Inverse Application of Age-Distribution Modeling Using Environmental Tracers $^3H/^3He$

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Abstract: As issues of source water protection of drinking water supplies have come to the forefront, the methodology to effectively manage semiconfined aquifers is still unclear. Commonly, the area around the wellhead is considered the most risk sensitive area, but in semiconfined settings the most sensitive areas may be located some distance away from the wellhead. This research employed the use of age-distribution modeling in concert with environmental tracers (tritium/helium-3), geochemical, and other hydrogeologic data. A synthetic test case was developed to determine the suitability of the technique for identifying localized areas of recharge to a wellhead in aquifers where evidence of modern water infiltration exists. Results of the model runs based on the synthetic test case indicate that the technique presented herein is capable of identifying localized areas of recharge contributing to a wellhead, in a semiconfined aquifer setting, with only a limited amount of required data. These results and the relative ease of application make this technique a valuable tool for obtaining a greater understanding of the flow regime at a wellhead, which in turn provides more information for risk assessment of public water supplies.

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Introduction

Source water protection strategies require detailed knowledge about the behavior of the surface water and/or groundwater system at a scale that reflects the risk to an intake or receptor. Confined aquifers are typically less susceptible to anthropogenic contamination than unconfined aquifers; however, their vulnerability should not be ignored due to the fact that confined aquifers are not always perfectly isolated systems. In many cases, source water protection plans for semiconfined aquifer settings consider the area immediately around the wellhead to be the most risk-sensitive zone requiring protection. In reality, the area requiring the more robust landuse management may be located some distance away from a wellhead at a localized recharge flux to the otherwise confined system. Aquitard windows, regions of focused recharge through an aquitard, can provide a direct conduit for potential contaminants from anthropogenic sources and elevated risk in otherwise confined hydrogeologic settings. The purpose of this research was to develop a successful method for identifying probable locations of localized recharge features to a semiconfined aquifer through the combination of geochemical, environmental isotope, and other hydrogeologic data sources. When data from these varied sources are used in conjunction with age-distribution modeling, a better understanding of the flow regime at a wellhead can be obtained. In a semiconfined aquifer, the flow contribution to a well from the various hydrogeologic pathways can be difficult to determine. The identification of an appropriate conceptual model for the age distribution of the water received at a well screen provides an estimate of the distance to the localized recharge source, along with its aerial extent. By combining data from multiple wells within a wellfield, one can identify subregions of areas contributing to recharge.

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Environmental Tracers

The environmental tracer tritium and the combined tritium/helium-3 system have been used extensively in groundwater studies to evaluate recharge rates, flow paths, flow velocities, and to ascertain the extent of contaminant plumes (Beyerle et al. 1999; Carmi and Gat 1994; Clark et al. 2004; Ekwurzel et al. 1994; Robertson and Cherry 1989; Shapiro et al. 1998; Solomon et al. 1993; 1995). The activity of tritium, a radioactive isotope of hydrogen, greatly exceeded natural levels due to above-ground nuclear weapons testing in the 1950s and early 1960s. The tritium level in the atmosphere peaked around 1963, at which time above-ground nuclear weapons testing was banned. Since the atmospheric peak, levels of tritium have steadily declined, so that current levels are essentially natural concentrations (Clark and Fritz 1997).

Tritium enters the groundwater system through recharge waters derived from precipitation. An analysis of tritium concentrations in groundwater samples can provide information concerning the time since the water was isolated from the surface. Because

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tritium has a half life of 12.43 years, water recharged near the bomb peak is difficult to evaluate in terms of age using tritium values alone (Clark and Fritz 1997). This is due to the fact that we are reaching the four half-life benchmark for tritium, meaning that metoric waters are now approaching prebomb concentrations of tritium. Tritium decays by beta particle emission to helium-3. Helium-3 is present in groundwater due to a variety of sources, including equilibrium solubility with the atmosphere, excess air above equilibrium solubility, tritium decay, nucleogenic, and mantle sources. It is necessary to isolate the tritiogenic helium-3, and this is typically achieved by calculating excess and atmospheric helium-3, and assuming nucleogenic and mantle sources are negligible for shallow systems. The combined measurement of tritium and helium-3 allows a determination of an apparent age that is independent of the tritium input function, and is instead based on the ratio of helium-3 to tritium. By measuring both the tritium and helium-3 concentrations in a water sample, a much less ambiguous age determination can be made (Clark and Fritz 1997; Solomon and Sudicky 1991).

