sections of PVC piezometers were installed at three sites: SCR2, SCR3, and SCR5 in the upper, middle, and lower sections of the study reach, respectively. For each cross section, piezometers were equally spaced, with three piezometers located in the river and three on the bank. Figure 3 provides a cross-sectional schematic of the relative piezometer positioning at each site, such that the piezometers formed a line perpendicular to the direction of streamflow. Each PVC piezometer had an internal diameter of 0.05 m with a length of ~1.25 m. Piezometers were capped with a vented top at the measurement point to reduce heat exchanges down the inside of the pipe. Each piezometer was screened at the bottom of the pipe, which varied between 0.5 to 0.7 m below the elevation of the streambed surface. The piezometer cross section at SCR2 and SCR3 was 8 m wide, with a spacing of 1.6 m between piezometers. For SCR5 the piezometer cross section was only 3.25 m wide, with a spacing of only

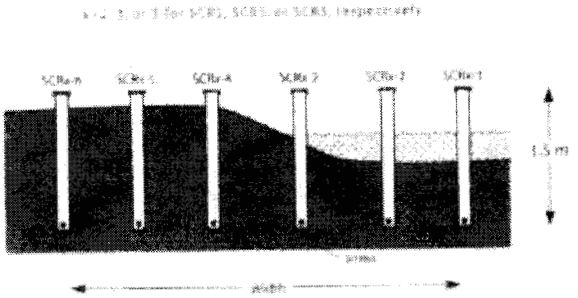

Figure 3. A cross-sectional configuration of a set of six PVC piezometers. Sites SCR2, SCR3, and SCR5 each contained one set of six piezometers. The width of the set of piezometers was ~8 m at SCR2 and SCR3 and ~3.25 m at SCR5 due to channel constraints. As depicted, circular-shaped, single-channel temperature loggers rested above each piezometer screen.

0.65 m between piezometers, due to a gradual decrease in channel width downstream of SCR3. Single channel, submersible temperature microloggers were placed in the bottom of each piezometer, and set to log temperature at five-minute intervals. For each cross section, one temperature logger was tethered to the outside of a piezometer in the river to monitor stream temperature. To obtain hydraulic gradients, depth-to-water was periodically measured inside and outside piezometers during the surface water bromide injection. Water levels were observed to be static during the measurement period. Background bromide samples on May 1 were determined to be 0.2, 0.2, and 0.3 mg/L at SCR2, SCR3, and SCR5, respectively. A steady source of bromide was believed to discharge into the stream at approximately SCR4 (Figure 2).

The surface water sodium bromide injection was performed May 2–4, 2000, above the study reach. At this time, piezometer measurements indicated the stream was neutral to slightly losing at SCR2 and increasingly losing downstream of this site. A tracer solution of sodium bromide (NaBr; 163 g/L) was introduced into the Santa Clara River using a constant rate injection method (Kilpatrick and Cobb 1985) for a 10-hour period at ~15 L/hour via the discharge from the Los Angeles County Sanitation District Valencia Water Reclamation Plant. Surface water samples were collected to observe the arrival, plateau, and departure of the NaBr tracer at SCR1, SCR2, SCR3, SCR4, and SCR5, as well as in three of the six piezometers at SCR2, SCR3, and SCR5. These sites ranged from 0.015 to 20 km below the injection site. Manpower and equipment constraints limited the total number of bromide samples that could be acquired during intensive four-day sampling, May 1–5, 2000. These operational limitations in sampling protocol caused a necessary reduction in the total number of piezometers that could be physically sampled for bromide from six to three piezometers at each cross section. As a consequence, only piezometers labeled #2, #4, and #6 (one in the river and two in the bank) were sampled for bromide (while all six piezometers were being sampled for temperature every five minutes). Bromide was sampled once an hour for the first 24 hours for SCR2, and once an hour for the first 36 hours for SCR3 and SCR5.

