Is it More Important to Characterize Heterogeneity or Differences in Hydraulic Conductivity Measurements?

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ABSTRACT

As a first step toward understanding the role of sedimentary structures in flow and transport through porous media, this work deterministically examines how transport simulations compare to observed transport through simple, artificial structures in a laboratory experiment. Small-scale laboratory-measured values of hydraulic conductivity were used to simulate transport in an intermediate-scale (10-m long), two-dimensional, heterogeneous porous medium (s^2_{lnK}=1.26, m_{lnK} = 4.18, where K is cm hr^{-1}). Results were judged based on how well the simulated transport matched observed transport through the tank. Permeameter and column experiments produced laboratory measurements of hydraulic conductivity for each of the five sands used in the intermediate-scale experiments. Despite explicit numerical representation of the heterogeneity, predictions using the laboratory-measured values under-estimated the mean arrival time by as much as 35%. The significance of differences between simulated and observed mean arrival time was investigated by comparing variability of transport predictions using the different measurement methods to that produced by different realizations of the heterogeneous distribution. Results indicate that the variations in measured hydraulic conductivity were more important to transport than variations between realizations of the heterogeneous distribution of hydraulic conductivity.

INTRODUCTION

Laboratory flow and transport experiments, beginning with simple column experiments more than a century ago, have gradually increased in complexity. Early heterogeneous experiments were primarily qualitative in nature[5] while later two and three-dimensional evaluations quantified the impact of simple heterogeneity[6]. Two-dimensional, two-media experiments by *Wood et al.*[7] and *Murphy et al.*[8] compared observed and simulated results for transport through simple heterogeneities in a one-meter long tank. Other recent efforts have focused on creating more complex heterogeneity with statistical properties similar to that found in natural systems[9,10,11]. Laboratory investigations of these more complex heterogeneities focused only on the observations of flow and transport and did not include comparison of the observations to numerical predictions, and were not large enough to prove that, for example, discrepancies were not a result of errors of constant-head boundary conditions.

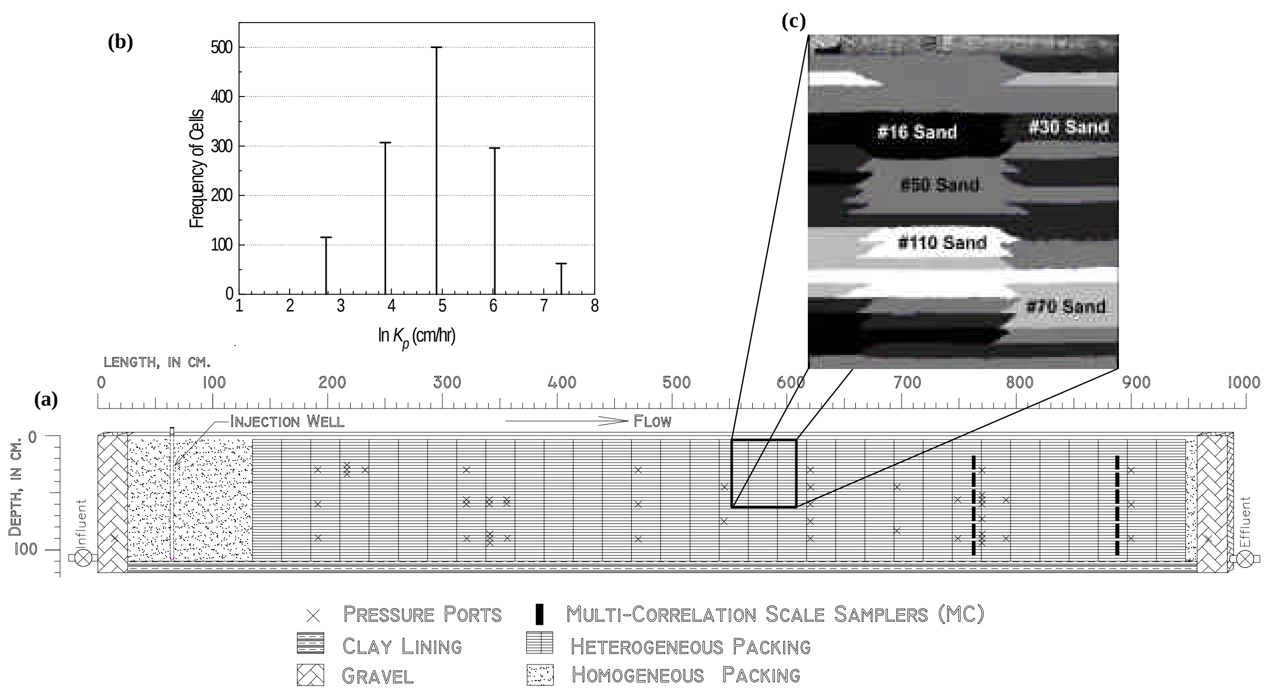
The work presented here is a critical step towards refining our understanding of the importance of measured hydraulic-conductivity variability compared to errors caused by inaccurate zonation of sedimentary features. A series of controlled, intermediate-scale tracer experiments are used to compare concentration observations to predictions simulated using measured hydraulic conductivity. The experiments were performed in a two-dimensional heterogeneous porous medium of sufficient correlation lengths to be statistically comparable to field-site heterogeneity. The experiments provide a complex, explicitly characterized system, that is simple enough to be controlled, definitive, and allow explicit numerical representation, yet complex enough to be relevant to field-site heterogeneity. The results demonstrate significant variability in transport predictions due to measurement-method differences in hydraulic-conductivity values. The significance of prediction variability, due to hydraulic-conductivity measurement variability, is evaluated by comparing it to the variability of transport predictions from 150 realizations of the heterogeneous distribution.

