doi: 10.17221/245/2016-SWR

Modelling Solute Transport in Homogeneous and Heterogeneous Porous Media Using Spatial Fractional Advection-Dispersion Equation

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Abstract

Moradi G., Mehdinejadiani B. (2018): Modelling solute transport in homogeneous and heterogeneous porous media using spatial fractional advection-dispersion equation. Soil & Water Res., 13: 18–28.

This paper compared the abilities of advection-dispersion equation (ADE) and spatial fractional advection-dispersion equation (sFADE) to describe the migration of a non-reactive contaminant in homogeneous and heterogeneous soils. To this end, laboratory tests were conducted in a sandbox sizing 2.5 × 0.1 × 0.6 m (length × width × height). After performing a parametric sensitivity analysis, parameters of sFADE and ADE were individually estimated using the inverse problem method at each distance. The dependency of estimated parameters on distance was examined. The estimated parameters at 30 cm were used to predict breakthrough curves (BTCs) at subsequent distances. The results of sensitivity analysis indicated that average pore-water velocity and dispersion coefficient were, respectively, the most and least sensitive parameters in both mathematical models. The values of fractional differentiation orders (α) for sFADE were smaller than 2 in both soils. The scale-dependency of the dispersion coefficients of ADE and sFADE was observed in both soils. However, the application of sFADE to describe solute transport reduced the scale effect on the dispersion coefficient, especially in the heterogeneous soil. For the homogeneous soil, the predicting results of ADE and sFADE were nearly similar, while for the heterogeneous soil, the predicting results of sFADE were more satisfactory in comparison with those of ADE, especially when the transport distance increased. Compared to ADE, the sFADE simulated somewhat better the tailing parts of BTCs and showed the earlier arrival of tracer. Overall, the solute transport, especially in the heterogeneous soil, was non-Fickian and the sFADE somewhat better described non-Fickian transport.

Keywords: fractional differentiation order; fractional dispersion coefficient; non-Fickian transport; scale effect

Increasing evidence shows that conservative solute transport in porous media, especially in heterogeneous ones, follows anomalous or non-Fickian processes, including early arrival, long tailing, and scale-dependent dispersion coefficient (Berkowitz *et al.* 2006; Berkowitz & Scher 2009; Gao *et al.* 2009; Wang *et al.* 2014). The classical advection-dispersion equation (ADE), which is based on Fick's law, cannot adequately describe a non-Fickian transport process (Benson *et al.* 2000b; Neuman & Tartakovsky 2009; Liu *et al.* 2017). Nonlocal space methods, such as space fractional advection-dispersion (sFADE), provide alternatives to characterize non-Fickian transport in porous media (Benson *et al.* 2000a; Chakraborty *et al.* 2009). The ability of sFADE to explain the solute transport in porous media was studied by various researchers over the past two decades, spanning laboratory to field scales. Benson *et al.* (2000a) applied sFADE to study the solute migration in relatively homogeneous porous media at laboratory and field scales. Notwithstanding the relative homogeneity of the porous media, they found

doi: 10.17221/245/2016-SWR

that the observed breakthrough curves (BTCs) in both cases were heavy-tailed. Applying sFADE to a highly heterogeneous aquifer (the MADE site at the Columbus Air Force Base in Mississippi) showed that, compared to ADE, the sFADE better simulated tritium BTCs (Benson *et al.* 2001). Experiments with a structured clay soil under near-saturated steady-state flow conditions showed better sFADE performance in comparison with that of ADE for a low flow rate, while the sFADE performance was more or less similar to that of ADE for a high flow rate (Pachepsky *et al.* 2000). Huang *et al.* (2006), Xiong *et al.* (2006), and Gao *et al.* (2009) evaluated the sFADE performance and the scale-dependency of its dispersion coefficient in 12.5-m long homogeneous and heterogeneous soil columns, representing a confined aquifer with thickness of about 9 cm. According to their results, the transport process was non-Fickian and the increasing rate of sFADE dispersion coefficient was generally smaller than that of ADE dispersion coefficient. Considering this fact that majority of alluvial aquifers are unconfined and highly heterogeneous in nature (Goosen & Shayya 1999), it is worthwhile to study the sFADE performance and variation of its parameters under controlled experimental conditions, representing a heterogeneous unconfined aquifer. Furthermore, to clarify the effects of the three parameters on sFADE outputs, it is necessary to carry out a parametric sensitivity analysis. However, to the authors' knowledge, the sFADE performance and the scale-dependency of its parameters have not yet been evaluated at a laboratory-scale which represents the heterogeneous unconfined aquifer.

Therefore, the main purpose of the present study was to compare the performances of sFADE and ADE for describing the conservative solute transport process through homogeneous and heterogeneous porous media in a sandbox wherein the heterogeneous packing resembled sedimentary pattern in nature. Moreover, this investigation attempted to analyze the variations of dispersion coefficients of sFADE and ADE with transport distance and perform the sensitivity analysis of ADE and sFADE parameters.

