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Groundwater age, life expectancy and transit time distributions in advective–dispersive systems; 2. Reservoir theory for sub-drainage basins

F. Cornaton *, P. Perrochet

CHYN, Institute of Geology, University of Neuchâtel, Emile-Argand 11, CH-2007, Neuchâtel, Switzerland

Abstract

Groundwater age and life expectancy probability density functions (pdf) have been defined, and solved in a general three-dimensional context by means of forward and backward advection–dispersion equations [Cornaton F, Perrochet P. Groundwater age, life expectancy and transit time distributions in advective–dispersive systems; 1. Generalized reservoir theory. Adv Water Res (xxxx)]. The discharge and recharge zones transit time pdfs were then derived by applying the reservoir theory (RT) to the global system, thus considering as ensemble the union of all inlet boundaries on one hand, and the union of all outlet boundaries on the other hand. The main advantages in using the RT to calculate the transit time pdf is that the outlet boundary geometry does not represent a computational limiting factor (e.g. outlets of small sizes), since the methodology is based on the integration over the entire domain of each age, or life expectancy, occurrence. In the present paper, we extend the applicability of the RT to sub-drainage basins of groundwater reservoirs by treating the reservoir flow systems as compartments which transfer the water fluxes to a particular discharge zone, and inside which mixing and dispersion processes can take place. Drainage basins are defined by the field of probability of exit at outlet. In this way, we make the RT applicable to each sub-drainage system of an aquifer of arbitrary complexity and configuration. The case of the well-head protection problem is taken as illustrative example, and sensitivity analysis of the effect of pore velocity variations on the simulated ages is carried out.

Keywords: Age; Life expectancy; Forward/backward reservoir theory; Flow systems; Capture zone probability; Protection zone

1. Introduction

In a previous work [2], three complementary groundwater characteristic temporal properties have been defined as random variables, for which the type definitions are related to the inlet and outlet boundaries of the aquifer system. Groundwater age (A) in the reservoir is defined as a relative quantity with respect to a starting location on the inlet boundary, where age is assumed to be zero. Groundwater life expectancy (E) corresponds to the time required prior to exiting at an outlet limit of the system. Life expectancy is therefore zero at the outlet. The transit time (T) is finally referred to as the time required to migrate from an inlet zone (where $T = E$) to an outlet zone (where $T = A$). The transit time from inlet to outlet is the sum at any point of the system of the variable age and the variable life expectancy ($T = A + E$). Cornaton and Perrochet [2] have shown that, for aquifers considered under steady-flow conditions, the reservoir theory (RT) [8] can be recovered by integrating forward

* Corresponding author. Address: Department of Earth Sciences University of Waterloo, CEIT Building 2052a, N2L 3G1 Waterloo, Ont., Canada. Tel.: +1 519 8884567; fax: +1 519 7467484.

E-mail addresses: fabien.cornaton@unine.ch, fcornato@scimail.uwaterloo.ca (F. Cornaton), pierre.perrochet@unine.ch (P. Perrochet).

Nomenclature

Abbreviations

ADE	advection dispersion equation
RT	reservoir theory
FRT	forward reservoir theory
BRT	backward reservoir theory
LTG	laplace transform Galerkin
pdf	probability density function
cdf	cumulative distribution function

Mathematical symbols

A	random variable "age"
E	random variable "life expectancy"
T	random variable "transit time"
g_A	age pdf, s^{-1}
g_E	life expectancy pdf, s^{-1}
p_n	probability of exit at outlet n
f_n	outlet n transit time cdf
m_n	outlet n drainage basin internal life expectancy cdf
F_n	outlet n cumulated flow rate, $m^3\,s^{-1}$
M_n	cumulative porous volume of age, or life expectancy, t or less, m^3
$\upsilon_A(t)$	groundwater volume of age t or less, and transit time superior to t, m^3
$\upsilon_T(t)$	groundwater volume of transit time t or less, m^3
$\upsilon_0(t)$	produced amount of water of transit time t or less at outlet, m^3
M_0	reservoir porous volume, m^3
F_0	reservoir steady-state discharge rate, $m^3\,s^{-1}$
$M_{0,n}$	outlet n drainage basin porous volume, m^3
$F_{0,n}$	outlet n steady-state discharge rate, $m^3\,s^{-1}$
$\mathbf{J}_U$	total mass flux vector ($U = A$ or E), $m\,s^{-2}$
D_m	coefficient of molecular diffusion, $m^2\,s^{-1}$
$\mathbf{q}$	Darcy flux vector, $m\,s^{-1}$
q_I	fluid source term, s^{-1}
q_O	fluid sink term, s^{-1}
$\mathbf{D}$	macro-dispersion tensor, $m^2\,s^{-1}$
$\boldsymbol{x}$	space position vector, m
$\boldsymbol{n}$	boundary outward normal unit vector
$\mathbf{I}$	identity matrix
$\hat{f}$	Laplace transform state of a function f
s	Laplace variable, s^{-1}
t	time, s

Greek symbols

Ω	reservoir aquifer
Γ_-	reservoir inlet boundary
Γ_+	reservoir outlet boundary
Γ_0	reservoir no flow boundary
Γ_n	outlet n boundary
∇	operator Nabla
φ	outlet or inlet transit time pdf, s^{-1}
ψ	internal age or life expectancy pdf, s^{-1}
$\delta(t)$	time-Dirac delta distribution, s^{-1}
ϕ	porosity or mobile water content
α_L	coefficient of longitudinal dispersion, m
α_T	coefficient of transverse dispersion, m
α	ratio α_L/α_T
τ_0	reservoir turnover time, s
$\tau_{0,n}$	outlet n drainage basin turnover time, s
τ_t	mean transit time at outlet, s
τ_i	mean internal age or mean internal life expectancy, s
τ_{it}	mean internal total transit time, s
σ	standard deviation, s
ξ	correlation length, m
ζ	separation distance

and backward advection–dispersion equations (ADE), associated to proper boundary conditions. In so doing, the RT has been generalized to systems with spatially distributed velocity fields and significant hydro-dispersive components. The RT enables the evaluation of a discharge zone transit time probability density function (pdf), as well as a recharge zone life expectancy pdf, $\varphi(t)$. Unlike direct evaluation methods of the breakthrough curves at an exit, or an inlet boundary, the RT makes use of the information on age or life expectancy in the entire reservoir, which is contained by the internal age or life expectancy pdf $\psi(t)$. The RT permits an accurate evaluation of the transit time pdf, for which the method ensures that the minimum and the maximum age in the aquifer are recovered at the inlet and outlet boundaries. However, the RT has been applied to the global system, thus considering as ensemble the union of all inlet boundaries on one hand, and the union of all outlet boundaries on the other hand. Therefore, more specific formulations are still required in order to be able to apply the RT to a specific outlet drainage basin.

The fundamental concept of groundwater flow systems originates from the works of Hubbert [11] and Tóth [25,26]. The groundwater flow systems are separated into different categories, mainly in relation to their spatial extend. The regional flow systems extend both from regionally and topographically elevated areas to lower regions, and beneath overlying local shallower watersheds within which smaller flow systems can further be distinguished. Regional flow systems are important in areas where the topographic gradients are significant, where recharge is limited, or where the rock basement has still a good permeability. The local flow systems are shallow, and the recharge waters rapidly reach the downstream discharge zones. In such flow systems, the interactions with the surface waters can prevail. These systems are often underlain by intermediate and regional flow systems. An outlet drainage basin can cover local and intermediate flow systems, but also regional flow systems. The discharge of the outlet is then potentially constituted of groundwater particles which have experienced various travel histories, from the restricted movement within the local flow system, to the long circulations within the regional flow system. Following the concepts of Tóth [25,26], Kiraly [15] defined the flow system as a fundamental hydrogeological unit, that can be compared to an equivalence class spatially connected (continuous) in the field of a dependent variable characterizing the quality, the quantity, or the movement of groundwater. To characterize this hydrogeological unit, the equivalence class in the field of the flow parameters, and the equivalence class in the field of the boundary conditions, must be properly defined. In the definition of Tóth, the flow system is defined as a set of flow lines for which any two adjacent flow lines at any point of the flow region remain adjacent throughout the whole domain. The hydrogeological flow system thus corresponds to an equivalence class in the set of the flow lines. This concept is fundamental, and has provided many insights in hydrogeology. However, it corresponds to a purely advective vision of the dynamics of groundwater flow. At macroscopic scale in porous media, dispersion moves water particles laterally from a flow line towards another. As a consequence, an advective–dispersive formulation of groundwater movement is more appropriate.