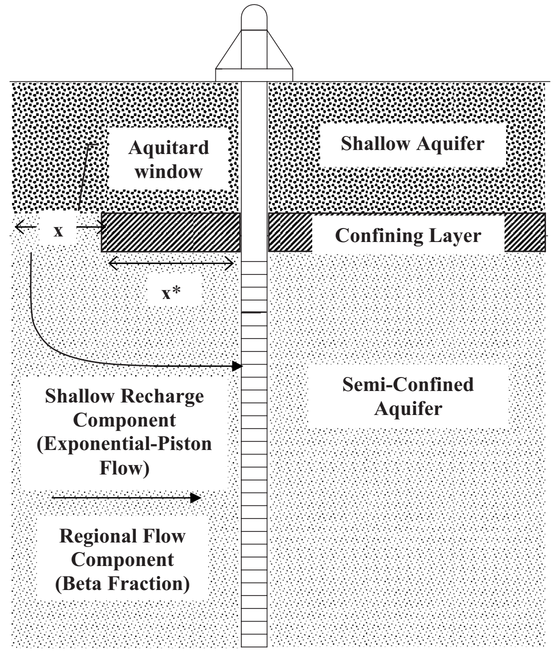
Age-Distribution Models

Age-distribution models are useful in determining the type of flow regime that best describes the makeup of the water received at a well screen. Cook and Böhlke (2000) describe four basic geometries or model types: (1) exponential; (2) linear; (3) exponential-piston flow; and (4) linear-piston flow. The benefits to these models are that less information is required than for typical modeling efforts, resulting in a less costly model development, and that the models themselves are relatively simple to implement. However, care should be taken in making sure that the conceptualized model agrees with the physical setting being modeled.

Age-distribution models are developed by assuming a function that expresses the transit time distribution of the tracer from the recharge area to its reception at a well screen or discharge site (Maloszewski 2000). The central parameter for all age-distribution models is the mean transit time, which represents a mass-weighted average of individual streamlines in the aquifer (Maloszewski 2000). Additionally, the function is normalized so that it is not dependent upon the amount of tracer that enters the system (Maloszewski and Zuber 1982). Environmental tracer data can be used to calibrate the models in order to determine which type of flow system is most reasonable (Cook and Böhlke 2000; Maloszewski 2000; Maloszewski and Zuber 1996, 1993).

Age-distribution models are simplified to assume that the system is at steady state and that spatial variations are minimal. The application of the models at individual wellheads results in the assumption of homogeneity and isotropy being more appropriate than for a model applied to a large-scale system. An additional constraint to the use of age-distribution models is that the mean transit time of a tracer will only be equal to the mean transit time of water if the tracer is injected and measured in the flux mode, and there are no zones of stagnation in the system. For environmental tracers that enter the system with recharge, this condition is automatically satisfied. Even with the simplifying assumptions required in the use of age-distribution models, the models can provide an estimate of hydrologic information that allows a meaningful interpretation of system parameters and environmental tracer transport (Zuber 1986).

Age-distribution models can provide additional insight into a system that cannot readily be obtained through other methods.



Note: Figure not to scale. Exponential age-distribution in unconfined (aquitard window location) volume; confined volume is represented by piston flow.

Fig. 1. Conceptual model of application of exponential piston model at wellhead

Most other methods require an extensive data set (which is often not available and impractical to obtain), in order to produce meaningful results. The advantage of this model type is that they are relatively easy to apply, and valuable insight can be obtained even from the interpretation of a very limited data set (Zuber and Ciezkowski 2002). Recent studies have shown that as few as two or three environmental tracer data points from only 1 year of data can be used in combination with other limited tracer data or prior knowledge to achieve a good model fit to the data (Zuber and Ciezkowski 2002).

Technique Application to Semiconfined System

For semiconfined aquifers, either the combined exponential-piston flow model or dispersion model is typically applicable due to the presence of both modern and prebomb water in the systems (Zuber 1986; Maloszewski and Zuber 1996). In the combined exponential-piston flow model (EPM), a system is modeled as having two components of flow: one having an exponential distribution of transit times, the other having piston flow distribution (Maloszewski and Zuber 1996). This is a more realistic approach for semiconfined aquifers, in that it allows for the introduction of younger waters; however those with extremely short transit times are eliminated. This model was selected for use in the current technique because it would be applicable for a typical layered semiconfined aquifer system commonly found in coastal plain geologic settings. The approach described in this paper was developed for use in the semiconfined Memphis Aquifer in Memphis, Tenn. Further details of the study site are given in the companion paper to this paper in this issue. A schematic showing the conceptual model for such a system near a wellhead receiving shallow recharge is shown in Fig. 1. The age-distribution, $g(t)$, of the EPM is represented by Cook and Böhlke (2000) as in Eq. (1)

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$$g(t)=\frac{R}{H\varepsilon}e^{[(x^*/x)-(tR/H\varepsilon)]} \quad \text{for } t>\frac{H\varepsilon x^*}{Rx} \tag{1}$$

where R=recharge through the confining unit breach (uniform, m/year); H=aquifer thickness (ft); ε=constant porosity; t=transit time (year); x=linear extent of recharge (ft); and x^*=distance to the recharge source (ft). The mean transit time, τ, is then determined from Eq. (2), given by Cooke and Böhlke (2000)

$$\tau=\frac{H\varepsilon(x+x^*)}{Rx} \tag{2}$$

The appropriate age-distribution function for the model can be used in combination with tracer information to approximate parameters for the flow system around a wellhead. The output tritium or helium-3 concentration for a water sample of mixed age in a system at steady state is determined from the use of the convolution integral. Convolution integrals are useful in many applications where the response of a system at a specified time is dependent not only on its current state, but also on its past behavior (Boyce and DiPrima 1992). This is the case for environmental tracers, where the solution is dependent upon the past history of tracer input to the system. The convolution integral represents the inverse Laplace transform of the product of the transforms of expressions for the weighting, or system response, and input functions, as shown in Eqs. (3) and (4) (Boyce and DiPrima 1992)

