CONTAMINANT TRANSPORT BEHAVIOR IN SAND-AND-GRAVEL AQUIFERS BASED UPON THE INTERPLAY BETWEEN POROSITY AND HYDRAULIC CONDUCTIVITY

Roger H. Morin, United States Geological Survey, Denver, Colorado USA

ABSTRACT

It is intuitive to think of hydraulic conductivity *K* as correlating positively with porosity *Φ* in coarse-grained porous media. However, at two study sites on Cape Cod, Massachusetts, USA, multivariate analyses of geophysical logs obtained from water wells revealed an inverse relationship between *K* and *Φ* in sand-and-gravel aquifers. Indeed, it has been demonstrated in laboratory experiments and also confirmed through field observations that hydraulic conductivity and porosity may be either positively or negatively correlated, depending on grain-size distribution and packing arrangement. Transport processes occurring within granular deposits are influenced by several factors, including fluid chemistry, mineral composition, and fluid interstitial velocity *V'*. This linear velocity describes the microscopic flow of water winding along pathways distributed through a mass of particles and, from Darcy's law, *V'* is proportional to the ratio *K/Φ*. Therefore, the nature of the interdependence (positive or negative) between these two material properties affects the range of possible values for *V'* and has fundamental implications regarding sorption reactions, aquifer dispersion, and the migration of contaminants.

RÉSUMÉ

La conductivité hydraulique *K* est intuitivement corrélée positivement à la porosité *Φ* dans les milieux poreux à granulométrie grossière. Cependant, à deux sites situés à Cape Cod, Massachusetts, USA, les analyses multi-variées des diagraphies de puits ont révélé une relation inverse entre *K* et *Φ* dans les aquifères de sables et graviers. En effet, il a été démontré en laboratoire et *in situ* que *K* et *Φ* peuvent être corrélés positivement ou négativement, en fonction de la granulométrie et du tassement. Les processus de transport survenant dans les dépôts granulaires sont influencés par plusieurs facteurs, incluant la chimie du fluide, la composition minérale et la vitesse interstitielle *V'*. Cette vitesse linéaire décrit l'écoulement microscopique de l'eau circulant à travers les pores et, à partir de l'équation de Darcy, *V'* est proportionnelle au rapport *K/Φ*. En conséquence, la nature de l'interdépendance (positive ou négative) entre ces deux propriétés influence l'intervalle de valeurs possibles pour *V'* et a donc des répercussions fondamentales sur les réactions de sorption et la dispersion, qui influencent la migration des contaminants.

1. INTRODUCTION

At two sites on Cape Cod, Massachusetts, USA, sets of geophysical logs were obtained in water wells that penetrated shallow sand-and-gravel aquifers prevalent in the region. The logs measured the natural gamma activity *γ*, hydraulic conductivity *K*, electrical resistivity *R*, and porosity *Φ* of the surrounding deposits. A typical log composite is presented in Figure 1 showing these four parameters as a function of depth.

A rigorous multivariate analysis of the log data found only slight interdependence among most of the four variables, but identified a strong inverse correlation between the hydraulic conductivity and the porosity (Morin, 2004). Conventionally, *K* and *Φ* are thought to be positively correlated (e.g., Chilingar, 1963; Nelson, 1994) in coarse-grained materials and the implications of this inverse relationship found on Cape Cod are considered within the context of contaminant transport.

2. *K*-*Φ* INTERDEPENDENCE

The interplay between hydraulic conductivity and porosity in granular materials may be investigated by first examining the correlation between *K* and some representative grain size *d* based upon experiments by Fraser (1935) and later elaborated upon by Marion et al. (1992) and by Kolterman and Gorelick (1995). In Figure 2a, a sprinkling of fine grains is gradually added to a collection of coarse grains represented by large *d* such that the overall representative grain size systematically decreases; the mixture shifts from coarse packed to fine packed (from left to right in Figure 2a). This experiment is illustrated in Figure 2b by a diagram depicting the corresponding relationship between the porosity and the average grain size. Both *Φ* and *d* initially decrease as the smaller grains fill the voids between the larger ones until a threshold is reached (Φ_{min}) where the voids are effectively filled. Beyond this stage, coarse grains begin to be suspended within a matrix of fine grains. Here, *d* continues to decrease but *Φ* now increases and we see a reversal in the relationship between representative grain size and porosity.