In this paper, we extend the RT to systems of arbitrary dimension, configuration, and spatial distribution of the inlet and outlet boundaries. In a first step, the applicability of the RT for a specific outlet drainage systems is theoretically demonstrated. In a second step, appropriate backward boundary value problems are defined in order to derive the RT for a given outlet drainage system. This specific sub-drainage system is characterized in terms of probability for the water particles to reach the outlet. Furthermore, we propose a quantitative approach for the design of outlet protection zones. We finally present results of calculated transit time pdfs at a pumping-well by generating random velocity fields. These simulations are used to make inferences on the effects of the spatial variability of velocity on the simulated age pdfs at the well.

2. Reservoir theory and advective–dispersive transport

We make the assumption that the classical ADE with time-independent transport parameters can model the groundwater evolutional transport of the age and life expectancy distributions under steady-flow conditions. The age probability distribution $g_A(\boldsymbol{x},t)$ [T^{-1}] at a position $\boldsymbol{x}=(x,y,z)$ in a groundwater reservoir Ω can be obtained as the solution of the forward-in-time ADE when a unit pulse of conservative tracer is uniformly applied on the recharge areas. The resulting breakthrough curve is the probabilistic age distribution [6,14]. The life expectancy pdf $g_E(\boldsymbol{x},t)$ [T^{-1}] is obtained by solving the formal adjoint model of the forward ADE [9,1], the so-called "backward-in-time" ADE [27,32,30]. Details concerning the specific features of the boundary value problems yielding the pdfs g_A and g_E are given in Cornaton and Perrochet [2]. Considering an aquifer domain Ω in the three-dimensional space with hydraulic recharge boundary Γ_- discharge boundary Γ_+, and impermeable boundary Γ_0, and given the age and life expectancy fields $g_A(\boldsymbol{x},t)$ and $g_E(\boldsymbol{x},t)$, one can define the function $\psi(t)$ as the internal age pdf, or internal life expectancy pdf:

$$\psi(t)=\frac{\partial m(t)}{\partial t}=\frac{1}{M_0}\frac{\partial M(t)}{\partial t}=\frac{1}{M_0}\int_\Omega \phi g_A(\boldsymbol{x},t)\,\mathrm{d}\Omega = \frac{1}{M_0}\int_\Omega \phi g_E(\boldsymbol{x},t)\,\mathrm{d}\Omega \qquad (1)$$

where $\phi=\phi(\boldsymbol{x})$ is porosity or mobile water content, M_0 is the total porous volume, and where the function $M(t)$ is the cumulated amount of mobile water in Ω with an age (or life expectancy) t or less, such that it corresponds to the internal age (or life expectancy) cumulative distribution function (cdf) $m(t)$, times the total porous volume M_0. The outlet (or inlet) transit time pdf $\varphi(t)$ is classically defined as a flux-weighted average of the mass fluxes events along the boundary, plus the integration of potential sinks (or sources):

$$\varphi(t)=\frac{1}{F_0}\int_{\Gamma_+}\mathbf{J}_A(\boldsymbol{x},t)\cdot\boldsymbol{n}\,\mathrm{d}\Gamma+\frac{1}{F_0}\int_\Omega q_{\mathrm{O}}(\boldsymbol{x})g_A(\boldsymbol{x},t)\,\mathrm{d}\Omega = \frac{1}{F_0}\int_{\Gamma_-}\mathbf{J}_E(\boldsymbol{x},t)\cdot\boldsymbol{n}\,\mathrm{d}\Gamma+\frac{1}{F_0}\int_\Omega q_{\mathrm{I}}(\boldsymbol{x})g_E(\boldsymbol{x},t)\,\mathrm{d}\Omega \qquad (2)$$

where $\boldsymbol{n}$ is a normal outward unit vector. The steady-state total flow rate is $F_0=F_{0,+}+F_{0,\mathrm{O}}=F_{0,-}+F_{0,\mathrm{I}}$, where $F_{0,+}$ is the flow rate through the outlet limits, $F_{0,-}$ is the flow rate through the inlet limits, $F_{0,\mathrm{I}}$ is the flow rate produced by internal sources of intensity q_{I} [T^{-1}], and $F_{0,\mathrm{O}}$ the flow rate related to internal sinks of intensity q_{O} [T^{-1}]. The total mass fluxes of age $\mathbf{J}_A$ [LT^{-2}] and life expectancy $\mathbf{J}_E$ [LT^{-2}] are classically defined by the sum of the convective and dispersive fluxes, $\mathbf{J}_A=\mathbf{q}g_A-\mathbf{D}\nabla g_A$ and $\mathbf{J}_E=-\mathbf{q}g_E-\mathbf{D}\nabla g_E$, with $\mathbf{q}$ denoting the Darcy flux vector [LT^{-1}], and $\mathbf{D}$ being the tensor of macro-dispersion [$\mathrm{L}^2\mathrm{T}^{-1}$].

The RT provides the intrinsic relationship between the distribution of ages (or life expectancies) in the reservoir Ω and at the boundaries [2]:

$$\varphi(t) + \tau_0 \frac{\partial \psi(t)}{\partial t} = \delta(t) \tag{3}$$

The turnover time τ_0 is the ratio of the aquifer porous volume M_0 to the steady flow rate F_0. The RT formulation (3) is referred to as forward reservoir theory (FRT) when the function $\psi(t)$ characterizes the internal age pdf. When $\psi(t)$ is the internal life expectancy pdf, Eq. (3) is referred to as backward reservoir theory (BRT). Letting $f(t)$ be the transit time cdf,

$$f(t) = \frac{F(t)}{F_0} = \int_0^t \varphi(\tau)\,d\tau \tag{4}$$

with $F(t)$ [L^3T^{-1}] denoting the cumulated outflow distribution of transit times, integration of Eq. (3) yields the following mass balance equation:

$$f(t) + \tau_0\psi(t) = 1 \tag{5}$$

or after multiplication by F_0

$$F_0 - F(t) = M_0\psi(t) \tag{6}$$

When the RT is applied to the global reservoir, the pdf $\varphi(t)$ represents the intensity of probability that the water particles have a transit time t at the outlet boundary Γ_+ corresponding to the union of each outlet of Ω. Accordingly, the pdf $\varphi(t)$ represents also the life expectancy pdf of the union Γ_- of each inlet boundary portion. In this state, Eq. (3) is of practical utility when aquifers with single recharge and single discharge zones are considered, in which case the pdf $\varphi(t)$ is the transfer function of the system. Numerical models are often used for the simulation of experimental data, such as data obtained from column experiments. The RT formulation (3) is an appropriate model for such kind of simulations, since they can be used to characterize solute transport by a transfer function approach, as earlier described by Jury [12], Dagan [3,4], Dagan and Nguyen [5], Jury et al. [13], White et al. [31], Sposito et al. [22], or Jury and Roth [14]. For more complicated, but realistic, aquifer flow configurations (e.g. several natural or artificial outlet zones connected to several recharge zones), more specific formulations are required in order to make the RT useful to deal with the common environmental problems that hydrogeologists face.

3. Reservoir theory for sub-drainage basins

In this section, we show how complex reservoirs of arbitrary configuration, and with several flow systems, can be characterized with the RT approach by treating each sub-system as a compartment model.

The drainage basin Ω_n of an outlet Γ_n can be defined as the union of all water molecules that will leave the system by Γ_n, eventually. This ensemble can penetrate through different flow units, since transverse dispersion can move water particles laterally. The backward probability approach represents an interesting alternative to the pure advective definition of outlet drainage basins. Backward ADEs have already been used for delineating pumping well capture zones, see e.g. [27,32,19–21]. The capture zone is defined in terms of probability of absorption of the water particles by a given outlet. In the following, we also make use of the backward transport modelling approach to delineate probabilistic drainage basins, for which the RT is developed to characterize the outlet transit time pdf, as well as the internal distribution of age within the probabilistic drainage basin.

