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Exact analytical solution of the convolution integral for classical hydrogeological lumped-parameter models and typical input tracer functions in natural gradient systems

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SUMMARY

This work presents the analytical solution to the convolution integral by taking into account the most widely used lumped parameter hydrogeological models (Piston, Exponential, combined Exponential-Piston and Dispersion model) and the eight most typical input tracer functions (Constant; Sinusoidal with linear trend; Sinusoidal with combined sinusoidal and linear trend; Instantaneous pulse injection; Step or Heaviside; Instantaneous pulse with exponential ending; Long pulse with sharp ending; Long pulse with exponential ending) naturally occurring or usually conducted in aquifer systems under natural gradient conditions. For such cases, the output tracer function is expressed in terms of mathematical elementary functions that only depend on the aquifer mean transit time and the parameters belonging to the assumed lumped model.

1. Introduction

Groundwater mean transit times have received increasing attention due to their interest for the management of water resources (Kinzelbach et al., 2003; McGuire and McDonnell, 2006), to manage groundwater vulnerability due to contamination of near surface recharge waters (Glynn and Plummer, 2005; Bethke and Johnson, 2008) or for applications in groundwater dating studies (McGuire et al., 2002; Stichler et al., 2008). It is defined as the first moment of a transit-time distribution (TTD) that may have complicated shapes (Etcheverry and Perrochet, 2000). Techniques for estimating these distributions can be grouped into three categories: (1) The geochemical techniques which combines environmental tracers with lumped parameter models (LPMs) (Corcho Alvardo et al., 2007; Knowles et al., 2010; Land and Huff, 2009; Genereux et al., 2009; Solomon et al., 2010; Stolp et al., 2010; Massoudieh et al., 2012). This is the most parsimonious approach since LPMs represent the mass transfer through the aquifer using parameterized analytical functions for describing the TTD. These functions explicitly explain how an input signal (recharge or pollution pulse for instance) is transformed as it travels through the aquifer system (Cornaton et al., 2011; Massoudieh and Ginn, 2011). (2) The numerical modelling approach, which allows understanding how TTDs behave in advective-dispesive dominated groundwater systems, regardless of the complexity of the internal spatial flow configuration (Kinzelbach, 1992; Varni and Carrera, 1998; Etcheverry and Perrochet, 2000; Sánchez-Vila et al., 2001; Cornaton and Perrochet, 2006; Cardenas and Jiang, 2010; Engdahl et al., 2012; Green et al., 2014). Issues with non-uniqueness may arise when TTDs are used to explain environmental tracer data for model validation (Varni and Carrera, 1998; Weissmann et al., 2002; Leray et al., 2012) because these concentrations can be fit by multiple transit time distributions. (3) The non-parametric free approach. This technique allows the determination of the TTD without imposing any predefined shape of the distribution function (Fienen et al., 2006; Liao and Cirpka, 2011; Liao et al., 2013; Massoudieh et al., 2013). It is a promising technique because it

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bypasses issues associated with model choice and parameterization. Nevertheless, it often relies on the use of large data sets to estimate TTDs.

Usually mean transit time is the main result of the above groundwater dating techniques, although it provides little information on skewed multimodal distributions. To infer transit time distributions in hydrogeological systems where data are limited (e.g., less developed countries, ungauged basins, karst and complex fractured systems where an internal detailed knowledge is not available) the geochemical technique has been widely used, mainly because LPMs do not require detailed hydrological characterization of the physical system. The lumped-parameter models treat the hydrogeological system as a whole, and assume the flow pattern to be in steady state or natural gradient conditions (Małoszewski and Zuber, 1996). They transform tracer inputs to output concentrations by solving a convolution integral which depends on both the input tracer function and the weighting function that lumps all the factors affecting groundwater flow and/or tracer transport (Małoszewski and Zuber, 1982; Zuber, 1986; Amin and Campana, 1996; among others).