INTERMEDIATE-SCALE EXPERIMENTS

Porous Medium Construction

The intermediate-scale porous medium was constructed in a tank approximately 10 meters long, 1.2 meters tall, and 0.06 meters inside width (Figure 1a). Each end of the porous medium consisted of a 20 cm section of pea gravel to provide constant-head boundaries for the system. The overall gradient and saturated zone thickness were adjusted with a set of constant-head tanks that controlled the water level in the pea gravel. The water table was level with the top of the sand packing at the up-gradient end of the tank. At the down-gradient end it was 15.7 cm below the top of the packing producing an overall gradient of approximately 0.016. Deionized water was supplied to the up-gradient constant-head tank. The gradient and resulting flow of approximately 3.2 L/hr were maintained throughout each experiment and the periods between experiments. Between experiments NaOCl was added to the deionized water supply to produce a one pore-volume pulse of 100 ppm NaOCl solution, eliminating the potential for significant microbial growth within the tank.

The packing within the tank consisted of two sections: a homogeneous section of coarse sand (#8 sieve) in the upstream 1.1 meters of the tank followed by an 8.1 meter heterogeneous section (Figure 1a). The heterogeneous section served as the laboratory analogy of random field-site sedimentary structure, was created using five different sands, and designed to support explicit representation in a numerical model. It was included to produce transport results with statistical properties similar to heterogeneous field sites. The heterogeneous zone approximated a log normal distribution of hydraulic conductivity (K) with a mean value of 4.18 (μ_{lnK}) and a variance of 1.22 (σ^2_{lnK}) where K has units of cm/hr. Each lateral and vertical correlation scale was 50.8 and 5.08-cm, respectively. A continuous distribution with a negative exponential covariance was



generated using a Fourier summation algorithm[12] and then discretized into five categories. Each category was assigned a particular sieve size sand: #16, #30, #50, #70 or #110 (Table 1). *Chao et. al.*[9] evaluated m_{lnk}, s^2_{lnk} and the correlation structure of the discretized distribution and verified that they matched the corresponding statistics of the original continuous distribution. The homogeneous zone provided a region to inject the tracer and promote initial mixing as it exited the injection well, producing a relatively consistent vertical line source. The coarser sand has a relatively high dispersivity reducing the effect of micro-heterogeneities in the packing and the potential for variation from the injection well.

A consistent packing procedure was used for the entire tank, details of the packing procedure have been reported in *Barth et. al.*[13] and *Barth et. al.*[14]. The sand was wet-packed in the tank to minimize consolidation and air entrapment. A total of 1280 cells were packed in the heterogeneous section: 32 columns and 40 layers producing 16 lateral and 20 vertical correlation scales. Vertical interfaces were avoided to reduce the chance for preferential migration of NAPLs used during other experiments (Figure 1c).

