Parameter Estimation for Fractional Transport

Paramita Chakraborty
Michigan State University, East Lansing, Michigan, USA
chakrab@stt.msu.edu
Mark M. Meerschaert
Michigan State University, East Lansing, Michigan, USA
mcubed@stt.msu.edu
Chae Young Lim
Michigan State University, East Lansing, Michigan, USA
lim@stt.msu.edu

The space-fractional advection-dispersion equation (fADE)

Non-Fickian transport of conservative solutes has been widely observed in laboratory and field data [1, 2, 8]. The resulting anomalous dispersion is not well described by the classical second-order advection-dispersion equation (ADE) without extensive site characterization [11]. The space-fractional advection-dispersion equation (fADE) provides an attractive alternative that can represent plume skewness and early arrivals:

$$(1)\ \frac{\partial C}{\partial t} = -v\frac{\partial C}{\partial x} + D\frac{1+\beta}{2}\frac{\partial^\alpha C}{\partial x^\alpha} + D\frac{1-\beta}{2}\frac{\partial^\alpha C}{\partial(-x)^\alpha},$$

where $C(x,t)$ is tracer concentration, v is the plume velocity, D controls rate of spreading, β is a skewness parameter ($-1 \le \beta \le 1$ with $\beta = 0$ for a symmetric plume) and the spatial fractional index $1 < \alpha \le 2$ codes the heterogeneity of the porous medium [Clarke et al, 2005].When $\alpha = 2$, (1) reduces the classical ADE with constant parameters. The fADE (1) has been successful at modeling unsaturated transport [10], transport in saturated porous media [12], and river flows [6, 7].

Parameter Estimation

This paper develops a general method of parameter estimation for the fADE parameters α, β, v, D from plume concentration data. Both spatial snapshots (observations of concentration $C(x,t)$ for t fixed and $x = x_1, \ldots, x_N$) and temporal breakthrough curves (measurements of $C(x,t)$ for x fixed and $t = t_1, \ldots, t_N$) are considered, since these are the data typically available. Naturally these data are contaminated by measurement error as well as model error (no model takes into account every source of variation].

For the fADE with point source initial condition, the underlying stochastic process is a stable Levy motion, a Markov process whose transition densities have no closed form in general, but can be efficiently computed by well established numerical methods [3, 4, 9]. Using a pseudo-particle approach, and equating the relative concentration of particles with stable density, we can equate the measured concentration with a histogram consisting of the observed number of particles in each bin, where bin size is chosen to represent the volume sampled in a concentration measurement, and the number of pseudo-particles is calibrated with plume roughness. A stable density $f_\theta(x,t)$ has a set of parameter $\theta = (\alpha, \beta, v, \sigma)$, where σ is related to D in such a way that $\sigma^\alpha = Dt|\cos(\pi\alpha/2)|$.

Several illustrative applications were fit to demonstrate the method on data sets representing field data: spatial snapshots from a tracer test at the MADE site in Mississippi; breakthrough curve data from tracer tests along the Grand River and the Red Cedar River in Michigan; and simulated ensemble snapshots from the Integrated Groundwater Modeling facility at Michigan State University.

References

[1] Benson, D. A., S. W. Wheatcraft and M. M. Meerschaert, “Application of a fractional advection–dispersion equation”, *Water Resour. Res*. (2000), 36(6), pp. 1403–1412.
[2] Benson, D. A., R. Schumer, M. M. Meerschaert and S. W. Wheatcraft, “Fractional dispersion, Levy motion, and the MADE tracer tests”, *Transp. Porous Media* (2001), 42(1/2), pp. 211–240.
[3] Bhattacharya, R.N., Gupta, V.K and Sposito, G. “On The Stochastic Foundation of the Theory of Water Flow Through Unsaturated Soil”, *Water Resources Research*, (1976), 12(3). pp. 503-512

[4] Chakraborty, P. (2008), “A Stochastic Differential Equation Model with Jumps for Fractional Advection and Dispersion”, *J. Statist. Phys.*(2008), in review. Available at http://www.stt.msu.edu/~chakrab/

[5] Clarke, D.D., M.M. Meerschaert, and S.W. Wheatcraft, “Fractal Travel Time Estimates for Dispersive Contaminants”, *Ground Water* (2005), 43(3), pp. 401–407.

[6] Deng, Z.-Q., V. P. Singh, and L. Bengtsson, “Numerical solution of fractional advection-dispersion equation”, *J. Hydraul. Eng.* (2004), 130(5), pp. 422–431.

[7] Deng, Z.-Q., L. Bengtsson, and V. P. Singh, “Parameter estimation for fractional dispersion model for rivers” *Environ. Fluid Mech.*,(2006) 6, pp. 451-475.

[8] Levy, M., and B. Berkowitz, “Measurement and analysis of non-Fickian dispersion in heterogeneous porous media”, *J. Contam. Hydro*. (2003), 64, pp. 203–226.

[9] Nolan, J.P. “An Algorithm for Evaluating Stable Densities in Zolotarev’s (M) Parameterization, *Mathematical and Computer Modeling*, (1999), 29, pp. 229–233

[10] Pachepsky, Y., D. Timlin, and D. A. Benson, “Transport of water and solutes in soils as in fractal porous media”, *Soil Sci. Soc. Am. J.* (2001), 56, pp.51–75.

[11] Zheng, C., and S. M. Gorelick, ”Analysis of the effect of decimeter-scale preferential flow paths on solute transport”, *Ground Water* (2003), 41(2), pp.142–155.

[12] Zhou, L., and H. M. Selim, “Application of the fractional advection-dispersion equation in porous media”, *Soil Sci. Soc. Am. J.* (2003), 67, pp.1079–1084.