Matemática Aplicada, Computacional e Industrial

ISSN 2314-3282

MACI

Vol. 4 (2013)

IV MACI 2013

4to Congreso de Matemática Aplicada, Computacional e Industrial

4th Congress on Industrial, Computational and Applied Mathematics

15 al 17 de mayo de 2013

May 15 to 17, 2013

Buenos Aires, ARGENTINA

G. LA MURA, D. RUBIO y E. SERRANO (Eds.)

ASOCIACIÓN ARGENTINA
DE MATEMÁTICA APLICADA,
COMPUTACIONAL E INDUSTRIAL

Matemática Aplicada, Computacional e Industrial

ISSN: 2314-3282

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ASOCIACIÓN ARGENTINA DE MATEMÁTICA APLICADA COMPUTACIONAL E INDUSTRIAL

Nonreactive solute transport in soil columns: Classical and fractional-calculus modeling

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Abstract: Vertical nonreactive solute transport data collected in three laboratory soil columns (made out of sediment samples from the Pampean aquifer located southeast of the Buenos Aires province) are contrasted with the explicit solutions of two model 1D linear PDEs: the classical advection–dispersion equation (ADE), and a *fractional advection–dispersion equation* (FADE) which has proven to be a useful modeling tool for highly inhomogeneous media exhibiting nontrivial scaling laws. Whereas two of the samples turn out to be quite homogeneous (thus requiring a fractional-derivative order $\gamma \to 2$), the third one is best described by a FADE with fractional-derivative order $\gamma = 1.68$. This example illustrates the FADE's ability to reveal self-similar geometric structures inside the sample.

Keywords: *Fractional partial differential equations - Smoothing, curve fitting - Sensitivity, stability, parametric optimization*
2000 AMS Subject Classification: 35R11 - 65D10 - 90C31

1 Introduction

The classical advection–dispersion equation (ADE) has been traditionally employed to model solute transport in soils (in Hydrology and Soil Science, the term "dispersion" does not imply waves but is a synonym of diffusion). In fact, the ADE captures adequately the behavior of a solute in a *homogeneous* medium. Its 1D version reads

$$\frac{\partial C}{\partial t} = v\left(\alpha\,\frac{\partial^2 C}{\partial x^2} - \frac{\partial C}{\partial x}\right), \tag{1}$$

where $C(x,t)$ is the solute concentration, v the average flow speed through the pores, $\alpha := D/v$ the *dispersivity*, and D the *longitudinal* dispersion coefficient (namely, along flow lines). Dimensionally, $[\alpha] = l$, hence its usefulness as a modeling parameter. The derivation of Eq. (1) in statistical physics assumes the solute particles to undergo Brownian motion, which is the composition of successive increments drawn from independent normally distributed random variables with identical finite variance.

We must recall however that a soil is a porous medium and will more likely exhibit heterogeneities at all scales, often leading to self-similar geometric structure. In 1990 some researchers [1] reported that the dispersivity showed scaling effects, tending to increase with distance. This type of process is often described as *anomalous dispersion*. During the 90's, transport models with fractional derivatives such as the *fractional advection–diffusion equation* (FADE) emerged, in which the scaling effects are accounted for by the order of the fractional derivative. Its 1D version with symmetric dispersion reads

$$\frac{\partial C}{\partial t} = v\left[\frac{\alpha_\mathrm{f}}{2}\left(\frac{\partial^\gamma C}{\partial_+ x^\gamma} + \frac{\partial^\gamma C}{\partial_- x^\gamma}\right) - \frac{\partial C}{\partial x}\right], \tag{2}$$

where $1 < \gamma \leq 2$ is the fractional-derivative order, $\alpha_\mathrm{f} := D_\mathrm{f}/v$ the "fractional dispersivity" ($[\alpha_\mathrm{f}] = l^{\gamma-1}$), D_f the fractional longitudinal dispersion coefficient ($[D_\mathrm{f}] = l^\gamma t^{-1}$), and $\partial_\pm$ a shorthand for the fractional derivatives to the left and to the right, defined as usual through Riemann–Liouville integrals.

Equation (2), which reduces to Eq. (1) for $\gamma = 2$, has been derived by assuming the solute particles to undergo the so-called Lévy motion, which is the composition of iid random variables with *infinite* variance. In Lévy motion, the persistence of the solute-particle motion, as well as significant deviations from the average, are much more likely than in Brownian motion. Hence there are particles that travel long distances above average speed, while others do so at lower speeds experiencing long waiting times before engaging the fluid motion. This has also been modeled by considering mobile and immobile zones (MIM) [2, 3].

At present, the articles which apply Eq. (2) to solute transport in porous media (and among them those which compare the results yielded by the classical and fractional models) are not few. Some research [4, 5] has concluded that the benefits of FADE with respect to ADE (which as already pointed out is a special case of the former) are not so evident in saturated sandy substrates, or clay substrates at high flow rates [4]. In the present study we too compare the goodness of both models, for sediment samples from the Pampean aquifer located southeast of the Buenos Aires province.

