

Perched Water Bodies in Arid Environments and Their Role as Hydrologic Constraints for Recharge Rate Estimation: Part 1. A Modeling Methodology

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The formation and temporal evolution of perched water bodies in arid environments is the theme of this article. Geological structure and effective recharge or net infiltration volume, which escapes the evapotranspiration capture zone, are the dominant factors controlling the phenomenon of perched water formation. An approach to use a combination of hydrological and geochemical data for present-day known occurrences of perched water bodies, cast in the form of hydrological and geochemical constraints, is proposed. These constraints are: present-day volume of perched water and attainment of steady-state behavior within a time period of less than 20,000 years (last pluvial), and present-day ^{14}C measurements.

Keywords: recharge, perched water, arid environment, hydrologic modeling.

Introduction

Perched water is defined as an unconfined saturated zone separated from an underlying saturated zone (water table) by an unsaturated zone, and is deemed significant with respect to infiltration and groundwater flux (USGS, 1981). Relative to a proposed waste disposal site, perched water bodies could occur: (1) above, (2) within, and (3) below the waste containment horizon. Of these three zones, perched water within the containment horizon itself would be of most concern because it is believed that waste canisters will last longer in unsaturated rock than under saturated conditions. The formation of perched water bodies in contact with or around waste canisters would likely increase the rate of waste canister failure, resulting in greater releases of contaminants.

Perched water is common in arid environments. For example, perched water flows from seeps into the U12n tunnel through the zeolitized Indian Trail Tuff at Rainier Mesa, 200 km northwest of Las Vegas, Nevada (Thordarson, 1965; Russell et al., 1987; Wang et al., 1993). Isotopic signatures (δD and $\delta^{18}\text{O}$) indicate that the perched waters at Rainier Mesa are similar to modern meteoric waters and recharge relatively quickly from local winter precipitation (Russell et al., 1987). Evidence also suggests that waters from the seeps in the zeolitized tuffs are chemically similar to water from the unsaturated zone below the perched water body but are distinct from shallower waters

(Wang et al., 1993). Preliminary field evidence from seeps and geophysical analyses suggest that perched water exists at the Peña Blanca natural analog site in Chihuahua, Mexico (Pearcy et al., 1993). A perched water zone at the Apache Leap Research Site (ALRS) in Arizona (Bassett et al., 1994) can be distinguished from other water bodies on the basis of $\delta^{34}\text{S}$ analysis. Perched water at the ALRS occurs within a tuff unit, and initial ^{14}C age dates suggest that the water may be as much as 3,000 years old. Finally, perched water has also been encountered at Yucca Mountain (YM), Nevada in air-drilled boreholes at depths of about 400 to 500 meters (Burger and Scofield, 1994; Yang et al., 1996). Perched water bodies tend to be long-term transient features that are formed where there is a contrast in hydrologic properties (Freeze and Cherry, 1979). Contrasts may result from differences between stratigraphic units. For example, hydraulic conductivity at various waste disposal sites tends to decrease with increased depth. Contrasts may also occur due to the juxtaposition of low conductivity strata adjacent to more permeable and conductive strata along a structural feature such as a fault or other persistent discontinuity.

Downey (1984) evaluated the geologic conditions and rock properties that produce a good seal when dealing with hydrocarbons, and some of these characteristics can be applied to evaluating the sealing properties of faults in relation to the trapping of water to form perched aquifers. Faults trap not so much by the properties of the fault itself but rather by placing a porous, permeable stratum adjacent to an impermeable stratum across the fault. However, an important instance where the fault itself may play a vital role in transporting or inhibiting water is where there is an overall tensional regional stress field that causes the fault to be much more likely to act as a conduit for flow. The