Theory

The one-dimensional sFADE for non-reactive solute with symmetric dispersion is (Benson *et al.* 2000b):

$$\frac{\partial C}{\partial t} = -v\frac{\partial C}{\partial x} + \frac{1}{2}D_f\left[\frac{\partial^\alpha C}{\partial x^\alpha} + \frac{\partial^\alpha C}{\partial(-x)^\alpha}\right] \quad (1)$$

where:
C – solute concentration (M/L^3)
v – average pore-water velocity (L/T)
D_f – fractional dispersion coefficient (L^α/T)
α – fractional differentiation order, $1 < \alpha \leq 2$
x – spatial coordinate (L)
t – time (T)

In sFADE, the heterogeneity degree of the porous medium and the scaling behaviour of the solute plume are characterized by the value of α (Benson *et al.* 2000b; Clarke *et al.* 2005). As $\alpha = 2$, the symmetrical sFADE reduces to the classical ADE:

$$\frac{\partial C}{\partial t} = -v\frac{\partial C}{\partial x} + D\frac{\partial^2 C}{\partial x^2} \quad (2)$$

where:
D – dispersion coefficient (L^2/T)

For a semi-infinite system with the initial condition of zero concentration and a step input at $x = 0$ with concentration C_0, the analytical solution to sFADE can be written as (Pachepsky *et al.* 2000):

$$C(x,t) = C_0\left[1 - F_\alpha\left(\frac{x - vt}{\left(\left|\cos(\pi\alpha/2)\right|D_f t\right)^{1/\alpha}}\right)\right] \quad (3)$$

where:
$F_\alpha(y)$ – standard symmetric Lévy probability distribution (Pachepsky *et al.* 2000):

$$F_\alpha(y) = C(\alpha) + \frac{\text{sign}(1-\alpha)}{2}\int_0^1 \exp\left(-y^{\frac{\alpha}{\alpha-1}}U_\alpha(\chi)\right)d\chi \quad (4)$$

where:
χ – integration variable
sign $(1 - \alpha) = -1$, and $+1$ for $\alpha > 1$ and $\alpha < 1$, respectively
$C(\alpha)$ = 1 and 0.5 for $\alpha > 1$ and $\alpha < 1$, respectively
$U_\alpha(\chi)$ – can be obtained as (Pachepsky *et al.* 2000):

$$U_\alpha(\chi) = \left[\frac{\sin(\pi\alpha\chi/2)}{\cos(\pi\alpha/2)}\right]^{\frac{\alpha}{1-\alpha}} \quad (5)$$

Similarly, for a semi-infinite system initially free of solute and a step input at $x = 0$ with concentration of C_0, the analytical solution to the classical ADE can be expressed as (Ogata & Banks 1961):

$$C(x,t) = \frac{C_0}{2}\left[erfc\left(\frac{x - vt}{2(Dt)^{0.5}}\right) + \exp\left(\frac{xv}{D}\right) \times erfc\left(\frac{x + vt}{2(Dt)^{0.5}}\right)\right] \quad (6)$$

where:
erfc (...) – complementary error function

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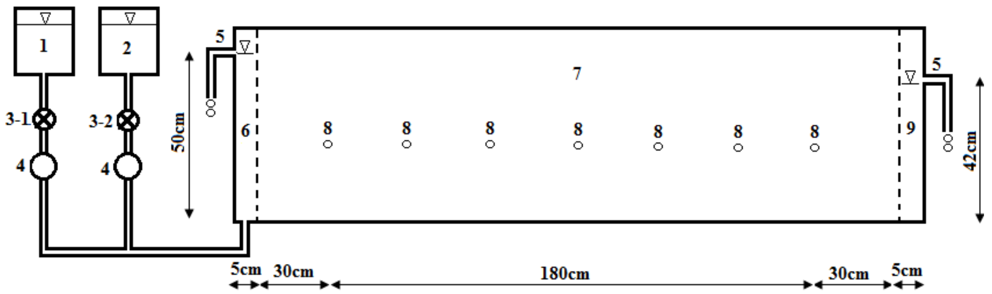

Figure 1. Schematic representation of the tracer test: 1 – tap water reservoir; 2 – NaCl solution reservoir; 3 – cut-off valves; 4 – flow meters; 5 – drainage ports; 6 – inflow part; 7 – porous medium part; 8 – sampling points; 9 – outflow part

It should be noted that to describe the solute transport in a heterogeneous porous medium using Eq. (2), a macroscopic mean transport equation with effective parameters is applied. In this case, it is assumed that the heterogeneous porous medium is macroscopically homogeneous and therefore the parameters of the solute transport are constant (Huang *et al.* 1995; Gao *et al.* 2009).

MATERIAL AND METHODS

Design of sandbox and construction of porous media. Tracer tests were conducted in a rectangular laboratory-scale stainless steel sandbox 2.5 m long, along which the main flow was imposed, 0.1 m wide and 0.6 m high. To provide the opportunity of visual observations, the front side of the sandbox was constructed of transparent Plexiglas plate 6 mm in thickness. As shown in Figure 1, the sandbox included three parts: inflow, porous medium, and outflow. The inflow and outflow parts were separated from the porous medium part by several layers of support screen. The Plexiglas wall of the sandbox included seven sampling ports with 5 mm diameter and 30 cm intervals. The water flow rate which discharges from cut-off valves was monitored by a flow meter (Micro-Flow FTB321D, OMEGA, USA).

The tracer tests were performed on homogeneous and heterogeneous porous media. The sands used in this study were taken from the deposits of a mountain river. They were cleaned and sieved by standard sieve series of American Society for Testing and Materials (ASTM, USA) (Table 1). In the homogeneous system, the sandbox was filled only with the sand S_5 (Figure 2a, b), whereas in the heterogeneous system, it was filled with seven different types of sand the properties of which are presented in Table 1 (Figure 2c, d). A total of 11 layers were packed in the heterogeneous system. To imitate the sedimentation pattern in nature, we filled each layer with several lenses, each lens having typical height of about 4 or 5 cm, width of 10 cm, and arbitrarily length. Before filling, the desired pattern was transferred to a transparent sheet, to scale, and attached to the Plexiglas plate to be used as a template for packing. Then, the sands were poured into the sandbox according to the template. Designing the sedimentation pattern of each layer was done carefully to prevent the formation of a continuous layer of higher permeability, thus, no preferential flow path occurred in the sandbox. In both systems: the packing was conducted under saturated conditions, the sand was packed using a rubber rod after pouring each layer, and the packing was continued to a height of 50 cm.