Ground water samples were taken at all three cross section sites in piezometers #2, #4, and #6 with manual pumping in the following manner: In an effort to sample water that more closely represented the chemistry of ground water passing a given piezometer at a given time, piezometers were purged 15 minutes prior to specified sampling times. This allowed the piezometers to reach hydrostatic conditions prior to collecting a ground water sample. (This purging of the well created a brief spike in temperature measurements that will be discussed later.) Both surface water and ground water samples were filtered through a "0.45 micrometer" in-line capsule filter to remove solid particulate before transfer to 250 mL bottles. Water samples were brought back to the laboratory for analysis of bromide concentration using an ion chromatograph. Companion stream and sediment temperature data were transferred to a computer in the field. After bromide analyses were completed, surface water temperature and bromide concentrations were used as part of the input set of parameters into VS2DH and VS2DT, respectively, and ground water temperature and bromide concentrations formed the basis for matches of simulated to observed results.

Results and Discussion

The steady NaBr injection for 10 hours created a step increase in bromide concentration as the reclamation plant discharge merged with the river. This resulted in a square-wave injection signal of bromide, as opposed to the sinusoidal-wave "injection" created by the diurnal stream temperature pattern. The bromide signal was dispersed downstream in a manner that resulted in an input pattern resembling the daytime stream temperature. The early morning timing of the sodium bromide injection led to peak downstream bromide concentrations appearing at each cross section slightly in advance of the natural daily temperature peak

As depicted in Figures 4a, 4b, and 4c, the resulting bromide surface water patterns were comparable in shape to water-temperature patterns, as concentration peaks reached SCR2, SCR3, and SCR5, respectively. In the figures, bromide concentration and temperatures for the surface water and piezometers #2, #4, and #6 are shown for each cross section. The piezometer observation (screen) depths varied slightly, as listed in the figure for each piezometer. Piezometers #1, #3, and #5 were not sampled for bromide due to manpower constraints, and as a consequence #1, #3, and #5 are not depicted to reduce redundancy of temperature data, as well as to enhance visibility of tracer comparisons. Briefly, temperature results for piezometers #1 and #3 were virtually identical to those observed results portrayed for piezometer #2 in Figures 4a, 4b, and 4c. Results for piezometer #5 plotted in a reasonable fashion midway between temperatures observed for #4 and #6 in Figures 4a, 4b, and 4c. Both vertical and horizontal migration of heat and bromide into the streambed are seen to increase from SCR2 progressive to SCR5 in the figures. Note that the periodic jagged appearance of the sediment temperature pattern is an artifact of pumping prior to each bromide sampling. There was concern that pumping might affect ground water flowpaths; however, the impacts on interpretation of results are likely to be small for two reasons. First, the volume of water pumped was small compared to the volume of pore water in the approximate region surrounding each piezometer. Specifically, the volume of water pumped out of each piezometer was in the range of 10^{-4} m^3 per sample, while the pore water volume surrounding each piezometer was in the range of 1 m^3. Second, any measurable impact on the ground water flowpath would be expected to affect the transport of heat and bromide in a similar manner. Further inspection of the three figures shows a clear downstream trend in both bromide concentration and temperature with respect to the degree to which surface water patterns were reflected in the sediments. This trend of increasing penetration of bromide and temperature is not in agreement with concurrently monitored hydraulic gradients. The time-averaged vertical hydraulic gradients observed at SCR2, SCR3, and SCR5 were 0.08, 0.04, and 0.11, respectively. This suggests the likelihood of a signif-