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sealing quality of a fault is determined by the minimum pressure required to displace connate water from void spaces of the fracture, thereby allowing leakage. The capillary pressure or sealing capacity of a rock is a function of the water-air interfacial tension, wettability, and size of the largest opening. The water-air interfacial tension is a constant, so the variability of the sealing capacity is dependent upon the remaining two properties, with the sealing capacity increasing as the size of the largest opening and the wettability decrease. In order for a seal to exist the total head pressure must be matched or exceeded by the capillary forces. In addition, the average sealing capacity is not the most important criterion to be met; rather, the least sealing capacity must match or exceed the total head pressure, because even a relatively small leak can allow a large amount of water to escape over a significant time period. Some of the conditions that affect the sealing property of a fault are orientation of the strata with respect to the fault, the regional stress field (as mentioned above), the offsetting of geopressures, and the effects of the fault movement on the geologic units. For example, differences in geopressures across a fault may enhance or diminish the sealing value of the fault. Within faulted blocks, pressure gradients usually run parallel to lithostratigraphic boundaries, and the pressure gradients across a fault may be offset by movement along the fault. Thus when high-pressured, impermeable strata are juxtaposed across the fault from and in the downdip direction of permeable, lower pressured strata, the sealing potential at the fault is enhanced. Another example is the case when under certain circumstances thick, undercompacted shales are interspersed between permeable layers. Then, movement along the fault may produce clay "smears" on the ends of permeable layers that inhibit movement of water across or along the fault (Downey, 1984).

When a permeable stratum overlays an impermeable stratum, the rotation of faulted blocks would cause any downward infiltrating water to be channeled in the downdip direction. If the flow in the downdip direction is inhibited (e.g., the juxtaposition of the impermeable layer against the permeable layer across a fault), a structural trap is produced that would permit the accumulation of infiltrating water and allow a perched aquifer to form. Perching will also depend on whether the fault/fracture zone acts as a barrier to fluid flow or a conduit. Preliminary numerical analyses of the role of fault zones have been presented by Wittwer et al. (1993), Bagtzoglou et al. (1994), and Ofoegbu et al. (1999, 2001) who indicated that, depending on the properties of the surrounding material, fault zones can interchangeably act as both barriers and conduits to flow. Similar behavior was observed by Berg and Haveman-Avery (1995) in Tertiary growth faults in the Texas Gulf coast. These faults were found to act as seals in the sheared zone and leak along the fault surface. Mineralogical changes within or between strata may also cause perched water due to a change in permeability. Such mineralogical changes within or between strata may also cause a change in permeability due to changes in volume during mineral formation. One example is the formation of relatively impermeable layers in response to alteration of primary phases,

such as feldspar to clays like kaolinite and smectite. Trends in mineralogy of this type point to areas of focused flow, and help to delineate paleohydrology. High concentrations of clays such as smectite may also serve to create low permeability zones that are favorable to the formation of perched water zones.

Perched water bodies would be more likely to form or expand under future, wetter, climatic conditions that cause increased recharge. It is possible that perched water bodies at a site under study are relict features formed by higher infiltration rates during former pluvial climates (i.e., the Pleistocene). Perched zones may also form where alluvial deposits underlie intermittent stream channels. When ephemeral stream flow saturates the alluvial material, the alluvium may remain saturated long after the stream channel is dry at the surface. Even though these perched zones would be located near the surface, the water could eventually drain through fractures to the water table below. More importantly, it is possible that water from these zones could find its way into the host rock by vertical and lateral flow along contacts at, or near locations where the waste containment horizon unit is exposed. Perched zones in alluvial material may be difficult to identify because they are probably infrequent and of short duration. However, like intermittent streams, they have the potential to form, drain, and form again.

This work addresses a specific mechanism that is known to promote the development of perched water, which is the lateral entrapment of water within dripping permeable zones due to faults or fault zones. Faults can affect groundwater in one of three general ways: (1) enhance flow rates, (2) inhibit flow, or (3) act in a neutral manner. Since this first part of a two-part paper is of a methodological nature, faults are considered to be neutral, thus only the effects of the relative positions of the layers of different, and perhaps sharply contrasted, hydrologic properties would affect the flow. Thus, the first question that needs to be answered is, *under such hydrogeological conditions, can a perched water body form and be sustained under a specific (and yet to be determined) spatially and temporally averaged recharge rate?* Furthermore, the second relevant question is, *under the aforementioned conditions, is the geochemistry of the water in the perched water body consistent with present day observations?* A modeling approach to estimate average recharge rates using a combination of hydrological and geochemical data for present-day known occurrences of perched water bodies, cast in the form of constraints, is proposed in this paper.