Numerous empirical investigations have shown the hydraulic conductivity of granular materials to be positively correlated in some manner to grain size (e.g., Hazen, 1911; Pryor, 1973). Shepherd (1989) summarizes this work by the general expression,

$$K = Cd^2 \qquad [1]$$

where C is a proportionality constant that may represent a variety of factors, including path tortuosity, particle shape, and pore shape. Considering Equation 1 within the context of the results presented in Figure 2b, the systematic decrease in representative grain size also implies a similar reduction in hydraulic conductivity. Thus, a condition is defined to the left of Φ_{min} (Case 1) where $K \sim \Phi$ and to the right of Φ_{min} (Case 2) where $K \sim 1/\Phi$, and we see a reversal in the relationship between K and Φ based upon grain-size distribution and packing arrangement. This inverse K-Φ behavior has also been recognized in various field studies (e.g., Beard and Weyl, 1973; Clarke, 1979).

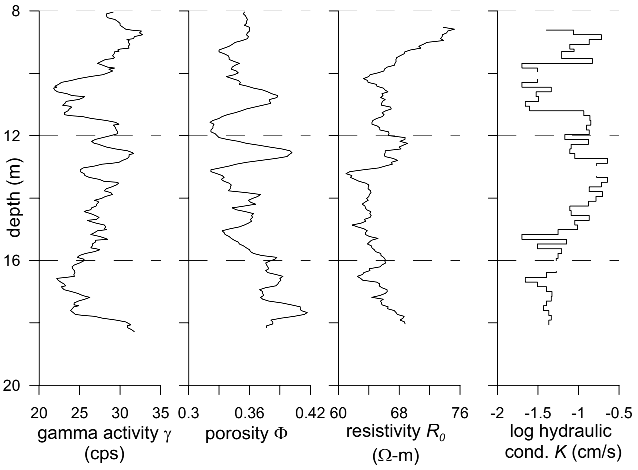

Figure 1. Composite of geophysical logs obtained from one well penetrating a sand-and-gravel aquifer on Cape Cod, Massachusetts.

3. TRANSPORT IMPLICATIONS

This basic change in the relationship between hydraulic conductivity and porosity has implications with respect to contaminant transport processes. Sorption reactions that take place within an aquifer are influenced by numerous physical factors, including fluid residence time t', grain surface area A_S, grain surface composition N_S, and fluid chemistry C_f (e.g., Zheng and Bennett, 1995).

$$\text{sorption reaction} = f\,(t', A_S, N_S, C_f, \ldots\ldots) \qquad [2]$$

The residence time t', or the time that the fluid is in contact with grains per unit path length, is the reciprocal of the interstitial velocity V'. This velocity, often referred to as the average linear velocity, describes the microscopic velocity of a fluid moving along pathways winding through a mass of particles. It is related to the macroscopic fluid velocity V (e.g., Freeze and Cherry, 1979) by the expression,

$$V' = V/\Phi \qquad [3]$$

According to Darcy's law,

$$Q/A = V = Ki \qquad [4]$$

where Q is the volumetric discharge measured through a sample having a cross-sectional area A and i is the hydraulic gradient. Substituting Equation 3 into Equation 4,

$$V' = [K/\Phi]\ i \qquad [5]$$

and

$$V' \sim K/\Phi \qquad [6]$$

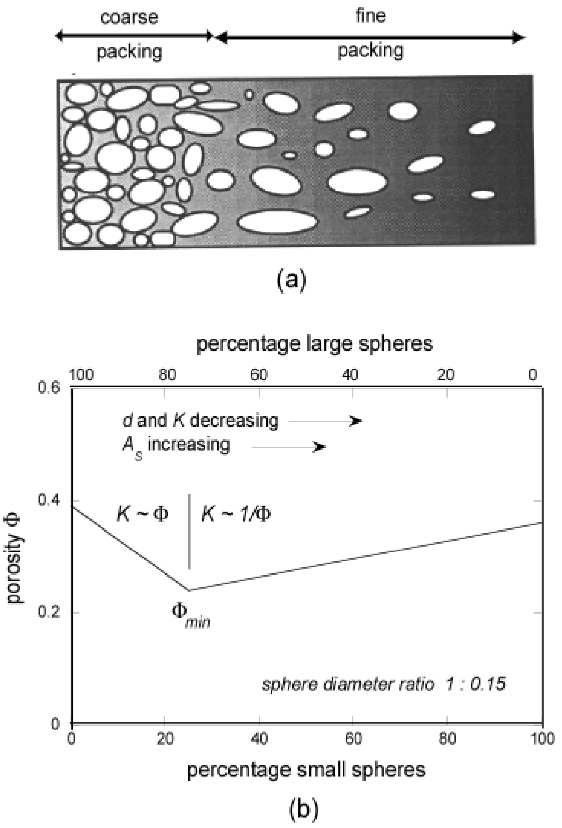

Figure 2. Ideal packing model based on a binary mixture of particles. (a) Diagram depicts gradual shift from a coarsely packed arrangement to a finely packed one as percentage of fine grains continually increases (after Marion et al. 1992). (b) Related diagram of porosity versus percentages of sphere sizes (after Fraser, 1935). Porosity Φ decreases with decreasing representative grain size d until it reaches a threshold porosity Φ_{min}. This is Case 1, where the hydraulic conductivity $K \sim \Phi$. After reaching Φ_{min}, porosity reverses trend and increases with further decrease in d. This is Case 2, where $K \sim 1/\Phi$.

