Calibration of models using groundwater age

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The need for groundwater age data

There have been substantial efforts recently by geochemists to determine the age of groundwater (time since water entered the system) and its uncertainty, and by hydrologists to use these data to help calibrate groundwater models. This essay discusses the calibration of models using groundwater age, with conclusions that emphasize what is practical given current limitations rather than theoretical possibilities.

From a research perspective, it can be argued that the conservation equations imposed in groundwater models make them most useful for providing fundamental insights into how systems operate. Yet from a water-manager perspective, water-use decisions must be made, and thus models are created as mathematical representations of aquifer systems in order to compile all of the available information into a tool that honors the physics and chemistry of the system. The compiled information will include prior knowledge of hydrogeologic framework parameters, but as the values and spatial distribution of those parameters are never completely known, hydraulic data are used to further constrain them during calibration. These hydraulic data can be divided into two categories: potentials (heads or water levels) and fluxes (direct measurements or indirect estimates). Having only head values will result in a nonunique answer with no optimal solution; flux information of some kind (whether prescribed or estimated) must be included during calibration.

Direct measurements of fluxes could include those of recharge, baseflow, or well pumpage. In many geographic regions (arid climates, for example), data or estimates for the first two are often not available. Pumpage data are frequently available, but the flow is often small compared to regional flow and, thus, although adding pumpage data may reduce nonuniqueness, large uncertainties in the estimated parameters often remain. Indirect estimates of fluxes could include those of recharge (using water budget methods) or environmental tracers. Tracers include data such as temperature, chemical concentrations, or apparent age interpreted from the chemistry. Age is proving to be a widely used (Kazemi et al. 2006; Bethke and Johnson 2008) flux indicator, although it is not independent of the effective porosity, which will be discussed shortly.

Advective-age simulation

Groundwater cannot be dated directly—only an "apparent" age can be obtained. For any idealized parcel of groundwater, hydrodynamic dispersion (mixing) always combines molecules that have individual ages that are unknowable. The apparent age is an interpretation of tracer concentrations that gives some average age of the molecules. In spite of this, neglecting dispersion is often still a useful first-order approximation. In one-dimension this is often called "piston-flow" or "hydraulic age" and can be calculated using Darcy's Law. Another analytical approximation assumes a specific two-dimensional flow field to obtain an "average" age for a well. An example is an exponential mixing model that assumes an even recharge distribution and a homogeneous aquifer with finite thickness (Cook and Bohlke 1999). The hydraulic-age approximation is often extended to two and three dimensions as an "advective age" using a pathline post-processing program (e.g., Pollock 1994) in conjunction with a flow model (e.g., Harbaugh 2005). Advective-age calculations provide a straightforward way to visualize approximate age distributions within flow systems. Simulated observations of advective age have been used to calibrate models, but differences between apparent-tracer and simulated-advective ages often remain unresolved (Weissman et al. 2002).

Simulations that include hydrodynamic dispersion should produce more realistic environmental-tracer (and thus age) distributions. One proposed method for this is "direct" age simulation, where assigning a uniform source term of unity to the advection-dispersion equation simulates "age" directly as the dependent variable (Goode 1996). This method is also known as the "age-mass" method because age mimics the role of chemical mass in the mass-balance equation (Bethke and Johnson 2002). Also, a value of zero age is assigned as an initial condition

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and to incoming fluids. The resulting simulation tracks the effect of dispersion on age, and at steady state yields the age distribution for a flow system.

Direct-age simulation

The advantage of direct-age simulation is its simplicity. The disadvantage is that it usually does not represent how a specific tracer disperses. The tracers used to estimate age are typically either those that decay exponentially over time, or have a transient input signal that is not linear in time. The nonlinear transient behavior causes the dispersive fluxes of these tracers to be different from those produced by the constant source in direct-age simulation. The error introduced by this can potentially be of similar magnitude to that of neglecting dispersion. An exception could be for tracers such as helium (in-grown) which behaves similar to the distributed source term. Solving the advection-dispersion equation for the specific tracer(s) of interest and then comparing simulated and observed tracer concentrations would be the most accurate calibration method, but given the substantial computational effort that simulating dispersion requires, neglecting it would be more computationally advantageous. So is neglecting dispersion a viable alternative?