Perched Water Body Modeling

The conceptual model proposed herein is that faulting may create traps by placing low permeability units in contact with higher permeability units across the fault plane. With a geologic and hydrostratigraphic framework of a particular site in place, it is possible to use first-level screening to identify regions within the model where faulting might lead to conditions favorable to the formation of localized perched water zones. These areas can also be focused on in more detail to establish whether the available hydrologic and geochemical data support the formation

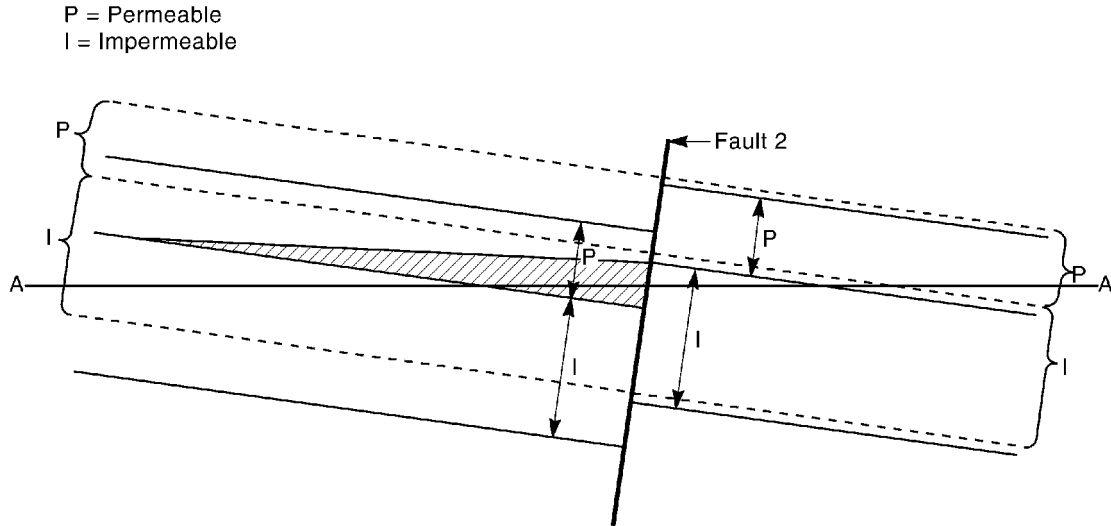


Figure 1. Cross-section (Allan Diagram) of a hypothetical normal fault-induced trap. Cross hatched areas represent potential perched water zones. The paper is the plane of fault 1 with the dashed lines representing contacts on the far side of fault 1 and the solid lines representing contacts on the near side of fault 1.

of perched water in the geologic past, present, or future. One method for evaluating fault-controlled traps has been developed for the petroleum industry (Allan, 1989). This approach focuses on constructing cross-sections in the plane of one of two intersecting faults. The volume of the trap geometry at the intersection (Figures 1 and 2) then gives an estimate of the maximum size of a potential perched water body formed by faulting. It is important to note that the use of Allan diagrams is simply an estimate of the volume contained within a geometry that is favorable to forming perched water. Depending on infiltration, a perched water zone may or may not form. Its sustainability and transient characteristics are also dependent on the infiltration and leakage rates. In unsaturated rock, there is an additional complication with the dependence of hydraulic conductivity on the degree of saturation. As saturation varies, the relative hydraulic conductivities of juxtaposed units will also vary, and because of differences in porosity and pore size, this variation is likely to be at different rates for different hydrogeologic units. At some level of saturation, the hydraulic conductivities will be equal, and as saturation decreases (or increases) past this point, the relationship between the relative hydraulic conductivities of the units in the trap may be reversed. In this fashion, the size and

occurrence of potential localized perched water bodies in unsaturated tuffs at a site may not only be a function of permeability (degree of welding, fracture density, etc.), but also a function of saturation level of the surrounding strata, which affects their hydraulic conductivity (Figure 3).