$$H(s)=F(s)G(s)=\mathcal{L}\{h(t)\} \tag{3}$$

$$h(t)=\int_0^t f(t-\tau)g(\tau)d\tau=\mathcal{L}^{-1}\{H(s)\} \tag{4}$$

where $F(s)$=Laplace transform of known function f (input function); $G(s)$=Laplace transform of known function g (weighting or system response function); and $h(t)$=convolution of f and g. The expression used for this research is given in Eq. (5), as represented by Cook and Böhlke (2000)

$$C_{\text{out}}(t_o)=\int_0^\infty C_{\text{in}}(t_o-t)g(t)e^{-\lambda t}dt \tag{5}$$

where C_{in}=input function for the environmental tracer; and λ=decay constant of the radioactive tracer. In cases where an older, tritium-free component of flow is known to contribute to the sample, an additional parameter, β, is used with a specified background concentration of tritium, c_β, and is added to the output concentration equation as given by Maloszewski and Zuber (1996) and shown in Eq. (6)

$$C_{\text{out}}(t_o)=\beta c_\beta+(1-\beta)\int_0^\infty C_{\text{in}}(t_o-t)g(t)e^{-\lambda t}dt \tag{6}$$

where β=fraction of water that is tritium free; and c_β=tritium concentration of the β fraction. Similarly, output concentrations for helium-3 can also be determined. Since helium-3 is produced by the beta decay of tritium, the equation is altered to account for ingrowth, as shown in Eq. (7)

$$C_{\text{out}}(t_o)=\beta c_\beta+(1-\beta)\int_0^\infty C_{\text{in}}(t_o-t)g(t)(1-e^{-\lambda t})dt \tag{7}$$

The limits of integration for the convolution integrals are chosen based upon the tracer being used in the study. In the case of tritium, it is acceptable to set the lower limit at a few years prior to the increase in atmospheric tritium in the mid 1950s (Maloszewski and Zuber 2002). The upper limit is set depending upon the expected mean transit times, to include all input data that might be contributing to the observed output concentrations. The upper limit can be determined experimentally by adjusting the value until negligible changes are observed in the solutions with the inclusion of additional years of input data (Zuber 1986).

For most real-world situations, it is common to have data available for the output concentration of environmental tracers, while certain input parameters are unknown. For such a case, the inverse problem is applied to determine appropriate parameter values. Thus, for this research, an inverse solution procedure was developed so that the technique would be suitable for real-world scenarios. It was assumed that for many cases, the parameters of interest (x, x^*, β, R) would be unknown, while measurements of tritium and helium-3 concentrations would be available for use as calibration targets. Additionally, geochemical modeling (equilibrium and mixing models) can be used to determine estimates of shallow water contribution to production wells, via an aquitard window. This would allow an estimate of the β parameter to be used as prior information. The use of estimates of x^* as prior information was also investigated, since locations of known surface or subsurface features that could provide pathways for hydraulic communication might also be available.

Inverse Code Implementation

The inverse procedure used in this research was UCODE, a universal inverse modeling code developed for the USGS by Poeter and Hill (1998). UCODE is universal in that it can be applied to any application model, as long as specific instructions are followed for extracting parameter values and running the application model. This code was selected for incorporation into this study because it is freely available and widely used by many groundwater professionals. Nonlinear regression is used to solve the parameter estimation problem by minimizing a weighted least-squares objective function. Weights reflecting measurement error are assigned to observations and prior information by the user. The form of the objective function used in UCODE is given in Eq. (8) (Hill 1998)

$$S(\mathbf{b})=\sum_{i=1}^{ND}\omega_i[y_i-y_i'(\mathbf{b})]^2+\sum_{p=1}^{\text{NPR}}\omega_p[P_p-P_p'(\mathbf{b})]^2 \tag{8}$$

where $\mathbf{b}$=vector containing values of each of the parameters being estimated; ND=number of observations; NPR=number of prior information values; y_i=ith observation being matched by the regression; $y_i'(\mathbf{b})$=simulated value which corresponds to the ith observation; P_p=pth prior estimate included in the regression; $P_p'(\mathbf{b})$=pth simulated value; ω_i=weight for the ith observation; and ω_p=weight for the P_p=pth prior estimate (Hill 1998). A modified Gauss–Newton method is employed within UCODE to adjust parameters to obtain a solution that minimizes the objective function (Poeter and Hill 1998). The modified version of the Gauss–Newton method used in UCODE is also called a Levenberg–Marquardt method. The Marquardt parameter is added to the regression to ensure that the parameter values used in successive iterations are better than the values in the previous iterations (Sun 1999). A damping parameter is also incorporated to damp oscillations and to make certain that maximum changes in parameter values remain within specified limits (Hill 1998). The form of the modified Gauss–Newton method used in UCODE is given in Eqs. (9) and (10) (Hill 1998)