2 Materials and methods

2.1 Experimental data

The experimental data $O(t)$ come from column tests made on undisturbed sediment samples from the Pampean aquifer, located southeast of the Buenos Aires province (mainly loessic, silt-clay and silt-sandy sediments). The samples are represented in a barycentric diagram in Fig. 1:
A: Taken on a site located along National Route 226, 15 km far from Mar del Plata city; average composition 18.62% fine sand, 65.29% silt and 16.08% clay [6].
B1: Taken on *cultivated soil* near La Dulce town, in the basin of the Quequén river; average composition 66.5% sand, 20.4% silt and 13.5% clay [7].
B2: Taken on adjacent *natural soil* near La Dulce town, in the basin of the Quequén river; average composition 76.5% sand, 10.4% silt and 12.5% clay [7].

The column tests consist in injecting a *ClNa* solution on top of the vertical columns (previously saturated with distilled water), so that its flow is due to gravity. Cl^- was chosen as a tracer for being unreactive with the medium. The conductivity of the eluted solution is then measured at regular intervals until it equals that of the injected one. Now, here enters another crucial hydraulic parameter: the *porosity* ρ. Different soils will differ in ρ values and that will lead to different flow times. In order to compare them, the regular intervals must be chosen as fractions of the estimated pore volume of the sample (i.e. $\rho_\mathrm{e} \times V$, where ρ_e is an estimation since determining ρ is one of our goals) and V the volume of the column. For each case and each time interval, several measurements are made and the average is taken.

2.2 Mathematical modeling procedure

The analytical solution of Eq. (1) for a column of length L and initial condition $C(x, 0) = C_i$ for $0 < x \leq L$ is given by [8]

$$C(L,t) = C_i + \frac{C_0 - C_i}{2}\left[\operatorname{erfc}\left(\frac{L - vt}{\sqrt{4v\alpha t}}\right) + \exp\left(\frac{L}{\alpha}\right)\operatorname{erfc}\left(\frac{L + vt}{\sqrt{4v\alpha t}}\right)\right], \quad (3)$$

where $C_0 = C(0, t)$, $t \geq 0$ is the boundary condition at the plane of the source. Hereafter we take $C_i = 0$. For $L/\alpha \sim 10^2$, the input from the transient in the second term can be safely neglected [8].

The analytical solution of Eq. (2) is obtained by Fourier transformation [9]. For the same conditions as in Eq. (3) it reads

$$C_\mathrm{f}(L,t) = C_0\left[1 - F_\gamma\left(\frac{L - vt}{\sigma}\right)\right], \quad (4)$$

where $\sigma = [v\alpha_\mathrm{f} t \cos(\pi\gamma/2)]^{1/\gamma}$ and F_γ is the γ-stable Lévy distribution function, which is evaluated numerically by means of a Matlab adaptation of the Fortran subroutine **cfastd** of Ref. [9]. The graphs of this solution look similar to those of Eq. (3).

Two optimization processes were separately conducted for each dataset [namely $O_\mathrm{A}(t)$, $O_\mathrm{B1}(t)$, and $O_\mathrm{B2}(t)$], choosing as objective functions the Euclidean distance between the experimental vectors and the corresponding analytical ones. For each, the corresponding Matlab script was written, using the minimization package **fmincon**. As fitness measures, the *relative distances* (the ratios between the absolute distances and the norm of the experimental data vector)

$$\delta = \frac{\min_{\alpha,\rho}\left(\sum_{i=1}^{n}[C(L,t_i) - O(t_i)]^2\right)^{1/2}}{\left(\sum_{i=1}^{n}[O(t_i)]^2\right)^{1/2}}, \quad \delta_\mathrm{f} = \frac{\min_{\gamma,\alpha_\mathrm{f}}\left(\sum_{i=1}^{n}[C_\mathrm{f}(L,t_i) - O(t_i)]^2\right)^{1/2}}{\left(\sum_{i=1}^{n}[O(t_i)]^2\right)^{1/2}} \quad (5)$$

are quoted in the inset of the figures.

2.3 Numerical results

Figures 1 and 2, which plot the Cl^- concentration as a function of time (expressed in pore volumes) summarize the results of the optimization process, exhibiting together with the experimental data the ADE and FADE solutions [Eqs. (3) and (4)] which best fit them. Quoted in the inset are the optimal parameters for the ADE (α and ρ) and FADE (γ and α_f) solutions, together with the respective relative distances and the initial concentration C_0 for each case.

For case **A** (Fig. 1), the best fit ($\delta_\mathrm{f} = 0.0167$ *vs.* $\delta = 0.0532$) is achieved by a FADE with $\gamma = 1.68$. We note moreover that the obtained values $\alpha_\mathrm{f} = 0.0294$ m$^{\cdot 68}$ and $\alpha = 0.00847$ m are consistent with the ones reported elsewhere. The flow speed for this case resulted to be $v = 3.814 \times 10^{-6}$ m/sec.

For cases **B** (Fig. 2), the differences between models are not remarkable (the optimal value of $\gamma \approx 2$). The recorded flow speeds ($v_{\mathrm{b}1} = 1.594 \times 10^{-5}$ m/sec and $v_{\mathrm{b}2} = 1.100 \times 10^{-5}$ m/sec) are higher than in case **A**, which is consistent with the observation at the end of Sec. 1.