The specific questions pertaining to a perched water body system are: (1) *Can the flow system be originating from relict perched water bodies that were formed during a much wetter initial condition in the distant past?* (2) *Can these perched water bodies be sustained at present-day levels (i.e., estimated reservoir volumes) under present-day recharge conditions?* (3) *Do such sustained perched water bodies agree with ¹⁴C residence times as inferred by Percent Modern Carbon (PMC) measurements at site boreholes?*

Modeling Methodology

Numerical Procedure and Constraints Imposed

Initially, a uniform suction head value, approximately equal to the bubbling pressure of the hydrogeologic units of the site, is assigned to the entire modeled region, which is then allowed to drain under gravity with no recharge flux added to the system. This provides the initial condition that will form the basis of all subsequent flux-based simulations. Solution of the flow equation in a transient mode produces pressure head results, which are transformed to saturation values. The volume of moisture within zones that exceeds an a priori selected percent saturation value (typically 99.95%) is then calculated, thus providing perched water volume as a function of time, $V(t)$.

Hydrologic Constraints

Once the $V(t)$ relationship has been obtained for the base-case state of the flow system (i.e., no recharge flux added) the point of maximum perched water volume is used as an initial

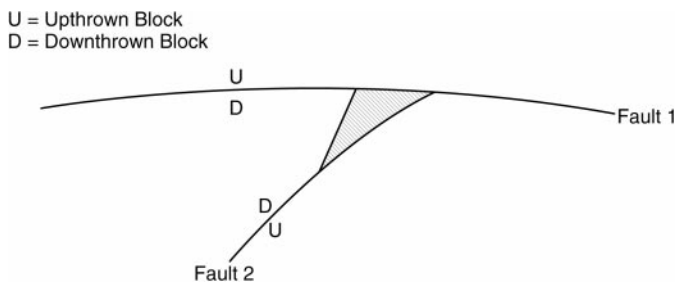


Figure 2. Plan view of the Allan Diagram at the level of A-A' in Figure 1.

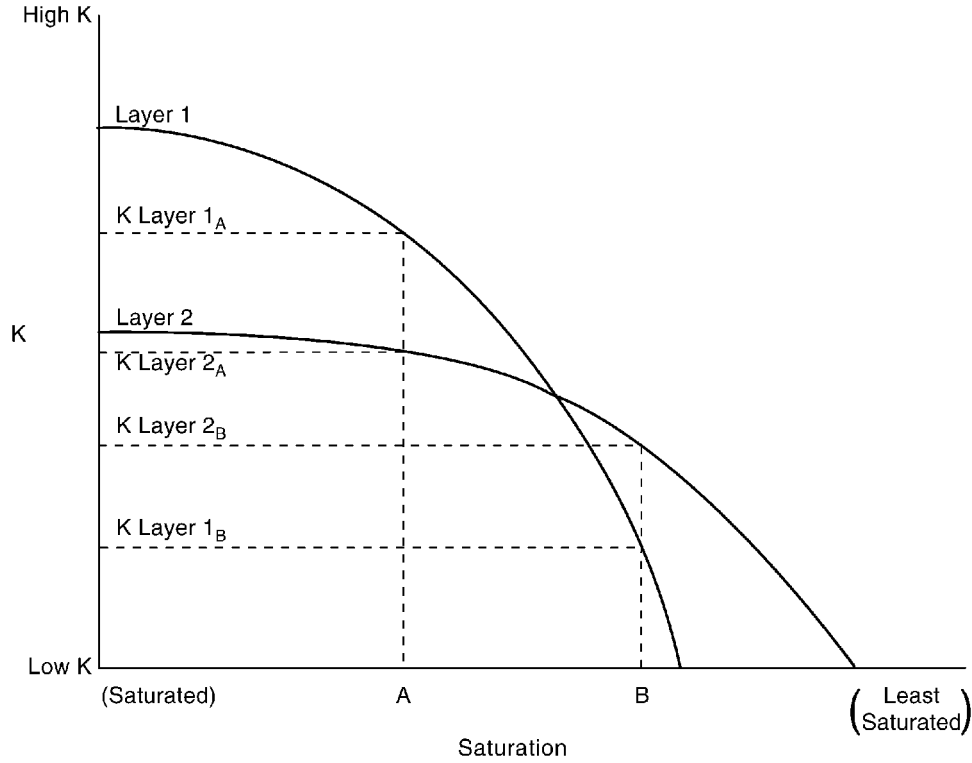


Figure 3. Schematic of unsaturated hydraulic conductivity as a function of saturation for two layers.

