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Direct simulation of groundwater transit-time distributions using the reservoir theory

David Etcheverry · Pierre Perrochet

Abstract Groundwater transit times are of interest for the management of water resources, assessment of pollution from non-point sources, and quantitative dating of groundwaters by the use of environmental isotopes. The age of water is the time water has spent in an aquifer since it has entered the system, whereas the transit time is the age of water as it exits the system. Water at the outlet of an aquifer is a mixture of water elements with different transit times, as a consequence of the different flow-line lengths. In this paper, transit-time distributions are calculated by coupling two existing methods, the reservoir theory and a recent age-simulation method. Based on the derivation of the cumulative age distribution over the whole domain, the approach accounts for the whole hydrogeological framework. The method is tested using an analytical example and its applicability illustrated for a regional layered aquifer. Results show the asymmetry and multimodality of the transit-time distribution even in advection-only conditions, due to the aquifer geometry and to the velocity-field heterogeneity.

Résumé Les temps de transit des eaux souterraines sont intéressants à connaître pour gérer l'évaluation des ressources en eau dans le cas de pollution à partir de sources non ponctuelles, et aussi pour dater quantitativement les eaux souterraines au moyen des isotopes du milieu. L'âge de l'eau est le temps qu'elle a passé dans un aquifère depuis qu'elle est entrée dans le système, alors que le temps de transit est l'âge de l'eau au moment où elle quitte le système. L'eau à la sortie d'un aquifère est un mélange d'eaux possédant différents temps de transit, du fait des longueurs différentes des lignes de courant suivies. Dans ce papier, les distributions des temps de transit sont calculées en couplant deux méthodes, la théorie du réservoir et une méthode récente de simulation des âges. Basée sur la dérivation de la distribution cumulées des âges sur tout le domaine, l'approche prend en compte le cadre hydrogéologique dans son ensemble. La méthode est testée sur un exemple analytique et son applicabilité est illustrée pour un aquifère stratifié régional. Les résultats montrent l'asymétrie et la plurimodalité de la distribution des temps de transit même dans des conditions uniquement d'advection, à cause de la géométrie de l'aquifère et de l'hétérogénéité du champ des vitesses.

Resumen El estudio de los tiempos de tránsito del agua subterránea es muy útil para (1) la gestión de los recursos de agua frente a la contaminación por focos no puntuales, y (2) la datación de aguas mediante isótopos ambientales. La edad de un agua subterránea es el tiempo que ésta ha permanecido en el acuífero contada desde el momento de su entrada, mientras que el tiempo de tránsito corresponde a la edad del agua en el momento en que abandona el sistema. En el punto de descarga en realidad se encuentra una mezcla de aguas con distintos tiempos de tránsito, debido a la yuxtaposición de líneas de flujo con diferentes recorridos. En este artículo se calculan las distribuciones de tiempos de tránsito mediante el acoplamiento de dos métodos ya existentes: la teoría de embalse y un método reciente de simulación de edades. El método se basa en la derivación de la distribución acumulada de edades, y es aplicable en todo el dominio hidrogeológico. El método se ha probado en un ejemplo analítico, y su aplicabilidad se muestra para un acuífero estratificado. Como resultado se obtiene que, aun en el caso de flujo exclusivamente advectivo, la distribución de tiempos de tránsito es asimétrica y multimodal debido a la geometría del acuífero y a la heterogeneidad del campo de velocidades.

Key words groundwater age · transit-time distribution · reservoir theory · numerical modeling · environmental isotope

David Etcheverry (✉) · Pierre Perrochet
Centre for Hydrogeology (CHYN), University of Neuchâtel,
2007 Neuchâtel, Switzerland

Present address:
David Etcheverry
Le Mollard,
38700 Le Sappey en Chartreuse, France
Fax: +33-0-438864019
e-mail: david.etcheverry@free.fr

Introduction

The mean age of water at the outlet of an aquifer is generally used to interpret environmental isotopic data; to assess groundwater pollution by radionuclides, organic compounds, or bacteria; to characterize the recharge; or to locate groundwater-protection zones. This mean age is the first moment of a transit-time distribution that may have various complicated shapes. For instance, multimodality and skewness of this distribution are to be expected in the case of layered aquifers, fracture porosity, or fault systems. However, groundwater dating often results in the determination of the mean transit time, a value that gives little information on skewed, multimodal distributions. Isotope hydrogeology makes common use of one-dimensional lumped-parameter models that are assumed to represent the transit-time distribution (Maloszewski and Zuber 1993). This transfer-function approach used for groundwater dating originates from chemical engineering and considers aquifers as black boxes that more or less represent hydrogeological reality. These transfer functions are usually used to solve inverse problems on the basis of tracer data and to calculate mean transit times or dispersion parameters.