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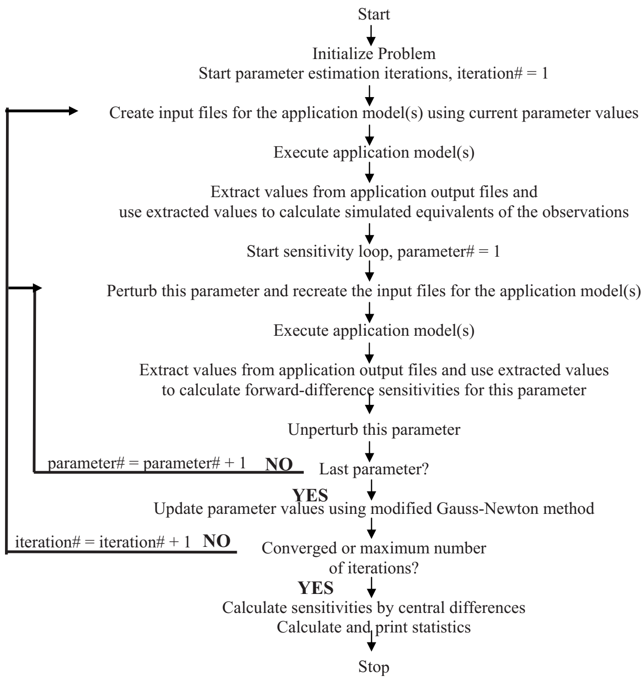
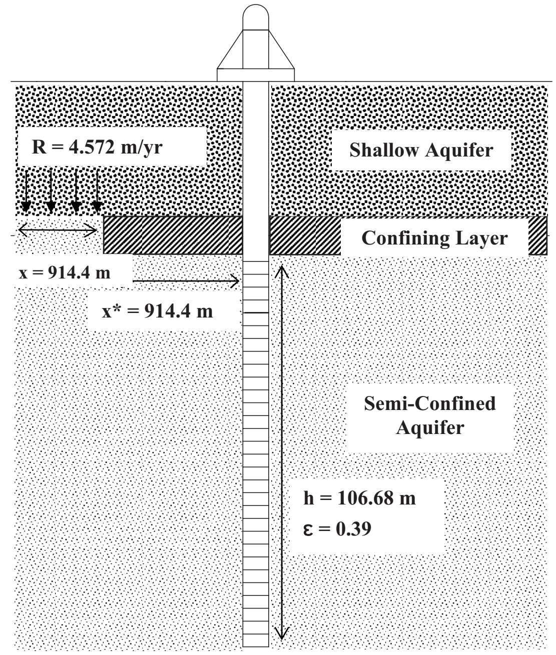


Fig. 2. Flowchart showing interaction between age-distribution algorithm and UCODE



Note: Figure not to scale. Exponential age-distribution in unconfined (aquitard window location) volume; confined volume is represented by piston flow.

Fig. 3. Semiconfined aquifer test case

$$(C^T X_r^T \omega X_r C + \mathrm{Im}_r) C^{-1} d_r = C^T X_r^T \omega (y - y'(b_r)) \tag{9}$$

$$b_{r+1} = \rho_r d_r + b_r \tag{10}$$

where r=parameter-estimation iteration number; X_r=sensitivity matrix evaluated at parameter estimates b_r, with elements equal to $\partial y_i' / \partial b_j$; ω=weight matrix; $(X^T \omega X)$=symmetric, square matrix of dimension NP (number of parameters) by NP that is used to calculate parameter statistics; C=diagonal scaling matrix with element c_{jj} equal to $[(X^T \omega X)_{jj}]^{-1/2}$; d_r=vector with the number of elements equal to the number of estimated parameters; I=NP dimensional identity matrix; y=observation being matched by the regression; y'=simulated value corresponding to the observation; m_r=Marquardt parameter; and ρ_r=damping parameter (Hill 1998). An algorithm compatible with UCODE requirements was written to solve the convolution integral for this research.

Numerical integration was incorporated to solve for output concentration values of tritium and helium-3 to be compared with available observations. The mean age of the water sample, as given by Eq. (2), was also computed for comparison with available age measurements. The mean age and output tritium and helium-3 concentrations were printed to a file for extraction by UCODE, so that parameter estimation iterations could be performed. A flowchart showing its connection to UCODE is shown in Fig. 2.

The numerical integration scheme employed within the age-distribution application model was the composite Simpson's 1/3 rule for equally spaced data, appropriate for the annual data used for this model. An additional requirement of this technique is that an even number of intervals be used in the approximation. A method with a lower error term was not necessary because of the anticipated accuracy limitations of the data to be used in the model. Simpson's 1/3 rule and its associated error term are given in Eqs. (11) and (12) (Hoffman 1992)

$$I = \tfrac{1}{3} h (f_o + 4f_1 + 2f_2 + 4f_3 + \dots + 4f_{n-1} + f_n) \tag{11}$$

$$\text{Error} = O\left(\frac{1}{n^4}\right) \tag{12}$$

where h=interval spacing; f_n=value of the function at point n; O represents a numerical coefficient for error associated with Simpson's 1/3 rule; and n=number of data points.

Synthetic Test Case

In order to evaluate the techniques capability of solving for various window recharge parameters, a synthetic test case was created. Thus, the system would be noise free and a demonstration of performance and utility could be assessed. The test case was developed to evaluate the ability of the age-distribution inverse method to estimate the window recharge rate (R), distance to the recharge source (x^*), extent of recharge feature (x), and fraction (β) of submodern water comprising a sample from a well receiving both modern and submodern components of flow, in a semiconfined aquifer. The test case was utilized to determine the number and type of observations required for a unique convergence. Additionally, it was important to evaluate the effect of using prior information available for certain parameters to determine if this information was necessary for model convergence. It was also important to determine whether or not parameter estimation would be significantly improved with the use of prior information. The goal of the synthetic test case was to determine the minimum amount of data required to effectively use the technique in a semiconfined aquifer setting, so that it could be applied by other investigators.

