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Transient age distributions in subsurface hydrologic systems

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SUMMARY

Transient age distributions have received relatively little attention in the literature over the years compared to their steady-state counterparts. All natural systems are transient given enough time and it is becoming increasingly clear that understanding these effects and how they deviate from steady conditions will be important in the future. This article provides a high-level overview of the equations, techniques, and challenges encountered when considering transient age distributions. The age distribution represents the amount of water in a sample belonging to a particular age and the transient case implies that sampling the same location at two different times will result in different age distributions. These changes may be caused by transience in the boundary conditions, forcings (inputs), or physical changes in the geometry of the flow system. The governing equation for these problems contains separate dimensions for age and time and its solutions are more involved than the solute transport or steady-state age equations. Despite the complexity, many solutions have been derived for simplified, but transient, approximations and several numerical techniques exist for modeling more complex transient age distributions. This paper presents an overview of the existing solutions and contributes new examples of transient characteristic solutions and transient particle tracking simulations. The limitations for applying the techniques described herein are no longer theoretical or technological, but are now dominated by uncertainty in the physical properties of the flow systems and the lack of data for the historic inputs.

1. Introduction

Despite decades of research, relatively few studies have expressly considered transient age distributions in subsurface hydrologic systems (Nir, 1973; Rodhe et al., 1996; Ozyurt and Bayari, 2005). Transience is ubiquitous in nature and every aspect of a system will change given enough time, including the age of the water. As with most of hydrology, the methods for describing age began as simple analytical models that approximate physical processes (e.g. Maloszewski and Zuber, 1982). A common, preliminary assumption throughout subsurface hydrology has been that a flow system occupies a steady-state, which simplifies the solution of the governing partial differential equations. These simple models guided the development of more complex models and numerical tools that allowed investigation of transient processes such as groundwater recharge and solute transport, but the steady-state assumption remains prevalent in many disciplines when considering age (McGuire and McDonnell, 2006). Curiously, the assumption has persisted without much quantitative investigation of the conditions for its validity. Recently, the subject of transient age has become more prevalent in groundwater (Woolfenden and Ginn, 2009; Cornaton, 2012; Gomez and Wilson, 2013), hillslope (Fiori and Russo, 2008; Duffy, 2010; Fiori, 2012; Ali et al., 2014) and catchment (Botter et al., 2011; Benettin et al., 2013) studies. Many of these studies used relaxation methods or transfer functions but this ignores the spatial redistribution of the water mass, which is itself a transient process. However, even these modeling techniques suggest that the role of transience can be significant.

Transience is not foreign to hydrology but the question of water age under transient conditions presents some unique conceptual and mathematical challenges. Many of these challenges arise due to a general lack of understanding about the relevant concepts and the most basic is that the age of any sample of water is a distribution. Here, age is defined as the elapsed time that a discrete volume (parcel) of water has been in a hydrologic system. Specifics of "the system" and its boundaries give rise to the many definitions of age in the literature, but the basic concept is the same in each application. Physical heterogeneities in the flow properties of a system, variability in the timing and spatial distribution of inputs, and a multitude of other factors create numerous pathways, moving at different speeds, that waters may take through the flow

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system. These different flow paths interact with each other and mix, creating a distribution of age. Naturally, if those processes change over time this will affect the age distribution so water collected from the same location at two different times might come from two different sources. The mathematical formalization of these concepts is admittedly more complicated. However, there have been advances in the age and residence time communities that allow both simplified and more robust solutions of transient age distributions for some cases.

To date, there are few articles that have dealt with the mechanics of transient age distributions. The authors believe that this is partially due to the unfamiliar form of the governing equations to a general audience and the counterintuitive nature of some of the associated concepts. This article is intended to shed some light on these unfamiliar constructions and, when possible, demonstrate their similarities to more familiar problems. Our goal is to provide an overview of the current state of modeling transient age distributions that should be accessible to a broad audience. A brief review of the background and governing equations is presented but much of our focus is on examples of the existing techniques and two new approaches. Most of our examples come from the work done on groundwater systems, reflecting our own backgrounds, but the concepts and solution techniques are independent of any particular model for the fluid velocity and are equally applicable to any fluid flow. The first examples are analytical and designed to contain as many similarities to the more familiar solute transport equations as possible, since similar techniques can be applied to both. The complexity of the problem is then increased and we shift our discussion to the application of solution techniques and offer some thoughts on promising avenues for future work.

2. Background

A detailed background on the derivation of the age equation can be found in a companion article in this same volume. Readers requiring more background are referred there, as well as to Ginn (1999), Cornaton and Perrochet (2006), and Ginn et al. (2009), as the background material here will be less technical.