Young-age tracers such as tritium and chlorofluorcarbons have time-varying input signals that often create relatively sharp concentration gradients in shallow aquifers. Dispersion in these environments has been shown to have an effect on the interpreted age (Plummer et al. 1993), and some error will be introduced if it is neglected. Old age tracers such as ^{14}C and ^{36}Cl, however, have input signals that changed very gradually with time (Kalin 2000; Park et al. 2002). In these cases, the decay produces a larger effect on the gradient than the input transients. These gradients are slight enough that longitudinal dispersion usually creates only minimal additional change in the concentrations (Johnson and DePaolo 1996). So neglecting dispersion for old-age tracers could be justified on these terms. Stagnant zones, however, such as aquitards and rock matrixes, can still create a loss of a long-lived tracer that is not accounted for by advection alone (Sudicky and Frind 1981; Sanford and Buapeng 1996; Sanford 1997).

Impediments to age-based calibration

One must also consider the certainty to which the values of dispersivity (and their distribution in space) are known for the setting and scale of the field site of interest. For regional-scale studies, dispersivities are often used based on measurements reported from wells (Gelhar 1986). More detailed studies (Leblanc et al. 1991), however, suggest the former may substantially overestimate dispersivity at the kilometer and greater scale. Given this uncertainty in scale-appropriate dispersivity values, does their inclusion improve model accuracy, or would neglecting dispersion be no less accurate? One could make an argument for the latter in many situations.

Age determination is also complicated by the mixing that occurs in conduits just before discharge, either in well casings or at springs. Water samples always contain molecules that have all taken different flow paths and distances to arrive at the sampling location. The mixing that occurs near the discharge site may often exceed that which has occurred within the flow system. This is especially true for long-screened wells and convergent flow fields. An attempt to account for this effect at wells is often made by backward tracking of multiple pathlines along the well-screen length or around the spring discharge location. Large pumping rates can also distort the flow field and age distributions (Zinn and Konikow 2007) and should be included in simulations when appropriate. Springs are typically focal points of highly convergent discharge, and therefore often contain "mixed" ages that can be identified when multiple tracers are used. One approach to calculate the age distribution within a sample would be to simulate the effects of dispersion in the flow system upstream of the sampling point (Varni and Carrera 1998; Perrochet and Etcheverry 2000; Cornaton and Perrochet 2006). This approach requires knowledge of the dispersivity upgradient from the sample location.

Given these potential impediments to accurate age determination and simulation, expectations for groundwater age as a calibration tool may need to be lowered. When age is used in model calibration, the fit virtually always appears to be poorer than a similar fit to hydraulic head. Examples of this difference for regional-scale models can be dramatic (Fig. 1), as even on a log-log scale the fit for age data is visually worse than that for head data. This is not unexpected, however, as hydraulic head is a relatively smoothly varying potential field, and age is based on the first derivative (velocity) of the potential field. Heterogeneity and rolling topography amplify this effect such that local groundwater divides can create large age gradients at scales that are too small to be incorporated into the model. So, given the difficulty in obtaining a "good" fit to observed ages, can ages still help improve estimates of model parameters? Before addressing this, the role of porosity in simulated-age calculations must be considered.