For a reservoir that owns several outlet and inlet zones, the global distributions $\varphi(t)$ and $\psi(t)$ can be regarded as a flux- and porous volume-weighted linear combination of the intrinsic distributions of each sub-drainage basin Ω_n and associated outlet Γ_n, $\varphi_n(t)$ and $\psi_n(t)$. Consider a reservoir Ω with N discharge areas Γ_n. Given that $M_0 = \sum_n M_{0,n}$ and $F_0 = \sum_n F_{0,n}$, with $M_{0,n}$ and $F_{0,n}$ being the outlet Γ_n drainage basin porous volume and discharge rate, respectively, and given that the cumulative mass of age t or less in sub-system Ω_n is the cdf $m_n(t)$ of the internal age pdf $\psi_n(t)$ scaled by the corresponding porous volume $M_{0,n}$, $M_n(t) = M_{0,n}m_n(t)$, the two following relations stand:

$$\psi(t) = \frac{1}{M_0}\sum_{n=1}^{N} M_{0,n}\psi_n(t) \tag{7}$$

$$\varphi(t) = \frac{1}{F_0}\sum_{n=1}^{N} F_{0,n}\varphi_n(t) \tag{8}$$

Eqs. (7) and (8) show that the pdfs calculated with the RT applied to the entire aquifer correspond to the superposition of each pdf calculated with the RT applied to each sub-system of the reservoir. The internal residence time distribution of the entire flow domain corresponds to porous volume-weighted mean of each internal residence time distribution of each sub-drainage basin, and the transit time distribution of the union of all outlets corresponds to flow rate-weighted mean of each outlet transit time distribution. A direct consequence of Eqs. (7) and (8) is that the global reservoir turnover time is $\tau_0 = \sum_n (F_{0,n}\tau_{0,n})/F_0$ and the global reservoir internal age is $\tau_i = \sum_n (M_{0,n}\tau_{i,n})/M_0$. Eqs. (4) and (5) can be used to define the transit time cdf $f(t)$ as a function of the linear combination of each $\varphi_n(t)$, or each $\psi_n(t)$. Furthermore, the internal groundwater volume functions defined in Cornaton and Perrochet [2] can also be characterized for each sub-system Ω_n. A drainage basin is considered here as a compartment within which the input amounts of age mass are transferred to its outlet. The compartment, therefore, is defined with respect to one of the global reservoir outlets, since the rate of mass transfer out of the compartment depends on the different possible paths of water particles within the compartment. It may be assimilated to an internal flow unit that connects a set of recharge zones to a specific discharge zone, and inside which the water particles motion is ruled by advection and dispersion processes. The limits of this compartment are not clearly defined, unlike in Eriksson [8], but they rather enclose a specific property. As will be developed in the following sections, this property is chosen as the occurrence of water particles with respect to the time they need to reach the outlet, sooner or later, so that the compartment corresponds to the field of probability of exit $p_n(\boldsymbol{x}, t)$ at outlet Γ_n. This field of probability can include dispersion-induced mixing processes, within the compartment and between compartments, which means that two different compartments can share their mass, as illustrated in Fig. 1. The uncertainty in the position of the groundwater particles is characterized by a general spreading of the probability of exit, this spreading being itself dependent on dispersion. In the sense of Kiraly's definition of a flow system as an equivalent class in the set of the flow lines [15], the outlet drainage basin is defined here as an equivalence class in the field of probability of absorption at outlet, for which and equivalence class in the field of velocity and dispersion tensor have to be defined.

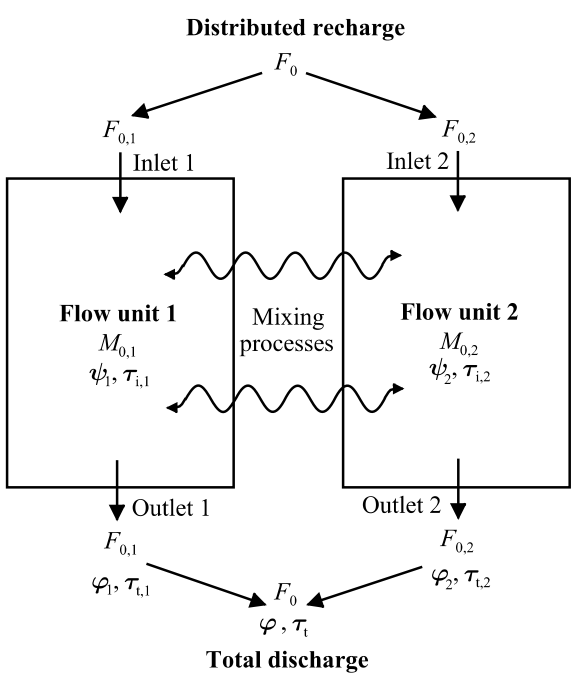

Fig. 1. Schematic illustration of a two-compartments reservoir.

3.1. Reservoir theory for a specific outlet drainage basin

To evaluate the pdfs $\varphi_n(t)$ and $\psi_n(t)$, we consider the backward-in-time ADE and set the boundary conditions in such a way that the dependent variable characterizes the density of probability that the water particles will exit the system at Γ_n, exclusively. This pdf can be calculated as a solution of the following boundary value problem:

$$\frac{\partial \phi g_E}{\partial t} = \nabla \cdot \mathbf{q} g_E + \nabla \cdot \mathbf{D} \nabla g_E - q_{\mathrm{I}} g_E \quad \text{in } \Omega \tag{9a}$$

$$g_E(\boldsymbol{x}, 0) = g_E(\boldsymbol{x}, \infty) = 0 \quad \text{in } \Omega \tag{9b}$$

$$\mathbf{J}_E(\boldsymbol{x}, t) \cdot \boldsymbol{n} = -(\mathbf{q} \cdot \boldsymbol{n})\delta(t) \quad \text{on } \Gamma_n \tag{9c}$$

$$\mathbf{J}_E(\boldsymbol{x}, t) \cdot \boldsymbol{n} = 0 \quad \text{on } \Gamma_+ \tag{9d}$$

$$-\mathbf{D} \nabla g_E(\boldsymbol{x}, t) \cdot \boldsymbol{n} = 0 \quad \text{on } \Gamma_0 \tag{9e}$$

The Cauchy type conditions on Γ_n and Γ_+ ensure that the calculated life-expectancy-to-outlet solution $g_E(\boldsymbol{x}, t)$ gives the intensity of probability that the water particles situated at the position $\boldsymbol{x}$ will be absorbed by Γ_n at time t. On any other outlet boundary Γ_+, this intensity of flux probability of exit is fixed to zero.

The internal life expectancy pdf ψ_n of sub-system Ω_n is defined by

$$\psi_n(t) = \frac{1}{M_{0,n}} \int_\Omega \phi g_E(\boldsymbol{x}, t)\, \mathrm{d}\Omega \tag{10}$$

The transit time pdf $\varphi_n(t)$ of the outlet Γ_n can be obtained by evaluating the inlet life expectancy pdf (see [2]):

$$\begin{aligned} \varphi_n(t) &= \frac{1}{F_{0,n}} \int_{\Gamma_n} \mathbf{J}_A(\boldsymbol{x}, t) \cdot \boldsymbol{n}\, \mathrm{d}\Gamma \\ &= \frac{1}{F_{0,n}} \int_{\Gamma_-} \mathbf{J}_E(\boldsymbol{x}, t) \cdot \boldsymbol{n}\, \mathrm{d}\Gamma + \frac{1}{F_{0,n}} \int_\Omega q_{\mathrm{I}}(\boldsymbol{x}) g_E(\boldsymbol{x}, t)\, \mathrm{d}\Omega \end{aligned} \tag{11}$$

Following Cornaton and Perrochet [2], the derivation of the BRT from (9) yields:

$$\varphi_n(t) + \tau_{0,n} \frac{\partial \psi_n(t)}{\partial t} = \delta(t) \tag{12}$$

with the observation zone drainage basin turnover time $\tau_{0,n} = M_{0,n}/F_{0,n}$. The transit time cdf f_n of the outlet Γ_n is defined by the integral of $\varphi_n(t)$, following Eq. (4):

$$f_n(t) = \int_0^t \varphi_n(\tau)\, \mathrm{d}\tau = 1 - \tau_{0,n} \psi_n(t) \tag{13}$$

For the drainage basin of outlet Γ_n, the life expectancy occurrence is given by $\psi_n(t)$. Eq. (13) allows decomposing the outflow of outlet Γ_n with respect to the arrival time.

