Residence Time Distribution in Dynamically Changing Hydrologic Systems

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1 Introduction

Age distributions (ADs) encapsulate the net flow and transport characteristics of natural reservoirs. In particular, ADs represent the time of exposure of water to the system’s biogeochemical conditions, and therefore are a key control on the transformations taking place. This research focused on quantifying the effect that dynamic flow conditions due, for example, to anthropogenic forcing or weather and climatic variability, has on modeled ADs of regional groundwater systems and hyporheic zones. For the purposes of this proposal we did not focus on anthropogenic effects but rather natural forcings. Here, age is defined as “the amount of time that has elapsed since a particular water molecule of interest was recharged [or entered the system] into the subsurface environment system until this molecule reaches a specific location in the system where it is either sampled physically or studied theoretically for age dating.” Closely related, residence time (RT) is “the time it takes for a parcel of water to travel from the recharge area to the discharge area in the system”. We refer to the age distribution (AD) or residence time distribution (RTD) when considering a representative fluid parcel, which cannot be defined by a single value but for a distribution.

Currently, there is a fundamental gap in the understanding of ADs for dynamically changing systems. With the exception of some recent applications (Kollet and Maxwell, 2008; Woolfenden and Ginn, 2009), steady-flow is generally assumed and modeled and/or measured ages neglect the transient nature of the forcings which is inherited by the system (e.g., Kirchner et al., 2000; McGuire and McDonnell, 2006; Cardenas, 2007). However, these hydrologic systems, particularly shallow aquifers, hillslopes, and hyporheic zones, can change dramatically at different time scales from
diurnal to decadal and longer. This gap translates into uncertainty for the interpretation of environmental tracer data, particularly it makes hard to quantify how much information about the real AD can be extracted from this data. This is crucial in several applications of groundwater age such as the evaluation of contaminant migration, design of nuclear repositories, inference of flow paths and recharge areas, evaluation of aquifers as storage reservoirs, and estimation of aquifer parameters, among others.

The NM WRRI student grant allowed the awardee to explore some of the fundamental aspects of theory and modeling of age distributions, leading to several conference presentations in national conferences and two proposals submitted to the National Science Foundation (NSF). Also, two publications are in preparation for peer-review journals. From a hydrologic perspective, this work has important implications at short spatial scales such as the hillslope scale (e.g., Fiori and Russo, 2008; Fiori et al., 2009) where the transport of solutes to the stream has an important control at the watershed scale; however, even though these systems respond to short time scale forcings and are strongly influenced by weather variability, the RTDs are estimated experimentally through tracer tests (e.g., McGuire and McDonnell, 2006) and numerically (e.g., Dunn et al., 2007; McGuire et al., 2007; Fiori and Russo, 2008) under the steady-flow assumption. Also, the hyporheic zone, which is a highly dynamic system, varying at different spatio-temporal scales, is explored under similar assumptions (Haggerty et al., 2002; Cardenas, 2008) with the exception of some restrictive applications (Boano et al., 2007). Furthermore, the knowledge produced in this proposed research can be transfered to atmospheric and oceanic sciences, where similar problems are encountered in the interpretation of environmental tracers or the estimation of ventilation rates with general circulation models (see Haine and Hall, 2002).

2 Mathematical and numerical modeling

In this section, the generalized age equation is introduced together with an application to regional groundwater flow systems.

2.1 Modeling of the groundwater age

The concept of age density or age distribution has been widely used to understand natural and man-made reservoirs in chemical engineering, and oceanic, atmospheric
and hydrologic sciences (e.g., Bolin and Rodhe, 1973; Delhez et al., 1999; Ginn, 1999). This function, defined as positive definite, splits the density of water into continuous age classes, then the age density function \( \rho(x, t, \tau) \) represents the contribution of material with an age \( \tau \) to the conventional water density \( \rho^T(x, t) \) so that

\[
\rho^T(x, t) = \int_0^\infty \rho(x, t, \xi) d\xi
\]

where \( x = (x, y, z) \) is the position vector at any point in the domain \( \Omega \), \( t \) is time \( (t \geq 0) \) and \( \tau \) is age \( (\tau \geq 0) \).

Ginn (1999) and others (e.g., see Delhez et al., 1999, for the case of pure fluid reservoirs) showed that \( \rho \) satisfies the partial differential equation

\[
\frac{\partial (\theta \rho)}{\partial t} + \mathcal{G}(\rho) + v_a \frac{\partial (\theta \rho)}{\partial \tau} = 0
\]

This expression is known as the governing equation for groundwater age (GWAE) in the hydrology literature and, as demonstrated by Ginn et al. (2009), it encapsulates previous equations for the transport of different measures of age such as the mean age equation (Goode, 1996), the percentile age and momentum equation (Varni and Carrera, 1998), and the aquitard age equation (Bethke and Johnson, 2002, 2008).

