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How much heterogeneity? Flow versus area from a big data perspective

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Abstract

Over the past 10 years, there has been an increased recognition that matrix diffusion processes are a significant factor controlling the success of groundwater remediation. New field techniques and modeling tools have, consequently, been developed to understand how contaminants diffuse into and then out of low-permeability ("low-k") zones and assess the resulting impact on groundwater quality. Matrix diffusion, in turn, is driven by one key factor: geologic heterogeneity. The importance of heterogeneity is being emphasized in the groundwater field by general rules of thumb such as "90% of the mass flux occurs in 10%-20% of the cross-sectional area" and conceptual models that show most of the groundwater flow occurs through the aquifer's "mobile porosity" which just a small fraction of commonly used effective porosity values (between 0.02 and 0.10 for mobile porosity vs. 0.25 for effective porosity). For this study, 141 boring logs from 43 groundwater remediation sites were evaluated to develop an empirically based estimate of the groundwater flow versus aquifer cross-sectional area to confirm or reject the general flow versus area rules of thumb. This study indicated that at these 43 sites, an average of 30% of the cross-sectional area carried 90% of the groundwater flow. Our flow-only analysis does provide moderate (but not confirmatory) support for the "mobile porosity" concept with an estimated representative mobile porosity value of about 0.11 at the 43 sites.

1 | INTRODUCTION

Because of matrix diffusion (which is explained well by Sale et al., 2014), understanding the dynamics of groundwater flow through various soil layers is essential to understand the transport and remediation of contaminants from groundwater in a natural setting. By using this information in groundwater contaminant remediation, efforts may be more focused around the areas of the subsurface known to be carrying the majority of the target contaminants. Depending on the remediation processes, focusing remedial efforts on these areas of higher mobility could save a substantial amount of time and operational costs by improving the efficiency of removal or treatment of the contaminant plume.

In groundwater media, a traditional conceptual model of groundwater flow relies on the concept of effective porosity. Effective porosity is generally defined as the portion of the soil through which groundwater moves or that portion of the media that contributes to flow. Effective porosity is also less than the total porosity because not all of the water-filled pores are interconnected or contribute to flow. Therefore, typical values of effective porosity used are 0.2 or 0.3 (e.g., see Newell, McLeod, & Gonzales, 1996; Payne, Quinnan, & Potter, 2008).

Recently, there has been an increasing focus on how geologic heterogeneity in aquifers makes remediation much more difficult due to effects such as matrix diffusion. In addition, there has been recognition that much of the groundwater flow and mass flux through the subsurface occurs in a relatively small fraction of an aquifer's cross-section. For

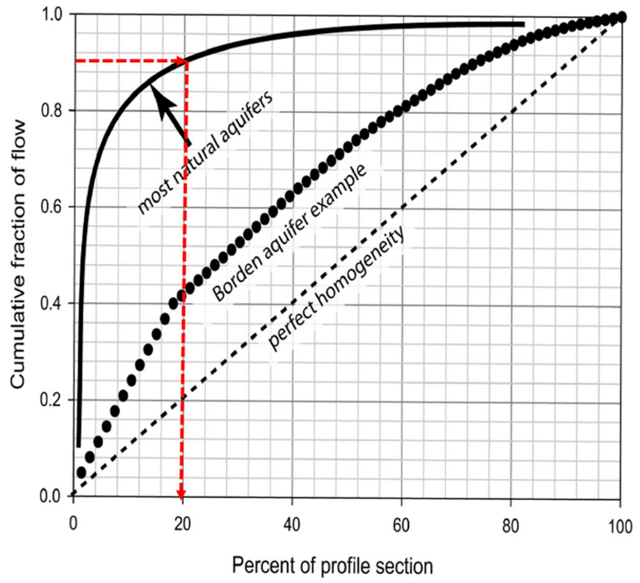


FIGURE 1 Distribution of flow in vertical profiles (Payne et al., 2008). The dashed line represents the flow distribution for a perfectly homogenous media, black circles show the flow distribution for the Borden aquifer (one of the most geologically homogeneous sand aquifers in the world), and the solid line shows most natural aquifers where flow will be concentrated in a smaller fraction of the aquifer pore space (Payne et al., 2008, fig. 8.2; Borden data from Rivett et al., 2001). The red arrows suggest that for "most natural aquifers" 90% of the flow occurs through about 20% of the aquifer cross-sectional area. Note the "most natural aquifers" line (solid black line) is conceptual, and not derived by data [Color figure can be viewed at wileyonlinelibrary.com]