The role of porosity

Simulated age is calculated by dividing the distance traveled by the seepage velocity, which is calculated by dividing the Darcy flux by effective porosity. Therefore, age can only be used to calibrate the ratio of the flux to the effective porosity. This flux is often controlled most directly by a specified recharge rate, and so if either fluxes or effective porosity are relatively well known, observed ages can help to constrain the other. Thus, the usefulness of age as a calibration tool depends on the environment where it is being applied. In humid environments, recharge is usually less difficult to estimate than in arid environments, where it is more variable in time and space. Likewise, the effective porosity of unconsolidated sediments is usually easier to estimate than that of fractured bedrock. So in a humid climate with uncon-

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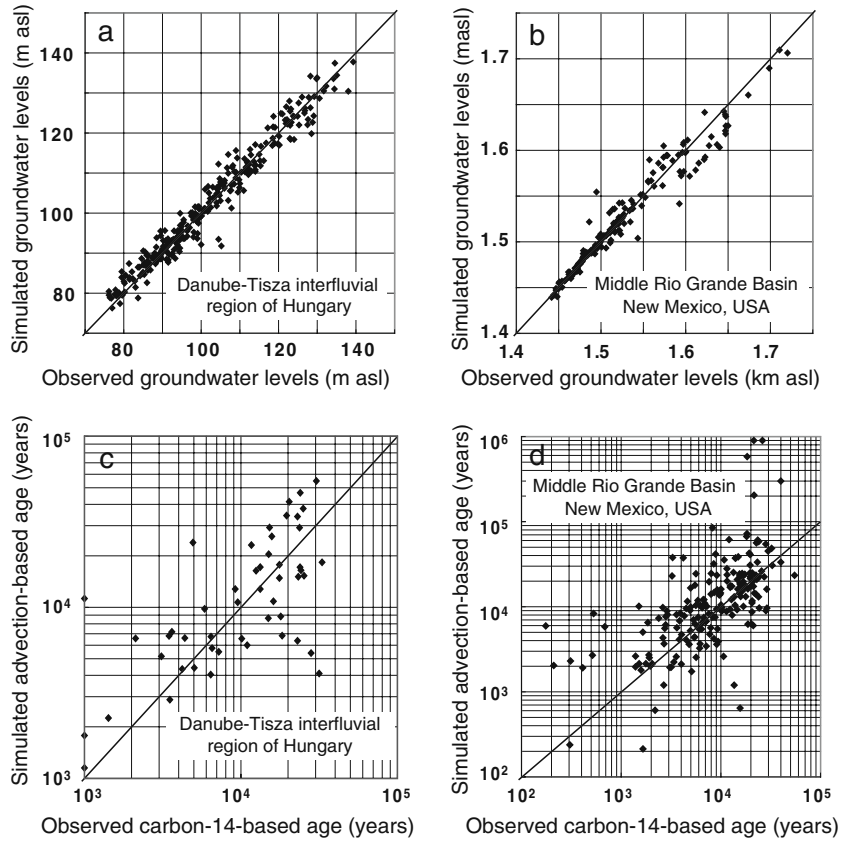

Fig. 1 Plots of observed versus simulated water levels in a regional flow system in **a** Hungary and **b** New Mexico, USA; and observed versus simulated ages in **c** Hungary and **d** New Mexico (Sanford et al. 2001, 2004)

solidated sediments, both recharge and porosity may already be somewhat constrained, and age may only add marginal improvement to the overall calibration (unless large-scale variability in recharge, porosity, or hydraulic conductivity exist). In a humid climate with fractured rock or an arid climate with unconsolidated sediments, age may substantially help to constrain effective porosity or recharge rates, respectively. This assumes the tracer ages are reliable given the problems of matrix diffusion and input signal variability. In an arid climate with fractured rock, age may not be useful in constraining either recharge or effective porosity, but only the ratio of the two.

Practical considerations

Given that ages have potential as a calibration tool, one needs to compare the benefit of different age-simulation