condition for a simulation with a uniformly distributed, prescribed flux added at the top of the domain. Depending on the value of this flux, any of the following situations is possible for the evolution of the perched water volume: (1) it could eventually go to zero (system drained), (2) it could eventually increase without bound (system flooded), and (3) it could be sustained at a steady-state level. Figure 4 depicts two cases in schematic form: (1) complete drainage and (2) attainment of a steady-state volume consistent with the observed present-day volume. Case (2) establishes the analogy between the numerical simulations and the present-day observations of the sustained character of the identified perched water bodies. Once such a match between

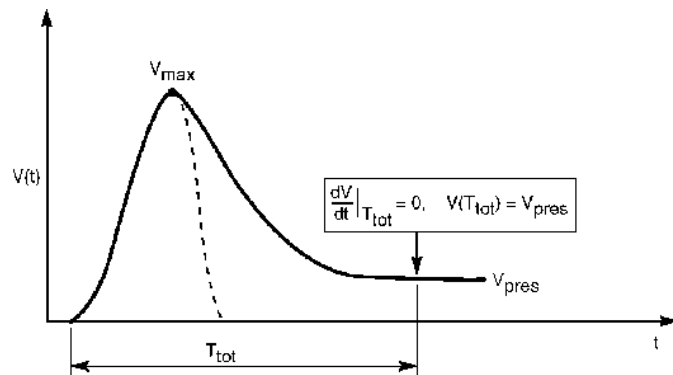


Figure 4. Schematic of perched water volume as a function of time for complete drainage and steady-state attainment simulations.

predicted and observed volumes are attained through repeated flow simulations with different input fluxes, the obtained flux is considered optimal and recorded.

As indicated in Figure 4, there exist two hydrological constraints that need to be satisfied. These are: (1) $dV/dt(t = T_{tot}) = 0$, and (2) $V(t = T_{tot}) = V_{pres}$, where V_{pres} is the observed (present-day) volume of the perched water reservoir and T_{tot} is the total simulation time. Finally, there exists an additional constraint, namely that since the present-day volume of the perched water reservoir is constant, a steady-state condition has been attained within a time period less than 18,000 to 20,000 years, which is the current-climate period. Thus, $T_{tot} \leq 20,000$ years is the third hydrological constraint that must be satisfied.

Numerical Model

In this work, all flow simulations are conducted with the BIGFLOW numerical code (Ababou and Bagtzoglou, 1993), which solves the local mass conservation equation in a slightly compressible and variably saturated porous medium without internal source/sink terms, expressed by

$$\frac{\partial}{\partial t} [M(h) + \theta(h)] = -\frac{\partial q_i}{\partial x_i} \quad (i = 1, 2, 3) \quad (1)$$

where q_i is the flux vector or specific discharge rate (L/T), h is the water pressure head, $\theta(h)$ is the volumetric water content (L^3/L^3) relative to the uncompressed soil matrix, and $M(h)$ is

an elastic storage term (L^3/L^3) due to the combined compressibility of water and solid porous matrix. $M(h)$ may be assumed negligible for unsaturated flow ($M = 0$ if $h < 0$), and proportional to pressure head for saturated flow ($M = S_s h$ if $h > 0$). S_s is the “specific storativity,” that is, the volume of water produced, per unit volume of the porous medium, for a unit decrease of hydraulic head ($L^3/L^3/L$).

The generalized Darcy equation for variably saturated flow is expressed in an arbitrary coordinate system as

$$q_i = -K(h) \frac{\partial}{\partial x_i} (h + g_j x_j) \quad (2)$$

where implicit summation on repeated indices is used. In this equation, $K(h)$ is the unsaturated hydraulic conductivity (L/T), h is the water pressure head relative to atmospheric pressure (L), negative in the unsaturated zone and positive in the saturated zone, and g_i is a cosine vector of unit length corresponding to the acceleration of gravity with a minus sign. Note that the water content $\theta(h)$ and the conductivity $K(h)$ are in general spatially variable functions of pressure head h . Inserting the Darcy equation into the mass conservation equation yields the Richards equation of unsaturated flow, here generalized to accommodate the case of a fully heterogeneous 3D porous medium

$$\frac{\partial \theta(h)}{\partial t} - \frac{\partial}{\partial x_i} \left[K(h) \left(\frac{\partial h}{\partial x_i} + g_i \right) \right] = 0 \quad (3)$$