Hydrogeological numerical models allow deterministic simulation of transit-time distributions principally thanks to three methods. The most common one is probably particle tracking. A collection of particle tracks gives a set of transit times from which the transit-time distribution is calculated (Tóth 1996; Nationale Genossenschaft für die Lagerung Radioaktiver Abfälle 1997; Oliveira and Baptista 1997). A disadvantage of the method is that the results are quite sensitive to the chosen path lines. In another approach, one calculates the turnover time for each stream tube of a model on the basis of the stream function (Deutscher Verband für Wasserwirtschaft und Kulturbau 1995). Because the stream function is only computable in two dimensions, the method cannot be applied to three-dimensional domains. Alternatively, the transit-time distribution can also be calculated by transport modeling of a conservative tracer (Kinzelbach 1992). This method requires full time-stepped simulations over sometimes very long periods, and it does not provide at once the age distribution on the whole domain, but a time-dependent concentration field. Moreover, in advection-dominated cases, this method may require excessive refinement in space and in time in order to properly capture the pulse function throughout the domain.

Goode (1996) presents a partial differential equation that makes it possible to simulate groundwater age as a continuous field. With this method, the transit-time distribution could be obtained by weight-averaging local fluxes and ages over the outlet. However, to be accurate, this method requires a very fine discretization of the outlet, which is not always desirable or affordable. Because the mesh density of a numerical model is necessarily limited, this treatment can lead to large uncertainties, particularly in the case of outlets like springs or boreholes, where the simulated mean transit time accounting for mixing is always lower than the maximal age in the aquifer.

This paper returns to the origin of lumped-parameter models, the reservoir theory, in order to solve the problem of transit-time distributions in a deterministic way. An earlier paper (Etcheverry and Perrochet 1999) used the reservoir theory to analytically calculate transit-time distributions for simple configurations, in order to verify the pertinence of the piston-flow and exponential model used in the lumped-parameter approach. In the present paper, the reservoir theory is combined with Goode's age-simulation method, to calculate the transit-time distribution, taking into account the age distribution over the whole groundwater flow system. The method is readily available in three dimensions and is particularly suited to assess transit-time distributions in complex hydrogeological configurations. If several discharge zones exist in the system, the transit-time distribution is that of the total discharge. If it is intended to calculate the transit-time distribution on a subsystem of the aquifer (a given well in a well field, for example), calculations have to be made on this subsystem alone. The corresponding subsystem can be simulated separately after graphical delimitation, for example. These efforts are not necessary in some ideal cases, where the bounds of the individualized transit-time distributions are not overlapping.

The objectives of this paper are to (1) deterministically calculate transit-time distributions to verify the applicability of lumped-parameter models in given configurations; (2) create new transfer functions on the basis of analytical or numerical solutions; and (3) solve cases impossible to treat with isotope dating, such as regional flow systems, for example. The intention is to demonstrate that the reservoir theory is well suited to these purposes. The basics of the reservoir theory are described, and how this theory can be applied to numerical models is explained. Some simple simulations give an insight into the complexity of transit-time distributions that could be expected in a regional flow system.

Reservoir Theory

The reservoir theory originates from chemical engineering and began appearing in the 1950s. The first important publications dealing with hydrology are by Eriksson (1961, 1971). The reservoir theory is an application of the Gauss theorem of the divergence on a fluid flowing through a delimited domain during a given period. The theory gives the intrinsic relation between the age distribution of water in a reservoir and at its outlets. The reservoir theory has not recently been applied in hydrogeology, which is why the next section presents the basics described by Bolin and Rodhe (1973), who summarized the results of Eriksson into a simple and rigorous form.

The Age of Groundwater

To avoid misunderstanding between "age," "residence time," and "transit time," these terms are defined as follows. The term "water element" denotes any conserved entity that is flowing through a delimited domain (reservoir). In this discussion, only groundwater ages are considered, but the definitions are appropriate for any substance flowing through a system. The *age* of a water element is the time that has elapsed since it entered the system, which is called the *residence time*. The age when it enters the system is then zero. When it exits the system, the age of the element is called the *transit time*. Because of the ambiguity between residence time and transit time, *water age in the reservoir* is used instead of residence time.

For water elements in an advection-only flow system, the ages and transit times are completely deterministic. If mixing occurs, or if considered at a macroscopic scale, the age of water is a stochastic variable that is subject to a probability density function. Let α be the age of water molecules in a given water element. If $\psi(\tau)$ is the normalized probability density function of molecule ages in this element, then the mean age, τ, of water in the element is the first moment of the distribution and reads

$$\tau = \int_0^\infty \alpha\psi(\alpha)d\alpha. \tag{1}$$

Relationship Between Transit Times and Water Ages in the Reservoir

A reservoir is considered as a bounded region in space through which matter (water in this case) is flowing. The system is considered in a steady state and no gain or loss of matter occurs by dispersion. The water elements of such a system can be arranged in a cumulative fashion whereby the age cumulative distribution function, $M(\tau)$, is the mass of water that has an age that is less than or equal to τ. If the total mass of the reservoir is M_0, then

$$\lim_{\tau\to\infty} M(\tau) = M_0. \tag{2}$$

The age probability density function, $\Psi(\tau)$, of water in the reservoir is by definition related to $M(\tau)$ as follows:

$$\Psi(\tau) = \frac{1}{M_0}\cdot\frac{dM(\tau)}{d\tau}\ (\textit{with the normalization condition}\ \int_0^\infty \Psi(\tau)d\tau = 1). \tag{3}$$

