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The frequency domain approach to analyse field-scale miscible flow transport experiments in the soils

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A new approach to the estimate of the parameters u (advective velocity) and λ (dispersivity) characterizing solute transport in soils is presented. The pair (u, λ) is estimated by matching in the *frequency domain* (FD) the theoretical expression of moments pertaining to the *breakthrough curve* (BTC) against to the one evaluated by means of the experimental data. In particular, we demonstrate that to reduce the impact of the random measurement-errors upon such an estimate, it is worth retaining in the Fourier's expansion of the moments only the harmonics associated to the smaller frequencies. This is due to the fact that the Fourier transform moves most of the measurement-errors affecting moments in the high-frequency range. As a consequence, by adopting a relatively small number of harmonics to compute the Fourier transform of the experimental moments, one may filter out most of the noise. It is also shown that the number of harmonics to retain (cut-off) depends upon the soil's water content as well as the magnitude of the characteristic length $\ell_{\mathscr{E}}$ of the error relative to the dispersivity λ.

The proposed methodology has been applied to a recently conducted plot-scale transport experiment. For comparison purposes, we have also estimated the pair (u, λ) by the classical *method of moments* (MM). Both the methods lead to the same value of the advective velocity u. This is explained by recalling that u depends upon the first-order moment, a quantity that is scarcely influenced by the measurement-errors. Instead, the estimate of the dispersivity λ (which is related to the second-order moment) is largely different (with the value achieved by the MM larger than the one obtained by the FD approach). Such a difference is addressed to the fact that in the MM the distortion-effect due to the measurement-errors amplifies with the increasing order of the moments, a phenomenon which is completely avoided in the FD approach by adopting the above mentioned cut-off.

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List of symbols and nomenclature

α dimensionless parameter
C [M L^{-2} T^{-1}] flux concentration
D [L^2 T^{-1}] dispersion coefficient
δ Dirac distribution
EP efficiency parameter
$\mathcal{E}_n$ [M L^{-2} T^n] noise affecting the n-order moment
$\tilde{f}$ Fourier transform of f
$\bar{f}$ Laplace transform of f
H Heaviside step function
K_m modified m-order Bessel function of the second kind
$\ell_{\mathcal{E}}$ [L] transverse length scale of the error-measurements
λ [L] dispersivity
M_0 [M L^{-2}] solute mass per unit area
M_n [M L^{-2} T^n] moment of n-order
$M_n^{(exp)}$ [M L^{-2} T^n] experimental moment of n-order
$\mathcal{M}_n$ dimensionless moment of n-order
Ω transport domain
ω [L^{-1}] spatial frequency
ϖ dimensionless spatial frequency
q [L T^{-1}] flux
ϑ [L^3 L^{-3}] volumetric water content
ϱ [M L^{-3}] soil's bulk density
t [T] time
t_c [T] time scale of transport
u [L T^{-1}] advective velocity
u_{eff} [L T^{-1}] effective velocity
$\bar{u}_{eff}$ [L T^{-1}] mean effective velocity
z [L] depth
ζ dimensionless depth

1. Introduction

The use of transport experiment(s) as a tool to identify the convective-dispersive properties of soils has been discussed in numerous studies (a wide review can be found in Rubin, 2003, and references therein). Classically, the identification of the transport parameters is carried out by the MM, first introduced by Aris (1958) and subsequently refined by many others (see, e.g. Gómez, Severino, Randazzo, Toraldo, & Otero, 2009; Köhne, Köhne, & Simunek, 2009; Severino, Santini, & Sommella, 2003, and references therein). A drawback related to such an approach is that moments are highly sensitive to their order, and therefore measurement-errors produce an enhancing distortion on the higher-order moments. Nevertheless, the MM is by far the most used method thanks to its ease of implementation. An alternative approach, based upon the Fourier analysis, has been proposed by Duffy and Al-Hassan (1988). In this case, the parameters' estimate is achieved by comparing the theoretical *vs* experimental BTCs in the FD. Unlike the MM, in the FD approach the dispersion mechanism *de facto* acts as a low pass-filter (Owen, 2007). As a consequence, if one can limit to a relatively small number of harmonics (low frequency range) the numerical computation of the Fourier transform of the experimental BTCs, then the parameters' estimate would be affected to a much lesser extent by the measurement-errors. One (technical) disadvantage is that the experimental BTCs must be Fourier transformed (by means of the fast Fourier transform). Nevertheless, such a drawback is compensated by the fact that in the FD simple (closed form) solutions are almost always available, whereas in the time domain they may not even exist, or result tremendously cumbersome (see, e.g. Sardin, Schweich, Leij, & Genuchten, 1991; Severino & Indelman, 2004; Severino, Monetti, Santini, & Toraldo, 2006).

So far the FD approach has been used (see e.g. Duffy & Al-Hassan, 1988) to determine the transport parameters at laboratory scale (samples of small sizes), where it is relatively simple to monitor the BTCs. However, at field (and even larger) scales this is not anymore the case due to the numerous limitations mainly related to the heterogeneity, which is a typical feature of the soils at that scale (see, e.g. Coppola et al., 2011; Fiori et al., 2010; Severino & Santini, 2005; Severino, Santini, & Monetti, 2009; Severino & Coppola, 2012; Severino, Tartakovsky, Srinivasan, & Viswanathan, 2012). In this case, the accessible information is the first and second order moment (see, e.g. Severino, Dagan, & van Duijn, 2000, 2007), and consequently the FD approach, as implemented at laboratory scale, does not apply.

Thus, a new approach dealing with moments rather than BTCs is required. To this aim, we refer to the following conditions (typical at field scale): a steady, one-dimensional flow takes place into a semi-bounded domain $\Omega \equiv \{z \in \mathbb{R} : z \geq 0\}$ which is initially solute free, i.e. $C(z,0) \equiv 0$, being C the flux concentration. A specific (per unit surface) mass M_0 is then applied at the surface $z = 0$ in the form of a pulse, and it is subsequently moved downward by advection. We also assume that at the very deep depths transport is immaterial. These translate into the following boundary conditions

$$C(0,t) = \frac{M_0}{u}\delta(t), \quad \lim_{z\to\infty} C(z,t) = 0, \tag{1}$$

being u the advective velocity. The n^{th}-order moment writes as:

$$M_n(z) = \int_0^\infty dt\, t^n\, C(z,t), \quad z \in \Omega. \tag{2}$$

Thus, if the concentration $C \equiv C(z,t)$ is determined in analytical form, one can compute (either analytically or numerically) moments (2). For the problem at stake, the concentration is obtained by solving (for details, see e.g. Jury & Roth, 1990, ch. 2.5.2) the advection-dispersion equation:

$$\frac{\partial}{\partial t}C + u\frac{\partial}{\partial z}C = D\frac{\partial^2}{\partial z^2}C \tag{3}$$

under the above initial/boundary conditions, the final result being:

$$C(z,t) = \frac{M_0 z}{2t\sqrt{\pi D t}} \exp\left[-\left(\frac{z-ut}{2\sqrt{Dt}}\right)^2\right]. \tag{4}$$

The dispersion coefficient D encompasses both diffusion and dispersive mechanisms, although the latter are always prevailing upon the former (a wide discussion upon such an

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