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# Travel time distributions under convergent radial flow in heterogeneous formations: Insight from the analytical solution of a stratified model

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ABSTRACT

We analyze conservative solute transport under convergent flow to a well in perfectly stratified porous media, in which the hydraulic conductivity is treated as a random spatial function along the vertical direction ($K(z)$). The stratified model provides a rare exception of an exact analytical solution of travel time distributions in the proximity of pumping wells, and it is used here to obtain insights about ergodic and nonergodic transport conditions under nonuniform flow conditions. In addition, it provides a benchmark for numerical models aiming to correctly reproduce convergent flow transport in heterogeneous media, such as indicating the minimum number of layers required to obtain ergodic travel time distributions using only one model realization. The model provides important insights about the shape of the depth-integrated concentrations over time measured at the well (breakthrough curves, BTCs), which are usually applied to obtain transport parameters of the subsurface. It can be applied to any degree of system's heterogeneity and using either resident or flux-weighted injection modes. It can be built using different probabilistic distributions of $K$. In our analysis, we consider a log-normal $K$ distribution, and the results indicate that, especially for highly heterogeneous systems, described by the log-$K$ variance ($\sigma_Y^2$), the minimum number of layers required for from one model simulation to reproduce ergodic travel time distributions can be prohibitively high, e.g., above $10^6$ for $\sigma_Y^2 = 8$ considering flux-weighted injections. This issue poses serious concerns for numerical applications aiming to simulate transport in the proximity of pumping wells. In addition, this simple solution confirms that stratification can lead BTCs to display strong preferential flow and persistent, power-law-like late-time tailing. Since the latter are common phenomenological macroscale evidences of other microscale hydrodynamic processes than pure advection (e.g., mass-transfer), caution must be taken when inferring aquifer properties controlling the anomalous transport dynamics in heterogeneous media from BTCs fitting.

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## 1. Introduction

Predicting solute transport behavior for optimal aquifer risk assessment and remediation is a challenging and uncertain task. The presence of hydraulic heterogeneities, which involve erratic spatial distributions of hydraulic properties controlling transport in the subsurface (e.g., the hydraulic conductivity, $K$) and the associated computational and technical difficulties, renders the spatio-temporal distribution of solute concentration amenable to be treated under a stochastic perspective [1]. Despite stochastic modeling in hydrogeology being a well-established discipline (e.g., [2–4]), there are still unexplored fields, such as the analysis of transport under radial convergent flow to a well, which require high attention for their practical utility.

Convergent flow is a very common configuration in groundwater applications. For instance, it applies under convergent flow tracer tests (CFTTs), which are routinely used to infer transport parameter and predict solute transport behavior in aquifers [5–10]. Despite their extended use, the interpretation of CFTTs is still problematic. For instance, obtaining information after breakthrough curve (BTC) fitting is cumbersome because of the fundamental difference between radial and uniform flow transport, which can be a source of error if not accounted for [11]. Analytical stochastic solutions are rarely applicable as they are usually based on weakly heterogeneous conditions ($\sigma_Y^2 < 1$, where $\sigma_Y^2$ is the variance of $Y = \ln K$) and under uniform flow conditions.

Numerical modeling provides a robust alternative to deal with highly heterogeneous transport (e.g., [12–14]), but they need to cope with problems of convergence and other numerical issues

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(like, e.g., the number of particles in Lagrangian models and the spatio-temporal discretization in Eulerian approaches), which can limit their extensive use in practical application.

The system becomes further complicated when radial flow is used to characterize heterogeneous formations. Most of the traditional analytical stochastic solutions for mean uniform flow (e.g., [4]) cannot be applied under nonstationary conditions, which are intrinsic in the radial flow configuration [15]. Approximate solutions assuming low heterogeneity and high anisotropy of aquifers have been applied to describe divergent transport in Multi-Gaussian fields of $Y$ [16–18]. However, such solutions cannot be applied in the case of convergent transport in highly heterogeneous formations. Very few numerical approaches have been reported in the literature to address this issue (e.g., [19–21]). In most cases, modelers have to face large computational domains in order to ensure ergodic transport conditions in their simulations. All these aspects leave the analysis of CFTTs in highly heterogeneous fields still a wide open field for research, despite its great relevance for practical purposes.

The main objective of this paper is to illustrate and analyze an exact analytical solution to describe travel time distributions in a heterogeneous stratified formation under radial convergent flow. Stratified models provide a powerful conceptual modeling framework of transport in confined aquifers consisting of layered geological bodies or for transport in single fractures close to physical boundaries. Stratified models have been widely explored in the literature from different perspectives since the 1960s (e.g., [22–28], even though the assumption of uniform flow conditions has been always considered. Stratified models provide exact analytical stochastic solutions for any degree of soil heterogeneity and type of $K$ distributions. As shown in the following section, this can be easily shown also for convergent radial flow configurations.