Equation (2) is analogous to the advection-dispersion equation (ADE) but in a five-dimensional space (3D space - time - age), where \( \mathbf{v}(x, t) = (v_x, v_y, v_z) \) is the pore velocity, \( \theta(x) \) is the porosity, \( v_a = 1 \) is the aging rate for the advective transport in the age dimension, and \( \mathcal{G}(\rho) = \nabla \cdot (\mathbf{v} \theta \rho) - \nabla \cdot (\theta \mathbf{D} \nabla \rho) \) is the transport operator that, in this example, includes advection, diffusion and dispersion, where the dispersion diffusion tensor \( \mathbf{D} = \{D_{ij}\} \) is defined as (Bear, 1972):

\[
D_{ij} = \alpha_T|\mathbf{v}| \delta_{ij} + (\alpha_L - \alpha_T) v_i v_j / |\mathbf{v}| + \omega D_m
\]

with \( \alpha_T \) and \( \alpha_L \) the transversal and longitudinal dispersivities, \( \omega \) the tortuosity, \( D_m \) the coefficient of molecular self-diffusion, and \( \delta_{ij} \) is the Kronecker delta function.

Eq. (2) assumes no internal sources (e.g., recharge) or sinks (e.g., withdrawals). The initial condition for age density in the time dimension, \( \rho_0(x, \tau) \), is generally unknown and depends on the system's geological evolution, presence of formation water, and flow history, which is dictated by climatic variability. In this regard, the influence of formation water is particularly important in geologically recent aquifers (e.g., sedimentary formations) where the initial condition becomes more important and uncertain (Varni and Carrera, 1998). The example for regional groundwater systems,
presented in the next subsection, assumes that all the water in the system has an initial age zero \( \rho_0(x, \tau) = 0 \), leading to the analysis of the evolution of groundwater age in a system forced with current climatic conditions and ignoring the flow and transport history. This assumption limits the generality of the conclusions, but it is still able to provide insights about the net flow and transport characteristics of the system. A more adequate approach would be to apply a transient forcing in spinup mode until a dynamic equilibrium is obtain, but this is computationally more demanding. Then, the initial condition is

\[ \rho(x, t = 0, \tau) = \rho_0(x, \tau) \]  

(4)

Also, the initial condition in the age dimension is given by

\[ \rho(x, t, \tau) = 0^- \]  

(5)

where the distinction of \( 0^- \) is made to acknowledge the possibility a discontinuity in the age distribution at zero due to a source of instantaneous material.

Initial conditions, boundary conditions and sources/sinks terms for physical interfaces depend on the flow characteristics, application and features to be highlighted. For instance, the age of incoming water flowing through a physical interface (e.g., recharge \( R \)) is prescribed to be zero (ignoring residence time in the vadose zone), defining age as the time since water entered the system, and then the boundary condition at the inflow area can be expressed as

\[ n \cdot (\nu\theta \rho - \theta D\nabla \rho) = -R\delta(\tau) \]  

(6)

where \( R \) is the incoming flux (or recharge), \( \delta \) is the delta Dirac function, and \( n \) is the outward unit vector.

If new water of age \( \tau_S \) is introduced into the aquifer, for example by an injection well, at a rate \( S \) in the location \( x_S \), a new production term \( p = S\delta(x - x_S)\delta(\tau - \tau_S) \) has

Figure 1: Schematic representation of the domain \( \Omega \). Boundaries are defined by the flow field as: (i) in-flow \( (\partial\Omega_1) \), (ii) out-flow \( (\partial\Omega_2) \), and (iii) no-flow \( (\partial\Omega_3) \).
to be added to the right hand side of Eq. (2). In general, the age of the new material is set to zero \((\tau_S = 0)\), but this term could be used to represent the introduction of water with a given age.

Similarly, new water entering the system through the inflow areas will have an age distribution concentrated at zero age, then the boundary condition mimics the introduction of an ideal tracer that marks the water at the inflow boundaries

\[
\rho(x, t, \tau) = \delta(\tau) \tag{7}
\]

The complete mathematical statement for modeling the groundwater age in a general domain (see Fig. 1) is:

\[
\frac{\partial (\theta \rho)}{\partial t} + \mathcal{G}(\rho) + \frac{\partial (\theta \rho)}{\partial \tau} = 0 \tag{8a}
\]

\[
\rho(x, t, \tau) = \delta(\tau) \quad \text{on } \partial \Omega_1 \tag{8b}
\]

\[
n \cdot (\theta D \nabla \rho) = 0 \quad \text{on } \partial \Omega_2 \tag{8c}
\]

\[
n \cdot (v \theta \rho - \theta D \nabla \rho) = 0 \quad \text{on } \partial \Omega_3 \tag{8d}
\]

\[
\rho(x, t, \tau = 0^-) = 0 \tag{8e}
\]

\[
\rho(x, t = 0, \tau) = \rho_0(x, \tau) \tag{8f}
\]

This model simplifies for steady-state flow (\(\mathcal{G}\) has no time-dependence), since the age density not longer depends on time \((\rho(x, t = 0, \tau) = \rho(x, t, \tau))\). Then, the derivative respect to time in Eq. (8a) and the boundary condition in time, expressed in Eq. (8f), disappear, leading to the traditional advection-dispersion equation (ADE) with time replaced by age.