Hydraulic conductivity measurements

Table 1 summarizes the sets of hydraulic-conductivity values for the 6 different Tyler Mesh sieve-size sands used in this work. The measured values were obtained using a flexible-wall permeameter (ASTM D 5084-90) and a constant-head column (ASTM D2434-68, 93). The constant-head column was packed using the same method as the intermediate-scale tank. The permeameter's flexible walls eliminate the potential for wall effects and the 8.9-cm diameter constant-head column was at least 50 times the mean grain diameter, exceeding the ASTM D2434 recommended minimum column diameter by a factor of 8-12. Flexible-wall permeameter samples were approximately 4-5 cm in length while the constant-head column values (K_c) are from hydraulic-head measurements with 20 or 40-cm separation in a 90 cm vertical column; thus K_c represents hydraulic conductivity measurements of column lengths close to the length of the lenses in the tank and under conditions of similar effective stress. Hydraulic-head measurements along the 90-cm column revealed no significant trend in hydraulic conductivity as a function of depth[14].

Table 1: Symbols Identifying Sets of Hydraulic-Conductivity and Respective Values

	Mesh Size (ASTM E-11)					
	#8[1]	#16[2]	#30[2]	#50[2]	#70[2]	#110[2]
[3]K_p (cm h^{-1})	NA	1550	417	133	48.6	15.1
[4]K_{cl} (cm h^{-1})	NA	2148	674	111	74.2	22.8
[5]K_c (cm h^{-1})	6077	2250	708	136	84.7	23.0
[6]K_{ch} (cm h^{-1})	NA	2360	780	165	92.5	23.2
[7]K_r (cm h^{-1})	NA	3170	716	156	104	45.1
[8]d_{50} (mm)	1.25	0.88	0.49	0.30	0.19	0.103
[9]d_{60}/d_{10}	1.56	1.72	1.50	1.94	1.86	~2.0

NA: not available.
[1]Sand in the homogeneous zone.
[2]Sands used to create the heterogeneous zone.
[3]Measured using flexible-wall permeameter.
[4]Lowest measured constant-head column values.
[5]Average constant-head column measured values.
[6]Highest measured constant-head column values.
[7]Values determined by regression.
[8]50% of grains are smaller.
[9]Uniformity coefficient (values < 4.0 indicate uniform soil).

The permeameter values (K_p) are from *Mapa et al.*[15], which reports only a single measured value for each sand. The constant-head column evaluations were conducted as part of the present study, and were repeated from 3 to 20 times to evaluate variability. Coefficients of variation for the column-measured values of hydraulic conductivity ranged from 0.04 to 0.11. The variability is reported using three sets of values: K_{cl}, K_c, and K_{ch}, consisting of the lowest, average and highest constant-head column measured values, respectively. K_c was determined by taking the arithmetic average of the individual K measurements

The values of conductivity for the different mesh-size sands span more than two orders of magnitude (Table 1). The sands evaluated were considered uniform because, based on the manufacturer's specifications, each sand satisfied the criteria of having a uniformity coefficient (d_{60}/d_{10}) of less than 4.0. Comparison of the column-evaluated values of hydraulic conductivity to those produced in a one-meter long, two-dimensional tank where flow was parallel to any potential packing-induced microheterogeneities, indicated that the individual mesh-size sands were isotropic.

The differences between K_p and K_c are attributed to large differences (~50 kPa) in the effective stress applied to the sample, and possibly the difference in sample size. The variation among the column values is attributed to differences in packing despite concerted efforts to avoid such differences. The column values are measured under conditions similar to those in the intermediate-scale tank and were expected to be closest to the *in situ* values. The variability of the column measurements is likely to be reproduced in the tank, and it was anticipated that the average column values, K_c, would be closest to the *in situ* values.