Next, consider a steady flux to and from this reservoir. Each water element leaving the reservoir is characterized by its transit time. These elements can be arranged in a cumulative fashion whereby the age cumulative distribution function, $F(\tau)$, is the flux of water that has an age that is less than or equal to τ. $F(\tau)$ satisfies Eq. (2) with a limit equal to F_0, which is the total flux leaving the reservoir. The age probability density function, $\Phi(\tau)$, of water leaving the reservoir is then related to $F(\tau)$ as

$$\Phi(\tau) = \frac{1}{F_0}\cdot\frac{dF(\tau)}{d\tau}\ (\textit{with the normalization condition}\ \int_0^\infty \Phi(\tau)d\tau = 1). \tag{4}$$

In a steady flow and ignoring mixing, the amount of water leaving the system with an age larger than τ must be balanced by the amount of water per unit time reaching the age τ, which can be formulated as

$$F_0 - F(\tau) = M_0\Psi(\tau) = \frac{dM(\tau)}{d\tau}. \tag{5}$$

Thus, assuming that $M(\tau)$ is known, the function $F(\tau)$ can be derived. From Eqs. (4) and (5), the relationship between the age distribution of water leaving the reservoir and the age distribution of water in the reservoir is

$$\Phi(\tau) = -\frac{M_0}{F_0}\frac{d\Psi(\tau)}{d\tau} = -\frac{1}{F_0}\frac{d^2M(\tau)}{d\tau^2}. \tag{6}$$

Shapes of the Distributions

As cumulative functions, $M(\tau)$ and $F(\tau)$ are by definition non-decreasing. It follows from Eq. (5) that $\Psi(\tau)$ is non-increasing, and from Eq. (6) that $\Phi(\tau)$ is non-negative. If $M(\tau)$ and $F(\tau)$ have some regular shapes, the complexity of $\Phi(\tau)$ has no theoretical limit. Nauman (1981) points out the utility of moments to characterize $\Phi(\tau)$ and $\Psi(\tau)$. The moments μ_n about the origin of a function $f(t)$ are given by

$$\mu_n = \int_0^\infty t^n f(t)dt. \tag{7}$$

Applied to $\Phi(\tau)$ and $\Psi(\tau)$, the moments of order zero are equal to one as a consequence of the normalization condition [Eqs. (3) and (4)]. The first moment of $\Psi(\tau)$ is the mean age of particles in the reservoir and is denoted as τ_a, whereas that of $\Phi(\tau)$ is the mean transit time and is denoted as τ_t. To describe the spread and skewness of the distributions, the second and third central moments, μ'_n respectively, are used:

$$\mu'_n = \int_0^\infty (t - \mu_1)^n f(t) dt. \tag{8}$$

Bolin and Rodhe (1973) prove that the mean transit time, τ_t, is strictly equivalent to the turnover time, τ_0, defined as

$$\tau_0 = \frac{M_0}{F_0}, \tag{9}$$

and they show that the comparison between τ_t and τ_a can help to characterize the behavior of reservoirs.

Transit Times and Masses in the Reservoir

Eriksson (1961) uses $F(\tau)$ to calculate the mass of water in the reservoir having an age less than or equal to a given value. Integrating Eq. (5) from zero to τ gives

$$M(\tau) = \tau F_0 - \int_0^\tau F(\alpha) d\alpha. \tag{10}$$

As can be seen in *Figure 1*, $M(\tau)$ is the surface represented by the surfaces (a) and (b) above the curve and on the left side of τ. The domain τF_0 is represented by (a), (b), and (c). This graphic representation shows that the quantity

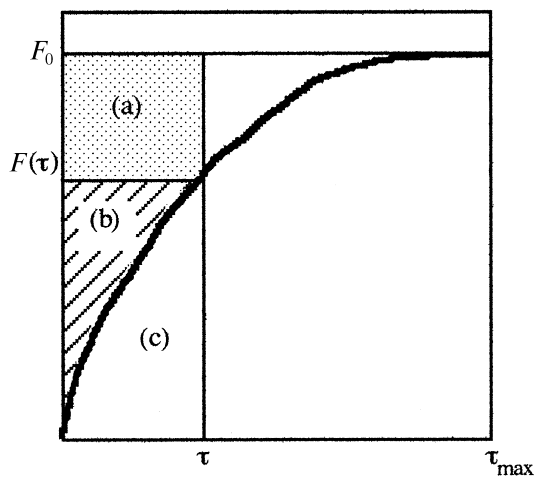


Figure 1 Cumulative flux, $F(\tau)$, at outlet versus transit time τ. **a** Amount of water in reservoir that has an age less than or equal to τ but that will experience a transit time greater than τ; **b** total amount of water in reservoir having an age less than or equal to τ but that will have left reservoir up to time τ; **c** amount of water leaving reservoir with an age less than or equal to τ

$$\int_0^{F(\tau)} \tau dF(\tau) \tag{11}$$

is the total amount of water in the reservoir (area b) having a transit time less than or equal to τ, and which will have left the reservoir up to time τ. The surface (a) is the amount of water in the reservoir that has an age less than τ, but that will experience a transit time greater than τ. One can calculate on this basis the duration of the contact between water and aquifer rocks.