The test case used for evaluation of the current research methodology consists of a fully penetrating well screened in a semiconfined aquifer adjacent to a recharge source. A schematic of the semiconfined aquifer test case is shown in Fig. 3. A forward model run for the application code was executed based on the

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Table 1. Forward Model Results for Semiconfined Aquifer Test Case

Observation dates and selected model output[a]	Forward model results
^{3}H-2002	1.918
^{3}H-2000	1.853
^{3}H-1998	2.054
^{3}H-1996	2.540
^{3}H-1994	3.311
^{3}H-1992	4.367
^{3}H-1990	5.707
^{3}H-1988	7.333
^{3}H-1986	9.243
^{3}H-1984	11.440
^{3}H-1982	13.918
^{3}He-2002	5.405
^{3}He-2000	6.206
^{3}He-1998	7.278
^{3}He-1996	8.553
Mean age (τ, years)	18.2

[a] ^{3}H and ^{3}He units are TU.

selected test case parameters. Model estimates for tritium and helium-3 were extracted from the output file, to be used as observations in the subsequent inverse model runs. The results of the forward model run for the semiconfined aquifer test case are shown in Table 1. Various scenarios were tested to determine the amount of information available from the observations to estimate each parameter. For scenario one, the inverse model only estimated the values of the window recharge and the extent of the window feature parameters (R, x). The next two scenarios were constructed to estimate three parameters each (x, R, β or x, x^*, R). The final scenario was created to estimate all four parameters of interest (R, β, x, x^*). In the initial inverse model runs for the various scenarios, no error in the observations or prior information on parameters was included. Additionally, a fairly large data set $(n=15)$ was used as observation data.

Results

Search Parameter Sensitivities

The two-parameter model converged with errors of less than 1% regardless of the starting parameters, resulting in a unique solution, as shown in Table 2. The standard error of the regression was very low, and the correlation coefficient was always nearly equal to 1. The inverse models that were constructed to estimate three or more parameters did not converge to a unique solution without the inclusion of prior information. Model input values were varied by 10–30% percent of the known values, and solutions converged to values with associated errors as much as 25%. Composite scaled sensitivities were calculated within UCODE for each model run, as shown in Fig. 4.

Model runs were next conducted using prior information on x^* and β. A unique calibration was achieved in both the three and four parameter models by using prior information on β for the model estimating x, R, β, and prior information on β and x^* for the four-parameter model. Convergence within 1% of known values was achieved for the three-parameter model with prior information on β, regardless of starting parameters. The use of prior

Table 2. Initial Model Results for Semiconfined Aquifer Test Case (No Observation Errors or Prior Information Included)

Observation dates and selected model output	Forward model results	Simulated values—model estimating x, R
^{3}H-2002 (TU)	1.918	1.919
^{3}H-2000 (TU)	1.853	1.853
^{3}H-1998 (TU)	2.054	2.054
^{3}H-1990 (TU)	5.707	5.708
^{3}H-1984 (TU)	11.440	11.440
^{3}He-2002 (TU)	5.405	5.405
^{3}He-2000 (TU)	6.206	6.206
^{3}He-1998 (TU)	7.278	7.278
x (m)	914.4	914.1
x^* (m)	914.4	NA[a]
R (m/year)	4.572	4.573
β	0.75	NA[a]
Standard error of regression	—	0.00352
r^2	—	1.000

[a] NA = not available.

information on x^* did not allow a unique calibration to be achieved for the model estimating x, x^*, R. For the four-parameter model, convergence within 5% of known values was achieved, regardless of starting parameters, with the use of prior information on β and x^*. When prior information on x^* was removed from the four-parameter model, unique convergence was still achieved, with the greatest error in parameter estimates being less than 6%. Although prior information was not specifically given for the values of x and x^*, reasonable maximum and minimum values were entered into the model to limit the search space based on known hydrologic and geologic data. The actual values for the observation data are shown in Table 3, along with the model estimates using prior information. The composite scaled sensitivity of β increased by 92% with the addition of prior information on the parameter, as shown in Fig. 5.

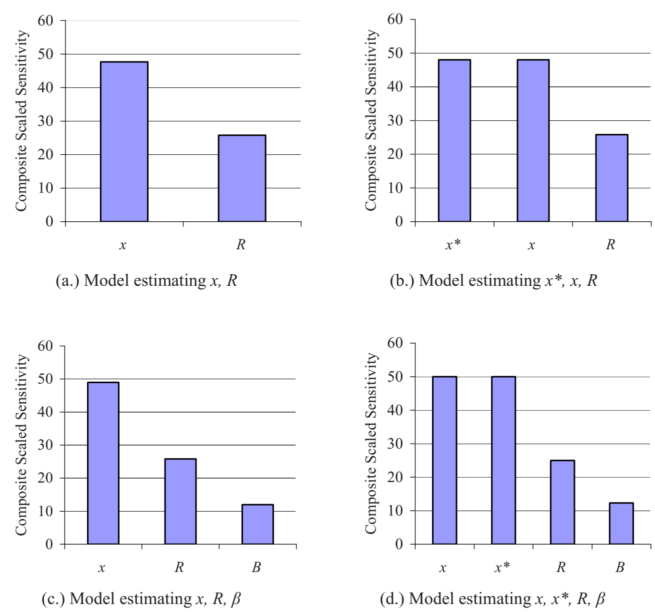

Fig. 4. Composite scaled sensitivities for semiconfined aquifer test case (no observation error, no prior information)