Tracer Experiments

A total of four tracer injections referred to as C7, C8, C9 and D1 were performed under very similar conditions. Aspects of some of the experiments listed were discussed by *Barth et. al.*[13], and the experiment names used here are consistent with the names used in that work. For each experiment the injection rate was approximately 3.0 L/hr, just slightly less than the nominal tank effluent rate, to avoid flow field disruption. Samples were collected every four hours, or approximately every 0.08 pore volumes until roughly 3.5 pore volumes had passed through the tank. Samples from the experiments using Potassium Bromide (KBr), experiments C7, C8 and C9, were analyzed using an Ion Selective Electrode. To verify the absence of density effects during C7, C8, and C9, the fourth tracer test (D1) was conducted using tritium. Tritium samples were analyzed with a liquid scintillation counter.

NUMERICAL SIMULATIONS

The finite-difference groundwater flow model MODFLOW[16] was used to simulate steady-state hydraulic head and flow in the tank. The free surface in the tank was represented with a no flow boundary that approximated the free surface elevation; testing using a calculated free surface indicated little error from the approximation, as expected given the steady-state flow field. To simplify data input the finite difference grid was oriented vertically so that depth in the single layer corresponded to thickness of the two dimensional packing. This made it possible to represent the two-dimensional tank as a single layer of 40 rows and 150 columns, for a total of 6000 finite difference cells, without any loss in accuracy of the numerical simulation. Each finite difference cell was approximately 2.5-cm tall and 6.4-cm long so that each 2.5-cm tall, 25.4-cm long sand cell was represented by four finite-difference cells. The upstream and downstream ends of the tank were represented as constant heads.

Transport was simulated using MT3DMS[17] and flows generated by MODFLOW[16]. The third order, Total Variation Diminishing (TVD) solver was used. Single values of porosity and dispersivity for each sand,reported in *Mapa et al.*[15] and *Szlag*[18], respectively, were used. As expected for the granular, silica sands used, porosity was very consistent across the five mesh sizes and dispersivity increased with increasing grain size. Tracer injection was represented as an initial concentration in two adjacent columns of finite-difference cells which corresponded to the height of the injection interval and the width of the source immediately following the injection period.

Simulated concentrations from finite-difference cells approximating the location of each sampler were integrated to provide simulated break-through curves (BTCs). Both simulated and observed solute transport BTCs were integrated by combining the flux-weighted concentration from each sampler in each of the two transects (Figure 1a). Simulated concentrations for each set of K values were weighted using the respective simulated flux. Observed concentrations from the physical experiments were weighted with flux values from simulations using the head and flow calibrated values of hydraulic conductivity, K_r[14]. Discrepancies between transport predictions using K from the different measurement methods were evaluated by analyzing the temporal moments of the integrated BTC from each transect. The nth absolute temporal moment (M_n) is defined as:

$$M_n = \int_0^\infty t^n C(x,t)dt \qquad (1a) \qquad\qquad m_n = \frac{M_n}{M_0} \qquad (1b)$$

where t is time and $C(x,t)$ is concentration as a function of space and time. The normalized absolute nth moment (m_n) is obtained by dividing M_n by M_0, and m_n represents the nth normalized central moment.

$$s_n = \frac{\int_0^\infty (t - m_1)^n C(x,t)dt}{M_0} \qquad (2)$$

For this paper m_1 and s_2 were evaluated for each BTC and are referred to simply as the first and second moments, respectively. The first and second moments provide summaries of the mean arrival time and the amount of tracer plume spreading, respectively, for the measured and regression values of hydraulic conductivity. These summaries do not capture all the subtleties of the tracer BTC but provide an efficient method of quantifying differences in transport results.

Simulating Flow and Transport for the 150 Realizations of the Heterogeneous Distribution

Discrepancies between the measured and regression-estimated values of hydraulic conductivity produce significant differences in simulated transport. Of concern is the importance of the variability produced by measured values of K, relative to other common types of variability. The variability of transport results due to different realizations of the heterogeneous distribution is used as a measure for that induced by the different hydraulic-conductivity measurement methods. Differences in transport results between realizations are used as an analogy for differences between repeated experiments at various locations in a stationary, heterogeneous aquifer, or the errors associated with improper zonation of heterogeneous, sedimentary features. Packing more than one realization of the heterogeneous distribution in the intermediate-scale tank was not practical, instead forward flow and transport was simulated in different realizations of the hydraulic-conductivity distribution. Variability of simulated flow and transport across the different realizations represents the variability expected for a given distribution of materials and provides a baseline against which the variability in transport predictions due to the different hydraulic conductivity measurement methods is compared.