3.2. Probability of exit at a specific outlet

The probability P_n that water particles exit through the boundary portion $\delta\Gamma_n$ prior to time t is related to the time integral of the probability flux [10]:

$$\mathrm{P}_n(\boldsymbol{x}_n, t)|\delta\Gamma_n| = \int_0^t [\mathbf{J}(\boldsymbol{x}_n, \tau|\boldsymbol{x}, 0) \cdot \delta\Gamma_n]\, \mathrm{d}\tau$$

where the probability flux $\mathbf{J}$ on an element $\boldsymbol{x}_n$ of $\delta\Gamma_n$ is conditional on the initial state $(\boldsymbol{x},0)$ in Ω. The total probability of exit through Γ_n is

$$\Pi_n(t)=\int_{\Gamma_n}\left(\int_0^t \mathbf{J}(\boldsymbol{x}_n,\tau|\boldsymbol{x},0)\cdot\boldsymbol{n}\,\mathrm{d}\tau\right)\mathrm{d}\Gamma_n$$

Following Gardiner [10], P_n also obeys the adjoint backward equation. Accordingly, we can formulate the following boundary value problem for the probability of exit $p_n(\boldsymbol{x},t)$ at Γ_n:

$$\frac{\partial\phi p_n}{\partial t}=\nabla\cdot\mathbf{q}p_n+\nabla\cdot\mathbf{D}\nabla p_n-q_1 p_n\quad\text{in }\Omega \tag{14a}$$

$$p_n(\boldsymbol{x},0)=0\quad\text{in }\Omega \tag{14b}$$

$$-\left[\mathbf{q}p_n(\boldsymbol{x},t)+\mathbf{D}\nabla p_n(\boldsymbol{x},t)\right]\cdot\boldsymbol{n}=-\mathbf{q}\cdot\boldsymbol{n}\quad\text{on }\Gamma_n \tag{14c}$$

$$-\left[\mathbf{q}p_n(\boldsymbol{x},t)+\mathbf{D}\nabla p_n(\boldsymbol{x},t)\right]\cdot\boldsymbol{n}=0\quad\text{on }\Gamma_+ \tag{14d}$$

$$-\mathbf{D}\nabla p_n(\boldsymbol{x},t)\cdot\boldsymbol{n}=0\quad\text{on }\Gamma_0 \tag{14e}$$

To characterize the probability for the position of water particles at a time t after recharge, the forward ADE has been assimilated to the Fokker–Planck equation, or forward Kolmogorov equation [16], which analyzes the random motion of water particles [17]. The backward equations (9a) and (14a) are related to the backward Fokker–Planck equation (or backward Kolmogorov equation) [27–29]. The function $p_n(\boldsymbol{x},t)$ corresponds to the cdf of the life-expectancy-to-outlet pdf defined in Eq. (9a), $p_n(\boldsymbol{x},t)=\int_0^t g_E(\boldsymbol{x},\tau)\,\mathrm{d}\tau$, and can also be assimilated to the fraction of the water particles situated at the position $\boldsymbol{x}$ that will reach Γ_n before time t. The total flux condition in Eq. (14c) ensures that the probability $\mathrm{P}_n|\delta\Gamma_n|$ of exit through Γ_n is certain. While Eq. (14c) ensures a maximum flux probability of exit at Γ_n (with $p_n=1$ in the right-hand side of the Cauchy condition formulation on Γ_n), Eq. (14d) prescribes a minimum flux probability of exit at any other outlet Γ_+. Since the flow velocity $\mathbf{q}$ and the dispersion tensor $\mathbf{D}$ are assumed to be independent of time, the function $p_n(\boldsymbol{x},t)$ approaches a limit at infinity. For the ultimate probability of exit $p_n^\infty(\boldsymbol{x})=p_n(\boldsymbol{x},\infty)$, one has to make the temporal derivative in Eq. (14a) vanish. With the boundary value problem (14a), we have defined the probabilistic drainage basin corresponding to the outlet Γ_n, $p_n(\boldsymbol{x},t)$, relatively to a particular travel time t. The ultimate, or steady-state probabilistic drainage basin is the field $p_n^\infty(\boldsymbol{x})$. Given the solution $p_n^\infty(\boldsymbol{x})$, the sub-drainage basin porous volume $M_{0,n}$ can be evaluated by integrating Eq. (10) over all time values:

$$M_{0,n}=\frac{\int_0^\infty\int_\Omega \phi g_E(\boldsymbol{x},t)\,\mathrm{d}\Omega\,\mathrm{d}t}{\int_0^\infty \psi_n(t)\,\mathrm{d}t}=\int_\Omega\phi\int_0^\infty g_E(\boldsymbol{x},t)\,\mathrm{d}t\,\mathrm{d}\Omega=\int_\Omega \phi p_n^\infty(\boldsymbol{x})\,\mathrm{d}\Omega \tag{15}$$

Because in both 2-D and 3-D domains there is a non-zero probability that the water particles will *not* be intercepted by the outlet Γ_n, $p_n^\infty(\boldsymbol{x})$ in Eq. (15) is less than one, $\int_0^\infty g_E(\boldsymbol{x},t)\,\mathrm{d}t<1$ for any $\boldsymbol{x}$. An iso-probability value $p_n^\infty(\boldsymbol{x})$ includes the domain for which the fraction $1-p_n^\infty(\boldsymbol{x})$ of its water amounts will reach the outlet Γ_n, sooner or later. The quantity $1-p_n^\infty(\boldsymbol{x})$ corresponds to the probability that the water particles located at the position $\boldsymbol{x}$ will not reach Γ_n.

3.3. Outlet capture zone and protection zone

In order to design an outlet capture zone from the probabilistic representation of the drainage basin, simple mass balance operations can be performed. We look for the minimum probability of exit, which provides an aquifer volume through which flow satisfies a given percentage of the total outlet discharge rate, $\varepsilon F_{0,n}$, with $\varepsilon\in[0;1]$. To do so, we derive the RT from the boundary value problem (14a), and obtain the following mass balance relation:

$$F_{0,n}-M_{0,n}\psi_n(t)=-\int_{\Gamma_-}\left[\mathbf{q}p_n(\boldsymbol{x},t)+\mathbf{D}\nabla p_n(\boldsymbol{x},t)\right]\cdot\boldsymbol{n}\,\mathrm{d}\Gamma+\int_\Omega q_1(\boldsymbol{x})p_n(\boldsymbol{x},t)\,\mathrm{d}\Omega=F_n(t) \tag{16}$$

where use has been made of Eq. (13) to express the outlet cumulated out flow function $F_n(t)=F_{0,n}f_n(t)$. Note that the inflowing limit Γ_- may be formed of several distinct boundary portions. The steady-state form of Eq. (16) is obtained by accounting for the pdf property $\psi_n(\infty)=0$:

$$F_{0,n}=-\int_{\Gamma_-}\left[\mathbf{q}p_n^\infty(\boldsymbol{x})+\mathbf{D}\nabla p_n^\infty(\boldsymbol{x})\right]\cdot\boldsymbol{n}\,\mathrm{d}\Gamma+\int_\Omega q_1(\boldsymbol{x})p_n^\infty(\boldsymbol{x})\,\mathrm{d}\Omega \tag{17}$$

The boundary integral term in the right-hand side of Eq. (17) provides the portion of the outlet total discharge rate which originates from recharge through the inflowing limits. The domain integral term provides the portion of the outlet total discharge rate which originates from recharge by internal sources. These quantities are time-dependent in Eq. (16). They relate to the different portions of the flow rate with respect to their infiltration origins, and that provide water particles which have travelled at a time t or less prior to exit. To design a capture zone, the value of probability ensuring the quantity $\varepsilon F_{0,n}$ to be balanced by natural recharge is then looked for by post-processing Eq. (17) for $\varepsilon F_{0,n}$, from the maximum probability towards the minimum probability. The obtained probability level can then be used to design the outlet capture zone.

Protection zones are in general designed with respect to a specific transit time from recharge to outlet. The definition of this transit time can vary from one country to one other, according to the laws on groundwater protection. Common reference values often range between 10 and 50 days. Other type of approaches are rather based on the choice of a relevant percentage of the outlet discharge rate to protect, and the protection zones are designed accordingly. With the function $F_n(t)$, one can pre-evaluate what time is relevant for the design of such protection zones. For example, if one decides that 90% of the total outlet discharge rate has to be protected ($\varepsilon = 0.9$), a simple reading on the cumulated outflow function $F_n(t)$ of the time t_{90} corresponding to $0.90F_{0,n}$ is required (see Fig. 2), $F_n(t_{90}) = 0.90F_{0,n}$. Eq. (17) can then be used to evaluate the probability isoline p_{90} which ensures the required mass balance. One can also fix a reference transit time to outlet, say t_{ref}, and design the outlet t_{ref}-capture zone by running the boundary value problem (14) for the duration t_{ref}. The value of probability inside which a chosen percentage of $F_n(t_{\text{ref}})$ is generated can then be evaluated on basis of Eq. (16).

