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Predictive modelling of flow in a two-dimensional intermediate-scale, heterogeneous porous media

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Abstract To better understand the role of sedimentary structures in flow through porous media, and to determine how small-scale laboratory-measured values of hydraulic conductivity relate to *in situ* values this work deterministically examines flow through simple, artificial structures constructed for a series of intermediate-scale (10 m long), two-dimensional, heterogeneous, laboratory experiments. Nonlinear regression was used to determine optimal values of *in situ* hydraulic conductivity, which were compared to laboratory-measured values. Despite explicit numerical representation of the heterogeneity, the optimized values were generally greater than the laboratory-measured values. Discrepancies between measured and optimal values varied depending on the sand sieve size, but their contribution to error in the predicted flow was fairly consistent for all sands. Results indicate that, even under these controlled circumstances, laboratory-measured values of hydraulic conductivity need to be applied to models cautiously.

INTRODUCTION

The heterogeneity of natural systems confounds attempts to achieve accurate groundwater flow models. In many instances hydraulic conductivity data consist of core-scale values collected at sparsely distributed locations. It is unclear how such core-scale values relate to larger scales, such as the scale of numerical grid blocks, thereby requiring field-site simulations to expend considerable effort on model calibration (Hill, 1998). An improved understanding of how measured, core-scale, hydraulic conductivity values relate to *in situ* values is needed to better constrain numerical simulation calibration, thus allowing more accurate assessment of groundwater flow and transport problems. The work presented here addresses the first step towards this objective, using a very controlled experiment to compare detailed flow and pressure observations to simulation predictions, and analysing discrepancies between measured hydraulic conductivity and optimal *in situ* values as determined by nonlinear regression. Intermediate-scale experiments provided a complex, explicitly characterized system. The experiments were simple enough to be controlled, definitive and allow explicit numerical representation, yet complex enough to be comparable to field site heterogeneity.

INTERMEDIATE-SCALE EXPERIMENTS

Hydraulic conductivity measurements

Table 1 summarizes the sets of hydraulic-conductivity values 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 permeameter values are from Mapa *et al.* (1994), 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 three to 20 times to evaluate variability. 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, for each sand. The values of conductivity for the different mesh-size sands span more than two orders of magnitude. The sands evaluated were considered uniform because each sand satisfied the criteria of having a uniformity coefficient (d_{60}/d_{10}) of less than 4.0.

Table 1 Symbols identifying sets of hydraulic conductivity and respective values.

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

NA: not available.
*Sand in the homogeneous zone.
† Sands used to create the heterogeneous zone.
‡ Measured using flexible-wall permeameter.
[a] Low constant-head column measured values.
[b] Average constant-head column measured values.
[c] High constant-head column measured values.
[d] Values determined by regression.

The differences between K_p and K_c are attributed to large differences 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, measured under conditions similar to those in the intermediate-scale tank, were expected to provide a better representation of flow in the intermediate-scale tank.

Construction of the intermediate-scale experimental tank

The porous media was constructed in a 10 m long, 1.2 m tall, 0.05 m inside-width tank with constant heads on each end, so that the flow field was essentially two-dimensional (Fig. 1(a)). The packing within the tank consisted of a homogeneous section of coarse sand (#8 mesh size) in the upstream 1.1 m of the tank, followed by an 8.1 m heterogeneous section. The heterogeneous section was designed to have properties similar to sedimentary structures at field sites, but was simple enough for explicit