From Equation 6, it can be seen that the range and magnitudes of the interstitial velocities associated with Case 1 ($K{\sim}\Phi$) will be different from those associated with Case 2 ($K{\sim}1/\Phi$), as illustrated in Figure 2b. Accordingly, sorption reactions that are affected by V' will also be different.

Actual values for hydraulic conductivity and porosity reported by Morin (2004) are manipulated to illustrate this point. In the study at Cape Cod, K varied over roughly an order of magnitude (0.02 – 0.22 cm/s) and Φ ranged from .32 to .42, but in an inverse sense. Thus, the hypothetical range of values for K/Φ is .06 to .52 for Case-1 conditions ($K{\sim}\Phi$) and .04 to .69 for the true Case-2 conditions ($K{\sim}1/\Phi$). A plot of K versus K/Φ for Cases 1 and 2 is shown in Figure 3, with the trends in K and K/Φ also symbolizing the behavior of d (Equation 1) and V' (Equation 6), respectively.

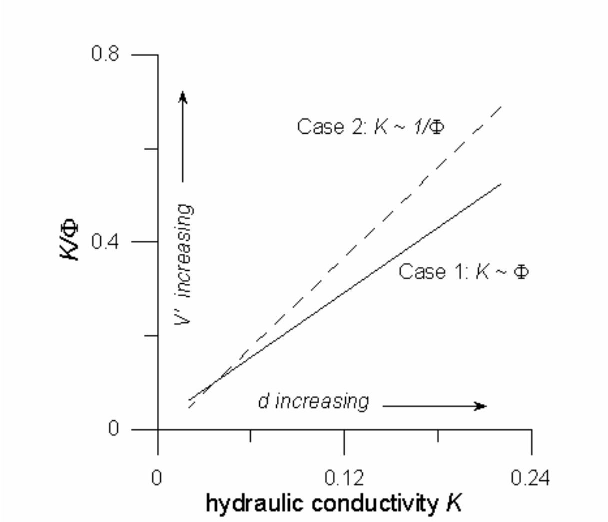

Figure 3. Relationship between K (proportional to d) and K/Φ (proportional to V') using field data from Morin (2004). K and Φ are positively correlated in Case 1 and negatively correlated in Case 2. Values from two Cases are similar at low K values but diverge at high K values.

When the hydraulic conductivity is low, values of K/Φ and, consequently, V' are small in both Cases 1 and 2 (Figure 3); the linear velocity V' is slow in fine-grained materials regardless of the Case. Therefore, materials that promote high sorption reactions (i.e., long fluid residence times, large grain surface area, etc.) continue to do so in either Case 1 or 2 with negligible differences. When the hydraulic conductivity is high, values of V' are fast in both Cases 1 and 2. However, a divergence in the trends between the two Cases at the highest values of K demonstrates that the linear velocity associated with Case 2 is even faster than that for Case 1 (Figure 3). Thus, conditions that tend to favor low sorption rates (i.e., short fluid residence times, small grain surface area, etc.) are even less amenable to these reactions when K and Φ are negatively correlated. There should be a more stratified and concentrated distribution of contaminants in Case-2 materials.

The coefficient of hydrodynamic dispersion D is comprised of two components (e.g., Freeze and Cherry, 1979).

$$D = \alpha V' + D^{*} \qquad [7]$$

where α is the dispersivity, an inherent physical property of the granular material, and D^{*} is the coefficient of molecular diffusion. For a given K, V' will be larger within the context of an inverse relationship between K and Φ. Consequently, the coefficient of dispersion will be larger when K and Φ are negatively correlated compared to when they are positively correlated. Although Case-1 materials can support fast values of V', Case-2 materials have even faster linear velocities. As such, these latter materials are more apt to have larger values of dispersion coefficient, particularly in zones of high hydraulic conductivity and low sorption.