3.4. Example: The well-head protection problem

We illustrate the application of the RT and of the definition of probabilistic capture and protection zones within the framework of the well-head protection problem (see Fig. 3). The resolution of the ADEs is performed using the Laplace-Transform Galerkin (LTG) finite element technique [23], which allows eliminating the time-derivative in the ADEs. Details about the LTG strategy are given in Cornaton and Perrochet [2]. However, more standard solution techniques using a time-stepping procedure can equivalently be used. We make use of a theoretical model, homogeneous with respect to hydraulic conductivity ($K = 5.0 \times 10^{-5}$ m/s), porosity ($\phi = 0.3$), longitudinal dispersivity ($\alpha_L = 10$ m), and transverse dispersivity ($\alpha_T = 2$ m). The model is similar to the one used by Neupauer and Wilson [20]. A hydraulic head $H = 50$ m is prescribed along the natural inlet limit Γ_-, and $H = 40$ m along the natural outlet limit Γ_+. The pumping-well is simulated by a hole of 0.5 m diameter in the finite element mesh (Γ_w), the center being at $\boldsymbol{x} = (200, 175)$. The extracted flow rate is $F_{0,w} = 8.64$ m^3/day. An additional infiltration (or irrigation) area of finite size (40 m × 40 m) is simulated here. The irrigation water contributes to the total inflow into the system, and the well flow rate contains a fraction of infiltrated water by irrigation, and a fraction of infiltrated water by the natural inlet limit Γ_-. The aquifer porous volume being $M_0 = 63{,}000$ m^3, and the steady flow rate being $F_0 = 30.456$ m^3/day, the aquifer turnover time τ_0 is 2068.558 days. The geometry, the boundary conditions and the resulting flow field are shown in Fig. 3a. The probabilistic time-dependent well capture zone (relative to a given temporal reference t_{ref}) is obtained by solving the boundary value problem (9), and by evaluating the life-expectancy-to-well-cdf $p_w(\boldsymbol{x}, t_{\text{ref}})$ at each node. This operation is straightforward when working in the Laplace domain, since the Laplace inversion for the single time value t_{ref} of the s-transformed function $s\hat{g}_E(\boldsymbol{x}, s) = \mathscr{L}\{\int_0^t g_E(\boldsymbol{x}, \tau)\,\mathrm{d}\tau\}$ yields the desired probability $p_w(\boldsymbol{x}, t_{\text{ref}})$.

Fig. 3b and c show the distribution of the life-expectancy-to-well pdf at $t = 3$ years and $t = 5$ years, which gives the intensity of probability for the position of the water molecules at the backward times 3 and 5 years (i.e. the most probable positions of the water molecules for having a travel time of 3 and 5 years before they reach the well). Fig. 3d gives a representation of the 3-years capture zone. These distributions are deformed by the presence of the infiltration area. In Fig. 3e, the 5-years capture zone is represented, as well as the probability isoline (isoline $p_w(\boldsymbol{x},5) = 0.465$) defining the pumping-well protection zone for a percentage of flow rate to protect of 90%. For $t = 5$ years, the well transit time cdf indicates that 86.5% of the flow rate produces water with this age or less (see Fig. 4c), $f_w(5) = 0.865$. The flow rate to protect is thus the 90% of 86.5% of the total steady-state discharge rate $F_{0,w}$. The pumping-well steady-state probabilistic capture zone porous volume $M_{0,w}$ is ~16.5% of M_0, and the corresponding turnover time $\tau_{0,w}$ is 1206.82 days. By enforcing Eq.

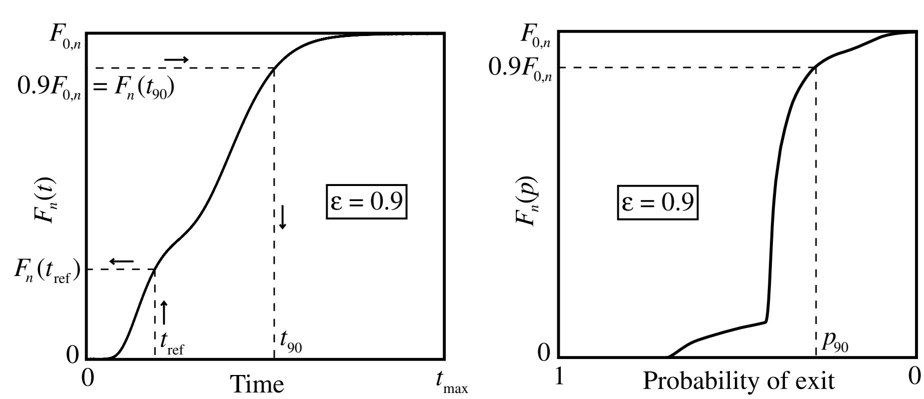

Fig. 2. Theoretical illustration of the protection zone definition procedure for $\varepsilon = 0.9$.

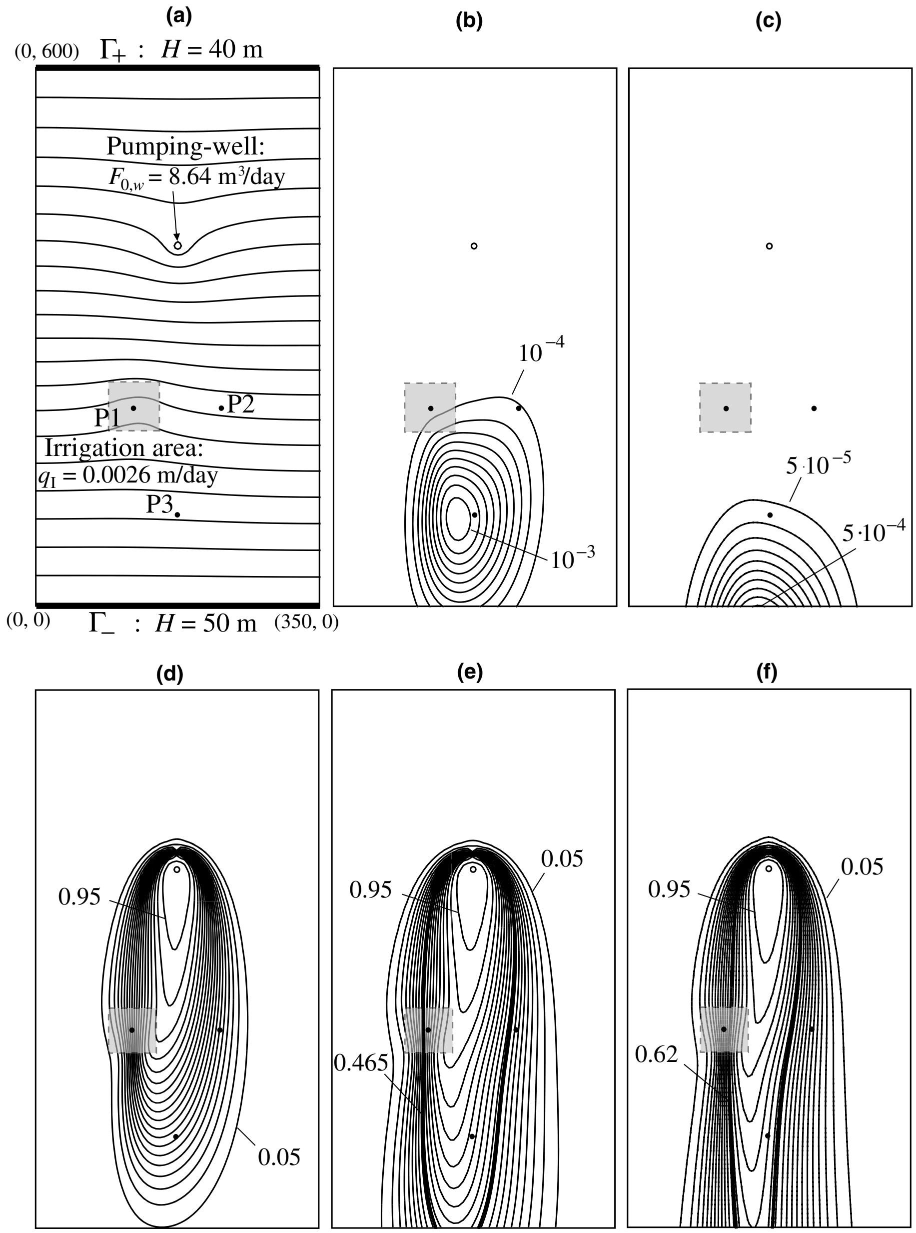

Fig. 3. Example of life-expectancy-to-outlet pdf and probabilistic capture zone calculations. (a) Geometry, flow boundary conditions, Laplacian field, and observation points location; (b) Life-expectancy-to-well pdf field in days^{-1} at time $t = 3$ years; (c) Life-expectancy-to-well pdf field at time $t = 5$ years; (d) Well 3-years probabilistic capture zone with contour interval 0.05; (e) Well 5-years probabilistic capture zone with indicated protection zone (thick line); (f) Well absolute probabilistic capture zone with indicated protection zone (thick line).