Direct Simulation of Groundwater Age

Following Eq. (6), it is possible to calculate $\Phi(\tau)$, if $\psi(\tau)$ or $M(\tau)$ is known. Goode (1996) developed a method to simulate the spatial distribution of groundwater age using a differential equation of the advective-dispersive type. To be consistent with the validity of the reservoir theory, only the advective case is considered here.

The mean age, A, of water in a steady-flow domain can be determined from the concentration, c, of a tracer injected as an impulse at time zero:

$$A = \frac{\int_0^\infty tc dt}{\int_0^\infty c dt}, \tag{12}$$

For transport by advection in a steady-flow field, the concentration satisfies

$$\theta \frac{\partial c}{\partial t} = -\vec{q} \cdot \nabla c, \tag{13}$$

where θ is the porosity, and $\vec{q}$ the Darcy velocity satisfying

$$\nabla \cdot \vec{q} = 0. \tag{14}$$

Multiplying Eq. (13) by time, integrating through all times, and dividing by the time integral of c yields

$$\vec{q} \cdot \nabla A = \theta. \tag{15}$$

Thus, the mean age of water at any point of a steady-flow system satisfies a steady-advection equation with porosity as an "aging" source.

From Ages in the Reservoir to Transit Times at the Outlet

Practical Procedure

The two methods presented above were combined to calculate transit-time distributions resulting from finite-element groundwater-flow models. Although the method is available for models of arbitrary complexity

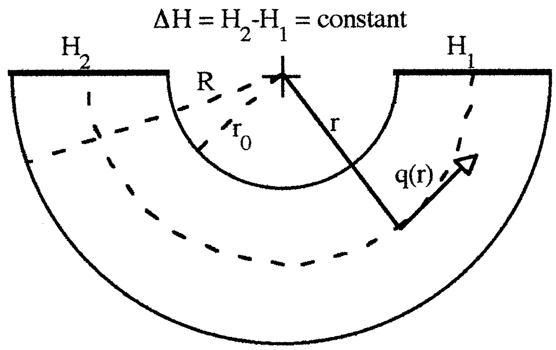


Figure 2 Geometry and boundary conditions for the verification example. $\Delta H = H_2 - H_1$, head difference; R and r_0, external and internal radii of the crown; r, distance to the center; $q(r)$, specific discharge

in one to three dimensions, in this first stage only simple two-dimensional conceptual models, with single inlet and outlet are considered.

After having defined the model geometry and properties and solved Eq. (14) under proper hydraulic boundary conditions, the advective age field is obtained by the solution of Eq. (15) with a zero age boundary condition on the inlet. From this solution, the cumulative-age mass distribution $M(\tau)$ is readily obtained by integrating the pore volume of age less than τ over the domain. The age probability density functions $\Phi(\tau)$ in the reservoir and $\Psi(\tau)$ at the outlet are then obtained from $M(\tau)$ by means of Eqs. (3) and (6).

Verification Example

A crown-shaped domain and the boundary conditions allowing for analytical solution of the functions $\Phi(\tau)$ and $\Psi(\tau)$ are first considered. The geometry, the boundary conditions, and the notation used to solve this problem are shown in *Figure 2*.

The analytical solution for this test example is given in the appendix. *Figure 3* shows that the schemes successively enforced to regionalize the ages, sort them in a cumulative manner, and find the age and transit-time distribution by first and second differentiation agree perfectly with the exact solution.

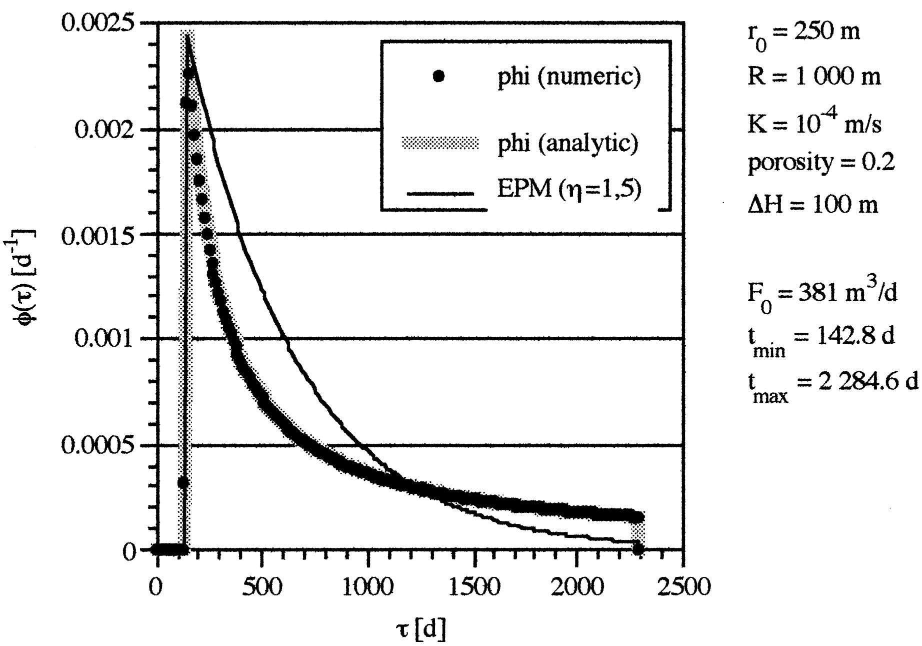
Many delayed decreasing functions could approximate the exact results. For example, the combined exponential piston-flow model (see, for example, Zuber 1986), calculated on the basis of the turnover time of the system [see Eq. (9)], could be a satisfying approximation, even if short transit times are overestimated. However, it would be necessary to adapt the definition of the η parameter that is equal to the total volume of the system divided by the volume with the exponential distribution of transit times, a definition that does not correspond to this case.