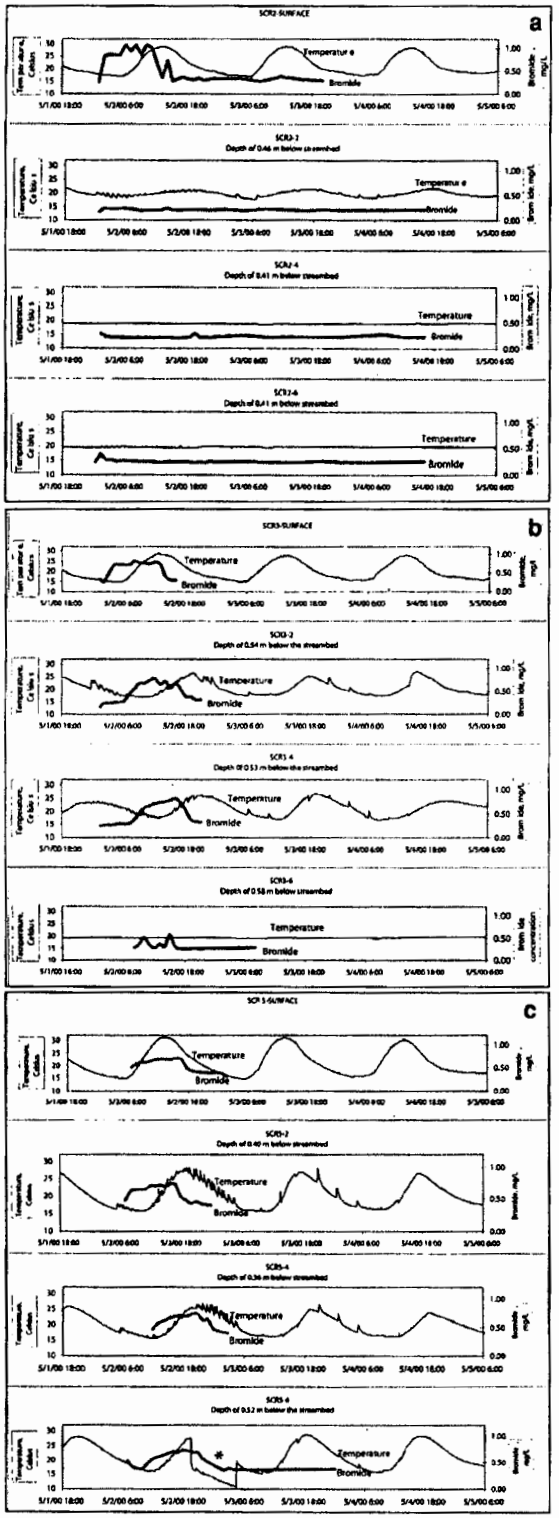

Figure 4. (a) Observed stream and sediment bromide concentrations and temperatures for SCR2–2, SCR2–4, and SCR2–6; (b) observed stream and sediment bromide concentrations and temperatures for site SCR3–2, SCR3–4, and SCR3–6; (c) observed stream and sediment bromide concentration and temperatures for site SCR5–2, SCR5–4, and SCR–6. Note that the asterisk located on SCR5–6 plot indicates a time period during which the temperature logger in SCR5–6 was erroneously removed and placed on the streambank.

icantly greater streambed K at SCR3 than SCR2, such that the resulting flux near SCR3 allowed deeper penetration of bromide and heat into the sediments.

These observed results form the basis for simulations of heat and bromide into the streambed using one-dimensional domains within VS2DH and VS2DT, respectively. Before performing these simulation analyses, a preliminary analysis of the travel times of the temperature and bromide peaks was performed to aid in establishing the viability of a one-dimensional approach to the problem. The rate of advancement of the temperature peak relative to the rate of advance of the bromide peaks observed in the laboratory column was calculated via Figure 1. This same calculation was determined based on data represented in Figures 4a, 4b, and 4c. These calculations yielded a travel-time ratio of bromide to temperature of ~1.4 for both the sand column and the streambed over the observed time period of the column experiment. Because the column experiment was macroscopically a one-dimensional flow system, this suggests that a one-dimensional approximation may be a reasonable approach to the Santa Clara River experiment. The one-dimensional simulation analyses were performed in the following sequence. Simulated sediment temperatures were manually fitted to observed temperature records for each site, by adjusting the hydraulic conductivity parameter within the model to minimize the difference between the simulated and observed temperature record. Once a best-fit hydraulic conductivity was determined, a vertical pore water flux could be estimated from the product of the measured hydraulic gradient and best-fit hydraulic conductivity for each site. These hydraulic parameters were then applied to simulations of bromide migration into the streambed, to determine if the hydraulic conductivity best fit to observed temperature measurements could predict the observed bromide concentrations using the temperature-based estimate of hydraulic conductivity for that site.