(17), we find that ~61% of the water extracted at the well originates from the natural inlet limit Γ_-, and that ~39% originates from the irrigation area. The isoline of probability within which 90% of the total discharge rate is attained is ~0.62 (see Fig. 3f). The corresponding area is ~10.7% of the total area. In Fig. 4a and b, the solutions of Eq. (10) and of the BRT (12) are given. The circles correspond to the verification of Eqs. (7) and (8). The BRT was applied to the natural outlet (Γ_+) capture zone, and the resulting pdfs were combined to the BRT results for the well (Γ_w), by enforcing Eqs. (7) and (8) to evaluate the global reservoir pdfs. The comparison with the FRT results for the global reservoir (considering the transit time pdf of the union $\Gamma_+ \cup \Gamma_w$ and the entire aquifer internal age pdf), shows a perfect agreement. The well transit time pdf shows two modes that are related to the two sources of infiltration. The irrigation area produces short transit times to the well (the minimum is $t \sim 500$ days), and thus corresponds to the major contribution to the first mode of the curve at $t \sim 500$ days. The second mode is mainly due to infiltration by the natural inlet (Γ_-). The intersection of the

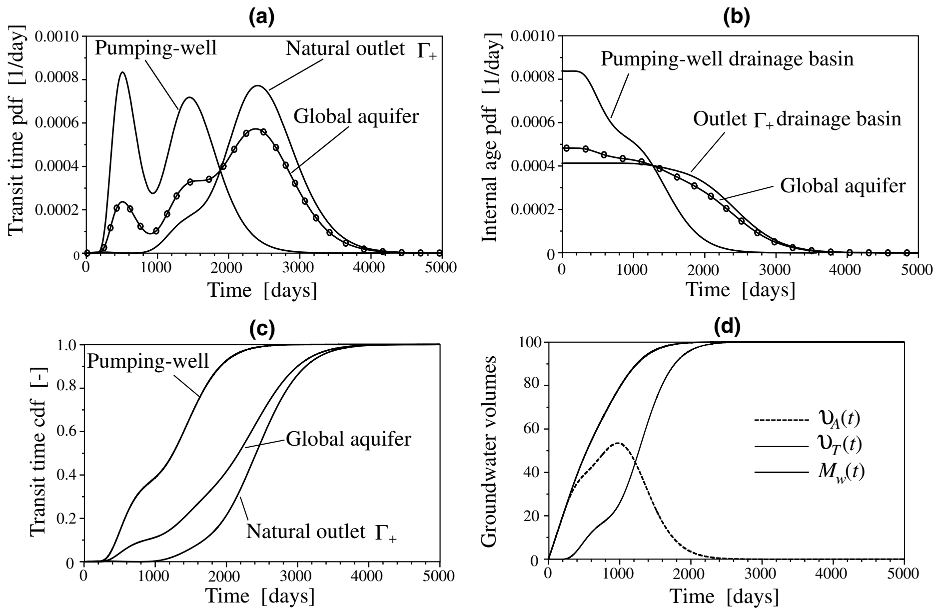

Fig. 4. RT for a theoretical pumping-well field. (a) Transit time pdf for the pumping-well Γ_w, the outlet Γ_+, and for the whole aquifer domain; (b) Internal age pdf for Γ_w, Γ_+ and for the whole aquifer domain; (c) Transit time cdf for Γ_w, Γ_+ and for the whole aquifer domain; (d) Internal groundwater volume functions for the pumping-well drainage basin in % of $M_{0,w}$. The circles in (a) and (b) correspond to the application of Eqs. (7) and (8).

life-expectancy-to-well pdf field at time $t = 3$ years with the inlet limit Γ_- (Fig. 3b) contains values up to 3.5×10^{-4} days^{-1}. This probability density magnitude must be present in the age distribution curve at the well, as shown in Fig. 4a. In a similar way, the observation point P1 (see Fig. 3a for the location) is concerned by a life expectancy value around 8.5×10^{-5} days^{-1} and P2 is around 10^{-4} days^{-1}, while P3 is around 9.5×10^{-4} days^{-1}. This shows that the effect of the irrigation area on the transit time distribution at the well is limited for ages superior to 3 years, and that the natural inlet limit is the main origin for the high probability of having arrival times at the well after this date. The analysis of the well transit time cdf $f_w(t)$ (Fig. 4c) indicates e.g. that 90% of the well discharge is concerned by water particles of 5.25 years old or less, ~63.10% by water particles of 3.95 years old or less (second mode), ~50% by water particles of 3.42 years old or less (median), ~46.75% by water particles of 3.26 years old or less (average age), ~42.25% by particles of 3 years old or less, ~14.15% by particles of 500 days old or less (first mode), and only ~4.25% by particles of 1 year old or less. The functions derived from the transit time cdf $f_w(t)$, and that describe the groundwater volumes in the reservoir as a function of age (or life expectancy), and transit time [2], provide interesting complement information on the dynamics of the system, in terms of groundwater amounts. We recall that the function $\upsilon_A(t)$ characterizes the porous volume with groundwater of age t or less, but that will experience an age superior to t at outlet. This function corresponds to the difference between the cumulated amount $M_n(t)$ of groundwater with an age t or less (cdf of the function $\psi_n(t)$ times the porous volume $M_{0,n}$) and the cumulated amount $\upsilon_T(t)$ of groundwater with an age t or less at outlet, $\upsilon_A(t) = M_n(t) - \upsilon_T(t)$. The function $\upsilon_A(t)$ informs on the quantities of water that contribute to the renewal of the groundwater stocks, and at the same time on the quantities that remain a long time within the system prior to exit. The function $\upsilon_A(t)$ relative to the pumping-well capture zone (Fig. 4d) equals the function $M_w(t)$ (volume of age t or less) until the approximate minimum transit time $t = 200$ days, indicating that the minimum arrival time at the well is around this date. The maximum of $\upsilon_A(t)$ is at time $t = 3$ years (~53% of M_0), and the relative rapid decrease that follows indicates that the water particles with an age superior to 3 years will not remain very long in the system, but will rather be rapidly absorbed by the well. An important tailing of the function $\upsilon_A(t)$ would at the contrary indicate that significant groundwater volumes remain a long time in the system before exit. The value of the function $\upsilon_T(t)$ at time $t = 3$ years is ~22% of M_0. The drastic increase of this function after 3 years indicates also that an important amount of groundwater flows rapidly to the well with a transit time superior to 3 years.

The RT applied to aquifer sub-systems (like the capture zone of a pumping-well), combined to the probabilistic definition of the domain that contributes to the outflow rate of a given observation zone, represents an interesting approach of groundwater resources protection. The FRT applied to the global system characterizes the entire environment in terms of residence and arrival times, by including each groundwater recharge and discharge zone, and the BRT enables the characterization of each specific outlet, and the identification of the associated drainage basin. The RT can help to refine the well-head protection study, by adding information obtained on the well and its drainage basin, to the well time-dependent and steady-state capture zones delineation. The functions $\upsilon_A(t)$, $\upsilon_T(t)$ and $M_n(t)$ allow characterizing the internal organization of age and of transit time to outlet, within the considered aquifer subdomain.