Tracer tests. Before starting the tracer tests, a steady water flow rate was established by imposing the constant water levels at two ends of the sandbox. The steady water flow rate was established when the fluctuations in the observed drainage rate at the outlet of the sandbox became negligible. The tracer test was started with a continuous injection of NaCl solution as the conservative tracer. To minimize density effects, in both tracer tests, the concentration of NaCl was 500 mg/l above the background concentration of NaCl in tape water. To continu-

Table 1. Classification of sands used in packing the sandbox

Sand classification	Mesh size	d_{50} (mm)
S_1	8/10	3.000
S_2	10/16	1.600
S_3	16/20	1.200
S_4	20/40	0.560
S_5	40/50	0.480
S_6	50/80	0.220
S_7	80/100	0.170

S_n – type of sand; d_{50} – size of the particle for which 50% of the soil particles are smaller

doi: 10.17221/245/2016-SWR

ously inject the NaCl solution, the valve 3-1 was switched off and the valve 3-2 (Figure 1) switched on simultaneously. The valve 3-2 was switched on so that the water flow rate, which discharges from the valve 3-2, was exactly equal to that from the valve 3-1. Sampling from ports was conducted at time intervals of 2 min. The electrical conductivity values of water samples taken from the sampling ports were measured using a calibrated electrical conductivity cell (Model: 130A, ORION, Germany). Then, they were converted to the concentration values utilizing the predetermined relationship between electrical conductivity and NaCl concentration. Measuring the tracer concentration at each port had continued until the concentration was steady and approximately equal to the inflow concentration.

Sensitivity analysis, parameter estimation and prediction. The sensitivity analysis is applied to discern the parameters which have the greatest influence over the model performance (Gan *et al.* 2014). The sensitivity analysis is defined as the rate of variation in the model outputs due to changes in the input parameters (Song *et al.* 2015). In this study, according to the previous studies (Mao & Ren 2004; Huang & Yeh 2007), the sensitivity analysis was performed on the parameters of ADE and sFADE using normalized sensitivity method defined as (Huang & Yeh 2007):

$$NS_i = P_i \frac{C(P_1,\ldots,P_i+\Delta P_i,\ldots P_n) - C(P_1,\ldots P_i,\ldots P_n)}{\Delta P_i} \qquad (7)$$

where:

NS_i – normalized sensitivity of i^{th} input parameter

P_i – i^{th} input parameter

ΔP_i – perturbation of parameter P_i

C – output function (i.e. the solute concentration)

Note that in this study, according to Mao & Ren (2004), the percentage of perturbation (i.e. $\Delta P_i/P_i$) in each parameter was set to 5%.

After the sensitivity analysis, the parameters of two mathematical models were estimated using the inverse problem method. To obtain the parameters of Eq. (3), an inverse model was developed with the objective function (*OF*) as follows:

$$OF = \frac{1}{N}\sum_{i=1}^{N}(c_i^{\text{calc}} - c_i^{\text{meas}})^2 \qquad (8)$$

where:

N – number of observation points

c_i^{calc} – calculated value of $C^{\text{calc}}(x,t)/C_0$ at i^{th} point

c_i^{meas} – measured value of $C^{\text{meas}}(x,t)/C_0$ at i^{th} point

To minimize *OF*, a version of the Levenberg-Marquardt algorithm (Khan *et al.* 2013) was applied. The integral in Eq. (4) was calculated using the trapezoidal integration with 10 000 nodes. The parameters of Eq. (6) were appraised by fitting the Eq. (6) to the observed BTCs. To this end, the software CXTFIT2.1 (Toride *et al.* 1999) was used. To check the goodness of fit, the statistical criteria, including determination coefficient (r^2) and root mean square error (RMSE), were used (Gao *et al.* 2009):

$$r^2 = 1 - \frac{\sum_{i=1}^{N}\left(c_i^{\text{calc}} - c_i^{\text{meas}}\right)^2}{\sum_{i=1}^{N}\left(c_i^{\text{meas}} - \bar{c}^{\text{meas}}\right)^2} \qquad (9)$$

$$\text{RMSE} = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(c_i^{\text{calc}} - c_i^{\text{meas}})^2} \qquad (10)$$

where:

$\bar{c}^{\text{meas}}$ – mean value of c_i^{meas}

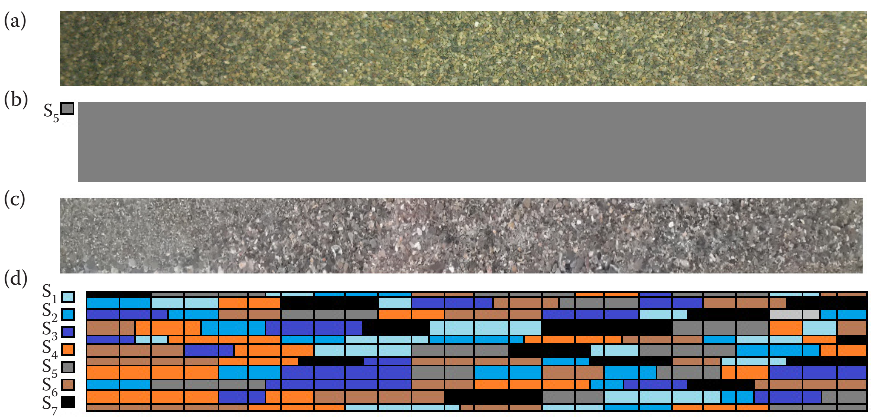

Figure 2. Distribution of sand types packed in the sandbox: photo, homogeneous soil (a); schematic representation, homogeneous soil (b); photo, heterogeneous soil (c); schematic representation, heterogeneous soil (d)

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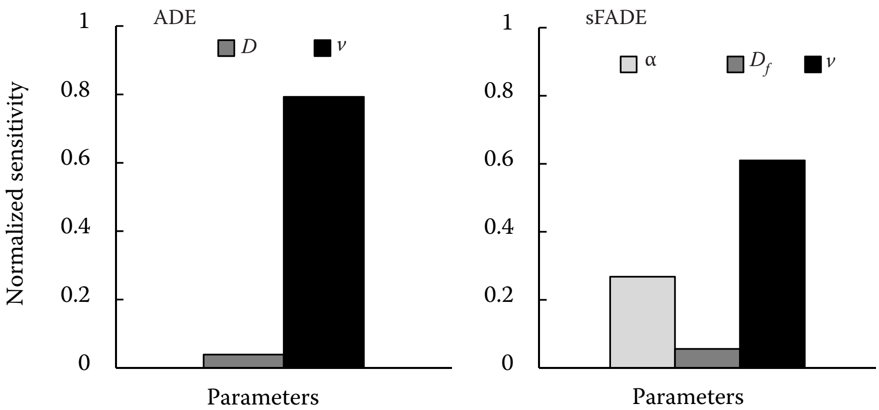

Figure 3. Normalized sensitivity of advection-dispersion equation (ADE) and spatial fractional advection-dispersion equation (sFADE) parameters (see Eq. (1))

To study the predictive abilities of ADE and sFADE, the estimated parameters by fitting the BTC at 30 cm were used to simulate BTCs at subsequent distances. The performances of ADE and sFADE were evaluated using the graphical display and the statistical criteria r^2 and RMSE. In the graphical display, the BTCs obtained from ADE and sFADE were compared to the observed BTCs.

RESULTS AND DISCUSSION

Sensitivity analysis of ADE and sFADE parameters. As shown in Figure 3, both in ADE and sFADE, the average pore-water velocity and dispersion coefficient have the most and the least effects on the variation of concentration, respectively. Mao & Ren (2004) also reported similar results in the sensitivity analysis of ADE parameters. Detailed investigation of normalized sensitivity results of parameters demonstrates that α, D_f, and D significantly influence the tails of BTCs, while ν strongly impacts the mean travel distance. The comparison of NS_i values related to ν indicates that the perturbation in ν influences the ADE outputs more than the sFADE ones.

Comparison of fitting results of ADE and sFADE. For the homogeneous soil, Table 2 shows the estimated

Table 2. Estimated parameters and statistical criteria for advection-dispersion equation (ADE) and spatial fractional advection-dispersion equation (sFADE) at various distances in the homogeneous soil

Distance (cm)	ADE				sFADE				
	v (cm/min)	D (cm^2/min)	r^2	RMSE	v (cm/min)	D_f (cm$^\alpha$/min)	α	r^2	RMSE
30	2.169	0.824	0.993	0.037	2.173	1.020	1.769	0.999	0.009
60	2.145	1.343	0.992	0.038	2.146	1.998	1.886	0.996	0.029
90	2.349	1.477	0.996	0.028	2.372	2.025	1.939	0.995	0.033
120	2.285	1.750	0.991	0.041	2.301	2.031	1.806	0.996	0.029
150	2.307	2.000	0.993	0.039	2.322	2.204	1.787	0.996	0.029
180	2.302	3.000	0.990	0.045	2.318	2.106	1.710	0.995	0.032
210	2.278	2.500	0.989	0.047	2.290	2.135	1.689	0.994	0.035
Minimum	2.145	0.824	0.989	0.028	2.146	1.020	1.689	0.994	0.009
Maximum	2.349	3.000	0.996	0.047	2.372	2.204	1.939	0.999	0.035
Max-to-Min ratio	1.095	3.641	–	–	1.105	2.161	–	–	–
Mean	2.262	1.842	0.992	0.039	2.275	1.931	1.798	0.996	0.028
SD	0.070	0.679	0.002	0.006	0.077	0.378	0.083	0.001	0.008

v – average pore-water velocity; D – dispersion coefficient; r^2 – determination coefficient; RMSE – root mean square error; α – fractional differentiation order; SD – standard deviation

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parameters and associated values of r^2 and RMSE. The fitting velocity values of ADE and sFADE are very close to each other at all distances and vary within the ranges of 2.145–2.349 cm/min and 2.146–2.372 cm/min, respectively. The estimated values of α at all distances are smaller than 2. This indicates that solute transport is non-Fickian. Similar results have also been reported by Xiong *et al.* (2006) and Huang *et al.* (2006). The variations in the fitting velocity values, the fluctuations in the values of α, and the non-Fickian transport behaviour can be attributed to non-uniformity in packing the homogeneous soil and pore-scale heterogeneity. The comparison of the dispersion coefficients at various transport distances shows that the dispersion coefficients of ADE and sFADE increase with the transport distance (see Table 2). Based on the estimated dispersion coefficients, the maximum to minimum ratio for the ADE dispersion coefficient is 1.685 times as much as that for the sFADE dispersion coefficient. This scale-dependency of dispersion coefficient is another evidence for non-Fickian transport in the homogeneous soil.