4. DISCUSSION

A multivariate analysis of geophysical log data obtained in shallow sand-and-gravel aquifers on Cape Cod revealed an inverse relationship between the hydraulic conductivity and the porosity of these coarse-grained unconsolidated deposits. Laboratory studies performed on a mixture of granular particles, as well as reports based on field observations, indicate the K and Φ can be either positively or negatively correlated, depending on grain-size distribution and packing scheme.

One of the primary factors controlling sorption reactions is the microscopic velocity of fluid moving around a mass of particles and this linear velocity V' is a function of the ratio K/Φ. Therefore, the interdependence of these two physical properties has some implications regarding contaminant transport behavior. Case 1 is defined here as a positive correlation ($K{\sim}\Phi$) and Case 2 as a negative one ($K{\sim}1/\Phi$). In zones where the hydraulic conductivity is low and grain size is small, there is a negligible difference between the two Cases in terms of linear velocity and sorption reaction. However, in zones where K is highest and grain size is relatively large, Case-2 materials support a significantly higher V' and sorption reactions are muted because of the shorter fluid residence time and smaller grain surface area.

Because dispersion is a function of V', the coefficient of dispersion in Case-2 materials may be greater than typically expected. Thus, two granular samples with identical values of hydraulic conductivity and porosity may have significantly different values of D, depending on whether K and Φ are positively or negatively correlated. This factor may, in part, account for the discrepancy between theoretical and measured values of D estimated at one of the Cape Cod sites (Garabedian et al. 1991; Hess et al. 2002). The interplay between particle size, shape, and packing with hydraulic conductivity and porosity influences contaminant transport, and an inverse K-Φ relationship presents another perspective on understanding these processes.

5. REFERENCES

Beard, D.C. and Weyl, P.K. 1973. Influence of texture on porosity and permeability of unconsolidated sand. AAPG Bulletin, Vol. 57, no. 2, pp. 349-369.

Chilingar, G.V. 1963. Relationship between porosity, permeability, and grain-size distribution of sands and sandstones. Proc., Int. Sedimentology Congress, Amsterdam, Netherlands, pp. 98-112.

Clarke, R.H. 1979. Reservoir properties of conglomerates and conglomeratic sandstones. AAPG Bulletin, Vol. 63, no. 5, pp. 799-803.

Fraser, H.J. 1935. Experimental study of the porosity and permeability of clastic sediments. J. Geology, Vol. 83, no.8, pp. 910-1010.

Freeze, R.A. and Cherry, J.A. 1979. Groundwater. 604 pp., Prentice-Hall, Englewood Cliffs, New Jersey.

Garabedian, S.P., LeBlanc, D.R., Gelhar, L.W., and Celia, M.A. 1991. Large-scale natural gradient tracer test in sand and gravel, Cape Cod, Massachusetts 2: Analysis of spatial moments for a nonreactive tracer. Water Resources Research, Vol. 27, no. 5, pp. 911-924.

Hazen, A. 1911. Discussion of “Dams on sand foundations” by A.C. Koenig. Trans., American Society of Civil Engineers, Vol. 73, p. 199.

Hess, K.M., Davis, J.A., Kent, D.B., and Coston, J.A. 2002. Multispecies reactive tracer test in an aquifer with spatially variable chemical conditions, Cape Cod, Massachusetts: Dispersive transport of bromide and nickel. Water Resources Research, Vol. 38, no. 8, 10.1029/2001WR000945.

Kolterman, C.E. and Gorelick, S.M. 1995. Fractional packing model for hydraulic conductivity derived from sediment mixtures. Water Resources Research, Vol. 31, no. 12, pp. 3283-3297.

Marion, D., Nur, A., Yin, H., and Han, D. 1992. Compressional velocity and porosity in sand-clay mixtures. Geophysics, Vol. 57, no. 4, pp. 554-563.

Morin, R.H. 2004. Inverse porosity-hydraulic conductivity relationship in sand-and-gravel aquifers determined from analysis of geophysical well logs, abs.,Transactions, American Geophysical Union, Spring Meeting Supplement, v. 85, no. 12, p. S322.

Nelson, P.H. 1994. Permeability-porosity relationships in sedimentary rocks. The Log Analyst, Vol. 3, pp. 38-62.

Pryor, W.A. 1973. Permeability-porosity patterns and variations in some Holocene sand bodies. AAPG Bulletin, Vol. 57, no. 1, pp. 162-189.

Shepherd, R.G. 1989. Correlations of permeability and grain size. Ground Water, Vol. 27, no. 5, pp. 633-639.

Zheng, C. and Bennett, G.D. 1995. Applied Contaminant Transport Modeling. 440 pp., Van Nostrand Reinhold, New York.