Spatial heterogeneity at laboratory scale: A corner stone in modeling contaminant transport in porous media

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A b s t r a c t

Modeling and computer simulation of contaminant transport has a long lasting history in groundwater hydrology. Various geo-hydrologists made an extensive effort to model and mimic the dynamics of both flow and contaminant transport in porous media. However, the unique feature of such efforts is the lack of proper justification concerning the mismatch obtained via comparing observed and simulated breakthrough curves. The current study is conducted under highly controlled experimental setup in uniform soil to enhance and better explain the rationality behind the failure emerging from reproduction of breakthrough curves by advection-dispersion equation (ADE) model. As the breakthrough curves obtained from the laboratory cannot be denied, it seems scientists should revise and perhaps revisit the ADE model for a better performance.
Keywords: Contaminant Transport, Sand-Box Model, Tracer Test, Pulse Injection, ADE Solution

1. INTRODUCTION

The fate and movement of dissolved substances in soils and groundwater has generated considerable interest to better manage the quality of the subsurface environment. The characteristics of solutes over relatively long spatial and temporal scales have to be assessed with the help of theoretical models as it is simply impossible to carry out experimental studies over sufficiently long distances and/or time periods. Mathematical models are often used to predict solute concentrations before management strategies are implemented. Advances in software and hardware now permit the simulation of subsurface transport using sophisticated mathematical models. Unfortunately, it is generally difficult to obtain reliable values for transport parameters such as the pore-water velocity, the retardation factor, the dispersion coefficient, and degradation or production parameters [1].

Laboratory sand-boxes are an important academic apparatus in the study of contaminant transport in porous media [2]. Traditionally, dispersion experiments were implemented in small size column test, as summarized by, e.g., Bear [3]. Utilizing sand-boxes set aside more capacity of producing soil structures with statistical properties similar to those found in nature. Employment of such sand-box in highly controlled laboratory tests is vital in ascertaining the limitations of method implemented in actual settings. Here experimental conditions are well defined and concentration and other data are much more accessible than in the field. Most published results fail to present the full evolution of the solute concentration is a common problem [4]. Consequently, quantification of the full evolution of the contaminant, particularly after peak tail (receding limb), should be recorded and studied in some detail as the signature is not symmetric. In this research, salt tracer transport conducted in uniform porous media to enhance our understanding of contaminat transport in porous media. The current report presents and documents the results obtained from very recent laboratory experimentations. Point contaminant movement for three different flow rates is monitored and then the observed data is utilized to evaluate the quality of results obtained from the analytical advection-dispersion equation.

2. ADVECTION-DISPERSION EQUATION THEORY

Solute transport process in porous medium is mainly governed by the processes of advection and dispersion. The advection-dispersion equation (ADE) for conservative solute transport in porous media is expressed as:

$$D_x \frac{\partial^2 C}{\partial x^2} + D_y \frac{\partial^2 C}{\partial y^2} + D_z \frac{\partial^2 C}{\partial z^2} - v_x \frac{\partial C}{\partial x} - v_y \frac{\partial C}{\partial y} - v_z \frac{\partial C}{\partial z} = \frac{\partial C}{\partial t}$$

(1)

Where D is the dispersion coefficient and v is the average linear velocity in respective direction, C is the solute concentration, x, y and z are Cartesian coordinate directions, and t is the time. Conservative solute means that the solute does not interact with the porous media or it does not undergo biological or radioactive decay.

The analytical solution applicable to mass transport in three dimensions assuming linear flow velocity in x-direction and boundary condition where an instantaneous point source $M = M_0$ injected at $(0, 0, z_s)$ and for $x = \infty$, $C = 0$ as well as, $\frac{\partial C}{\partial x} = 0$, together with the initial condition when $t = 0$ and $0 < x < \infty$, $C = 0$, can be written as:

$$C(x,y,z,t) = \frac{M_0}{n} X(x,t) \, Y(y,t) \, Z(z,t)$$

(2)

with

$$X(x,t) = \frac{e^{-\frac{(x-v_x t)^2}{4D_x t}}}{\sqrt{4\pi D_x t}} \qquad Y(y,t) = \frac{e^{-\frac{(y)^2}{4D_y t}}}{\sqrt{4\pi D_y t}} \qquad Z(x,t) = \frac{e^{-\frac{(z-z_s)^2}{4D_z t}} + e^{-\frac{(z+z_s)^2}{4D_z t}}}{\sqrt{4\pi D_z t}}$$

where M_0 is the initial contaminant mass at $x=0$, $y=0$ and $z=z_s$, n is the porosity, x is the distance from the source to a calculation point in the downstream direction, y is the lateral distance from the source to the calculation point, and z is the distance from the water table to the calculation point.

