



# On the use of late-time peaks of residence time distributions for the characterization of hierarchically nested groundwater flow systems



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## ARTICLE INFO

### Article history:

Available online 22 April 2016

### Keywords:

Hierarchically nested groundwater flow systems

Residence time distributions (RTDs)

Late-time peaks

The Dosit River Watershed

## SUMMARY

Previous studies on the characterization of hierarchically nested groundwater flow systems have mainly been based on the spatial distribution analyses of groundwater pathways. In this paper, by considering the discrete nature of the temporal behavior induced by different hierarchical flow systems, a new approach is proposed. The core of this approach is to use the critical residence times defined by the late-time peaks of residence time distributions (RTDs) to divide the groundwater flow field into local, intermediate and regional systems as described by Tóth (1963). We first introduce Tóthian basins of a 2D cross section and a 3D domain as synthetic test cases. The feasibility of the approach is demonstrated by comparing the partitioning results given by the dividing streamlines associated with internal stagnation points in the 2D Tóthian basin and by the hydraulic connections between recharge and discharge zones in the 3D Tóthian basin. Then, the Dosit River Watershed in Northwestern China is introduced as a field case study. Using the calibrated 3D groundwater flow model, one distinct late-time peak is identified from the RTD and indicates that the Dosit River Watershed can generally be regarded as a two-order nested flow structure with local and regional flow systems. This approach can be used to identify the volumes occupied by different orders of flow systems in 3D, and therefore opens up a new perspective in the study of the 3D nature of basin-scale groundwater flow.

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## 1. Introduction

Groundwater circulation is one of the most important hydrological processes (Alley et al., 2002). At the basin scale, it is extremely sophisticated due to the multi-scale undulation of the water table, which generally induces a hierarchically nested flow structure formed by local, intermediate and regional flow systems (Tóth, 1963). Generally, groundwater moves rapidly along short and shallow pathways within local flow systems and slowly along long and deep pathways within intermediate or regional flow systems. These pathways affect the amount of time during which groundwater and rock interact, and subsequently determine the physical and chemical properties of groundwater and influence the simultaneous geologic processes (e.g., Batelaan et al., 2003; Cardenas,

2007; Domenico and Palciauskas, 1973; Garven, 1995; Gassiat et al., 2013; Gomez and Wilson, 2013; Jiang et al., 2010, 2012; Schwartz et al., 1981; Tóth, 1999; Wang et al., 2015a; Wang et al., 2015b). Identifying the spatial distributions of local, intermediate and regional flow systems in groundwater basins is, therefore, of great significance.

The concepts of local, intermediate and regional groundwater flow systems have been extensively examined and verified using simplified, 2D cross-sectional basin models (e.g., Freeze and Witherspoon, 1967; Jiang et al., 2011; Robinson and Love, 2013; Tóth, 1963; Wang et al., 2011; Zlotnik et al., 2011). However, the Earth's ground surface is composed of diverse hydrologic landscapes (Winter, 2001), the vast majority of which are much more complex having typical 3D features. Since it has long been recognized that complex topography can result in a more complex groundwater flow structure (Wörman et al., 2006; Winter, 2001; Zijl, 1999), a thorough understanding on the nature of groundwater circulation should be based on 3D analyses (e.g., Gleeson and Manning, 2008; Goderniaux et al., 2013; Marklund and Wörman, 2011; Wörman et al., 2006, 2007; Zijl, 1999).

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Modeling is essential for investigating complex groundwater flow systems. On the basis of calibrated groundwater models, previous characterizations of hierarchically nested groundwater flow systems have mainly been based on the spatial distribution analyses of groundwater pathways. Two methods are usually applied. The first is to find dividing streamlines (separatrices) around internal stagnation points, which has been found quite effective in a 2D cross section of a basin (e.g., Anderson and Munter, 1981; Jiang et al., 2011; Robinson and Love, 2013; Wang et al., 2014). However, due to the mathematical definition of stagnation points as singularities of the solution, it is difficult to accurately locate internal stagnation points in a complex 3D flow field, not to mention locating stagnation points based on field data only. Even if accurately located, it is also a challenge to determine the corresponding 3D dividing surfaces. Thus, stagnation points, in 3D, have mainly been shown in well-studied synthetic or simplified cases (e.g., Townley and Trefry, 2000; Winter, 1978). By tracing groundwater pathways, the second method is to link recharge zones to discharge zones based on their hydraulic connections (e.g., Batelaan et al., 2003; Vissers and van der Perk, 2008; Welch and Allen, 2012). However, delineating recharge (or discharge) zones of each individual flow system is a challenge in itself. In practice, attempts to this approach take continuous discharge zones as a basis for defining each flow system. This does not yield a rigorous identification of flow systems in the Tóth sense, because a single continuous discharge zone can encompass the discharge zone of several distinct flow systems (Tóth, 1963).