Temperature Simulations

Simulations of streambed temperature were compared to measured streambed temperatures at piezometers SCR2–2, SCR3–2, and SCR5–2 (the only piezometers sampled for bromide beneath the stream channel) by using VS2DH with a one-dimensional vertical simulation approach. The observed upper and lower thermal and hydraulic conditions were chosen as upper and lower boundary conditions, using temperature/pressure data from the stream and shallow piezometers, as well as data from deeper observation wells to determine the regional ground water temperature. The simulation domain and boundary conditions are shown in Figure 5, and the properties for the sand texture sediments are given in Table 1. The thermal properties in the table are based on the literature cited in the table for sand textured material. For saturated conditions, thermal properties for a given texture vary little relative to variations in hydraulic properties for the same texture, because saturated thermal properties vary only ± 50% for a given texture. This uncertainty in assignment of thermal properties may be important in conduction-dominated heat flow, but becomes less significant as advection increasingly contributes to the total heat flow. As discussed in the pro-

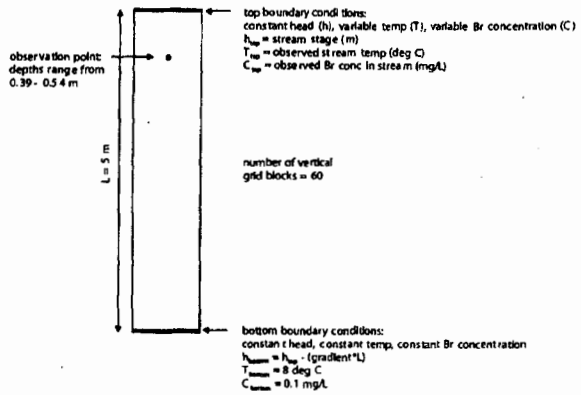

Figure 5. Graphical domain and boundary conditions applied for VS2DH and VS2DT simulations of heat and bromide ground water transport, respectively.

Table 1

Porosity = 0.37
Water retention parameters: alpha = 1.04 m^{-1}, beta = 6.9, and residual saturation = 0.072 $m^3\ m^{-3}$
Heat capacity of air = 1.2×10^3 J/(m^3 °C)
Heat capacity of dry solids = 2.18×10^6 J/(m^3 °C)
Heat capacity of water = 4.18×10^6 J/(m^3 °C)
Thermal conductivity = 1.0 W/(m °C)
Absorption coefficient = 0.0
Porosity is from field observations; thermal properties are from Healy and Ronan (1996), and solute properties are from Healy (1990).

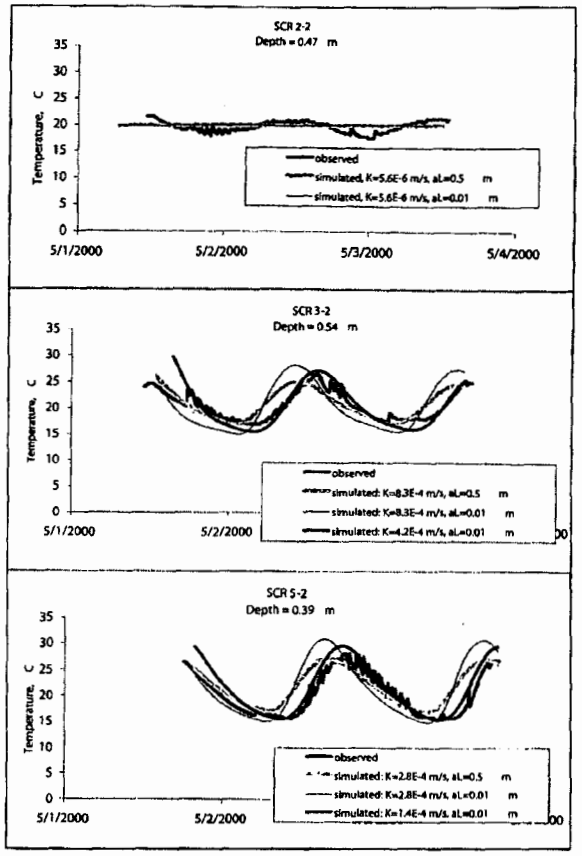

Figure 6. Comparison of observed and simulated sediment temperatures for SCR2–2, SCR3–2, and SCR5–2.

cedure section, site inspection suggested that advection would be significant beneath the Santa Clara River.