The above ADE with constant parameters is still the most commonly used method to characterize movement of a plume in an aquifer [4]. Within an aquifer of minimal degree of heterogeneity, the ADE had been verified to offer fairly precise picture of contaminant movement [5].

3. MATERIALS

The experiment is conducted in a lab scale sand-box filled with uniform clean fine sand material. The uniformity coefficient of the sand is 1.52 with d_{50} equal to 0.232 mm and the porosity of the packed material is calculated to be 45 percent [Table 1]. The internal dimension of the sand-box is 130×48×70 cm^3 in x-, y- and z-directions, respectively. To ensure minimal impact of wall effects on experimental set up, both side of sand material are filled and covered by clay soil with 4 cm tick and compacted so that no creeping occurs along the walls of the box. The dominant flow direction is along the x-axis of the apparatus. An inflow and outflow reservoirs is located at each end of the box separated by a lattice plate covered with fine mesh fabric net from the sand material. Three 30 cm PVC pipe (as injection and sampling points) with internal diameter of 0.8 cm, perforated at one end (5 cm long) is installed 35 cm apart from each other along the center line in x- direction [Figure 1]. The center of perforated part of the pipes is adjusted at the level of 45 cm from the bottom of the box. Water held at constant elevations at both upstream and downstream reservoirs via adjustable overflows to keep hydraulic gradient at desired values in different tests.

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Table 1- Properties of the sand used

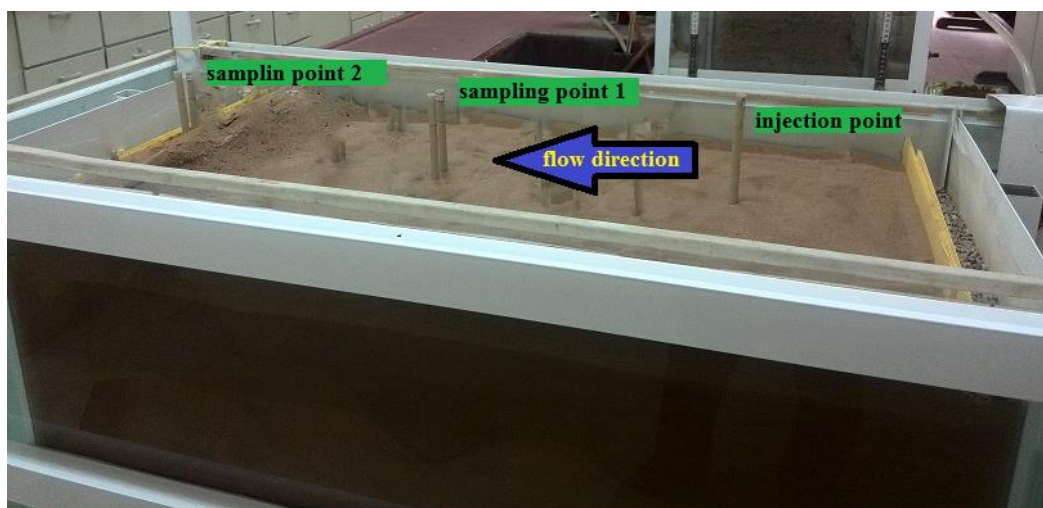| C_U	Porosity	d_{50}, mm	Hydraulic conductivity
1.52	0.45	0.232	0.024 cm/s

Figure 1. Sand-box view and location of injection and sampling points

4. METHODS

Sodium chloride (NaCl) tracer is injected to saturated zone as a pulse injection. In all tests, the NaCl concentration was 10 g/l above the NaCl background concentration of the tap water. This concentration of NaCl was chosen to provide a sufficiently distinct range over which significant concentration measurements could be made. Preparations are made to introduce an instantaneous pulse injection, with little disruption of the background flow. This is accomplished by inserting a serum hose via pipe at injection point at the depth of 10 cm below water table. For monitoring tracer concentration along the box, samples are taken through aforementioned pipes from the aquifer at 2 points downstream located at 35 and 70 cm from the injection point. Electrical conductivity of each sample is measured via conductivity meter. The EC-meter is calibrated over all tests. The EC measurements are then converted to concentration values utilizing the calibration curve. Data for analyses consist of breakthrough curve measurements, in the form of pairs of concentration versus time values.