One hundred fifty realizations of the heterogeneous packing were generated using a Fourier summation algorithm and then discretized using the K_r values to produce 150 discretized realizations with m_{lnK} = 5.33 and s^2_{lnK} = 1.07, where K is in cm/hr. Transport was simulated in the 150 realizations to generate BTCs and the results used to estimate the ensemble average transport moments and their 95% linear confidence intervals. Variability of the results as a function of the hydraulic-conductivity measurement method was compared to the 95% confidence intervals for transport produced by the different realizations.

RESULTS

Simulation of transport using K_r values in 150 realizations of the heterogeneous distribution provided perspective for the large variations in transport predictions caused by the differences in measured hydraulic conductivity. Figure 2 plots the simulated BTCs for the realization packed in the tank, reflecting the variation caused by the differences in measured values of hydraulic conductivity. Also shown are the BTCs from 150 realizations of the correlated random field using K_r. The variability of simulated BTCs is of the same order for both sources of variation in transport.

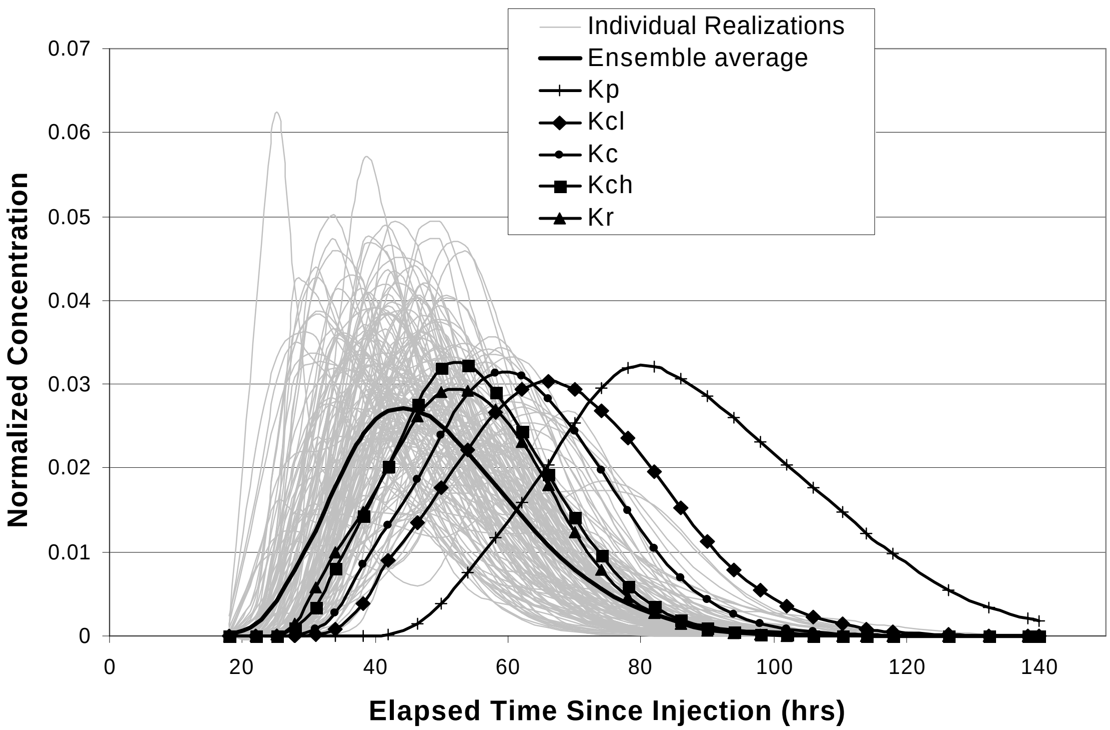


Figure 2: Simulated BTCs at transect 2 using experiment C7 boundary conditions: impact of realization variability compared to differences in measured value of hydraulic conductivity. K_r values were used to generate the unlabeled thin-line BTCs for individual realizations and the bold line without symbols representing the ensemble average. Curves with symbols identify the simulated BTCs for the realization that was packed in the tank.