As discussed earlier, appropriate values for thermal dispersivity are a subject of active debate, with some researchers arguing that in principle thermal dispersivity values should be comparable to solute dispersivity (de Marsily 1986), while more recently most researchers argue that thermal dispersivities should be negligible as a result of the retardation of thermal dispersion due to dissipation of heat into the solid matrix (Ingebritsen and Ward 1998). A value of 0.01 m is recommended in the documentation for VS2DH (Healy and Ronan 1996); as discussed later, a value of 0.5 m is the upper range examined for solute dispersivity in this work. Thus for comparative purposes, thermal dispersivity values of 0.01 and 0.5 m were both examined throughout heat simulations. (Transverse dispersivities were assumed 0.1 of the longitudinal dispersivity, though the transverse dispersivity had no impact on one-dimensional simulations.)

Figure 6 provides a comparison of simulated with observed sediment temperatures at SCR2–2, SCR3–2, and SCR5–2 during the period of elevated bromide concentrations in the streambed. For SCR2–2, the best-fit value for K of 5.6×10^{-6} m/sec produced a similar fit for both values of dispersivity, suggesting that thermal dispersion is absent due to the inherent lack of thermal dispersion as a significant factor or the low water fluxes at this site (since the dispersion tensor approaches zero as the flux velocity is zero, regardless of the magnitude of the dispersivity value). For SCR3–2 and SCR5–2, a completely different image results from comparison of simulated to observed sediment temperatures. In both these cases, the dispersivity value produced a clear effect on the simulated sediment temperature, with a value of 0.01 m producing the best fit. In preliminary simulation runs, comparison of dispersivity values of 0.01 and 0.00 m produced no discernible differences in the simulated sediment temperatures within the spatial scale of interest (i.e., 1 m). In a laboratory column with a length of 0.036 m, the longitudinal dispersivity was reported to be 0.00221 m (Hopmans et al. 2002). Table 2 lists the observed hydraulic gradients, m/m, the best-fit temperature-based estimates of K between the streambed surface and the piezometer screen, m/sec, as well as the resulting temperature-based estimate for streambed percolation rate, m/sec. The predicted K values for SCR3 and SCR5 are considerably greater than the value for SCR2. Resulting temperature-based estimates of percolation rate agree well with the

Table 2

Streambed Sediment Properties	SCR2-2	SCR3-2	SCR5-2
Observed vertical hydraulic gradient, m/m	0.08	0.04	0.11
Hydraulic conductivity (best fit), m/s	5.6×10^{-6}	4.2×10^{-4}	1.4×10^{-4}
Percolation rate, m/s	4.5×10^{-7}	1.7×10^{-5}	1.5×10^{-5}

trend in depth-penetration of heat and bromide depicted in Figures 4a, 4b, and 4c. Detailed inspection of Figures 4b and 4c reveal that although the predicted percolation rate is slightly higher for SCR3 than SCR5, the resulting diurnal pattern in sediment temperature appears slightly higher at SCR5. The reason for this may be due to the larger diurnal magnitude in measured stream temperature at SCR5 compared with SCR3.

Bromide Simulations

VS2DT simulations were run in the following manner. The observed surface water bromide concentrations and stream stage were input as upper boundary conditions, while the background ground water bromide concentration and observed hydraulic gradients were used to formulate the lower boundary conditions. VS2DT simulations of sediment bromide concentration were run for SCR2–2, SCR3–2, and SCR5–2 during the period of raised concentrations of bromide as shown in Figures 4a, 4b, and 4c. As with the temperature simulations, input parameters from Table 1 were used, with the grid shown in Figure 5. The temperature-based, best-fit hydraulic conductivity values listed in Table 2 were assigned to VS2DT, such that there was no parameter fitting except for solute dispersivities. Solute dispersivities were selected based on documentation for VS2DT (Healy 1990) using the scale of the experimental regime delineated by the SCR piezometer cross sections (~1 m vertical and 8 m horizontal). Based on this information, solute dispersivity values ranging from 0.1 to 0.5 m were examined. Figure 7 provides the predicted bromide sediment concentrations compared with the observed bromide sediment concentrations for SCR2–2, SCR3–2, and SCR5–2 during the period of augmented bromide concentrations within the stream channel. For SCR2–2, SCR3–2, and SCR5–2, the best-fit bromide concentration is obtained using the temperature-based, best-fit K value and a solute dispersivity of 0.1 m. As shown for SCR3–2 and SCR5–2, a K value other than the best-fit K value is necessary to obtain a good fit if a solute dispersivity of 0.5 m is used in simulations. These results suggest a value of solute dispersivity of 0.1 m appears to be the best choice for a 1 m spatial scale.