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Table 3. Model Results for Semiconfined Aquifer Test Case (Prior Information Included, No Observation Error)

Observation dates and selected model output	Forward model results	Simulated values—model estimating x, R, β	Simulated values—model estimating x, x^*, β, R	Simulated values—model estimating x, x^*, β, R (no prior on x^*)
^{3}H-2002 (TU)	1.918	1.919	1.919	1.919
^{3}H-2000 (TU)	1.853	1.853	1.853	1.853
^{3}H-1998 (TU)	2.054	2.054	2.054	2.055
^{3}H-1990 (TU)	5.707	5.708	5.708	5.709
^{3}H-1984 (TU)	11.440	11.440	11.440	11.441
^{3}He-2002 (TU)	5.405	5.405	5.405	5.405
^{3}He-2000 (TU)	6.206	6.206	6.207	6.207
^{3}He-1998 (TU)	7.278	7.278	7.278	7.278
x (m)	914.4	914.1	868.7	968.7
x^* (m)	914.4	NA	867.1	969.1
R (m/year)	4.572	4.573	4.573	4.573
β	0.75	0.750	0.750	0.750
Standard error of regression	—	0.00353	0.00496	0.00387
r^2	—	1.000	0.998	0.998

Impact of Number of Observations

Once it had been determined that the method in this research was capable of uniquely estimating all four parameters of interest, the remainder of the model runs were focused on this scenario, since all four parameters were likely to be of interest in future investigations. Subsequent model runs were developed to determine the minimum number of observations that would be required to estimate all four parameters, and the effect of observation error on the resulting solutions. The effect of observation error was evaluated by introducing a random error to each observation that ranged from 0 to 10%. The upper limit of 10% was used because of the expected high accuracy and precision of the methods used in determining the tritium and helium-3 values from field samples in the Memphis aquifer. It should be noted that this value was chosen based upon values measured from the Memphis aquifer, and the precision could be less in hydrogeologic conditions differing from the Mississippi Embayment, where geogenic sources of ^{3}He may be much more significant. The conditions and precision of the methodology are presented in detail by Bayer et al. (1989) and Solomon and Cook (2000).

The model converged uniquely when estimating all four parameters and the above described observation error was included. The values obtained from the model simulation including observation error are shown in Table 4, along with the actual values for the test case. Dimensionless sensitivities are shown in Table 5.

In the next set of model runs, observations were removed from the input data set in order to determine the minimum required data set. The observation data for tritium from 1984 and 1990 were both removed, along with the observation for helium-3 in 1998. These were removed because they represented older historical data which carry a significant amount of information, but that

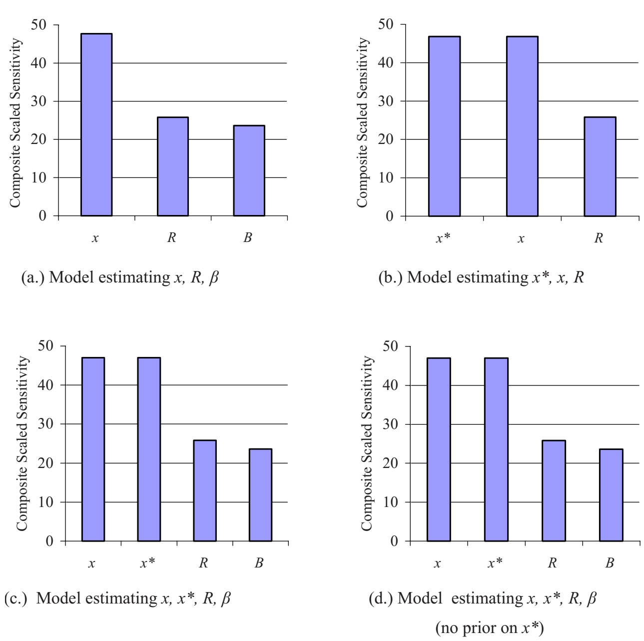

Fig. 5. Composite scaled sensitivities for semiconfined aquifer test case (prior information included; no observation error)

Table 4. Model Results for Semiconfined Aquifer Test Case (Observation Error and Prior Information Included)

Observation dates and selected model output	Forward model results	Simulated values—model estimating x, x^*, R, β
^{3}H-2002 (TU)	1.918	1.967
^{3}H-2000 (TU)	1.853	1.922
^{3}H-1998 (TU)	2.054	2.144
^{3}H-1990 (TU)	5.707	5.856
^{3}H-1984 (TU)	11.440	11.606
^{3}He-2002 (TU)	5.405	5.762
^{3}He-2000 (TU)	6.206	6.618
^{3}He-1998 (TU)	7.278	7.736
x (m)	914.4	916.6
x^* (m)	914.4	933.9
R (m/year)	4.572	4.414
β	0.75	0.750
Standard error of regression	—	0.18420
r^2	—	0.998