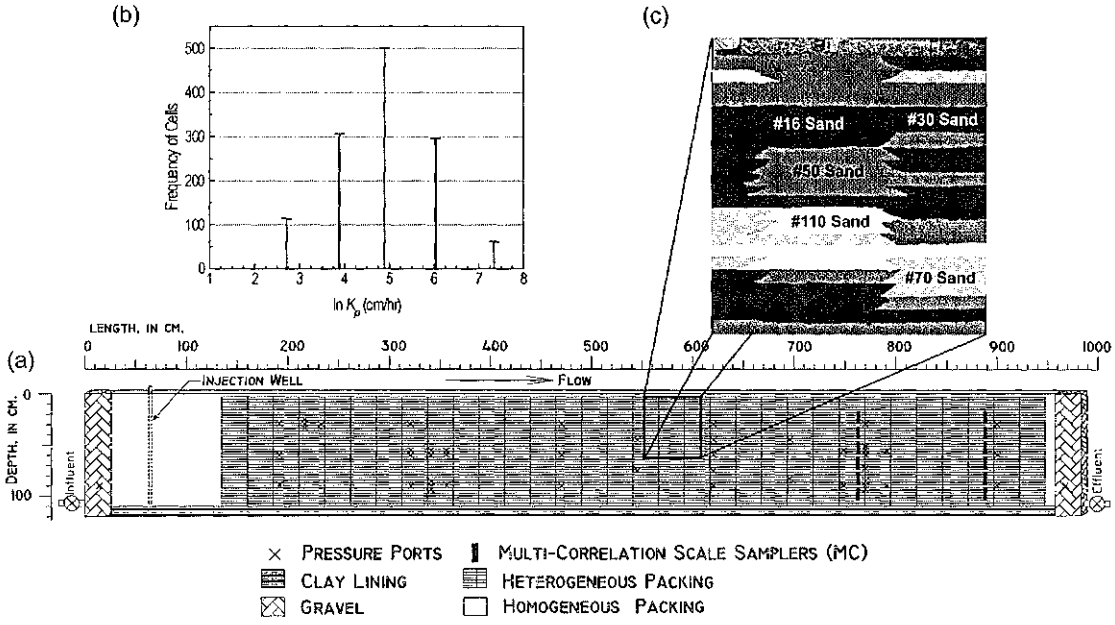

Fig. 1 Intermediate-scale tank design showing (a) the dimensions of the entire tank including a simplified representation of the sand-cell packing and the pressure and sampling ports, (b) the frequency distribution of the five sands packed in the tank categorized using the natural log of their permeameter values, and (c) an enhanced grey-scale detail of the tank packing. Each sand lens is 2.54 cm tall and 25.4 cm long, and is tapered at the ends as shown in (c).

numerical representation. The heterogeneous section approximated a log-normal distribution with a mean of 4.84 (Fig. 1(b)), equivalent to 126 cm h^{-1}. The variance of the log-transformed K_p values was 1.26 ($\sigma^2_{\ln K}$), significantly larger than at Cape Cod ($\sigma^2_{\ln K} = 0.26$; LeBlanc *et al.*, 1991), but smaller than at MADE ($\sigma^2_{\ln K} = 4.5$; Boggs *et al.*, 1990). Sand was packed as tapered cells (Fig. 1(c)), approximately 2.54 cm by 25.4 cm, with a total of 32 columns and 40 layers. The vertical and lateral correlation scales of 5.08 and 50.8 cm, respectively, resulted in 20 vertical and 16 lateral correlation lengths packed in the tank.

Four data sets, referred to as C7, C8, C9 and D1 were collected under very similar conditions. The data sets consisted of the flow rate leaving the tank, or effluent rate, and pressure at 46 ports (Fig. 1(a)). Effluent rates typically were 3200 $cm^3 h^{-1}$. Repeated pressure measurements indicated typical standard deviations of less than 0.08 cm of water pressure.

NUMERICAL SIMULATION DESIGN AND REGRESSION ANALYSIS

The finite difference groundwater flow model MODFLOWP (Hill, 1992) was used to simulate steady-state pressure and flow in the tank. The model grid consisted of 40 rows and 150 columns. Row width corresponded to the 2.54 cm sand layer thickness. The up- and down-gradient boundaries were simulated as constant heads. The location of the free-surface boundary was, as verified by simulation, accurately approximated.

The heterogeneous section was represented using a finite difference grid of four columns per sand column and one finite difference row per sand row.

Inverse modelling was performed because, as noted below, simulations using laboratory-measured hydraulic conductivities did not reproduce flow and pressure observations as well as expected. Inverse modelling and associated sensitivity analyses were performed as described by Hill (1998). Simultaneous regression of the four pressure and effluent data sets produced optimal values of hydraulic conductivity for the five sands in the heterogeneous packing reported as K_r in Table 1. Hydraulic conductivity of the homogeneous section, the #8 sieve size sand, was not estimated because of insensitivity. Observation weights are based on the variability about mean observation values quantified as a standard deviation of 0.08 cm for pressure and 21 $cm^3\ h^{-1}$ for effluent.