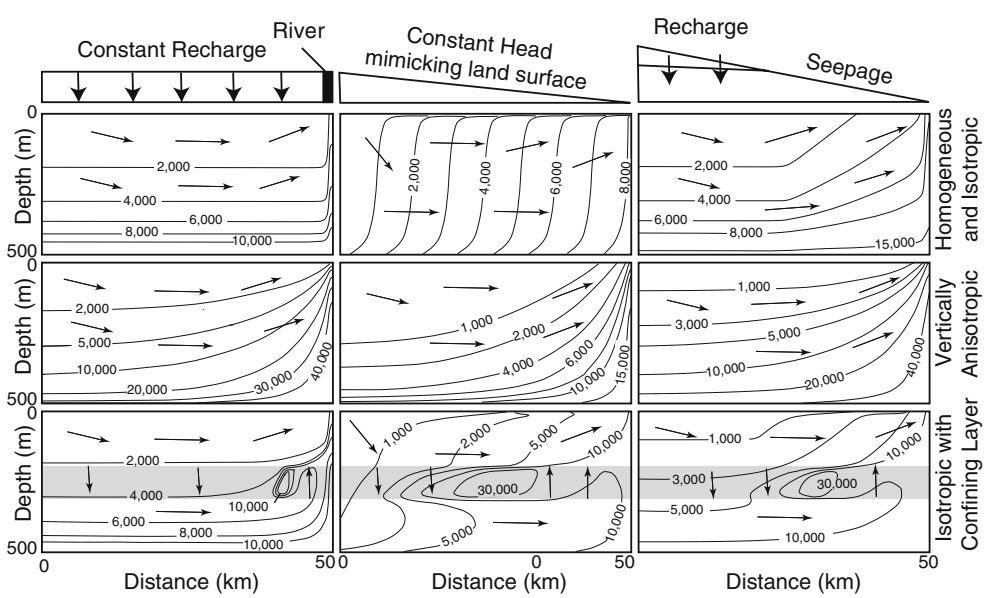

Fig. 2 Spatial patterns of groundwater age as a result of various distributions of recharge and hydraulic conductivity (*K*). *Contour values* are age in years. *Arrows* show general direction of flow. The vertical anisotropy ratio in the middle set of simulations is 10,000:1 (horizontal to vertical). The confining-layer contrast in *K* in the lower set of simulations is 1000:1

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techniques with their computational requirements. Simulation of the advection-dispersion equation requires grid resolution criteria to be met in order to obtain numerically stable and accurate results. One- or two-dimensional simulations can usually be discretized to a fine enough degree to incorporate realistic dispersivity values (given they can be estimated somehow). Three-dimensional simulations are much more challenging. To incorporate horizontal dispersivities on the order of meters and vertical dispersivities of <1 m into a regional model of tens of kilometers across or more by hundreds of meters deep is intractable with today's computers (Sanford and Pope 2010). Also, the simulation of dispersion is not an option for current local-grid refinement techniques. But because dispersion may not be critical for old-age tracers, regional models with coarser discretization could still be useful coupled with advection-only age simulation.

Spatial variability in recharge or hydraulic conductivity will create markedly different age distributions (Fig. 2). For example, constant recharge in space leads to horizontal isochrones (lines of equal age), but variable recharge can create substantial vertical gradients in age. Some of these patterns can also be seen in simple previous models of expected age distributions (Goode 1996; Cook and Bohlke 1999). Also, if the model paradigm is one of a homogeneous, anisotropic system, then age gradients will exist both horizontally and vertically, but overturned ages (younger underlying older water) cannot exist (Fig. 2). Such overturned ages have been observed at field sites, and can only exist where substantial vertically layered heterogeneity is present (Fig. 2). This sensitivity of age to vertical hydraulic conductivity is fortuitous, because vertical conductivity is usually much more poorly constrained than horizontal conductivity. It is clear from these arguments that even when neglecting dispersion, tracer ages are still data that are valuable for model calibration.

In conclusion, the mixing of ages within flow systems and in wells have forced geochemists and hydrologic modelers alike to consider and address how one might include dispersion in the simulation of tracers and apparent ages. This inclusion is feasible today in one or two dimensions, but tracer simulation in three dimensions on regional scales is not practical with realistic dispersivities (assuming they are known in the first place) on today's computers. However, the great sensitivity of age to heterogeneity within flow systems means that advection-only simulation of age is still a very valuable approximation in many situations. Therefore, development of new and better techniques for both measuring and simulating groundwater age should continue.

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