In the case of saturated flow ($h \geq 0$), a new variable H for the total hydraulic potential is introduced

$$H = h + g_j x_j \quad (4)$$

where the summation of repeated indices is over the three dimensions. The BIGFLOW code is based on a low-order, seven-point centered finite difference scheme in space, and a fully implicit one-step (Euler backwards) finite difference scheme in time. It suffices to say that, even though the numerical model of choice here is BIGFLOW, any other code capable of simulating variably saturated flow processes could be used instead.

Although the assumptions of hydraulic and thermodynamic equilibrium inherent in volume-averaging processes—for example the equivalent continuum model (ECM)—render these models nonapplicable for simulating episodic fracture flow, the ECM is useful for evaluating critical aspects of flow and transport at fractured rock sites. In the work of Klavetter and Peters (1986) the fracture porosity, ϕ_f , can be defined as the ratio of the fracture volume to the total bulk rock volume. The matrix porosity, ϕ_m , can be defined as the ratio of the volume of the voids in the matrix (excluding fracture void space) to the volume of the matrix. An equivalent bulk hydraulic conductivity is then given by

$$K_c = K_m(1 - \phi_f) + K_f \phi_f \quad (5)$$

The ECM is based on the assumption that the pressure heads in the fractures and the matrix are identical in a plane perpendicular to flow. The more the fracture orientations become preferential, or consistent, the more this conceptual model will suffer due to the lack of anisotropic characteristics. Equation (5) implies that having identified an optimal recharge rate q , which is areally averaged over a computational cell with some (finite) support Ω (computational pixel scale), one could infer a flux rate through the fracture continuum, which is assumed here to act like a continuous porous medium with van Genuchten-Mualem unsaturated behavior (Mualem, 1976; van Genuchten, 1978), given the fracture porosity. Therefore, the recharge rates calculated by the numerical procedure, described above, could be deconvolved to matrix and fracture rates given some simplifying assumptions.

Geochemical Constraints

A means of refining computer models of flow at a site is to use available water and mineral chemistry to identify where perched water might have occurred in the geologic past. Hydrochemical facies and environmental tracers such as the stable isotopes have long been used to distinguish water bodies and to identify potential flow paths (National Academy of Sciences, 1992). Radiometric age dates can be determined for both mineral deposits and groundwaters and used to estimate rates of fluid flow and timing of changes in paleohydrological conditions.

An obvious next step in the work, presented herein, is to investigate whether ^{14}C data from the site could corroborate or refute hydrologically conditioned simulation results. Consider the mass balance of ^{14}C within a well-mixed reservoir (Pearson and Truesdell, 1978), expressed in $\text{PMC} = C/C_i$:

$$\frac{d(CV)}{dt} = Aq_i C_i - AqC - \lambda CV \quad (6)$$

where C_i is the PMC of young (present-day) water, $\lambda = 1.2097 \times 10^{-4} \text{ yr}^{-1}$ is the radioactive decay constant for ^{14}C , A is the horizontal cross-sectional area of the perched water body, and the rest of the symbols are indicated in Figure 5. The

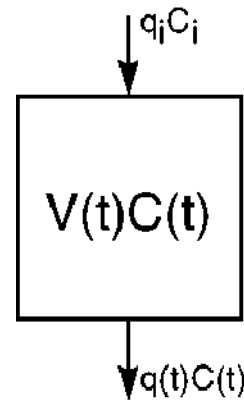


Figure 5. Schematic depicting water and ^{14}C mass balance parameters for a well-mixed perched water reservoir.