Figure 4 illustrates the observed and fitted BTCs at different distances. As can be seen in Figure 4, the observed BTCs in the homogeneous soil are relatively smooth and sigmoidal. The sigmoidal shapes of the observed BTCs stem from the nature of homogeneity of porous medium packed in the sandbox (Huang *et al.* 1995; Gao *et al.* 2009). As evident from Table 2 and Figure 4, the sFADE and ADE have nearly the same fitting results in the homogeneous soil, so that the r^2 and RMSE values of ADE and sFADE are very close to each other and the shapes of fitted BTCs with ADE and sFADE are nearly indistinguishable.

For the heterogeneous soil, the estimated parameters and associated values of r^2 and RMSE are summarized in Table 3. Similar to the homogeneous soil, the fitting velocity values of ADE and sFADE are very close to each other at all distances. Nevertheless, due to the heterogeneity of the soil, the fitting velocity values of ADE and sFADE vary dramatically with distance in the ranges of 0.599–1.242 cm/min and 0.602–1.286 cm/min, respectively. These results are in agreement with the findings from the study conducted by Gao *et al.* (2009). As shown in Table 3, the estimated α values are within the ranges of 1.166–1.374, and are consistently smaller than those of the homogeneous soil. A smaller α value implies a highly heterogeneous porous medium and a greater deviation from Fickian transport (Schumer *et al.* 2001; Huang *et al.* 2006; Xiong *et al.* 2006). Table 3 shows that the dispersion coefficients of ADE and sFADE increase with distance. The maximum to minimum ratio for the ADE dispersion coefficient is 3.798 times as much as that for the sFADE dispersion

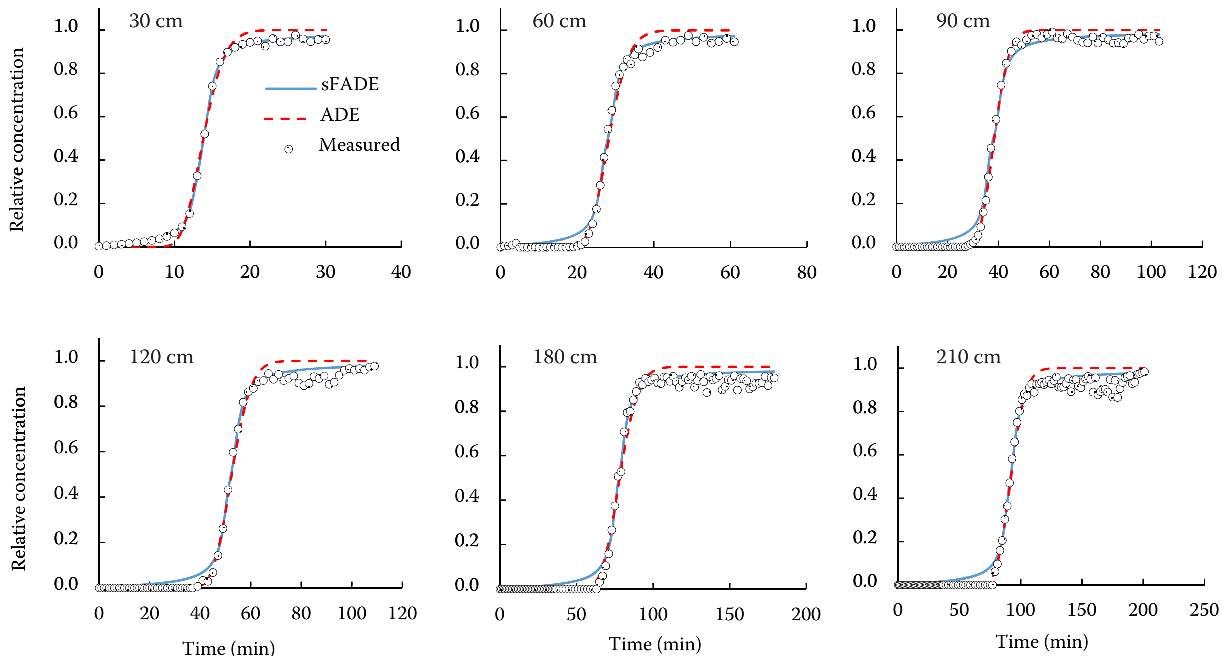

Figure 4. Comparison of the observed breakthrough curves with those fitted by advection-dispersion equation (ADE) and spatial fractional advection-dispersion equation (sFADE) for homogeneous soil at different distances

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Table 3. Estimated parameters and statistical criteria for advection-dispersion equation (ADE) and spatial fractional advection-dispersion equation (sFADE) at various distances in heterogeneous soil