The variability depicted in Figure 2 can be summarized and quantified by plotting the average m_1 (Figure 3a) and s_2 (Figure 3b) from simulated BTCs for all four experiments. The top five sets of values depicted in each graph reflect the difference between the moments calculated from the observed BTCs and the simulated BTCs based on K_p, K_{cl}, K_c, K_{ch} and K_r. Error bars signify the range of values over the four experiments. The bottom set of values in each graph depict the mean moments of simulated transport using K_r in 150 realizations of the distribution. The error bars for these values indicate the 95% confidence intervals. The range of first and second moments due to measurement-method variability is on the same order as that produced by between-realization variations in sedimentary structure.

DISCUSSION/CONCLUSIONS

This investigation, especially because of its size and complexity, provides unique insight into processes that cannot be controlled or explicitly evaluated at field sites. The experiments, simulations and analysis produced a unique perspective on our understanding of sedimentary structures, measured hydraulic conductivities, and their role in controlling flow and transport through porous media. The experiments provided results free from the effects of scaling and parameterization. The data presented illustrate limitations on the application of laboratory-measured hydraulic-conductivity values to predictive modeling of heterogeneous systems.

Typically, the reported mean and variance of a heterogeneous distribution represent the magnitude and variability of sedimentary structures but do not represent the variations that occur for either repeated measurements or use of alternate measurement methods on a single sedimentary structure. Even under the ideal conditions of the reported experiments the variability of transport predictions, as a function of the hydraulic conductivity measurement methods, was significant compared with that produced between realizations of a heterogeneous distribution of hydraulic conductivity. The results show that the variability in measured values of hydraulic conductivity contributes as much or more to the uncertainty in transport simulations as the random variations between realizations of the heterogeneous distribution. This suggests that the statistical parameters summarizing a heterogeneous distribution should be reported with confidence intervals that reflect the variability of hydraulic-conductivity measurements.

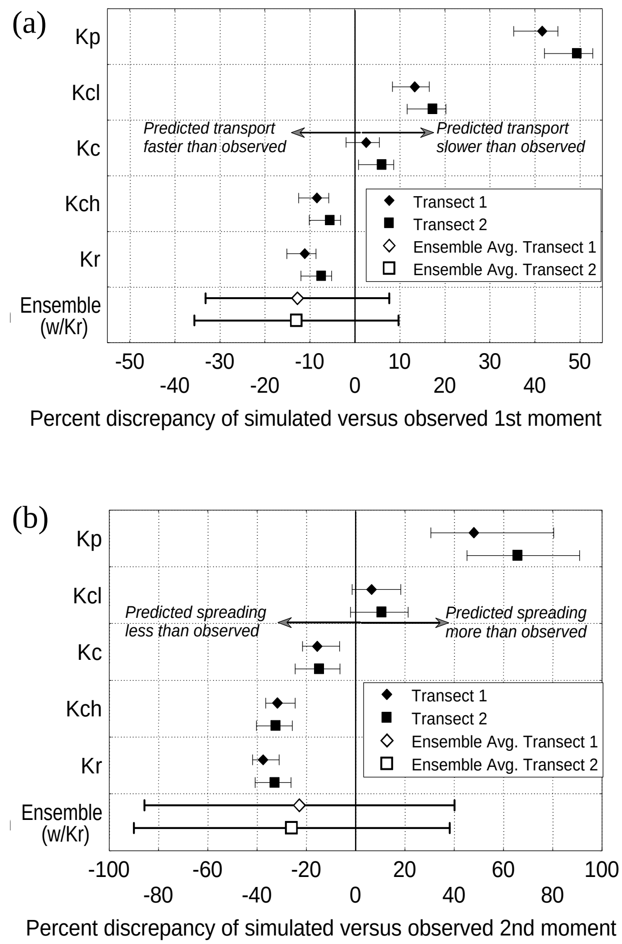


Figure 3: Discrepancies between observed and predicted BTC (a) first moments and (b) second moments for each set of measured hydraulic conductivity values and the ensemble average of the distribution using Kr. Error bars on the ensemble average indicate 95% confidence intervals based on the 150 realizations. All other error bars indicate the low and high values derived using measured moments for the four experiments.

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