well-mixed model assumes that all sources of water input to the reservoir (fracture and matrix flow) are completely mixed with the water already in the reservoir. The lefthand side of this equation can be written as

$$\frac{d(CV)}{dt} = V \frac{dC}{dt} + C \frac{dV}{dt} \quad (7)$$

Since mass balance of water must be conserved, we have

$$V = V_o + \frac{\Delta V}{\Delta t} t \quad (8)$$

where V_o is the starting volume and

$$\frac{\Delta V}{\Delta t} = A(q_i - q) \quad (9)$$

Finally, rearranging we get

$$\begin{aligned} \frac{dC}{dt} \left(V_o + \frac{\Delta V}{\Delta t} t \right) + \frac{\Delta V}{\Delta t} C \\ = -AqC - \lambda C \left(V_o + \frac{\Delta V}{\Delta t} t \right) + Aq_i C_i \end{aligned} \quad (10)$$

and

$$\frac{dC}{dt} = - \frac{\frac{\Delta V}{\Delta t} + Aq + \lambda V_o + \lambda \frac{\Delta V}{\Delta t} t}{V_o + \frac{\Delta V}{\Delta t} t} C + \frac{Aq_i C_i}{V_o + \frac{\Delta V}{\Delta t} t} \quad (11)$$

Setting $A_1 = V_o$; $B_1 = A(q_i - q) = \frac{\Delta V}{\Delta t}$; $A_2 = Aq_i + \lambda V_o = \frac{\Delta V}{\Delta t} + Aq + \lambda V_o$, and $B_2 = \lambda \frac{\Delta V}{\Delta t}$, we get

$$\frac{dC}{dt} = - \frac{A_2 + B_2 t}{A_1 + B_1 t} C + \frac{A C_i q_i}{A_1 + B_1 t} \quad (12)$$

This equation is an ordinary differential equation that, unfortunately, has no closed form solution. In the process of arriving at this equation for ^{14}C , the following assumptions were made: (1) the influx rate (q_i) is not changing with time; (2) optimal flux estimates represent the areal average of a matrix-fracture continuum; (3) there is no daughter product contribution ($C_{\text{tot}} = {}^{12}\text{C} + {}^{13}\text{C} + {}^{14}\text{C}$); (4) the transport system is lumped, exhibiting no spatial characteristics; and (5) no ^{14}C is partitioned in liquid and gas phases. Murphy (1995) presented an exact formulation, whereby such partitioning could be incorporated in Equation (12) if so desired. Integration of Equation (12) is performed numerically using a fourth and fifth order Runge-Kutta-Fehlberg algorithm with a self-adapting time step.

The geochemical constraint that must be satisfied is that after a period of time equal to T_{tot} the ^{14}C in the perched water body cannot be substantially different than a target value, PMC_{pres} , which is what has been observed at site boreholes.

Variability in Hydrologic Properties and Latin Hypercube Sampling

In order to determine the likelihood of developing localized perched water zones, the potential for trapping and the areal extent of that perched water zone must be exhaustively evaluated. To do this, the hydraulic conductivity must be determined for all the hydrogeologic units involved at all possible saturation levels. The hydrologic effects of the difference in hydraulic conductivities of various units must also be evaluated to determine the trapping potential of all the units at all saturation levels.

Ideally, to make the best final probability estimate for the perching potential, an infinite number of combinations of hydraulic conductivity to saturation level and different saturation levels of different beds should be considered. For each of these combinations the areal extent of the region likely to become perched should be calculated. This task, however, would involve a vast number of calculations. In order to obtain sufficiently accurate results without using all possible combinations, a statistical method known as *Latin Hypercube Sampling* (LHS) was employed, within the framework of Monte Carlo simulations, to determine the overall probability of the site developing localized perched water zones.

LHS is a method of predicting the probability of an event Y that is a function of several other variables X_1, X_2, \dots, X_K . In order to obtain a representative sampling of the data without having a vast number of samples and thus calculations, certain constraints are placed upon the choice of samples. Each of the X_k variables (representing the hydrogeologic units in this case) is divided into n nonoverlapping intervals (representing permeabilities). A random sample is selected from each of these n intervals of X_1 . Likewise, a random sample is selected from each of the n intervals of X_2 . The values from the n intervals of X_1 are then paired randomly with the values of the n intervals of X_2 . This produces n paired values, which are then paired randomly with the values of the n intervals of X_3 , and so on. This process continues with the rest of the X variables to produce a representative value of permeability for the entire unit (Iman and Shortencarier, 1984).