Example Simulation

The method is applied to modelized vertical cross sections of regional groundwater flows that are equivalent to those of Tóth (1962, 1963) but with several layers. *Figure 4* shows the domain structure, the boundary conditions, and the recharge and the discharge zones.

In the following examples, only the permeability contrast between layers is varied. The porosity and the boundary conditions are constant to enable easy interpretation based on flow-line lengths and velocity.

Figure 3 Verification of the method by comparing numerical and analytical results. The combined exponential piston-flow model (EPM) is shown because of its similarity to the results presented herein



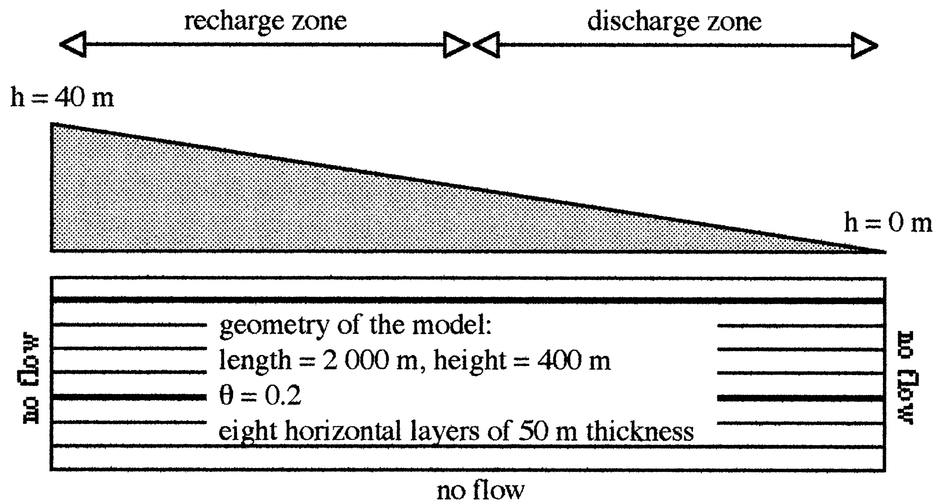


Figure 4 Conceptual layered model used for simulation examples

The locations of the recharge and the discharge zones do not change for all cases.

Homogeneous case

Equations (14) and (15) are solved for a homogeneous hydraulic conductivity of 10^{-4} m/s. *Figure 5* shows the calculated distributions $M(\tau)$, $\Psi(\tau)$, and $\Phi(\tau)$. This very simple case demonstrates that even in purely advective conditions, the transit-time distribution spreads about the mean. For this reason, the dispersion model commonly used in isotope hydrology could be a good approximation of this type of groundwater flow system. The dispersion parameter would have to