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Table 5. Dimensionless Scaled Sensitivities for Semiconfined Aquifer Test Case (Observation Error and Prior Information Included)

Observation date	x^*	x	β	R
^{3}H-2002	14.3	−14.3	−7.07	−6.21
^{3}H-2000	13.9	−14.0	−6.89	−7.72
^{3}H-1998	15.7	−15.7	−7.78	−9.57
^{3}H-1990	44.8	−45.0	−22.6	−18.9
^{3}H-1984	90.0	−90.3	−45.6	−28.0
^{3}He-2002	44.1	−44.2	−22.2	−35.4
^{3}He-2000	50.8	−51.0	−25.7	−40.6
^{3}He-1998	59.6	−59.8	−30.1	−45.6

are less likely to exist in typical settings. It was important within this research to identify minimum data requirements for successful model calibration. The models resulted in a unique solution regardless of starting parameters; however, the loss of the observation data from the earlier years resulted in reduced composite scaled sensitivities for the parameters, and increased error in the parameter estimates. This is due to the fact that a large amount of information for estimating x, x^*, and β had previously been obtained through the tritium observations from 1984 and 1990. The greatest contribution for the estimate of R had been obtained from the helium observation from 1998, which was also removed for this simulation. The simulations were run with and without observation error. The observation error had a greater effect on the model with fewer observation points than it had with that containing the early-year data. The model results from the simulations with the early-year observation data removed are shown in Table 6. Dimensionless scaled sensitivities are shown in Table 7.

An evaluation of sensitivities indicated that, as with previous model runs, the greatest amount of information from the observations was available for the estimation of x and x^*, while the least amount of information was available for β. The helium-3 observation from 2000 provided the most information toward the estimation of all four parameters. A final set of model scenarios was evaluated to determine the impact of removing an additional tritium or helium-3 observation. If starting parameters were fairly close to the true values (within 15%), models converged to values that were within about 5% of actual parameter values. However, if starting parameters were much different than actual values, the models converged to parameter values that had very large (more than 50%) errors in the estimate of x. Thus, a unique convergence was not achieved when additional tritium or helium values were removed, indicating that a minimum required data set had been identified.

Table 7. Dimensionless Scaled Sensitivities for Semiconfined Aquifer Test Case (Early Observation Data Removed; No Observation Error)

Observation date	x^*	X	β	R
^{3}H-2002	17.6	−17.3	−7.46	−7.20
^{3}H-2000	16.7	−16.5	−7.08	−8.86
^{3}H-1998	18.6	−18.3	−7.89	−11.0
^{3}He-2002	52.5	−51.6	−22.6	−38.9
^{3}He-2000	60.5	−59.5	−26.1	−45.2

Results of the test case runs, as shown in Tables 2–7, indicate that it is not necessary to have a long record of tritium input values for the estimation of all four parameters in question (R,β,x,x^*), as long as helium-3 measurements and prior information on β are available. It is not possible to uniquely determine the four parameters without the combination of tritium and helium-3 values. Because helium-3 is the daughter product of tritium decay, the concurrent measurements provide a great deal of information as to the age of the water, which restricts the possible solutions. Without the information provided by helium-3, the solution cannot be determined because the concentrations could be observed in several types of flow regimes. Helium-3 observations pinpoint whether the system in question has rapid or slow turnover times, thus marking the point in time at which recharge occurred.

Discussion

Data Requirements and Model Convergence

For the test case, a minimum of two helium-3 measurements, and three tritium measurements were required for a unique solution when estimating all four parameters. This represents data collected over only 3 years. This makes this approach very attractive, in that a minimal amount of observation data is required. In

Table 6. Model Results for Semiconfined Aquifer Test Case (Early Observation Data Removed)

Observation dates and selected model output	Forward model results	Simulated values—model estimating x, x^*, R, β (no observation error)	Simulated values—model estimating x, x^*, R, β (observation error included)
^{3}H-2002 (TU)	1.918	1.939	2.064
^{3}H-2000 (TU)	1.853	1.842	1.969
^{3}H-1998 (TU)	2.054	2.026	2.172
^{3}He-2002 (TU)	5.405	5.408	5.854
^{3}He-2000 (TU)	6.206	6.210	6.726
x (m)	914.4	914.5	818.2
x^* (m)	914.4	835.1	937.3
R (m/year)	4.572	4.733	4.673
β	0.75	0.750	0.750
Standard error of regression	—	0.0215	0.0841
r^2	—	0.999	0.999

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many cases, a good portion of this data may already exist, requiring the collection of only a small amount of additional data in order to apply the technique.