2.1. Governing equation

The various transient age equations are all almost entirely encompassed within the original derivation of Ginn (1999). For a single component, the governing equation of the aqueous phase mass density over space, time, and age is:

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho}{\partial a} + \nabla \cdot \mathbf{V}\rho - \nabla \cdot \mathbf{D}\nabla\rho = F \quad (1)$$

where $\rho = \rho(\mathbf{x}, t, a)$ is the mass density of the fluid, $\mathbf{x}$ is a position vector, t and a denote time and age coordinates, respectively, $\mathbf{V} = \mathbf{V}(\mathbf{x}, t)$ is the vector field of velocity, $\mathbf{D} = \mathbf{D}(\mathbf{x}, t)$ is a tensor field of hydrodynamic dispersion coefficients, and F is a source/sink/reaction term that can be used to represent a wide range of processes. Both $\mathbf{V}$ and $\mathbf{D}$ may vary spatially and temporally but neither is a function of age; transience changes the speed that water moves through a system, which in turn effects dispersion, but not the "age velocity." Dispersion does not occur in the time or age dimensions, only in the spatial dimensions. By definition, steady-state age distributions occur when there is a dynamic equilibrium in the age of the water molecules flowing past a fixed point in space. The transient case might mean that older water is being displaced by younger water and that their relative fractions are changing. In many cases this suggests that sources are transient; for example, flow paths that may be cutoff under dry conditions can be reconnected given a large enough event, providing an influx of young water.

Several other forms of the age equation are often encountered in the literature. These include Goode (1996), Delhez et al. (1999), and Duffy (2010), who present mass balance approaches for simulating the mean age in groundwater, oceans and catchments, respectively. Other forms of the age equation exist and this is not intended to be a complete list since that would be excessive for our purposes. The important point is that nearly every derivation or application of an age equation has assumed a steady-state flow system prior to solving the age equation. The list of studies that have done the opposite is short and those references may be found in the later sections of this article. However, one final, noteworthy variant of an age distribution is the integrated response model, such as Botter et al. (2011), which has been compared to Eq. (1) by Benettin et al. (2013). These models are common in catchment hydrology and seek to address the difficulty in applying physically-based advection–dispersion models by simplifying the system to the point where it is treated as a single reservoir. The outflow rate from the reservoir is considered as a function of age and a series of relaxation equations are applied to an initial condition to distribute age in the effluent, or the "age export" from the system. Probability density functions and cumulative distributions can be considered in these kinds of approaches but the main point is that they do not directly model the physical redistribution of water within the system. Our focus is on physically based models so we do not consider these methods further.

Most models for age can be related to (1), usually by volume averaging, and several equivalences are explained by Ginn et al. (2009). However, simulated and observed age distributions may deviate from solutions of (1) because important heterogeneities may have been omitted from the upscaled model. This can result in the system having "memory" or otherwise falling into the class of a non-Fickian equation. One example of a non-Fickian age equation is:

$$\frac{\partial^\alpha \rho}{\partial t^\alpha} + \frac{\partial^\alpha \rho}{\partial a^\alpha} + \nabla \cdot \mathbf{V}\rho - \nabla \cdot \mathbf{D}\nabla\rho = 0 \quad (2)$$

where ∂^α denotes the Riemann–Liouville fractional derivative and α is the order of fractional differentiation, which recovers the classical equation when $\alpha = 1$. Eq. (2) is nonlocal in time and age, but a space nonlocal or fully nonlocal form can also be written following the solute transport literature. The non-Fickian age equation was suggested by Ginn (1999) and derived by Engdahl et al. (2012) in an effort to describe the expected dynamics of systems that deviate from (1). The deviations in question typically arise due to unresolved heterogeneities in the velocity field or multi-domain mass transfer into stagnant regions. Nonlocal equations are more difficult to solve than their local counterparts and there is no work to date involving transient, direct solutions of non-Fickian age equations. As such, our discussion of them will end here but the solutions of these non-local equations can produce a wide range of solutions that can otherwise only be generated by highly resolved, distributed parameter models.

The reason for bringing up equations like (2) is that transient solutions of Eq. (1) will take on different forms than those often seen in the literature for steady-state age distributions. The same is true for 1-D and 2-D variations of (1) compared to their respective steady-state approximations. One might call such deviations non-Fickian, but this is not strictly correct since the mechanism describing the flux in (1) is Fickian, whereas the flux in (2) is not. For example, distributed parameter models can easily create situations where the age distributions do not fit a simplified 1-D analytical model that assumes a Fickian model of dispersion (Engdahl et al., 2012). This represents a violation of the assumptions of the 1-D model, not a breakdown of Fickian behavior in the distributed model. Thus, many "non-Fickian" behaviors are due to a lack of characterization and represent a deficiency in an upscaled or