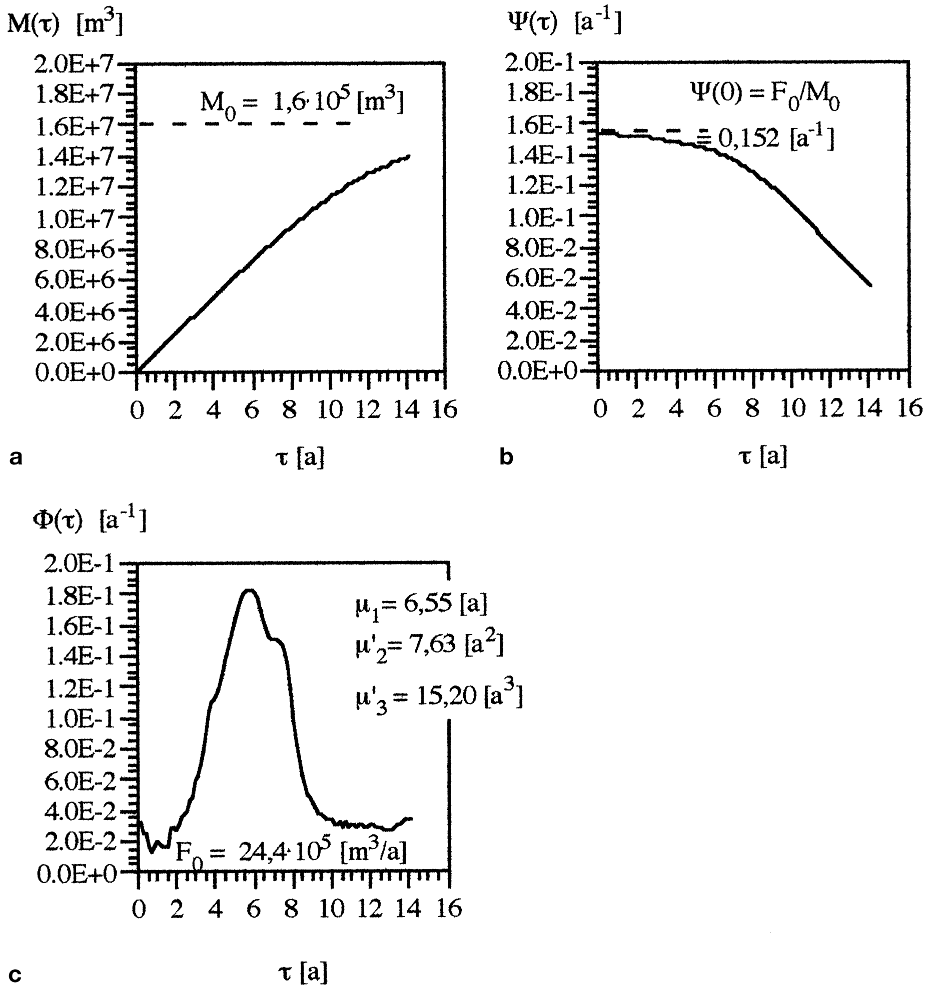


Figure 5 **a** Age mass-cumulative distribution, **b** age distribution in the aquifer, and **c** transit-time distribution for homogeneous case. Hydraulic conductivity is 10^{-4} m/s. Moments are given for the transit-time distribution. $\Phi(\tau)$ exhibits high frequency oscillations due to error propagation after two differentiations from $M(\tau)$

be redefined for that purpose on the basis of the "geometric dispersion" generated by advective circulations, and not on the basis of molecular diffusion or hydrodynamic dispersivity. The dispersion here is related to the different flow-line lengths and to the heterogeneity of velocities.

Heterogeneous case with two layers
The thickness of the high-conductivity (10^{-6} m/s) lower part of the aquifer is increased until its upper boundary reaches the surface of the reservoir. *Figure 6* shows that the mean age of water and the age dispersion at the outlet varies dramatically for successive configurations.

The transit-time distribution is very sensitive to the thickness of the low-permeable layer, particularly when the top of the latter is between a depth of 0 and 50 m.

Heterogeneous case with three layers
A layer with reduced hydraulic conductivity (10^{-5} m/s) is introduced in the domain. The transit-time distributions are calculated for six successive positions of the low-permeability layer shown in *Figure 7.* An objective study of this case can be performed with the first three statistical moments. *Figure 8* gives the mean, the variance, and the skewness of the transit-time distributions for successive positions of the low-permeability layer.

When the low-permeability layer is at the top of the aquifer, the transit-time distribution is characteristic of a delayed decreasing function. The low-permeability layer acts as a retardation factor on transit times. The strong skewness accounts for the maximal influence of old groundwater. The distribution becomes bimodal as soon as a high-permeability zone appears on the top of the aquifer. The mean transit time decreases as the influence of old groundwater reduces. When the low-permeability layer is at the bottom of the aquifer, its slight influence on the transit-time distribution is characterized by a unimodal distribution, by a low mean transit time, by a low variance, and by a low asymmetry.

Conclusions

The reservoir theory allows for analytical and numerical deterministic calculations of transit-time distributions and is particularly suited to complex hydrogeological configurations. The intrinsic relationship between age distribution in the aquifer and transit-time distribution allows the extrapolation of one to the other, by simple differentiation or integration. Thus, masses in the reservoir or fluxes at the outlet corresponding to a given age class can be calculated. The good resolution of the transit-time distribution is made possible on numerical models, because the computation is based on the domain age distribution and does not depend on a somewhat arbitrary refinement of the discharge zone. One major aspect is that the "geometric dispersion" within the system can be fully captured, even though mixing occurs at the outlet. Results demonstrate that the mean transit time alone