Composite scaled sensitivities, correlation coefficients, calculated error variance and linear confidence intervals on the parameter estimates (Hill, 1998) were used. To quantify the difference between measured and regression values of hydraulic conductivity, the percent discrepancy is calculated as in equation (1). The m indicates measurement type (Table 1), and j refers to the sand sieve number. Linear 95% confidence intervals for the percent discrepancy were determined by using the plus- and minus two standard deviation values of K^j_r in equation (1) to produce the corresponding high and low values of percent discrepancy:

$$\varepsilon = \frac{K^j_m - K^j_r}{K^j_r}(100) \tag{1}$$

Equation (2) indicates the potential effect of differences between measured and regression values of hydraulic conductivity on flow predictions as a flow-relevant scaled discrepancy:

$$\varepsilon^* = \frac{\left(K^j_m - K^j_r\right)}{\overline{Q}}\frac{\partial Q}{\partial K^j_m}(100) \tag{2}$$

The $\overline{Q}$ is the mean observed effluent for the four experiments and $\partial Q/\partial K^j_m$ is the sensitivity of calculated flow through the tank to K^j_m evaluated at the measured value of K using MODFLOWP.

RESULTS

Despite the controlled nature of these experiments, effluent predictions were considerably different from observations. Figure 2(a) compares predicted effluent to values measured for the four data sets. Predictive simulations using K_p, K_{cl} and K_c values under-predicted the effluent rate by about –40% and –20%, and from –9.9% to –14.7% with a mean value of –13.0%, respectively. Predictions using the K_{ch} values had a mean error of –2.2% (Fig. 2(a)). The discrepancy for K_c, which was expected to be almost zero, is surprisingly large and prompted the use of sensitivity analysis and nonlinear regression to relate the flow discrepancy to variations in hydraulic conductivity.

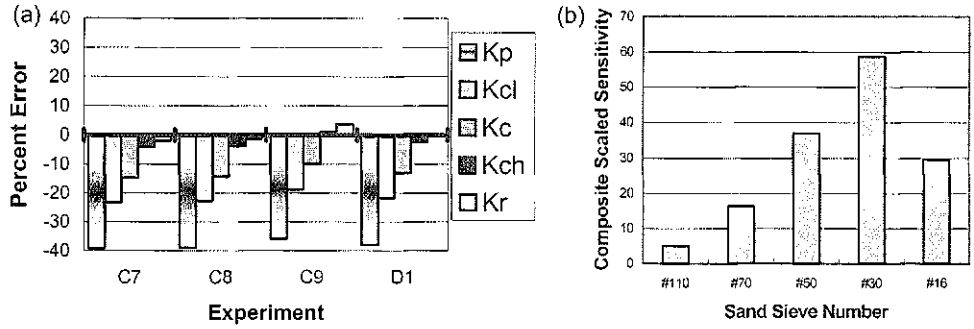

Fig. 2 (a) Percent error of simulated tank effluent compared to that observed for data sets C7, C8, C9 and D1, for permeameter values (K_p); low (K_{cl}), mean (K_c) and high (K_{ch}) values of column measurements, and estimated by the regression (K_r). (b) Composite scaled sensitivities of the five different sieve size sands based on simultaneous optimization of hydraulic conductivity for C7, C8, C9 and D1.

Composite scaled sensitivities from the sensitivity analysis (Fig. 2(b)) are based on simultaneous consideration of the pressure and effluent data from all four data sets. The fact that sensitivities are all within an order of magnitude of each other and all correlation coefficients are less than 0.88 indicates that optimal values of hydraulic conductivity for each sand can be estimated (Hill, 1998). Regression results confirm this; regression values (K_r) are listed in Table 1.

Figure 3(a) shows the percent discrepancy between regression and measured values of hydraulic conductivity. Significance of discrepancies for all permeameter-measured values of hydraulic conductivity is illustrated by the fact that the 0% discrepancy is not within the linear 95% confidence intervals. For all measurement methods, the percent discrepancies for the #110 and #16 sands were significant. For the #70, #50 and #30 sands the confidence intervals for the larger values tend to include zero, so that these regression values are not significantly different to the measured values.