This analysis serves to illustrate that this simple solution is able to show how the shape of the BTCs depends directly (a) on stratification and especially on vertical variability (heterogenity) of the soil structure, (b) on the type of tracer injection, and (c) on the ergodic conditions where the solute travel time distributions are generated from, and that mainly depend upon the number of layers used for the aquifer discretization.

The first goal is to illustrate that a simple model based on a perfectly stratified radial flow configuration is able to generate anomalous travel time distributions (i.e., BTCs showing highly positively or negatively skewed travel time distributions) with similar features than those commonly observed on depth-integrated non-Fickian BTCs (i.e., non symmetric distributions of concentrations measured over time at a fixed controlling section) from field experiments. This similarity is of fundamental importance since commonly aquifer hydrodynamic properties are sometimes inferred from specific patterns on BTCs. It has been shown that the latter patterns depend directly on the conceptual and physical conceptual model used to simulate microscale aquifer structures. Examples include the spatial distribution of porosities [9], presence of inclusions (e.g., [29]), fractional derivative approaches to transport [30], mass-transfer processes (e.g., [31]), nonstationary correlation structures in multiGaussian stochastic models (e.g., [32]) or conditional connectivity [33].

A classic example is for instance the apparent power-law late-time scaling of BTCs, which has been sometimes observed in field experiments. In this case, several physical-based models can be used to fit the BTCs, such as those simulating diffusive-based mass-transfer mechanisms following a power-law memory function (e.g., [31]). However, there are other mechanisms leading to power-law-shaped BTCs. Pedretti et al. [21], using 3D numerical simulations based on unconditional multiGaussian fields, showed that under convergent radial flow configurations the late-time behaviors on BTCs can scale as a power-law function because of the underlying stratified flow distributions. Contrarily to Pedretti et al. [21], in this work we explicitly start from an analytical solution based on a stratification conceptual model to illustrate the relationship between stratification and anomalous BTCs under a radial convergent flow configuration.

A second goal is that this analytical model indicates the conditions for which incomplete sampling occurs, e.g., when the injection well is not fully penetrating or is screened over a limited subset of the stratified medium. Such conditions may lead to nonergodic transport, for which the BTC is subject to uncertainty. We better define the concept of ergodicity later in the text.

In this same line, the third goal is to show that this model can be used as a benchmark for numerical simulations aiming at reproducing radial convergent transport in highly heterogeneous media, emphasizing possible problems related to incomplete sampling or numerical deficiencies in handling strong $K$ contrasts. It suggests the minimum required resolution (in terms of number of layers) that a simulation requires to adequately reproduce the impact of the underlying heterogeneous soil structure on the BTCs.

The paper is structured as follows. We first describe the conceptual model (Section 2.1), the mathematical derivation of the travel time distributions (Section 2.2) and and their analytical solutions using a log-normal distribution of the hydraulic conductivity in terms of resident or flux-weighted injection modes. The results are presented in the following manner: first, the ergodic case of travel time distributions, depending on the type of injection (Section 3.1). Afterwords, we analyze the nonergodic case, involving the limited sampling of $K$ (Section 3.2). We also evaluate here the global errors between analytical and numerical results depending on the degree of subsampling. Finally, the paper concludes with a discussion and the main conclusions drawn from this work.

## 2. Methodology

### 2.1. Conceptual model

A conceptual sketch of the aquifer configuration is depicted in Fig. 1. We consider a formation characterized by thickness $b$ (constant in space) and divided into a number of layers $N_L$. All layers are characterized by the same constant thickness $L$, proportional to the vertical integral scale of $K$, such that $L_i = b/N_L$, where $i$ ($i = 1, \ldots, N_L$) indicates the generic layer of the formation. The formation is perfectly stratified, meaning that the hydraulic conductivity $K$ is homogenous in each of the layer composing the formation, but heterogeneous along the vertical axis ($K = K(z)$). We treat $K(z)$ as a stationary random function, with given univariate distribution $f(K)$.

The stratified formation is very useful in grasping the main features of transport in heterogeneous media, leading to an exact solution for flow and transport; for this reason it has been employed in the past, although mainly for transport under mean uniform flow. Such a conceptual model may also be adopted to model flow and transport in more realistic three-dimensional formations, provided that the solute is injected at a close distance from the pumping well, say at distances of the order of the horizontal integral scale of $K$ (e.g., [2,21]).

To simulate transport in a CFTTs scheme, we account for an extraction well with radius $r_w$ and a passive well at a radial distance $r_0$ from it. The pumping well is fully penetrating and screened along the full aquifer, while the passive well may sample a more limited section of the porous medium. The extracting well is discharging for sufficient time at a constant rate Q to generate steady-state conditions at the passive well area.

An injection of a conservative solute of total mass $M$ takes place as a pulse injection from the passive well, acting as an injection

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