Distance (cm)	ADE				sFADE				
	v (cm/min)	D (cm^2/min)	r^2	RMSE	v (cm/min)	D_f (cm$^\alpha$/min)	α	r^2	RMSE
30	0.762	0.985	0.981	0.056	0.779	0.557	1.260	0.993	0.034
60	0.728	0.809	0.991	0.041	0.736	0.369	1.339	0.994	0.034
90	0.721	1.859	0.994	0.031	0.727	0.576	1.302	0.996	0.027
120	0.599	1.179	0.997	0.023	0.602	0.367	1.253	0.994	0.030
150	0.844	4.210	0.994	0.029	0.856	0.909	1.201	0.986	0.045
180	1.098	4.802	0.984	0.053	1.119	1.241	1.374	0.989	0.045
210	1.242	13.933	0.977	0.060	1.286	1.664	1.166	0.983	0.051
Minimum	0.599	0.809	0.977	0.023	0.602	0.367	1.166	0.983	0.027
Maximum	1.242	13.933	0.998	0.06	1.286	1.664	1.374	0.996	0.051
Max-to-Min ratio [a]	2.073	17.222	–	–	2.136	4.534	–	–	–
Mean	0.856	3.968	0.991	0.042	0.872	0.812	1.271	0.991	0.038
Standard deviation	0.213	4.328	0.007	0.013	0.225	0.453	0.068	0.004	0.008

[a]Max-to-Min ratio denotes the ratio of the maximum value of a parameter to its minimum value; v – average pore-water velocity; D – dispersion coefficient; r^2 – determination coefficient; RMSE – root mean square error; α – fractional differentiation order

coefficient. Comparing Table 2 to Table 3, it can be found that the increasing rate of the dispersion coefficient in heterogeneous soil is significantly larger than that in homogeneous soil. The more scale-dependent dispersion coefficient in the heterogeneous soil reveals a greater degree of non-Fickian behaviour in comparison with the homogeneous soil. Similar results were also found by Huang *et al.* (2006) and Xiong *et al.* (2006).

Figure 5 depicts the observed and fitted BTCs at different distances of the heterogeneous soil. The observed BTCs at distances of 30, 60, and 90 cm show relatively regular shapes, while those at distances of 120, 180, and 210 cm exhibit very irregular and

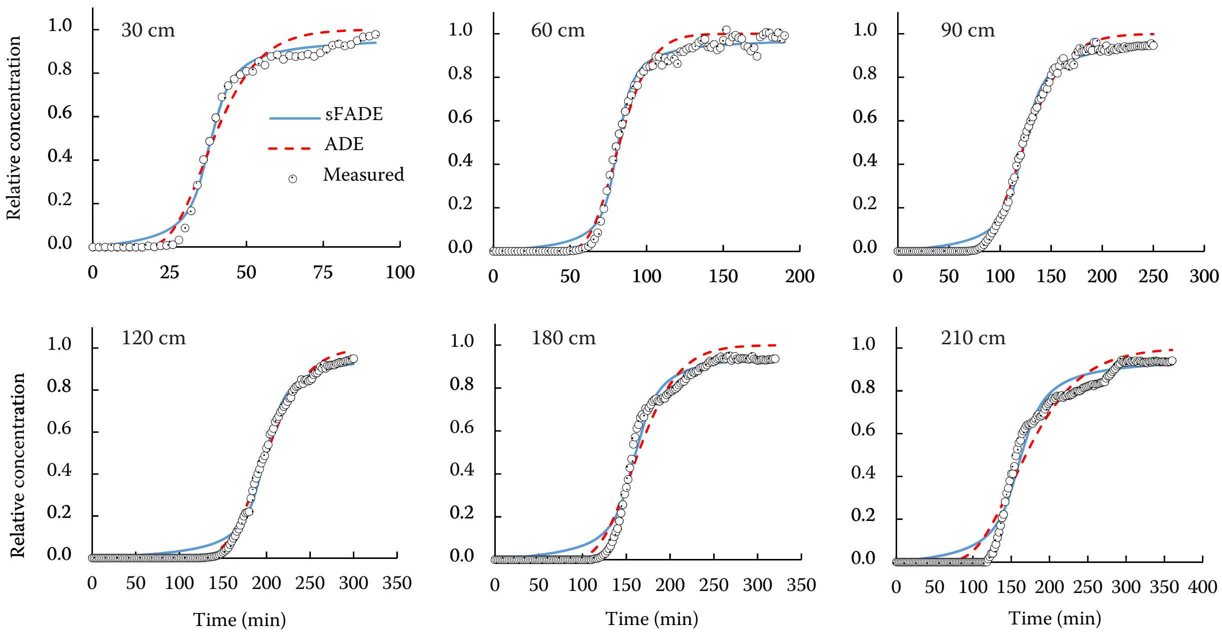

Figure 5. Comparison of the observed breakthrough curves with those fitted by advection-dispersion equation (ADE) and spatial fractional advection-dispersion equation (sFADE) for heterogeneous soil at different distances

doi: 10.17221/245/2016-SWR

Table 4. Values of statistical criteria as the indicators of performance for advection-dispersion equation (ADE) and spatial fractional advection-dispersion equation (sFADE) at subsequent distances using the best estimated parameters at 30 cm