The numerical procedure of estimating the recharge rate that would sustain a perched water body of specified volume and PMC at a site could be repeated for as many LHS property set replicates (Figure 6). By calculating statistics on the inferred recharge rate, one could make assertions regarding the variability in this rate and its sensitivity to the hydrologic property variability.

Limitations of Proposed Methodology

Climatic changes may not be the only mechanism controlling groundwater flux. It has been hypothesized that heat effects due to either reactions within the waste or near-surface diurnal processes may cause perched water zones to form. This process involves the vaporization of water around the heat source from waste heat. Water vaporized by waste heat moves away until it

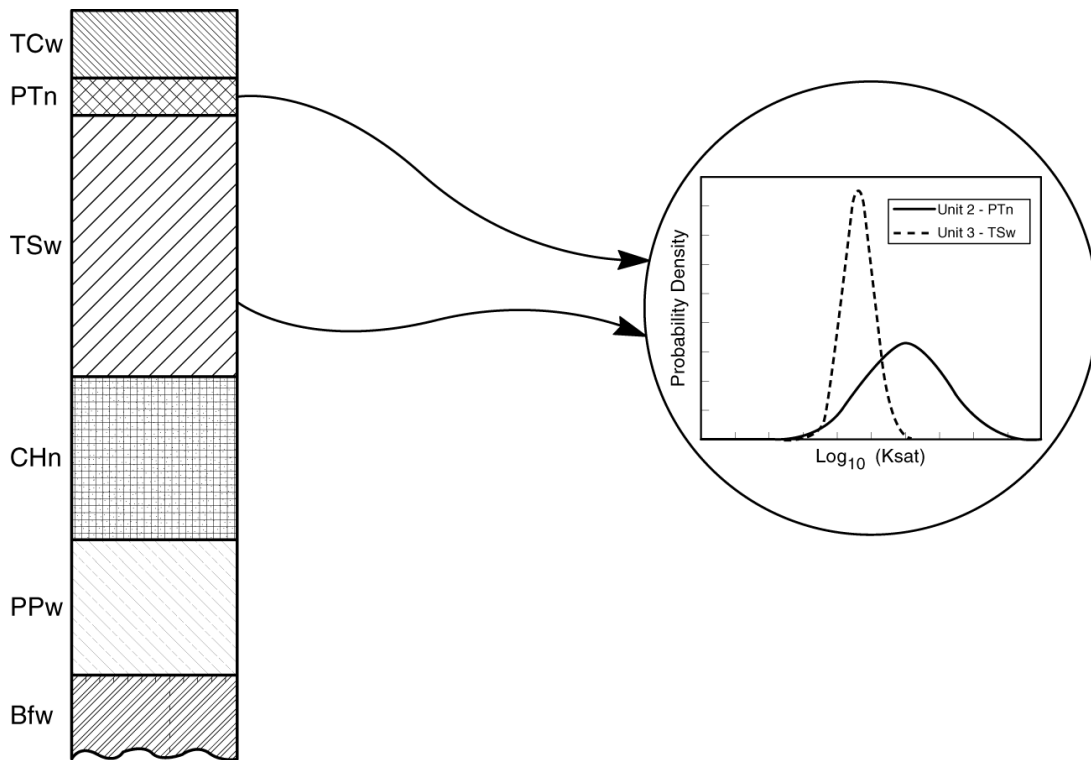


Figure 6. Schematic of LHS-based hydrogeologic unit parameter sampling.

reaches a location where the rock temperature is low enough to cause condensation. If the condensed water encounters low permeability material, rock water saturations may increase and form a perched zone. In a recent study, Ofoegbu et al. (1999) have evaluated the effects of repository-induced elevated temperatures on the formation and/or dissipation of perched water bodies. Thus, it seems that the methodology presented herein should and could be readily enhanced to account for nonisothermal effects and processes.

The transport system should be unlumped by conducting detailed transport simulations. This way, some of the simplifying assumptions, inherent in the lumped approach, will be relaxed and a more detailed ^{14}C transport process can be investigated.

Finally, another obvious area of improvement is the incorporation of fracture processes by repeating these analyses following a double porosity or stochastic approach, which could be improved by incorporating hydrologic anisotropy either within individual rock units, or within the fault zone.

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