example, Cramer, Shultz, Plank, and Levine (2018) indicated that "90% of the mass flux contaminant transport at Superfund sites has been shown to move through only 10% of aquifer material."

A related concept is described by the term "mobile porosity" which explains the preferential flow of fluid through "the segments of the aquifer with the highest permeability" (Payne et al., 2008, p. 67). In subsurface plume migration, contaminants can more easily be traced and remediated by "recognizing that the flow is concentrated in the mobile porosity" (Payne et al., 2008, p. 48). In Figure 1, Payne et al. (2008) plotted "Cumulative Fraction of Flow" versus "Percent of Profile Section" (e.g., the percent of the cross-sectional area to flow). They depicted how perfectly homogenous soils can follow a path along the dashed line, with no variation in flow over the entire cross-section. The Borden aquifer, a very homogeneous natural aquifer, followed a more convex line (dots). Most natural aquifers, however, were shown to follow a path like the solid line, where flow varies across the different soil layers. Based on this line, 90% of the groundwater flow occurs through approximately 20% of the cross-sectional area at a site. In particular, Payne et al. (2008) note that "for the purpose of assessing plume migration rates, assuming mobile porosities between 0.02 and 0.10 would be more appropriate than using the common 0.20 value" (p. 67).

Therefore, mobile porosity represents the portion of total porosity that contributes to advective flow and transport in aquifers (Payne et al., 2008).

$$\Theta_t = \Theta_m + \Theta_i \, , \tag{1}$$

where

Θ_t = total porosity (%),
Θ_m = mobile porosity (%), and
Θ_i = immobile porosity (%).

Mobile porosity can be determined through tracer studies, as shown in Table 1. In different locations, likely with unique adjacent soil compositions, mobile porosity of sandstone aquifers range from 0.08% to 5%, and from 1.7% to 9% in aquifers with gravel mixtures. Similarly, the calculated mobile porosities from 73 tracer tests summarized by Suthersan et al. (2014) indicate that "for about half the sites, the derived Θ_m value was 0.09 or less and for about 80% of the sites, the derived Θ_m value was 0.15 or less" (Suthersan et al., 2014).

2 | EVALUATION OF FLOW DISTRIBUTION

The distribution of flow (and/or mass flux) versus the cross-sectional area of the aquifer can better inform remediation efforts. As such, a planning-level empirical study was performed to determine the distribution of flow versus cross-sectional area by compiling actual site data.

In this study, 287 boring logs from 56 sites were obtained from the California GeoTracker database (GeoTracker, 2018) and analyzed to determine the percent of cross-sectional area carrying the majority of groundwater flow.

2.1 | Implications

The groundwater flow versus area is becoming a more important part of the groundwater remediation conceptual site model. Sites, where more of the groundwater flow is transmitted through a smaller area, have these attributes:

- They are likely to be more prone to impacts from matrix diffusion processes because there are likely more interfaces between transmissive and stagnant or effectively stagnant low-permeability units where contaminants can first diffuse into low-permeability zones, then back diffuse out when the concentrations in the transmissive zone drop;
- They may be better candidates for partial source zone treatment where dense nonaqueous phase liquid source zones feeding the high groundwater flow zones are targeted for treatment. More flow through a small cross-sectional area means the targeted zone for partial source zone remediation may be smaller; and

TABLE 1 Summary of mobile porosity estimates based on tracer studies (Payne et al., 2008, table 3.2)