As an analysis of goodness-of-fit for simulated fits to observed data, a root-mean-square-error (RMSE) analysis was performed. Analyses were performed to determine the absolute difference between simulated and observed values over the duration of monitoring. Figure 8 shows the RMSE for the best-fit temperature and bromide simulations. For temperature, the RMSE was 0.92°, 1.23°, and 1.74°C for SCR2–2, SCR3–2, and SCR5–2, respectively, while the range in observed temperature at the sediment surface was approximately 14°, 15°, and 17°C for SCR2–2, SCR3–2, and SCR5–2, respectively. For bromide concentrations in the streambed, the RMSE was 0.021, 0.076, and 0.15 mg/L for SCR2–2, SCR3–2, and SCR5–2, respectively, while the range in bromide concentration at the sediment surface was 0.89, 0.65, and 0.60 mg/L for SCR2–2, SCR3–2, and SCR5–2, respectively. Thus, the residuals are small for all cases relative to the respective ranges in temperature and bromide at the upper boundary of the model. A second measure of fit is presence or absence of a temporal trend in the residual. Absence of a trend, that is, a residual line which tends to randomly wander above and below zero, suggests a robust fit through time. Residuals lacked temporal trends for all of the temperature fits. In contrast, residuals for two bromide fits (SCR2–2 and SCR2–5) showed positive slopes, though relative to their ranges in bromide concentrations these trends are small. For both temperature and bromide fits, RMSE values increase downstream, reflecting the challenge in fitting the more abrupt increase at depth in both temperature and bromide at SCR3 and SCR5.

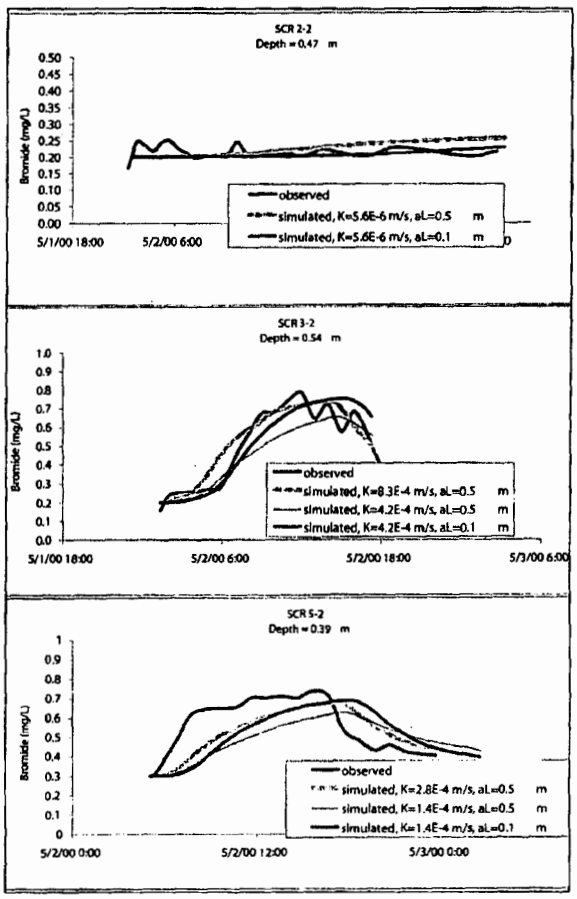

Figure 7. Comparison of observed and simulated sediment bromide concentration for SCR2–2, SCR3–2, and SCR5–2 during the period of the surface water bromide injection.

Conclusions

Both tracers provided qualitatively similar hydraulic information at all three cross sections of this reach of the Santa Clara River. For SCR2, the relatively low K value caused most bromide tracer to pass downstream without being entrained in slowly infiltrating stream water; and in a similar fashion, the large diurnal stream-temperature pattern failed to significantly penetrate in underlying sediments. For SCR3 and SCR5, higher K values contributed to greater streambed infiltration, resulting in significant advection of both bromide and heat into underlying sediments. Analysis of simulation results suggests that bromide