Distance (cm)	Homogeneous soil				Heterogeneous soil			
	ADE		sFADE		ADE		sFADE	
	r^2	RMSE	r^2	RMSE	r^2	RMSE	r^2	RMSE
60	0.989	0.044	0.994	0.032	0.985	0.052	0.982	0.059
90	0.963	0.088	0.969	0.080	0.974	0.067	0.978	0.061
120	0.970	0.076	0.977	0.066	0.608	0.239	0.626	0.234
150	0.966	0.084	0.973	0.074	0.879	0.133	0.935	0.097
180	0.961	0.089	0.969	0.079	0.353	0.336	0.510	0.292
210	0.964	0.085	0.973	0.073	0.020	0.395	0.241	0.348
Minimum	0.961	0.044	0.969	0.032	0.020	0.052	0.241	0.059
Maximum	0.989	0.089	0.994	0.080	0.985	0.395	0.982	0.348
Mean	0.969	0.078	0.976	0.067	0.636	0.204	0.712	0.182
SD	0.009	0.016	0.008	0.016	0.355	0.130	0.278	0.115

r^2 – determination coefficient; RMSE – root mean square error; SD – standard deviation

asymptotic shapes. The measured maximal concentrations at most of the sampling ports are less than the inlet concentration within the experimental time period. This result reveals non-Fickian transport and arises from the heterogeneous nature of soil. The observation of the slightly late tails and the early arrivals in the measured BTCs can be attributed to the heterogeneity patterns of porous medium. According to the observed BTCs, the heterogeneous soil packed in the sandbox only has micro-heterogeneity, arising from grain-size distribution. This heterogeneity pattern leads to the insignificant preferential paths. This causes that the number of the paths with low and high velocities decreases and, consequently, the number of occurrences of the late tails and early arrivals decreases. Similar to the homogeneous soil, the shapes of BTCs fitted by sFADE at different distances of the heterogeneous soil are nearly similar to those fitted by ADE (Figure 5). This result is also supported by checking their r^2 and RMSE values (see

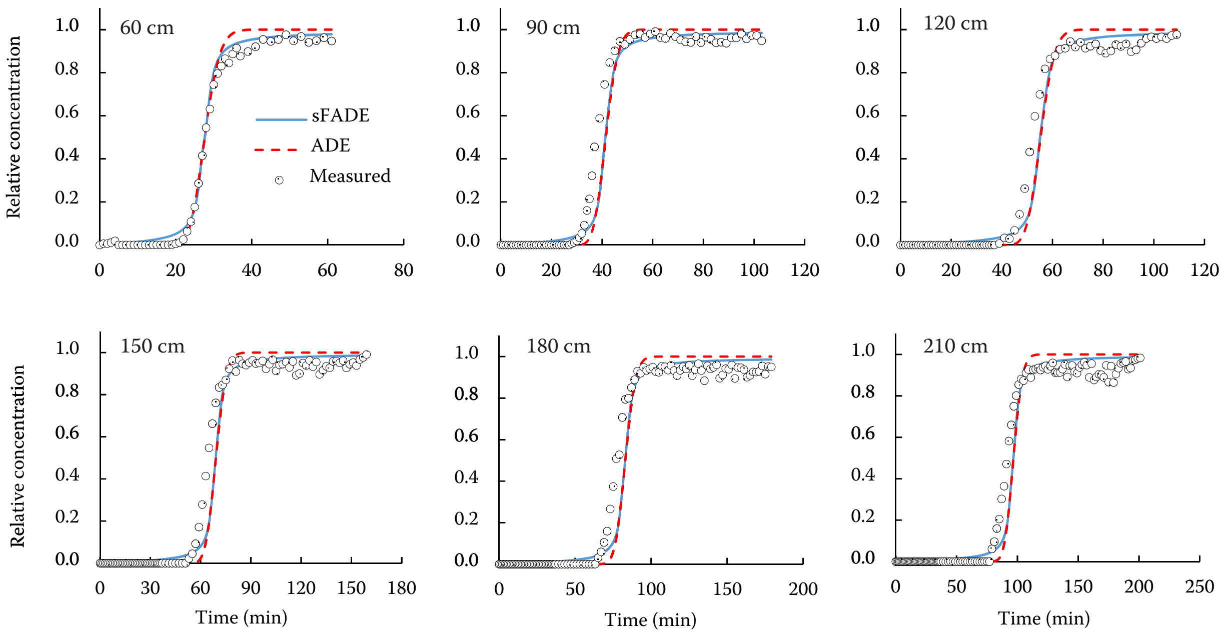

Figure 6. Predicted breakthrough curves in the homogeneous soil at different distances by advection-dispersion equation (ADE) and spatial fractional advection-dispersion equation (sFADE) using parameters determined at 30 cm

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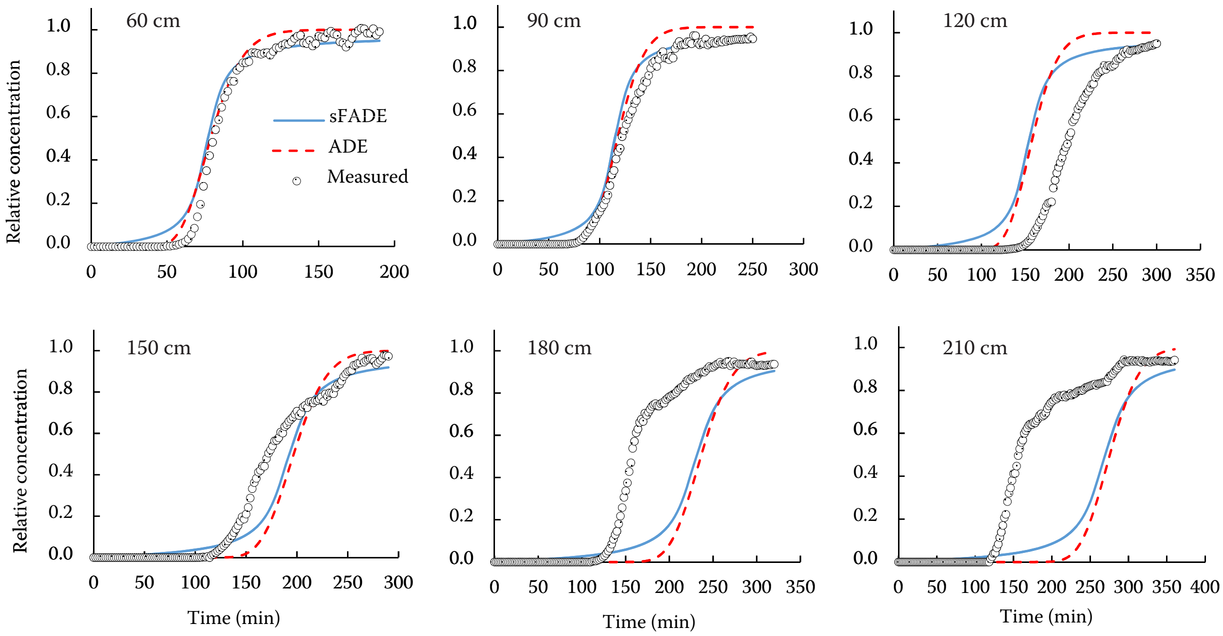

