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Approximating groundwater age distributions using simple streamtube models and multiple tracers



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ABSTRACT

We use a streamtube based decomposition and a recently developed, simple relationship between tracer concentrations and ages to estimate groundwater age distributions. The decomposition assumes that an age distribution can be approximated using a superposition of linearly independent streamtubes. Transport in each streamtube is modeled with inverse Gaussian functions, the parameters of which are inferred from radiometric tracer concentrations. Three simple sampling methods are considered for weakly and moderately heterogeneous aquifers and the method gives reasonable approximations in both systems. The method is sensitive to errors in the measured concentrations but some of these errors are easily identifiable and a range of plausible age distributions can still be found. The method was then tested in a highly heterogeneous system and reasonable estimates of the age distribution were also obtained. The simplicity of this method and its insensitivity to the heterogeneity structure suggest that this approach may be an effective tool for obtaining estimates of age distributions in natural systems.

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1. Introduction

Groundwater age distributions have a wide range of potential applications in hydrogeology, including model calibration, reactive transport, risk assessment, sustainability studies, and reservoir characterization (e.g. [21,41]). Age distributions are useful in all of these applications because the same hydrodynamic processes that affect the migration of dilute solutes also affect age distributions ([19]). The age of an individual water molecule of groundwater can be defined as the amount of time that has elapsed since it was last exposed to the atmosphere. Any sample of water is a collection of molecules and represents a mixture of water of different ages; the age distribution is simply the histogram (or probability density function) of all the ages present in the sample. The shape of an age distribution reflects many of the heterogeneities in the subsurface that can usually only be inferred from an artificial tracer test and this has substantial implications for parameter estimation and high-resolution groundwater modeling [16,21]. However, the real problem lies in identifying the age distributions in natural systems and this practical challenge limits their application in hydrologic problems.

Age distributions can be generated analytically by solving the age equation in simple cases [19] or from numerical flow and

transport models [37,39,45,47]. The numerical models can include complicated processes, such as mass transfer, reactions, and transient conditions such as pumping or seasonal flow variations [10,20]. Detailed models must be realistic to be useful but they will still have large uncertainties associated with their parameter specification and these uncertainties may cause the results to be unreliable [44]. Even in a well-defined, realistic model there is still no guarantee that the modeled ages reflect the actual distribution because age cannot be directly measured and validating the model based on tracer concentrations can also be difficult.

Measured concentrations of geochemical tracers can also be used to determine ages but they are not without complications. Many different tracers can be used, including radiogenic isotopes and anthropogenic compounds, and the way ages are determined is dependent on the tracer [8]. Geochemical tracers are often assumed to give an estimate of the mean age (first moment of the age distribution) under an assumption of piston or plug flow, but this will be inaccurate is the higher moments of the distribution are non-zero [46]. The term "apparent age" is often used to describe tracer ages because many unknown or unaccounted for factors, like dilution or borehole mixing, may have affected the measured tracer concentration or the interpretation of the concentration as an age [2,45,49]. The effects of dilution and mixing on measured concentrations are difficult to isolate and even the installation of monitoring wells can affect the age distribution [48]. Lumped parameter models (LPMs) (see [51]) are able to

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account for some of these complicating factors by assuming the form of an age distribution and then use multiple tracers to constrain the parameters of that distribution (e.g. [1,3,9,50]) but it should be noted that the distributions are assumed. The simplified models often cannot represent broad distributions with heavy, old age tails (i.e. high positive skew), or multi-modal distributions (e.g. [25]) but LPMs can still be useful, particularly when coupled with a mixing model that accounts for some of these effects. Multiple tracers acting on different time scales or measured at different times can be used to improve age estimates [9] and Bayesian inference can also provide improvements, as demonstrated by Massoudieh et al. [36]. The obvious limitation to geochemical methods is that, in most cases, we are limited to using whatever tracers are already present in an aquifer because forced or injected tracers cannot provide the same extent of characterization [30] and may alter the flow field in the natural system. Furthermore, if time series data has not already been collected, a single sampling event may not be sufficient for a LPM, even if multiple tracers are sampled.

Mechanistic connections between the age distributions and measured tracer concentrations are also powerful tools. The difference between these studies and the LMPs are that transport processes are not treated solely as a "black-box" that produces an assumed distribution, and a model is used to generate age distributions and tracer concentrations which are then compared. For example, Weissmann et al. [47] simulated CFC concentrations and age distributions in a heterogeneous aquifer. The concentrations were used to estimate the mean age and those were then directly compared to the simulated mean age distribution. Other mechanistic studies include Varni and Carrera [46], Castro and Goblet [7], Loáiciga [33], Larocque et al. [28], and Eberts et al. [15] but most require detailed flow and transport models and are time consuming to construct. Despite the progress that has been made through these studies, there is still no single methodology that can provide reliable estimates of age distributions across the full range of complex heterogeneity structures present in natural aguifers. New methods continue to be developed to address this problem and it is important to consider the circumstances that they perform well under so that more progress can be made toward the accurate identification of groundwater age distributions.