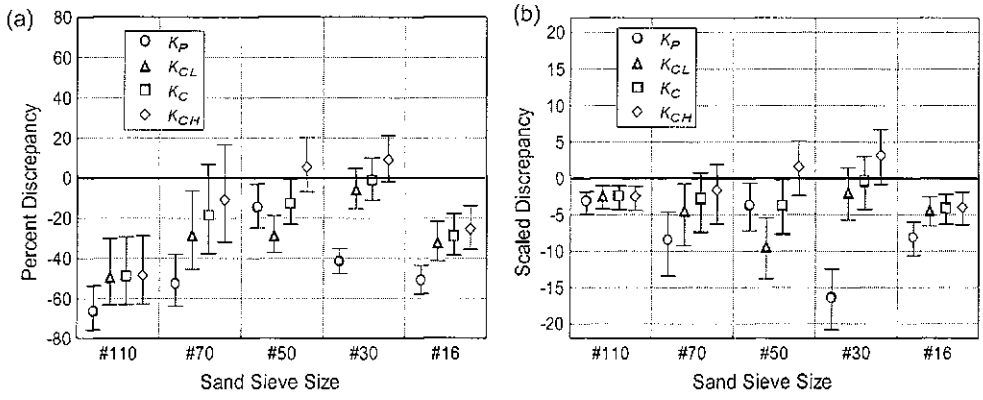

Fig. 3 Differences, expressed as (a) percent, and (b) flow-relevant scaled discrepancies, between optimized (K_r) and measured (K_p, K_{cl}, K_c, K_{ch}) hydraulic conductivity values for each of the five sands. Error bars reflect the linear 95% confidence intervals of K_r values.

For equation (2) $\partial Q/\partial K^j_c$ for the #110, #70, #50, #30 and #16 sands was 3.5, 4.6, 6.1, 1.5 and 0.1 cm^2, respectively. The sensitivities evaluated for the other measurement-method values of hydraulic conductivity were similar. The magnitudes of percent discrepancy for the #110 and #16 are significant for all measurement methods and relatively large (Fig. 3(a)), while the flow-relevant scaled discrepancies (Fig. 3(b)) are fairly consistent for a particular method of measurement. Although the confidence intervals indicate that many of the constant-head column scaled discrepancies are not significant, there does appear to be a bias. Measured hydraulic conductivity usually contributed to the under-prediction of flow.

POTENTIAL SOURCES OF DISCREPANCIES

Potential sources of the effluent discrepancies can be attributed to hydraulic conductivity measurement errors, pressure and effluent measurement errors, and model errors, described in detail by Barth (1999). The factors suspected of contributing to hydraulic conductivity measurement errors include variability of measured values, wall effects and consolidation. Errors in pressure and effluent measurement were primarily a function of the measurement technique precision. Sources of model errors included accurate representation of the tank-wall deflection, porous-media consolidation, boundary condition representation, and grid refinement, which were all investigated numerically.

The analysis indicated that the greatest potential for error was produced by the variability of constant-head column hydraulic conductivity measurements. However, it is unclear why predicted flow using the mean measured values (K_c) and the highest constant-head column measured values (K_{ch}), differs from the observed flow by an average of –13% and almost matches the observed flow, respectively. Similarity in packing methods and effective stress suggest that the tank *in situ* values should be equal to or less than the mean constant-head column measured values. The contribution from wall effects was negligible. The only other significant error source was grid refinement, which reduced the predicted effluent error on the order of only 1–2% (Mehl, 1998). In summary, none of the issues examined were likely to have contributed sufficiently to explain the –13% discrepancy between the mean constant-head column predicted and observed flow. Even if all potential sources were assumed to increase the flow prediction, the error in predicted effluent would be about 10%.

DISCUSSION/CONCLUSIONS

Despite careful construction of the porous media, the detailed information available and an exhaustive consideration of possible errors, tank effluent predictions using mean column-measured hydraulic conductivity were 13% less than the observed, while the highest column-measured values closely reproduced the effluent rate. For the mean constant-head column values the scaled discrepancies were comparable for all sands indicating that the measured values of each sand had similar contributions to the under-prediction of flow. The data presented illustrate limitations on the application of

laboratory-measured hydraulic conductivity values to predictive modelling of heterogeneous systems, even in the absence of scaling and zonation issues.

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