The age density of water leaving an outflow boundary \(\Gamma\) is calculated as the flux-weighted average of \(\rho\) over the boundary

\[
R_\Gamma(t, \tau) = \rho(x, t, \tau) \bigg|_{x \in \Gamma} = \frac{\int_\Gamma (\mathbf{n} \cdot \mathbf{v}) \rho(x, t, \tau) dx}{\int_\Gamma (\mathbf{n} \cdot \mathbf{v}) dx}. \tag{9}
\]

### 2.2 Regional groundwater systems

The classical regional groundwater system (RGS) is represented by a cross-sectional Tothian-like domain (Tóth, 1962, 1963, 2009), filled with a homogeneous and isotropic porous media (See Figure 2). The system is bounded by the water table at the top
and impermeable boundaries on the other three sides. Ignoring the effects of storage for this application (assumes transport time constant $\gg$ compressible storage time constant; verified by simulation using typical parameters), the porous media flow will be modeled by Darcy’s law and the continuity equation for incompressible flow in a non-deformable media (groundwater flow equation):

$$\nabla \cdot (K \nabla h) = 0$$

(10)

where $h(x, t)$ is hydraulic head, $t$ is time, $x = (x, y)$ is the spatial location vector, and $K$ is the hydraulic conductivity tensor. No-flow, $n \cdot v = 0$, boundary conditions are used for the bottom and sides ($\Omega_3$ for age modeling). The pore velocity is derived from Darcy’s law as $v = -(K/\theta) \nabla h$, $\theta$ is porosity, and $n$ is an outward unit normal vector.

At the top of the domain, boundary conditions are prescribed in order to resemble a transient climatic forcing, imposing the hydraulic head distribution as a Dirichlet boundary, which implies transient zones of in-flow ($\Omega_1$) and out-flow ($\Omega_2$) for the transient forcing. The following harmonic head distribution is used for this purpose:

$$h(x, t; y = 0) = mx + h_{amp} \cos \left( \frac{2\pi}{T} t \right) \sin \left( \frac{2\pi}{\lambda} x \right)$$

(11)

where $m$ is the regional head (or topographic) gradient, $h_{amp}$ is the amplitude of the local fluctuations, $T$ is the period of the temporal fluctuations, and $\lambda$ is the wavelength of the spatial fluctuations.

Figure 2 shows the harmonic forcing applied at the top boundary for three different times (top figure) and a snapshot of the flow field (bottom figure). Arrows indicate inflow and outflow zones at the snapshot time and the streamlines show a nested behavior going from local to regional flowpaths.

In this example, the period for the transient forcing is 10 years (decadal fluctuations), the wavelength of the spatial fluctuations is 2 km, and the domain is 10 km by 1 km, with origin at the upper left corner. Figure 3a shows the spatial variability of groundwater age distributions (GWADs), scaled with respect to the conventional water density $\rho^T$, for points at $x = 6,000$ m and depths 100, 300, 600, 900 m after 100 years of simulation. These points capture the general behavior of short, intermediate, and long flow paths. It is interesting to notice the complex multi-modality, in particular of the intermediate flow paths, represented by the point at 600 m depth, which contain a mixture of different ages due to its time-varying interaction with re-
Figure 2: Snapshot of the regional flow field at $t = 0$ and general properties of the system. Keep in mind the dramatic changes of the flow field with time, which drive the system from regionally to almost locally dominated.

gional and short flow paths. Figure 3b presents the temporal variability of the scaled GWADs at a point ($x = 6,000$ m and $y = -300$ m) for different times. Given the initial condition chosen for this example, the distribution at a particular time $t$ does not have contributions from water older than $t$. Also, these distributions tend to reach a dynamic equilibrium with time under this periodic forcing, similar to the expected state after a spinup run. Finally, Figure 3c integrates the scaled GWADs over all the time-varying discharge areas for different times. At the early times, e.g., 2.5 years, most of the water is young, coming from local flow paths, then as time progresses, contributions of different ages arise showing as small bumps in older ages. Again, after a long time with this periodic forcing, the system converges to a dynamic equilibrium state. Now the question is, what happens if the system’s forcing is not periodic, but irregular or chaotic? How will the GWADs evolve over time and what does it tell us about the interpretation of age data? This are questions that are being explored by the awardee and represent the main contribution of his PhD dissertation.

3 Funding Products

3.1 Conference Presentations

Preliminary results of this research were presented at the following conferences:
Figure 3: (a) Modeled groundwater age distributions at different depths after 100 years of simulation, (b) modeled groundwater age distributions at different times for a point (6000m, -300m), (c) flux-weighted groundwater age distribution at different times integrated over all the discharge areas.


3.2 Proposals

The following proposals were submitted to NSF and are pending. The awardee contributed with a considerable part of these proposal, which are based on the findings of this research.


References