As calibration is an inevitable part of any modeling exercise, an effort was made to tune the associated parameters in the current application [4]. The dispersion coefficient of the analytical solution of ADE model is considered to be an explicit and potential tuning parameter. As a result, this parameter is used for matching purposes. The average velocity is estimated specifically, and is used as a fix parameter in the ADE curve fits to the data. Furthermore, due to the limitation of the ADE model, the average tracer velocity is being considered as essentially equal to the average fluid velocity. In such cases, for the ADE solution, computation of the average fluid velocity was achieved by dividing Darcy velocity (Q/A) by porosity. The observed breakthrough curves were analyzed by comparison to the fitted solution of the ADE formulation. For the ADE, the early time portion up to central region of the breakthrough curves (where the relative concentration is raised from 0 to peak concentration) was used as the basis for obtaining optimal fits. Current investigation emphasizes the use of ADE model. Thus, in spite of the fact that other parameters are involved in the ADE fits, we focus here on the overall fit of ADE solution, as characterized by, dispersion coefficient.

5. RESULTS AND DISCUSSIONS

The tests carry out with the uniform sand system and analysis of tracer movement in the sand box led to noticeable results. Three tests are performed altogether, at three flow rates. In all experiments, precise measurements are done during the total development of the contaminant plume, including near the beginning and after peak breakthrough concentrations. All three terminated experiments' breakthrough curves are plotted as relative concentration versus time graphs [Figure 2 and 3]. The experiment outputs are judged against the ADE solution which is shown as thin solid lines in all figures. The produced solution demonstrated here corresponds to best fit solution. All ADE solutions with a different dispersion coefficient are data-calibrated for which all data points were considered when fitting the curves. The ADE model generates weak outputs in the receding limb of the curves in each case.

Six typical breakthrough curves are shown here for both sampling points. The observed and calculated ADE breakthrough curves associated with sampling point 1 and 2 at flow rate of 33 ml/min, 71 ml/min and 144 ml/min are demonstrated in Figure 2 and 3, respectively. The curves present a divergence among the observed and ADE outputs. The discrepancy between the fit is quite apparent toward the end of breakthrough curves. Normally, it is supposed that the contaminant transport in a uniform porous media, similar to this, will follow analogous processes, but a number of research do not support these general assumptions. In fact, some studies within homogeneous geologic materials report preferential flow paths (influencing water flow and tracer transport) (e.g., [6], [7]). These occur due to macro-structures, caused by processes such as bridging effects, and also due to micro-structures, reflecting grain-shape heterogeneities [4].
In sharp contrast to the ADE solution, field and laboratory analyses demonstrate that the dispersion coefficient is not constant but is dependent on the time and length scale of measurement [8]. This is shown in tests output that long-time tails is noticeably different from those of ADE fitting curves. Such scale-dependent dispersion coefficient is what refers to as anomalous transport in related literature. Anomalous behavior is often argued to be the result of heterogeneities, at all scales, which cannot be ignored [4]. Even as high a resolution as possible to define aquifer properties, analyses have not been capable to capture the dynamics of contaminant movement (e.g., [9]). Nevertheless, unresolved heterogeneities exist even at relatively small scales [4].