Residence time distributions (RTDs) have been widely used to understand natural or man-made reservoirs in chemical engineering, oceanic, atmospheric and hydrologic sciences (e.g., Bird et al., 2007; Danckwerts, 1953; Levenspiel, 1999). When considering basin-scale groundwater studies, the groundwater residence time is the total time required by one groundwater particle to move from recharge to discharge zones, and the RTD is mathematically equivalent to a probability density function (PDF) that describes the amount of time groundwater spends within a basin (Fig. 1). Knowledge of the RTD provides relevant insights regarding the renewal time of the resource and the time required for elements to be transported and react with the rock (Kazemi et al., 2006; Suckow, 2014; Turnadge and Smerdon, 2014). Moreover, as the RTD bears the signature of the system characteristics (flow and transport properties, geometry, boundary conditions), it can be used to understand the system as a whole. In the field, dating methods based on natural or man-made tracers can be used to constrain the RTD (Kazemi et al., 2006; Suckow, 2014; Turnadge and

Smerdon, 2014). Therefore, this approach is ideal for hydrogeologists to explore the basin-scale groundwater flow.

Recently, Goderniaux et al. (2013) proposed a framework for partitioning a groundwater basin into shallow local and deep regional flow compartments. Their partitioning method assumed that the RTD of deep regional groundwater flow fits an exponential distribution, which was proven to arise under the Dupuit assumption (Haitjema, 1995). In fact, several studies showed that RTDs of basin-scale groundwater flow generally exhibit a power-law distribution if the vertical groundwater movement is considered (Cardenas, 2007, 2008; Cardenas and Jiang, 2010; Wörman et al., 2007). In Cardenas's (2007) and Cardenas and Jiang's (2010) studies on the RTD in 2D Tóthian basins, a finding was that in addition to an early-time peak, there are late-time peaks, which were ascribed to the arrival of solutes taking long pathways of intermediate-to-regional flow systems. Thus, the current study aims to examine the relationships between the hierarchically nested flow systems in space and the occurrence of late-time peaks in time, and to evaluate the feasibility of using late-time peaks to partition groundwater flow into local, intermediate and regional systems. In this paper, we first introduce synthetic 2D and 3D Tóthian basins as test cases to show the framework and its feasibility. We then use the Dosit River Watershed in Northwestern China as a field case study. Note that Tóthian basins refer to basins of hierarchically nested groundwater flow systems, and this term is widely adopted in the community of Tóthian flow cell organization.

## 2. Methods

### 2.1. Principle

A common approach to calculate the RTD consists of solving groundwater flow and solute transport in an Eulerian framework (Cardenas, 2007; Cardenas and Jiang, 2010). However, for basin-scale groundwater studies, one drawback is that a very fine discretization of time and space is required to fulfill the Courant criterion of solute transport to avoid numerical dispersion (Zheng and Bennett, 2002), which results in a considerable computational effort. Moreover, as the concept of groundwater flow systems proposed by Tóth (1963) is based on the spatial distribution of groundwater pathways, dispersion or diffusion, which significantly impacts on the configuration of RTDs (Cardenas, 2007; Cardenas and Jiang, 2010), especially the late-time peaks, should be eliminated. Therefore, by assuming pure advective solute transport (i.e., without dispersion and diffusion), the forward (or backward) particle-tracking technique, which tracks large quantities of groundwater particles released at recharge (or discharge) zones, is often chosen as an efficient alternative (Basu et al., 2012; Goderniaux et al., 2013; Wörman et al., 2007).

In this study, steady groundwater flow is numerically simulated using the 3D modular finite difference groundwater flow model MODFLOW (Harbaugh, 2005). Groundwater pathways, i.e., the resulting pathway lengths, penetration depths and residence times, are calculated using the particle-tracking code MODPATH (Pollock, 1994). Specifically, we release groundwater particles at the top border of each discharge cell for backward tracking. Treating the resulting groundwater residence times as statistical samples, we use classic methods of the probability and statistics to calculate the PDF, which is also the RTD. Note that according to Cardenas (2007) and Cardenas and Jiang (2010), to get a correct RTD, the groundwater discharge rate should be taken into account. Generally, two approaches could lead to the correct RTD: either releasing a number of particles spatially distributed along the top border of every discharge cell, the number of which is chosen

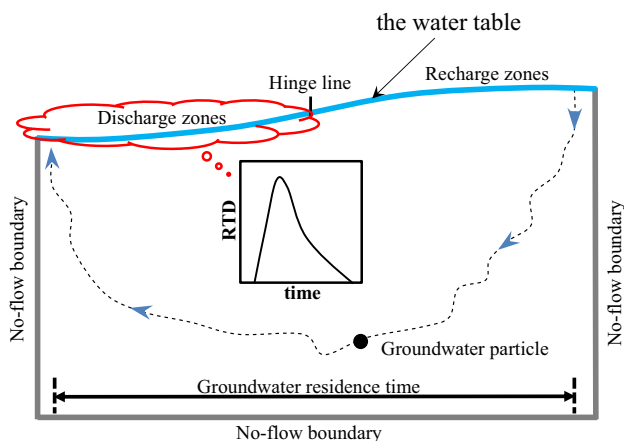


Fig. 1. Schematic diagram showing boundary conditions, concepts of residence time distributions (RTDs) and groundwater residence times.

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