Locations	Aquifer	Aquifer material	Mobile porosity (%)	Notes
Quebec, Canada	–	Poorly sorted sand and gravel	8.5	6.4 m^3 injection in 7.25 hr
Central Valley, California	–	Poorly sorted sand and gravel	4–7	575 m^2 injection over 30 days; arrival monitored in seven wells
Northern Texas	Ogallala	Poorly sorted sand and gravel	9	1460 m^3 injection over 28 days
New Jersey	Passaic Formation	Fractured sandstone	0.1–0.7	24.6 m^3 injection over 2 days
Los Angeles, California	Gaspur aquifer	Alluvial formation	10.2	17 m^3 injection over 8 hr
Northern New Jersey	–	Glacial outwash	14.5	7.57 m^3 in 3 days
Northern Missouri	–	Weathered mudstone regolith	7–10	4.54 m^3 in 9 days
Sao Paulo, Brazil	–	Alluvial formation	7	18.9 m^3 injection over 2.5 days
Phoenix, Arizona	–	Alluvial formation	7	2.27 m^3 in 8 hr
Savannah River Site, South Carolina	Atlantic coastal plain	Silty sand	5	Model calibration
Kaiserslautern, Germany	Trifels Formation	Fractured sandstone	0.08–0.1	Multiple injections and volumes 0.1–5 m^3
West Texas	Rio Grande River Valley	Alluvium, sand, and gravel	1.7	18.9 m^3
Northern Texas	Ogallala	Alluvium, poorly sorted sand and gravel	0.3–1.7	Dipole test, 61.3 m^3
Central Colorado	Cherry Creek	Alluvium, sand, and gravel	11–18	Two injection tests, 4.9 and 7.6 m^3
Central Colorado	Denver Formation	Siltstone, sandstone, mudstone	1–5	Monopole—tracer injected in monitoring well/pumping well

- They are characterized by having only a small fraction of the contaminated aquifer volume that is easily reached by injection-based treatment technologies.

3 | METHODOLOGY

3.1 | Initial data set

The boring logs used in this study were obtained from the California State Water Resources Control Board GeoTracker database (GeoTracker, 2018). At least five boring logs were downloaded and analyzed from each site selected at random from the database, with all sites located in California. Before further selection criteria were applied, 287 boring logs from 56 sites were analyzed. Here, each soil section per the Unified Soil Classification System (USCS) was recorded along with exact depths of occurrence throughout the boring log. Fractured rock sites were not included in the analysis.

Additionally, the approximate depth to water in feet below ground surface (bgs) was recorded for each boring log. From the initial data set of 287 boring logs, 33 did not have specific depth to water information available. As such, for this subset, the depth to water was assumed to be 15 ft bgs based on the median value from various sites in the Hydrogeologic Database (Newell, Hopkins, & Bedient, 1990). Additionally, only soil layers within the boring logs in the saturated zone at each site were retained for further analysis.

3.2 | Groundwater flow and cross-sectional area

Following Payne et al.'s fig. 1, data for each soil section and soil type in a boring log were analyzed to generate a curve showing the "Cumulative Fraction of Flow" versus "Percent of Profile Section." Literature values for hydraulic conductivity were used for each USCS soil type recorded in boring logs (Table 2). In cases where two soil types were recorded in a single section, the average hydraulic conductivity of the combination was used.

The next step was to partially randomize each hydraulic conductivity estimate to account for the natural variation in hydraulic conductivity in an individual boring. As discussed in Schultz, Cramer, Plank, Levine, and Ehman (2017), natural depositional environments almost always exhibit vertical heterogeneity in grain size and hydraulic conductivity, even within individual packets of sediments. To account for the variability within each soil type above (e.g., variability within sands vs. silts vs. clays), the general range of estimated hydraulic conductivities for each row in table 3.2 in Domenico and Schwartz (1997) was first calculated, and showed that "coarse sand" had a potential range of ×6700 between the low- and high-end estimates, "fine sand"