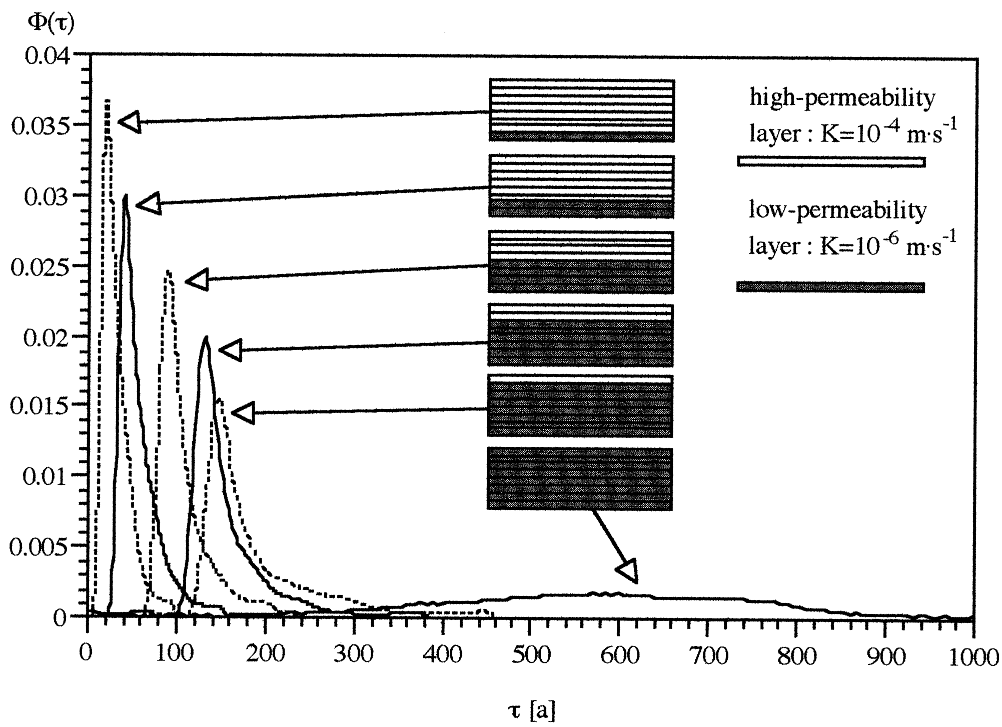
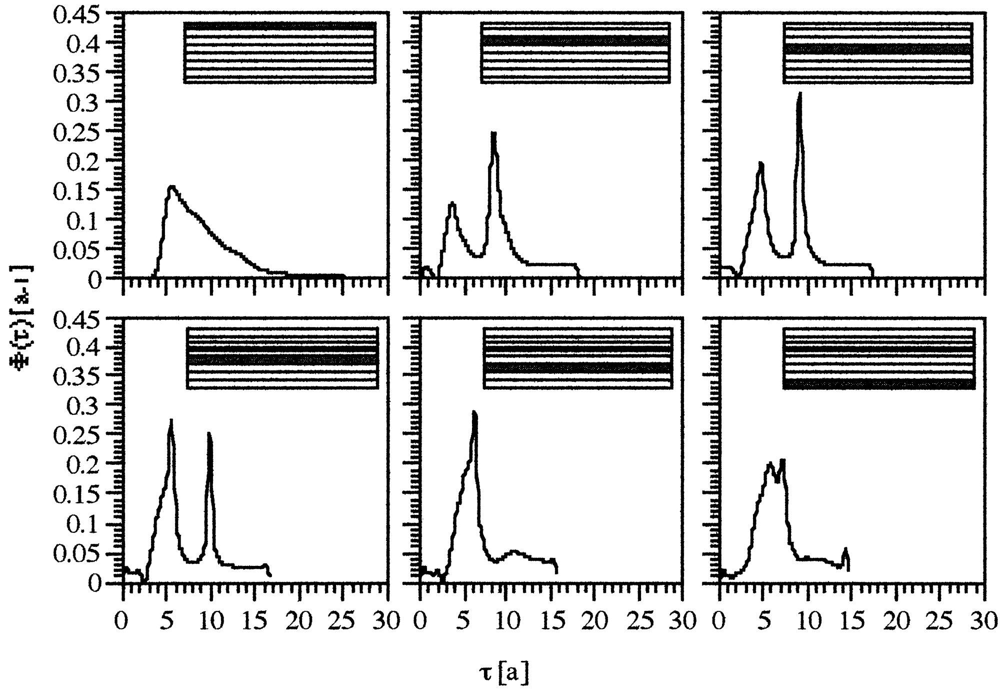