The solution of convolution integrals is not an easy task despite it being a well-known technique since the 19th century. Often, hydrologists have to resort to numerical methods for accounting complex time varying input tracer functions when evaluating convolution integrals. There is a number of software codes specifically developed to numerically solve the convolution integrals (Zoellmann and Aeschbach-Hertig, 2001; Małoszewski and Zuber, 2002; Bayari, 2002; Ozyurt and Bayari, 2003, among others), but their use is not easy and requires some expertise from the user. Additionally, these codes typically use a user defined constant time length scheme (i.e. monthly or annual) to solve the convolution integral. The input tracer function is therefore accommodated to follow the defined time step discretization, which is done by averaging the available input tracer concentration measurements over the corresponding time step regardless of the input tracer measurement sampling frequency (i.e. daily, monthly or annual measurements). Such averaging process might generate errors when estimating the model lumped parameters, especially in the case of scarce input tracer data measurements. Nevertheless, in some cases the input tracer functions can be mathematically described by using elementary functions. The latter makes the convolution integral to be analytically solved for some lumped-parameter models. Analytical solutions of the convolution integral can be found for some simple input tracer functions: Małoszewski and Zuber (2002) solved the convolution integral for a constant tracer injection function and by considering the Piston flow Model (PFM), the Exponential Model (EM), the combined Exponential-Piston model (EPM) and in some cases the Dispersion model (DM), which are the most widely used lumped-parameter models used for quantitative interpretation of tracer data in hydrologic systems (McGuire and McDonnell, 2006). Amin and Campana (1996) extended the previous work to include the case of the Partial Mixing lumped-parameter Model (PMM). In this model the weighting function is expressed in terms of a three-parameter gamma function, ranging the model applicability from near EM to near PFM, but never reaching these extremes. Małoszewski et al. (1983) considered a simple sine-wave which is another time invariant injection tracer function. In this case they modelled the output tracer concentration by acknowledging the fact that the convolution integral of a sine input function mathematically produces a sine output function, which is delayed and buffered with different strength in terms of the assumed lumped model. They provided the mathematical expressions to relate the expected output changes in amplitude and time-shift for both, EM and DM. Kubota (2000) formally derived the latter expressions by explicitly integrating the convolution integral with a sinusoidal input tracer function for the same lumped models. Custodio and Custodio-Ayala (2013) focused in the problem of considering a piecewise input tracer function. They solved the convolution integral for the EM case by considering an instantaneous tracer pulse followed by an exponential decreasing tracer tail injection.

The preceding injection functions are only a subset of the input tracer functions found in the available literature related to tracer data interpretation in hydrologic systems. In fact, input tracer functions in natural gradient systems show other typical configurations (i.e. Novakowski et al., 1995; Gerasopoulos et al., 2003; Gooddy et al., 2006; Vincenzi et al., 2011; Farlin et al., 2013; among others) which can be easily expressed in terms of elementary mathematical functions. Although evaluating convolution integrals is not easy and often error prone, especially when discontinuous functions are involved, these analytical input functions might be used to obtain the analytical solution of the convolution integral for the classical lumped parameter models (i.e. PFM, EM, EPM and DM) which have not been obtained yet.

This study aims to obtain the exact solution of the convolution integral by accounting eight synthetic input tracer functions (Constant; Sinusoidal with linear trend; Sinusoidal with combined sinusoidal and linear trend; Instantaneous pulse injection; Step or Heaviside; Instantaneous pulse with exponential ending; Long pulse with sharp ending; Long pulse with exponential ending) and the four classical lumped parameter models PFM, EM, EPM and DM.

2. Background

Lumped parameter models are useful to estimate the mean residence time of groundwater in complex and poorly characterized groundwater flow systems. They are convenient because no spatially distributed detailed information is needed from the aquifer system (i.e. transmissivity, porosity, boundary conditions, etc.) which is typically required for numerical models based on Darcy's Law.

The lumped-parameter approach appeared initially in the field of chemical engineering (Levenspiel, 1962, 1999), but their use has been extended to other disciplines including hydrogeology (see Małoszewski and Zuber, 1982, 1996; Zuber, 1986; Amin and Campana, 1996, among others). In the lumped-parameter approach the groundwater system is treated as a whole and the flow pattern is assumed to be in steady state. In the general case, the lumped parameter models transform the tracer input concentrations C_{in} to output concentrations $C(t)$ according to Eqs. (1) or (2), which are equivalent, and known as convolution integrals (see Małoszewski and Zuber, 1982; Kwakernaak and Sivan, 1991; Soliman and Srinath, 1998 or Olsthoorn, 2008, among others),

$$C(t) = \int_{-\infty}^{t} C_{in}(t')g(t-t')e^{-\lambda(t-t')}dt' \quad (1)$$

$$C(t) = \int_{0}^{\infty} C_{in}(t-t')g(t')e^{-\lambda t'}dt' \quad (2)$$

where λ is the radioactive (or chemical) tracer decay constant (i.e. if no chemical tracer degradation nor radioactive tracer is used then $\lambda = 0$), t is the time of entry, t' is the integration variable and $g(t')$ is the system response function, also called the weighting or the transit time distribution (TTD) function. This function describes the exit-age mean residence time of tracer concentrations, which entered into the aquifer system at various times in the past. It is ascertained by the response of the system to a pulse injection of tracer. It may have various complicated shapes and it is not easy to calculate. In fact, the inference of TTDs is an active research issue (Fienen et al., 2006; Cirpka et al., 2007; Liao and Cirpka, 2011;