6. CONCLUSIONS

The three tests conducted under highly controlled experimental settings give proper justification as how and why the analytical solutions of advection–dispersion equation cannot effectively describe the entire observed breakthrough curves trend. The critical after peak tail behaviors of the breakthrough curves are not properly captured by the ADE analytical solution. Several published studies using the ADE report merely tolerable fits of breakthrough behavior due to divergence of data at the after peak zone. Such differences become significant, for example, in the analysis of issues related to groundwater remediation [4]. The sand box apparatus we used here permits study of the hydraulic of the contaminants transport. In addition, uniform structure cannot be assumed in the field and heterogeneity is present at all spatial scales. Thus, analytical solution emerged from ADE model does not manage to reproduce contaminant movement even for uniform soils based on observed data collected in the lab under highly controlled experimental set up.
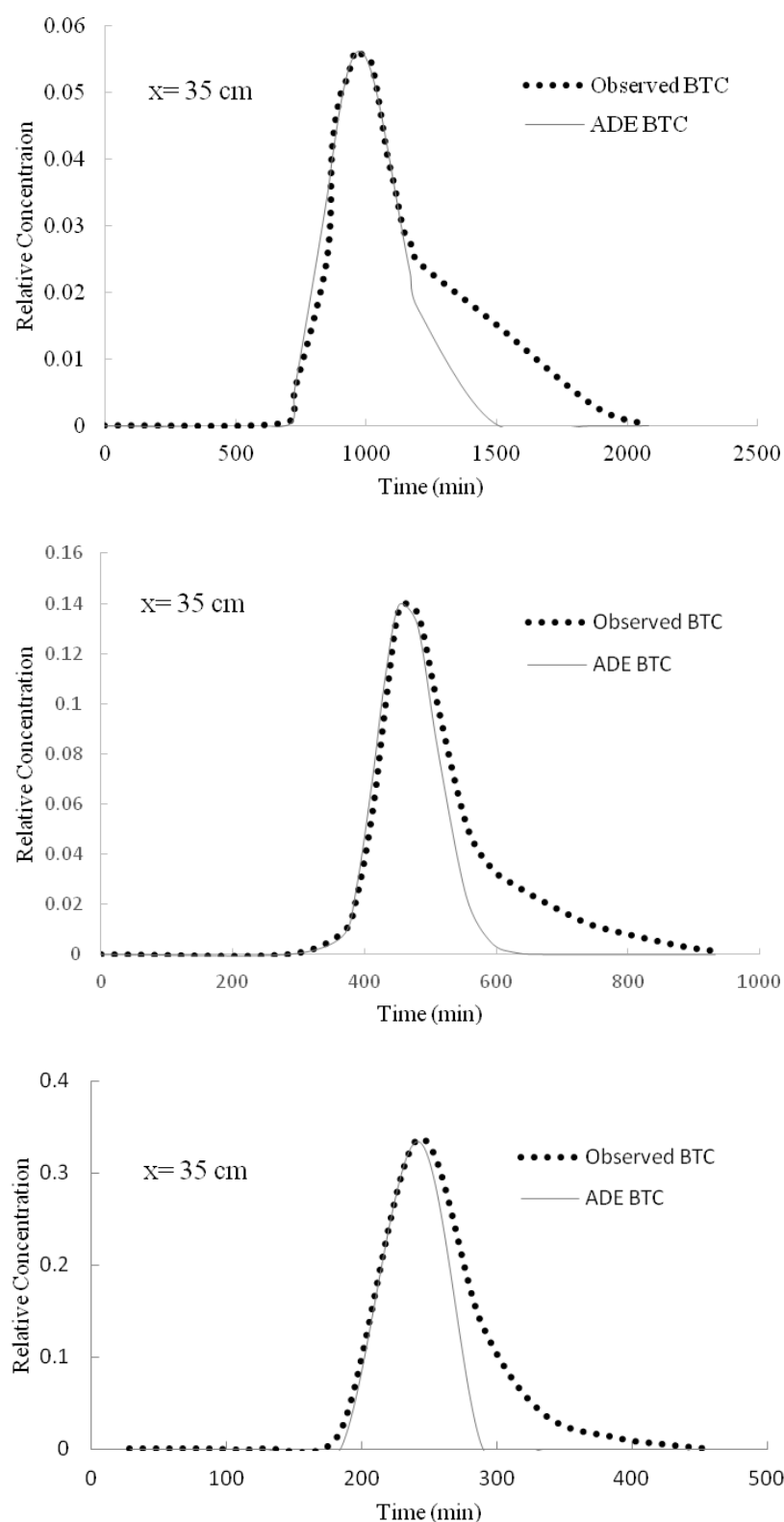
7. ACKNOWLEDGMENT