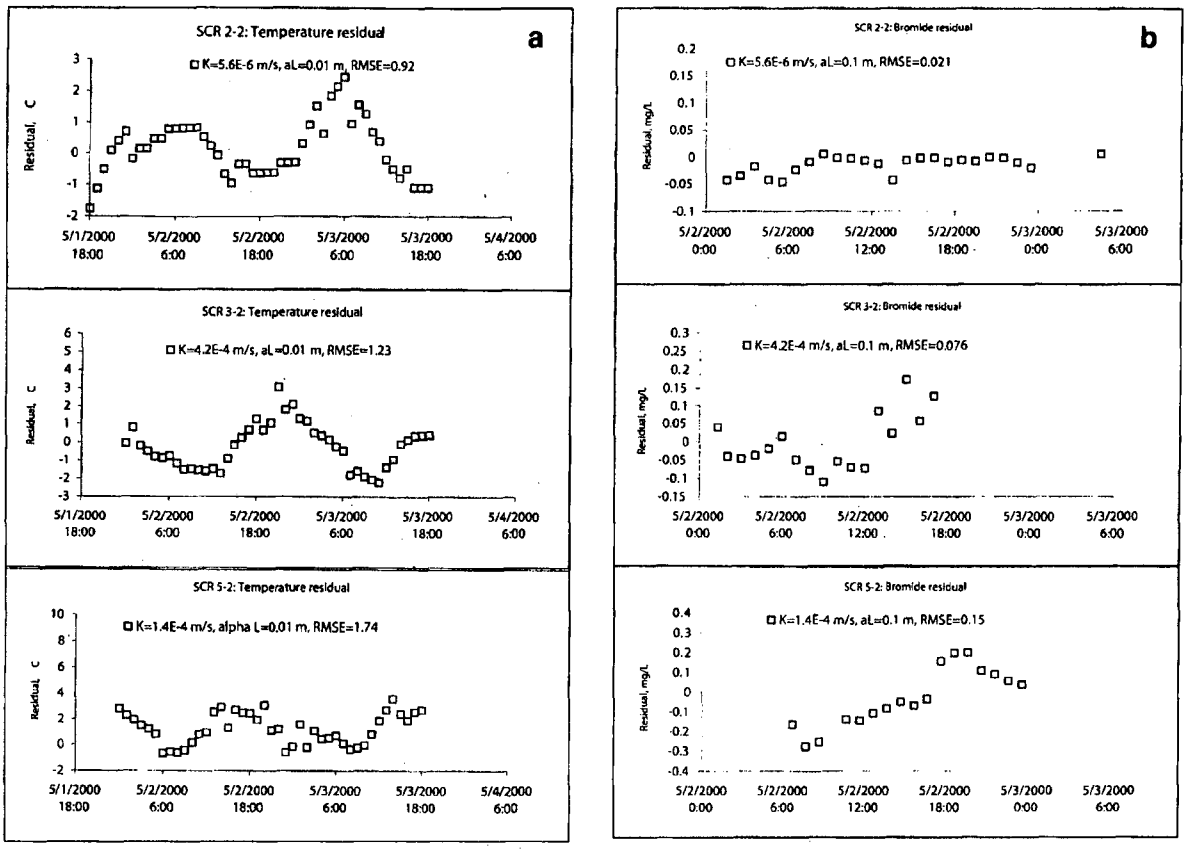

Figure 8. (a) Residuals between observed and simulated sediment temperature for SCR2–2, SCR3–2, and SCR5–2. RMSE is root-mean-square-error. (b) Residuals between observed and simulated bromide sediment concentrations for SCR2–2, SCR3–2, and SCR5–2. RMSE is root-mean-square-error.

and temperature are of comparable quantitative value in characterizing shallow ground water flow as well. Specifically, the ability to simulate bromide sediment concentrations from observed temperature patterns indicates that heat and bromide appear to possess comparable utility in predicting hydraulic parameters for this type of hydrological setting. However, caution should be used due to differences in the nature of conservative (bromide) versus nonconservative (heat) tracers, particularly when preferential flowpaths are present. In this case, heat will dissipate into the surrounding "edges or walls" of the preferential flowpath and potentially "mask" the presence of the preferential flowpath, while bromide will travel unabated with flowing ground water through the preferential flowpath. In the future, this distinctive difference between conservative and nonconservative tracers may afford improved characterization of multiple flowpaths in the near-stream environment.

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