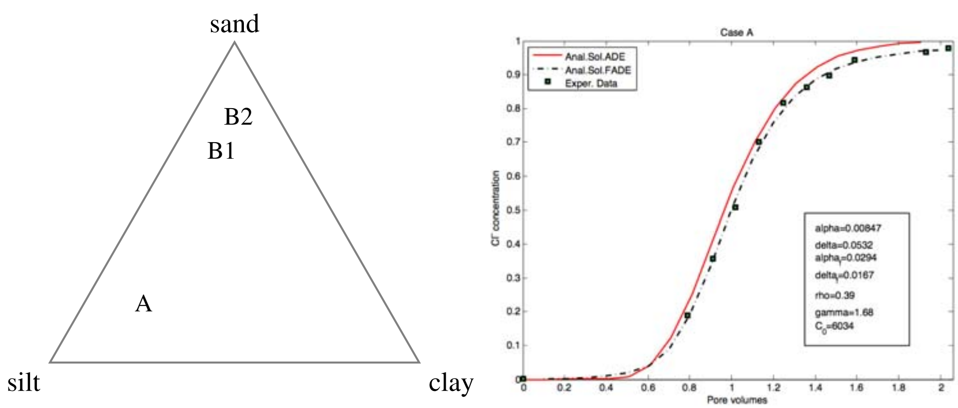

Figure 1: Parameter optimization results for case **A**. A FADE with $\gamma = 1.68$ better fits the data.

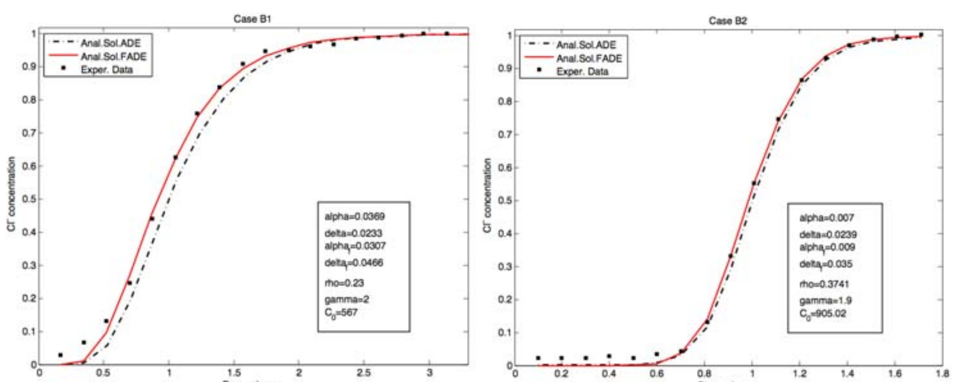

Figure 2: Parameter optimization results for cases **B**. Either an ADE or a FADE with $\gamma \approx 2$ fit the data.

3 Conclusions

In this work, the classical (ADE) and fractional (FADE) advection–dispersion equations have been applied to model nonreactive solute transport in soil columns, in three different cases. It is noteworthy that in all cases, the curve fitting was excellent.

Case A: The best fit ($\delta_{\mathrm{f}} = 0.0167$ *vs.* $\delta = 0.0532$) was achieved by a FADE with $\gamma = 1.68$, and the measured flow speed was $v = 3.814 \times 10^{-6}$ m/sec. The optimal FADE ($\alpha_{\mathrm{f}} = 0.0294\ \mathrm{m}^{.68}$) and ADE ($\alpha = 0.00847$ m) dispersivities are consistent with the ones reported before.

The important differences between both theoretical breakthrough curves are those at the beginning and especially at the end. An almost parallel deviation at the center is of lesser importance, and may be due to a small difference in the optimal porosity, which could result in different advective components for both models. We are now undertaking a sensitivity analysis of the results to the values of ρ.

The fact that the transport of a solute in a porous medium is well described by a FADE is potentially of great importance, as it would allow to follow the plume of contaminant in the field, using directly the parameters found in laboratory soil columns.

Cases B: In these cases, the initial and final tails of the breakthrough curves appear superimposed. Together with the fact that the optimal $\gamma \approx 2$, this indicates that the differences between both models are not relevant, and the FADE would not offer advantages. Again, we note that the flow speeds are in these cases higher than in case **A**, so we find consistence with what was pointed out at the end of Sec. 1 [4, 5].

The explanation for the differences between cases **A** and **B** would reside primarily in the different compositions of the respective sediments, since those of case **B** have an overwhelmingly higher proportion of sand. Whereas this is conceivably relatively monodisperse, compact clay grains may be highly polydisperse, thus leading to statistically fractal geometric structures. We have also noted the difference in flow speeds.

Despite the existence of residual Cl^- after washing the columns, we have chosen to model with zero initial condition in order not to introduce noise in the comparisons. This fact should be taken into account when interpreting the results.

Finally it should be added that these investigations are at an early stage and need to be validated by field studies.

ACKNOWLEDGMENTS

R.D. acknowledges support from UNMdP, through grant EXA544/11.

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