Figure 2. Measured breakthrough curves with fitted ADE solution (thin solid lines) for the sampling point 1. Flow rates for each test is 33 ml/min (top), 71 ml/min (middle) and 144 ml/min (bottom). Related values of dispersion, D_x, for the ADE fits are (top) 1.90E-4, (middle) 1.99E-4 and (bottom) 1.85E-4 cm^2/sec.
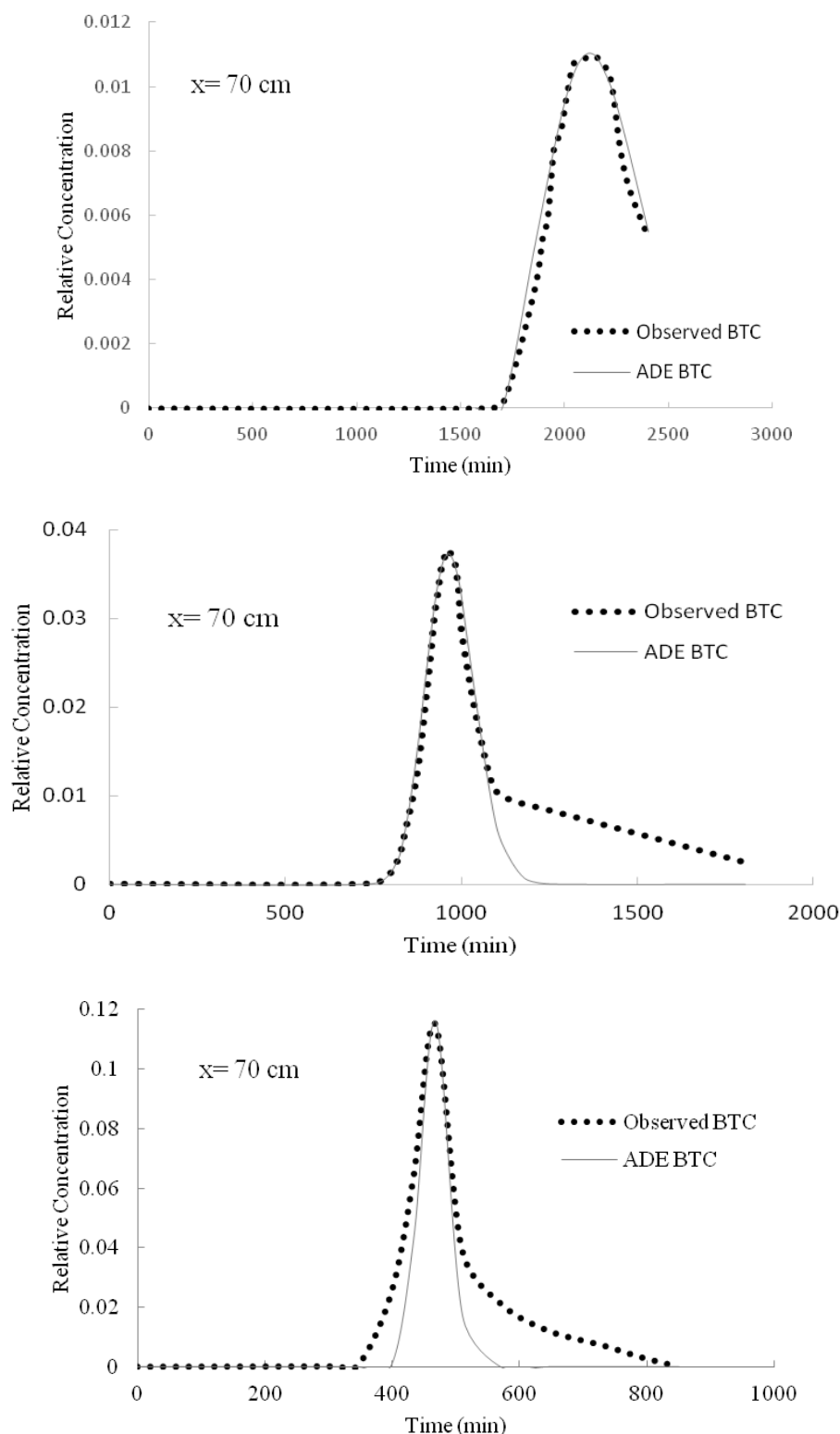
Figure 3. Measured breakthrough curves with fitted ADE (thin solid lines) solution for the sampling point 2. Flow rates for each test is 33 ml/min (top), 71 ml/min (middle) and 144 ml/min (bottom). Related values of dispersion, D_x, for the ADE fits are (top) 2.12E-4, (middle) 2.17E-4 and (bottom) 2.02E-4 cm^2/sec.

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