4. Analysis of pore velocity effects on the ages at a pumping-well

Transit time uncertainties depend primarily on uncertainties in hydraulic conductivity and pore velocity. In this section, we focus on the exclusive effect of pore velocity on the calculated transit time pdf at a pumping-well. To analyze the sensibility of the transit time pdf to the spatial variations of velocity, hundreds of realizations of an unconditional Log-normal random hydraulic conductivity field $\log(K)$ have been performed, following the spectral generation procedure of Mejía and Rodríguez-Iturbe [18]. The method makes use of a stationary random phase model to obtain asymptotically Gaussian and ergodic processes, by addition of harmonics of random frequencies, which are sampled from a spectral density function. The number of harmonics is the main factor that governs the quality of the generated process.

The geometry of the model corresponds to a 1200×700 m confined horizontal flow domain with a single pumping-well. The model consists of 33,600 bilinear quadrangles of size 5×5 m. The flow boundary conditions are indicated in Fig. 5a. On the western out flowing boundary a constant hydraulic head is assigned ($H = 0$ m). The pumping-well is located at $\boldsymbol{x}_\mathrm{w} = (400; 350)$ with an extraction flow rate $Q(\boldsymbol{x}_\mathrm{w}) = 5.0 \times 10^{-5}$ m^3/s. On the eastern inflowing boundary, a constant flux $q = 5.0 \times 10^{-7}$ m/s is imposed, rather than a prescribed hydraulic head, to ensure that the aquifer turnover time remains unchanged between each realization of the $\log(K)$-field. The northern and southern boundaries are impervious. Dispersion is uniformly fixed to the minimum acceptable, in relation to the possible numerical instabilities ($\alpha_\mathrm{L} = \Delta \boldsymbol{x}/2 = 2.5$ m, $\alpha_\mathrm{T} = \alpha_\mathrm{L}/10$, $D_\mathrm{m} = 2.3 \times 10^{-9}$ m^2/s). The $\log(K)$ generations were carried out for two relative separation distances $\zeta = L/\xi$, with L being the characteristic domain length in the x- and y-directions, and ξ being the correlation length. One example of generation is given in Fig. 5. The pumping well transit time pdf $\varphi_\mathrm{w}(t)$ is calculated for each realization using the BRT. The groundwater volumes $\upsilon_A(t)$, $\upsilon_T(t)$ and $M_\mathrm{w}(t)$ relative to age and transit time within the well capture zone Ω_w are also evaluated by post-processing the transit time cdf $f_\mathrm{w}(t)$, following Cornaton and Perrochet [2]. For each realization of the $\log(K)$ field, $\varphi_\mathrm{w}(t)$, $f_\mathrm{w}(t)$, $\upsilon_A(t)$, $\upsilon_T(t)$ and $M_\mathrm{w}(t)$ were calculated by assuming a physical dependency between the hydraulic conductivity K and the porosity ϕ (see Appendix A). The same realizations have also been carried out with a uniform porosity distribution, by taking the mean of the calculated heterogeneous porosity fields. The simulations for the relative separation distance $\zeta = 200$ show very small fluctuation of the calculated well transit time pdfs and groundwater volume functions, as illustrated in Figs. 5 and 6. Including the K–ϕ relationship (A.4) has the effect of reducing the differences between the simulated curves. Since pore velocity is proportional to the ratio K/ϕ, using Eq. (A.4) instead of a uniform porosity has the effect of homogenizing the velocity field, and consequently the spreading of the results is minimized. The results of the simulations with the relative separation distance $\zeta = 20$ show far more important differences between the calculated curves. This was expected because of the different types of generated $\log(K)$ fields, depending on ζ. The case $\zeta = 20$ results in marked zones of permeability, which can easily create separated preferential flow paths, as attested by the shape of the pumping-well capture zone in Fig. 5a. The case $\zeta = 200$ presents smoother permeability contrasts, which induce a more homogeneous transport. The effect of the K–ϕ relationship (A.4) for the case $\zeta = 20$ is even more pronounced than for the case $\zeta = 200$. When a uniform porosity is used, the simulated transit time pdfs and groundwater volume functions have contrasted shapes between each realization, and they all present important tails. When Eq. (A.4) is used, tailing is highly diminished, and the differences between the realizations are far less apparent.

The effect of the K–ϕ relationship on the dispersion of the results is obvious, when the tail of the curves simulated with a uniform porosity is compared to the tail of the curves simulated with the K–ϕ dependency. In this section, we have shown by means of numerical experiments, that a correlation between porosity and hydraulic conductivity has striking effects on age transport, particularly through the smoothing effect that this correlation induces on the age distribution, yielding more homogeneous-like transport phenomena. With even small spatial variations in porosity, the resulting velocity fields produce far less different age transport solutions than velocity fields which are only proportional to the Darcy flux vector. In porous media settings, it is reasonable to consider that the solutions which account for the K–ϕ dependency are physically more consistent. In such cases, pore velocity will depend only on the hydraulic gradient as in homogeneous medium, which is a much smoother function than hydraulic conductivity, in rela-

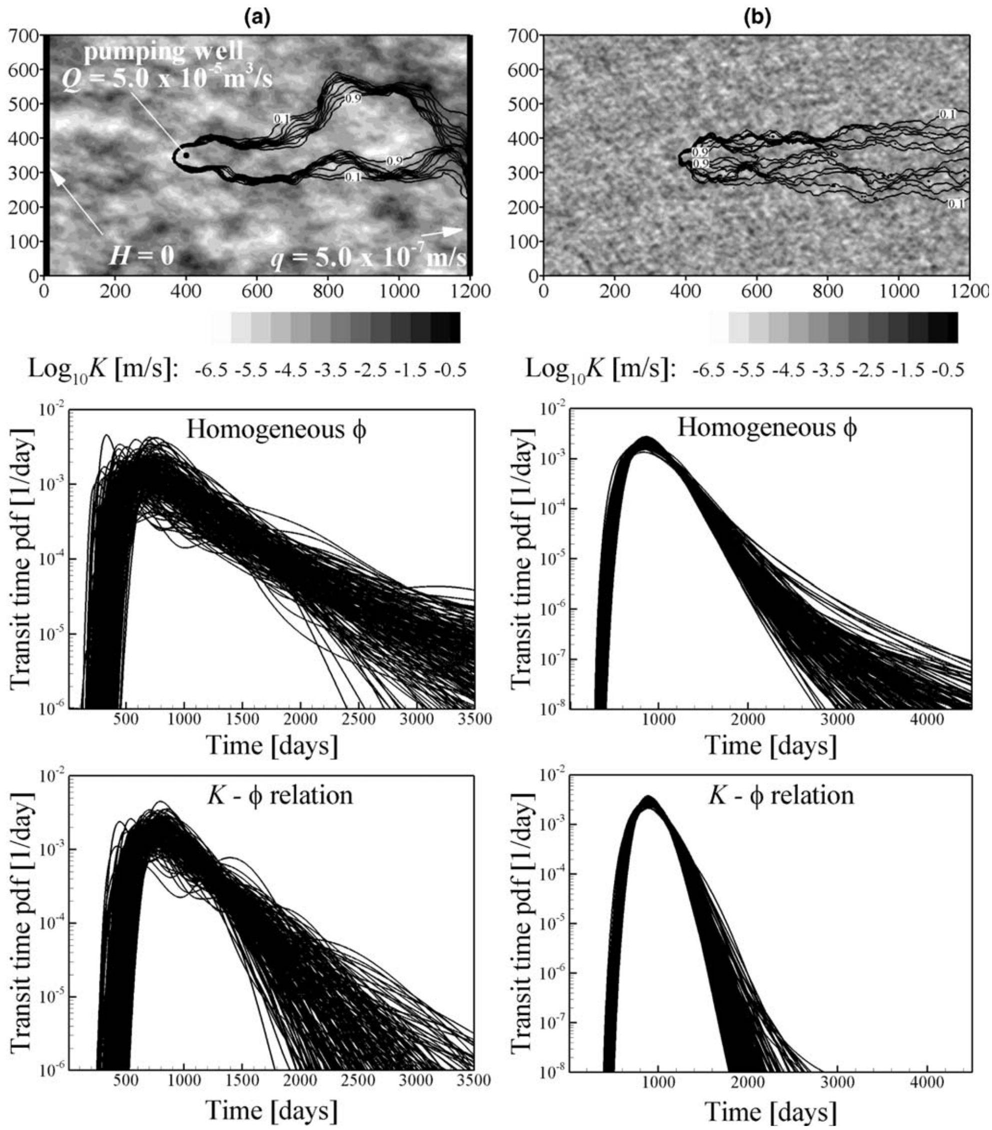

Fig. 5. Example of log(K) hydraulic conductivity field realization (simulated mean $\mu = -4.0$ and standard deviation $\sigma = 0.9$) and corresponding well absolute capture zones. Well transit time pdf for 200 random realizations of the log(K) field. (a) Relative separation distance $\zeta = 20$; (b) Relative separation distance $\zeta = 200$.

tion to the diffusive nature of the flow equation. We may argue that since porosity is generator of age during the water particles travel history, the ratio K/ϕ is a main factor that governs age transport. The knowledge of the spatial distribution of porosity is of high importance when dealing with age transport processes, because the uncertainty on porosity distribution has a direct effect on the uncertainty of the results. For mean age simulations which are carried out using a uniform distribution of porosity, one must be aware of the fact that multiplying porosity by two will yield twice as old simulated ages, or similarly dividing porosity by two will yield twice as young simulated ages. Depending on the available field data information on the couples K–ϕ, the number of parameters may be reduced by one by adopting an appropriate permeability/porosity relationship, as suggested in Appendix A.