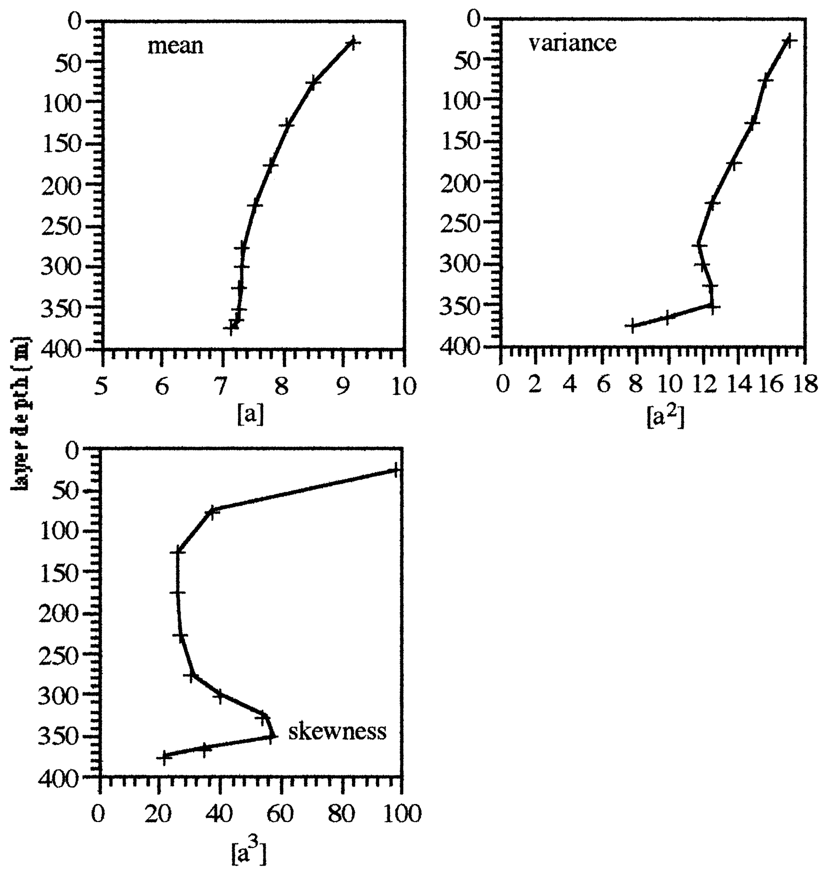
Figure 6 Transit-time distributions for increasing thickness of the low-permeability layer

Figure 7 Transit-time distributions for increasing depths of the low-permeability layer



gives little information on the whole distribution. An asymmetry of the transit-time distribution is encountered even in advection-only conditions due to the aquifer geometry and to the velocity-field heterogeneity. Multimodality appears when the aquifer is divided into two horizontal parts by a low-permeability layer.

Figure 8 Mean, second, and third central moments of transit-time distributions versus depth of the low-permeability layer



Appendix

Analytical Solution of Transit-Time Distribution for a Semi-circular Crown-Shaped Aquifer

The geometry of the model domain is given in *Figure 2*. Two-dimensional, vertical groundwater steady flow with homogeneous conductivity and porosity is considered. R and r_0 are the external and internal radii of the crown. To obtain semi-circular flow lines, the hydraulic heads are set constant at the inlet and at the outlet. The head difference is constant and is denoted ΔH. Since πr is the total length of a flow line, the specific discharge $q(r$ at a distance r of the center of the crown is

$$q(r) = \frac{K\Delta H}{\pi r}. \tag{A1}$$

The total flux F_0 through the aquifer is

$$F_0 = \int_{r_0}^{R} q(r)dr = \frac{K\Delta H}{\pi} ln\left(\frac{R}{r_0}\right), \tag{A2}$$

and its total volume is

$$M_0 = \theta \frac{\pi}{2}\left(R^2 - r_0^2\right). \tag{A3}$$

The transit time $\tau(r)$ of water along each flow line is a function of the porosity and reads

$$\tau(r) = \frac{\theta\pi r}{q(r)} = \frac{\theta\pi^2 r^2}{K\Delta H}, \tag{A4}$$

with minima and maxima given by

$$\tau_{min} = \frac{\theta\pi^2 r_0^2}{K\Delta H} \text{ and } \tau_{max} = \frac{\theta\pi^2 R^2}{K\Delta H}. \tag{A5}$$

Since $\tau(r)$ is monotonically increasing with r, the cumulative flux $F(\tau)$ at the outlet is

$$F(\tau) = \int_{r_0}^{r(\tau)} q(r)dr, \tag{A6}$$

namely

$$F(\tau) = \frac{K\Delta H}{\pi} ln\left(\frac{r(\tau)}{r_0}\right). \tag{A7}$$

Substituting $r(\tau)$ from Eq. (A4) yields

$$F(\tau) = \frac{K\Delta H}{2\pi} ln\left(\frac{K\Delta H}{\theta\pi^2 r_0^2}\tau\right). \tag{A8}$$

From Eqs. (2)–(6) the distributions $\Psi(\tau)$ and $\Phi(\tau)$ are solved:

$$\Psi(\tau) = \frac{F_0}{M_0} = \frac{1}{\tau_{max} - \tau_{min}} ln\left(\frac{\tau_{max}}{\tau_{min}}\right), \text{ with } 0 < \tau \leq \tau_{min},$$

$$\Psi(\tau) = \frac{1}{\tau_{max} - \tau_{min}} ln\left(\frac{\tau_{max}}{\tau}\right), \text{ with } \tau_{min} < \tau \leq \tau_{max},$$

and

$$\Phi(\tau) = 0, \text{ with } 0 < \tau \leq \tau_{min},$$

$$\Phi(\tau) = \frac{1}{ln\left(\frac{\tau_{max}}{\tau_{min}}\right)\tau}, \text{ with } \tau_{min} < \tau \leq \tau_{max}. \tag{A9}$$

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