Recently, Massoudieh and Ginn [35] (abbreviated as M&G hereafter) showed that a unique relationship exists between the measured concentration of a radiogenic tracer and the groundwater age distribution, specifically that a measured, normalized concentration of a decaying tracer defines one point on the Laplace transformed age distribution (see Section 2.1). Conceptually, this result is similar to the relationships shown by Varni and Carrera [46], but this relates concentrations directly to age distributions and not the moments of the age distribution (however, we note that if a distribution is Gaussian the first two moments are sufficient for describing it). If the shape of an age distribution can be parameterized, the number of different tracers required to uniquely define the age distribution is exactly the number of parameters that describe the distribution. This relationship provides a direct link between an analytical model of tracer migration and the groundwater age distribution. The approach is promising and could potentially be used to construct age distributions more easily than previous approaches, but the method was only outlined by M&G and remains untested.

The purpose of this article is to evaluate the method of estimating age distributions that was outlined by M&G in a practical context for several synthetic aquifers with increasingly complicated heterogeneity structures. This departs from many of the previous studies on age because we focus exclusively on approximating the entire age distribution at a sampling location, as opposed to the mean age at a point or the distribution of mean ages in an aquifer. Moreover, the method differs from LPMs because only a single

sampling event in time will be used. Our approach uses a streamtube ensemble based conceptual model for flow and transport, which is then used to generate estimates of the age distributions (Section 2). The example applications herein are based on numerical simulations in synthetic aquifers to eliminate uncertainty about the structure, sources, or boundary conditions of the example problems; however, we do consider how the introduction of measurement and model error will affect the results. Different combinations of tracers and sampling schemes are evaluated in our efforts to improve the results obtained from the basic M&G method while maintaining a focus on simplicity. This study shows that reasonable estimates of groundwater age distributions can be found using the M&G approach for all the heterogeneity structures we consider.

2. Groundwater age

Groundwater age emerges as a special case within the general concept of residence time or exposure time. Residence time received its first rigorous treatment in the chemical engineering literature decades before making its way into hydrology (e.g. [11,32]). In the 1980's, additional developments by Maloszewski and Zuber [34] and Campana [5], amongst others, highlighted some of the applications of age in a hydrologic context. More recently, age has been used in a variety applications ranging from groundwater (e.g. [22,30,45,47,49]) and watershed modeling (e.g. [4,14,40]) to ocean circulation and mixing (e.g. [12,13]). However, regardless of the physical processes being considered (i.e. ocean, aquifer, or watershed), the fundamental concepts of an age or residence time distribution remain the same, and the governing equations are almost identical. This article exclusively focuses on the case of groundwater age but the concepts can certainly be applied elsewhere.

The governing equation of groundwater age describes how the mass density of water is distributed over space, time, and age. The method we are evaluating uses 1-D effective representations of age and the corresponding form of the governing differential equation for the age distribution of a single aqueous phase is:

$$\frac{\partial \rho(x,t,a)}{\partial t} + \frac{\partial \rho(x,t,a)}{\partial a} + \upsilon \frac{\partial \rho(x,t,a)}{\partial x} - D \frac{\partial^2 \rho(x,t,a)}{\partial x^2} = 0 \tag{1}$$

where ρ is the distribution of the aqueous phase mass density, x is the spatial coordinate, t is time, a is age, v is the velocity (m/d), and D is a hydrodynamic dispersion coefficient (m^2/d) [17]. This equation describes how the water mass itself is distributed over the space, time, and age dimensions and the conventional mass density is recovered by integrating (1) over the age dimension. Ginn [19] derived a more general, multi-dimensional form of Eq. (1) that included spatially variable velocity and dispersion coefficients, and other forms of the age equation are given by Goode [22], Varni and Carrera [46] but our focus is on the solutions of Eq. (1) for simplicity. Note that if the mass density has reached a steady state, the time derivative in Eq. (1) is zero and the resulting equation is the constant coefficient transport equation with age substituting for time and the mass density replacing concentration.

Basic connections between age and transport can be established conceptually with nothing more than a rudimentary understanding of flow and transport. If it is assumed that a dilute tracer moves with a discrete packet of water, and an ensemble of those packets represents a distribution over age, it is straightforward to recognize that the solute mass will also be distributed over the age dimension [42]. More rigorous connections involve the moments of transport and age [23] or the physical mechanics of flow [19,21], but the close relationship between transport and age is, potentially, a very powerful link.

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