5. Summary and conclusions

(1) The reservoir theory was first popular for its utility in chemical engineering, and was later introduced in the Earth Sciences by Eriksson [8], after having attempted to quantify the relations between the carbon amounts and fluxes in nature by assuming a simple linear relation [7]. In the reservoir theory, Eriksson assumes that no mixing may occur within the reservoir. This theory was made applicable to hydro-dispersive aquifer systems by Cornaton and Perrochet [2], there-

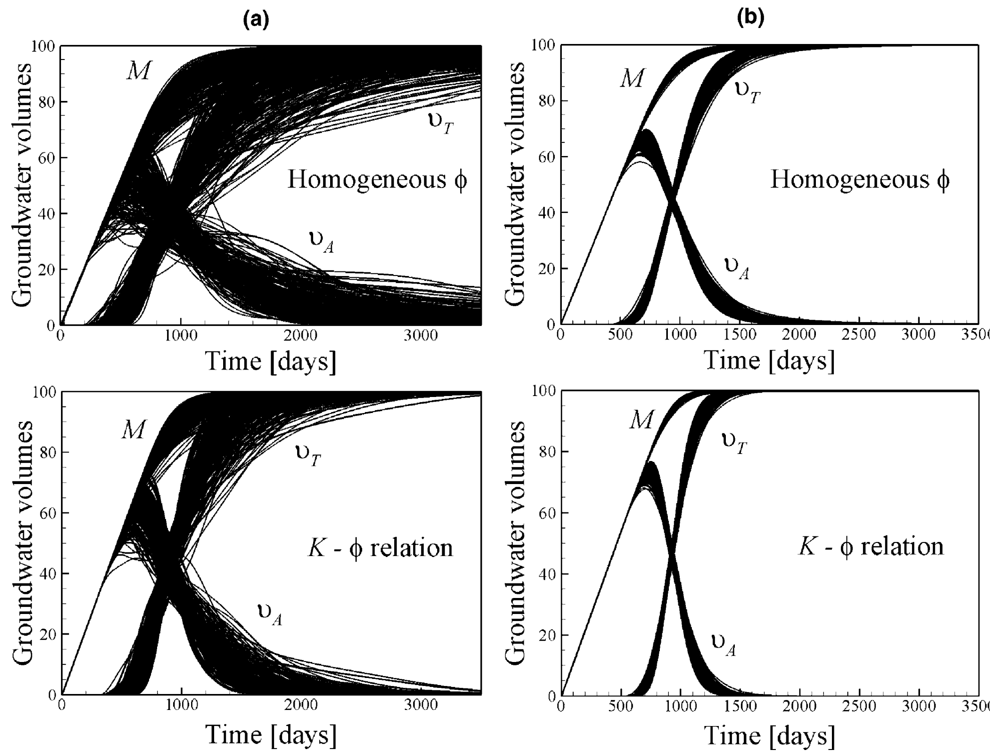

Fig. 6. Well capture zone groundwater volume functions (in % of $M_{0,w}$) for 200 random realizations of the log(K) field. (a) Relative separation distance $\zeta = 20$; (b) Relative separation distance $\zeta = 200$.

fore allowing mixing processes to be taken into account. In the present paper we have extended these results to any internal sub-drainage basin of a reservoir, by using the backward transport modeling approach. For any natural or artificial outlet of a reservoir of arbitrary geometry and flow complexity, the transit time distribution can then be calculated by relating the life expectancy occurrence at inlet to the life expectancy occurrence in the outlet drainage basin. Furthermore, the drainage basins of the reservoir individual outlets are also characterized in terms of probability.

(2) The application of the generalized reservoir theory has been illustrated with synthetic numerical experiments related to the well-head protection problem, by considering homogeneous and heterogeneous velocity fields. The backward transport modeling approach has been used to define capture zones, as it has already been done in previous works, but further linked to the RT approach. The combination of both approaches, which are based on similar forward and backward equations, can be helpful in aquifer and outlet vulnerability studies.

(3) The spatial heterogeneity of velocity was modeled by generating Lognormal random permeability fields, and by adopting a physical relationship between porosity and permeability. Simulation results for the well transit time pdf illustrate the effects of velocity fluctuations on the arrival times. Under advection-dominated regimes, the simulations generally showed important tailing effects, and join the idea already forwarded by several authors who considered the effects of dispersion on age transport (see e.g. [30]), that the representation of groundwater age by a single time value (generally this time is a mean age) can be misleading. However, as it has been illustrated in a previous work [2], dispersion is only one factor among others that creates unrepresentative mean ages. The spreading of the results for the well transit time pdf, based on hundreds realizations of the velocity field, is very much lowered when permeability and porosity are linked by a physical relationship. This points out the importance of porosity as a governing parameter for age transport, since it acts as an age generator. Therefore, particular attention should be given to the spatial distribution of this parameter.

(4) The RT allows for the simulation of the transit time pdf of outlets and inlets with better accuracy than direct evaluation methods, and provides fundamental transient information which can be added to many hydrogeological studies, like the groundwater resources vulnerability and protection analysis.

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Appendix A. Permeability–porosity relation

We consider the well-known Hagen–Poiseuille law, which expresses the geometric permeability κ [L^2] in granular media by the following general formulation:

$$\kappa = \frac{\phi^3}{\omega\theta^2 A_s^2} \tag{A.1}$$

where ω is a dimensionless geometrical factor depending on the morphology and distribution of the grains, θ is tortuosity [$-$], ϕ is porosity [$-$], and A_s [L^{-1}] is the specific surface of the grains, which can be defined by

$$A_s = \frac{3(1-\phi)}{G_0}\int_0^{+\infty}\frac{1}{r}\frac{\partial G_{\mathrm{cum}}(r)}{\partial r}\,\mathrm{d}r = 3(1-\phi)\int_0^{+\infty}\frac{g(r)}{r}\,\mathrm{d}r \tag{A.2}$$

with $G_{\mathrm{cum}}(r)/G_0$ being the grain size cdf (G_0 is the total dry soil weight), and thus the function $g(r)$ being the corresponding grain size pdf. Once the κ-field has been generated, the medium porosity is calculated by solving

$$\kappa = \frac{\phi^3}{\gamma(1-\phi)^2}, \quad \gamma = 9\omega\theta^2\left(\int_0^{+\infty}\frac{g(r)}{r}\,\mathrm{d}r\right)^2 \tag{A.3}$$

for ϕ, with the important assumption that the factor γ is a constant over the entire domain. This assumption implies that the grain-size distribution, the shape and arrangement of the grains are uniform functions of space. However, for $\log(K)$ fields showing variations up to four orders of magnitude, we verified that Eq. (A.3) yields smoothly varying porosity fields (e.g. between 5% and 25%), which belong to an acceptable range of porosity in porous medium. Note that Eq. (A.3) is close to the Fair–Hatch equation for non-uniform soils (see e.g. [24]), although it is expressed in a more general form. Assuming e.g. that the grain size pdf $g(r)$ is Lognormal with the mean μ and the standard deviation σ, Eq. (A.3) simplifies in:

$$\kappa = \frac{e^{2\mu-\sigma^2}}{9\omega\theta^2}\frac{\phi^3}{(1-\phi)^2} \tag{A.4}$$

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