Backward Probabilities for Contaminants undergoing Fractional Dispersion

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Introduction

When contamination with an unknown source history and/or prior location is detected in rivers or aquifers, one important question to the hydrologic community is when and/or where the contaminant originated. This problem is addressed by backward probability, which is an inverse advection-dispersion modeling problem. Particularly, the backward location probability describes the contaminant's possible location at a previous time, and the backward travel time probability describes possible time for it to reach the sampling location from an upgradient location. They have been used extensively in many water quality related studies, including the identifications of pollutant sources and the delineation of well-head protection zones. Previous methods typically rely on the inverse of the classical advection-dispersion equation (ADE) to calculate the backward probabilities. The natural media heterogeneity however can not be represented adequately by a local transport model. This study extends and inverts stochastic descriptions of solute dynamics based on the space fractional advection-dispersion equation (fADE) model to address the influence of heterogeneity in fractal media on backward probabilities.

Inverse model of the space fADE

Superdiffusion of a passive tracer in a flow field with spatially-varying velocity v and dispersion coefficient D can be modeled by the following space fADE

$$\text{(1)} \qquad \frac{\partial C}{\partial t} = -\frac{\partial}{\partial x}(vC) + \frac{\partial}{\partial x}\left(D \frac{\partial^{\alpha-1} C}{\partial x^{\alpha-1}} \right) + q_I C_I - Q_O C$$

with a general initial condition

$$\text{(2)} \qquad C(x, t=0) = C_i(x)$$

where C is the resident concentration, t is time, x is the spatial coordination, $1 \le \alpha \le 2$ is the order of a Riemann-Liouville fractional derivative, and q_I and Q_O is the source inflow and sink outflow rate, respectively. We start to derive the inverse model of fADE with infinite boundaries

$$\text{(3)} \qquad C(x,t)|_{x=+\infty} = 0 \,, \qquad \frac{\partial^{\alpha-1}}{\partial x^{\alpha-1}} C(x,t)|_{x=-\infty} = 0 \ .$$

By combining the adjoint probability method developed by *Neupauer and Wilson* [1] and the fractional-order adjoint operator proposed by *Zhang et al.* [2], we construct the backward model for the space fADE

$$\text{(4)} \qquad \frac{\partial \Phi}{\partial s} = \frac{\partial}{\partial x}(v\Phi) - \frac{\partial^{\alpha-1}}{\partial (-x)^{\alpha-1}}\left(D \frac{\partial \Phi}{\partial x} \right) - q_I \Phi + \frac{\partial h}{\partial C}$$

$$\text{(5)} \qquad \Phi(x, s=0) = 0$$

$$\text{(6)} \qquad \Phi(x,s)|_{x=+\infty} = 0 \,, \left[D \frac{\partial}{\partial x} \Phi(x,s) + v\Phi(x,s) \right]\Bigg|_{x=-\infty} = 0$$

where Φ is the adjoint state, h is the performance function, s=T-t is the backward time, and T is the detection time.

Other forms of the space fADE are possible, and the corresponding inverse models can be built using the same methodology developed in this study.

Numerical solutions and examples

We solve the backward probability model numerically using a random walk particle tracking scheme. The solution is cross-verified by an implicit Eulerian finite difference method. Fig. 1 compares backward ADE and fADE solutions for one example aquifer.

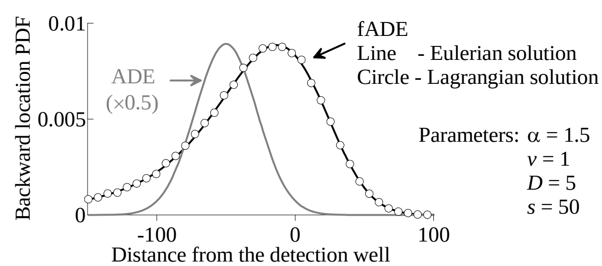

Figure 1. Backward location PDF at backward time *s*=50, with the detection well located at *x*=0.

References

[1] Neupauer, R.M., and J.L. Wilson, Adjoint method for obtaining backward-in-time location and travel time probabilities of a conservative groundwater contaminant, *Water Resources Research*, 35(11), 3389-3398, 1999.

[2] Zhang, Y., D.A. Benson, M.M. Meerschaert, and H.P. Scheffler, On using random walks to solve the space-fractional advection-dispersion equations, *Journal of Statistical Physics*, 123(1), 89-110, 2006.