Convergence problems can occur if composite scaled sensitivities for any parameter are less than about 0.01 times the largest sensitivity value (Poeter and Hill 1998). This difficulty was not encountered in any of the model scenarios tested. The composite scaled sensitivities for the various model types indicate that the tritium and helium-3 observation data provide the most information toward estimating x and x^*, and the least amount of information in the estimation of the β parameter. Dimensionless scaled sensitivities provide information about the importance of each observation to each of the parameters. In general, the early-year tritium and helium-3 data provided more information for the estimation of the parameters. Tritium observation data from the 1980s and early 1990s in the test case yielded much higher dimensionless scaled sensitivity values for x, x^*, and β. This is due to the variability of the tritium input function, and its continued decline from peak values after the ban on above ground nuclear weapons testing. Observations from these years would have recharge components with a much stronger tritium signal, thus the information provided by these values is less ambiguous than tritium observations from more recent years. It should be noted that an independent estimation of β may be used to constrain the inverse model by comparing the tritium value from the ${}^3H/{}^3He$ to the tritium input function (Manning et al. 2005). This may provide further stability in the overall estimation of the remaining parameters.

Helium-3 observations were only used in the test case for the years 1998, 2000, and 2002. This is due to the fact that the technique of age dating with tritium/helium-3 is relatively new, so it is unlikely that data would actually be available for helium-3 for years prior to the mid 1990s. Thus, simulations were performed for the test case with only the observations that were likely to exist in real-world scenarios. Regardless, the helium-3 values from all three dates provided a significant amount of information to the estimation of the parameters, with all four values having high dimensionless scaled sensitivities to helium-3 observations. As the tritium signal continues to decay, it will become increasingly important to collect combined tritium/helium-3 data to avoid ambiguity from a weak tritium signal.

Impact of Prior Information

The test case results also indicate that it is important to have prior knowledge about the composition of the water sample in terms of the percentage of submodern water. Prior information on β improved the regression significantly. This type of information can readily be estimated using major ion water chemistry and free equilibrium geochemical and mixing software, such as NETPATH (Plummer, et al. 1991), to determine the percentage of shallow water and unaffected semiconfined aquifer water that comprise a particular sample. In the test case, a lower weight indicative of a standard deviation of 10% was applied to the prior information for the β parameter. This weight was applied so that the model was allowed to converge to β values within the range of expected accuracy of the estimate, rather than being required to converge to a specific value of β.

Prior information on x^* did little to improve the regression results, as shown in Tables 2–7 and Figs. 4 and 5. This is mainly due to the fact that observation data already provided a significant amount of information toward the estimation of that parameter. The additional information provided by the prior information only reduced errors by about 1%. Because prior knowledge about the location of the recharge source is not required, the applicability of this method is broadened to incorporate systems where little hydrogeologic information is available. It is much more expensive to obtain the data necessary to identify sources of recharge to serve as prior information, whereas it is relatively inexpensive to collect geochemical data in order to obtain prior information on β. Although prior information was not specifically given for the values of x and x^*, it is necessary to constrain the search space to reasonable maximum and minimum values based on known hydrologic and geologic data.

Conclusions

Several conclusions can be drawn from the results of this investigation. The EPM, when used in combination with environmental tracer data and geochemical information, is capable of identifying the location of a source of recharge to a well screened in a semiconfined aquifer. Using two helium-3 measurements and three tritium measurements, all four parameters of interest: (1) linear extent of recharge region $[x]$; (2) distance from the well to the recharge source $[x^*]$; (3) fraction of tritium free water $[\beta]$; and (4) the recharge flux $[R]$, can be uniquely determined in the presence of observation error as long as prior information is available for β; however, it is not necessary to have prior information on x^* for a unique solution to be obtained. Additionally, the number and type of observations (tritium or helium-3) available for calibration have a direct impact on the ability of the technique to converge to a unique solution.

The benefit of this technique is that recharge locations can be reliably identified with only a small amount of observation data. The minimal data requirement makes the technique unique, in that most modeling efforts require extensive data sets over long periods of record. The results of this study as applied to wellheads screened in the Memphis aquifer in Memphis, Tenn., will be presented in a subsequent paper. The study will demonstrate how multiple wells may be used in conjunction to identify the most probable locations of leakage features.

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Notation

The following symbols are used in this paper:

- $\mathbf{b}$ = vector containing values of each of parameters being estimated;
- C = diagonal scaling matrix;
- $C_{\mathrm{in}}(t)$ = input function for environmental tracer;
- C_{out} = output concentration of environmental tracer;
- c = tritium concentration;
- d_r = vector with number of elements equal to number of estimated parameters;
- $F(s)$ = Laplace transform of known input function;
- $G(s)$ = Laplace transform of known system response function;

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$g(t)$ = age-distribution function;
H = aquifer thickness;
$H(s)$ = system response function;
$h(t)$ = input function;
m_r = Marquardt parameter;
ND = number of observations;
NPR = number of prior information values;
P_p = Pth prior estimate included in regression;
$P_p'(b)$ = pth simulated value;
R = recharge through confining unit breach;
R = parameter estimation interation number;
T = mean transit time;
t = transit time;
X_r = sensitivity matrix evaluated at parameter estimates;
$(X^T \omega X)$ = matrix used to calculate parameter statistics;
x = linear extent of recharge;
x^* = distance to recharge source;
y_i = ith observation being matched by regression;
$y_i'(b)$ = simulated value which corresponds to ith observation;
β = fraction of water that is tritium free;
ε = constant porosity;
λ = decay constant of radioactive tracer;
ρ = damping parameter;
ω_i = weight for ith observation; and
ω_p = weight for pth prior estimate.

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