Figure 7. Predicted breakthrough curves in the heterogeneous soil at different distances by advection-dispersion equation (ADE) and spatial fractional advection-dispersion equation (sFADE) using parameters determined at 30 cm

Table 3). As depicted in Figures 4 and 5, both in the homogenous soil and in the heterogeneous soil, the sFADE gives somewhat better fitting results at the tailing parts of BTCs. Furthermore, it shows an earlier arrival of tracer. The relatively higher capability of sFADE, with respect to ADE, for describing the heavy-tails has also been observed in other research studies (e.g. Benson *et al.* 2000a; Pachepsky *et al.* 2000; Gao *et al.* 2009).

Comparison of ADE and sFADE predictions. As mentioned before, the obtained transport parameters at the distance of 30 cm were used to predict the BTCs at subsequent distances. For the homogeneous and heterogeneous soils, the measured and predicted BTCs at several distances are shown in Figures 6 and 7, respectively. Also, the associated r^2 and RMSE values are listed in Table 4.

For the homogeneous soil, the predicted BTCs with ADE and sFADE at different distances are more or less in good agreement with the observed BTCs. The performances of ADE and sFADE at any given distances are approximately the same, with the exception that sFADE provides somewhat better predicting results in the late-time tails and shows an earlier arrival of tracer (see Figure 6 and Table 4).

For the heterogeneous soil, in general, with increasing distance from point 30 cm, both ADE and sFADE make weak predictions. As evident from Figure 7 and Table 4, the performances of two models at proximal distances to point 30 cm are almost similar to each other, while at distal distances from point 30 cm the sFADE provides better predicting results than ADE. These results can be attributed to two factors. First, the ADE is more sensitive to the variation of the pore-water velocity, compared to sFADE. Second, the variation of the ADE dispersion coefficient in the heterogeneous soil is much greater than that of sFADE. Similar to the homogeneous soil, the sFADE better predicts tailing parts of BTCs and indicates the earlier arrival of tracer (Figure 7). As described in previous sections, the early arrivals and late-time tails in BTCs demonstrate a non-Fickian transport, which increases with the increasing heterogeneity degree of porous medium. The predicting results indicate that, compared to ADE, the sFADE somewhat better captures non-Fickian transport. Similar results have also been reported by Gao *et al.* (2009) and Huang *et al.* (2006).

CONCLUSION

This study examined the capabilities of advection-dispersion equation (ADE) and spatial advection-dispersion equation (sFADE) to describe the solute transport process in homogeneous and heterogeneous porous media. Moreover, a sensitivity analysis was

doi: 10.17221/245/2016-SWR

performed on the parameters of ADE and sFADE. The results of sensitivity analysis indicted the average pore-water velocity and dispersion coefficient had the greatest and the smallest effects on ADE and sFADE outputs, respectively. The observed breakthrough curves (BTCs) for the homogeneous soil had relatively smooth and sigmoidal shapes, whereas those for the heterogeneous soil had very irregular and non-sigmoidal shapes. The fitting velocity values of ADE and sFADE at a certain distance, for both soils, were very close to each other. In the homogeneous soil, the fitting velocity values of ADE and sFADE varied in the ranges of 2.145–2.349 and 2.146–2.372 cm/min, respectively, whereas in the heterogeneous soil, they changed in the ranges of 0.599–1.242 and 0.602–1.286 cm/min, respectively. The average values of fractional differentiation orders (α) estimated for sFADE were 1.798 and 1.271 in the homogeneous and heterogeneous soils, respectively. The dispersion coefficients of ADE and sFADE, for both soils, increased with transport distance. The increasing rate of the sFADE dispersion coefficient, especially in the heterogeneous soil, was significantly smaller than the ADE dispersion coefficient. For the homogeneous soil, the predicted BTCs by sFADE and ADE at all distances were nearly similar to each other, whereas for the heterogeneous soil, the BTCs predicted by sFADE were more accurate than those by ADE, especially when the transport distance increased. Overall, the results demonstrated that the solute transport in both soils was non-Fickian, the deviation from Fickian transport was much more significant in the heterogeneous soil and the sFADE somewhat better captured non-Fickian transport.

Acknowledgements. This research was financially supported by University of Kurdistan. The authors appreciate the support provided.

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Received for publication December 11, 2016
Accepted after corrections July 18, 2017
Published online September 27, 2017