TABLE 2 Hydraulic conductivity values used in the study

Soil type symbol	Classification	Hydraulic conductivity (cm/s)	Data source
GW/GM/GP/GC	Gravel	3×10^{-1}	Median D&S table 3.2
SW	Sand, clean, well-graded	5.5×10^{-2}	Payne fig. 3.9 for $n = 0.35$
SP	Sand, clean, poorly graded	5.5×10^{-3}	
SM	Sand, silty	1×10^{-3}	
SC	Sand, clayey	1.2×10^{-4}	Geomean SM, SC
ML	Silt, sandy/silt	1.4×10^{-5}	Payne table 3.1
MH	Silt, clayey	1.1×10^{-6}	Geomean ML, CL
CL	Clay, sandy/silty, low plasticity	1×10^{-7}	Estimated
CH	Clay, high-plasticity	2.1×10^{-8}	Median D&S table 3.2

Abbreviations: D&S, Domenico and Schwartz (1997); Payne, Payne et al. (2008).

had a range of ×1000, and silt had a range of ×20,000. To evaluate the range due to grain size and sorting in sands, fig. 3.9 in Payne et al. (2008) was evaluated, and it showed that generally there was a factor of ×1000 or more between fine and coarse sand; and a factor of ×10 to ×100 range between “very well sorted” and “very poor sorted.”

Therefore, to capture this variability in hydraulic conductivity, a ×100 “random multiplier term” was added to the hydraulic conductivity for each soil type presented in Table 2 for each of the discrete soil types in each well log used for this analysis. For example, if a particular segment of a boring log indicated the presence of 5 ft of silty sand (SM), Table 2 indicated that a representative middle-range hydraulic conductivity was 1×10^{-3} cm/s. The random multiplier term then increased or decreased this value in the range between 1×10^{-4} and 1×10^{-2} cm/s. This random multiplier term, while constrained to a factor of ×100, was different for each time SM was identified in a particular boring.

The contributing transmissivity based for each soil type in the boring and corresponding thicknesses and hydraulic conductivities were then was calculated using Equation 2.

$$T = k \cdot b, \tag{2}$$

where

T = transmissivity (ft^2/year) for each soil type;
k = hydraulic conductivity of the soil types (ft/day); and
b = cumulative thickness of each of the soil type (ft).

3.3 | Percent of flow and cross-sectional area

Within each boring log, the transmissivity was calculated for each soil section, then the percent of total transmissivity across the entire vertical length of the boring log was determined. Soil sections were sorted from highest to lowest percent of transmissivity per foot to calculate cumulative percent of transmissivity across the boring section.

$$T_c = (T/T_t), \tag{3}$$

where

T_c = cumulative transmissivity across boring log (%);
T_t = sum of transmissivity across all soil sections in a boring log (gal/year); and
T = transmissivity across single soil section (gal/year).

Note that transmissivity will be proportional to the groundwater flow through each boring so that the “Cumulative Fraction of Flow” could be calculated for each boring.

The cumulative aquifer cross-sectional flow area within each boring section was also calculated to find the percent of the total cross-sectional area that is receiving the majority of the flow.

$$A_c = (A)/A_t, \tag{4}$$

where

A_c = cumulative flow area (%);
A_t = sum of cross-sectional areas of all soil sections in a boring log (ft^2); and
A = cross-sectional area of a soil section (ft^2; thickness × cross-sectional width).

Figure 2 depicts a single boring log used for this study and indicates: (a) individual soil sections with soil types and (b) layers that carry >1% of the overall flow through the cross-section (blue arrow and corresponding calculated percentage of transmissivity). The image shows the groundwater transmissivity through the heterogeneous mixture of soils. Larger arrows indicate more transmissivity and therefore more groundwater flow. As previously discussed, the flow will be distributed among the layers, finding the path of least resistance based on thickness and soil type. In this example, about 16% of the cross-sectional area carries 90% of the cumulative groundwater flow (Figure 3).

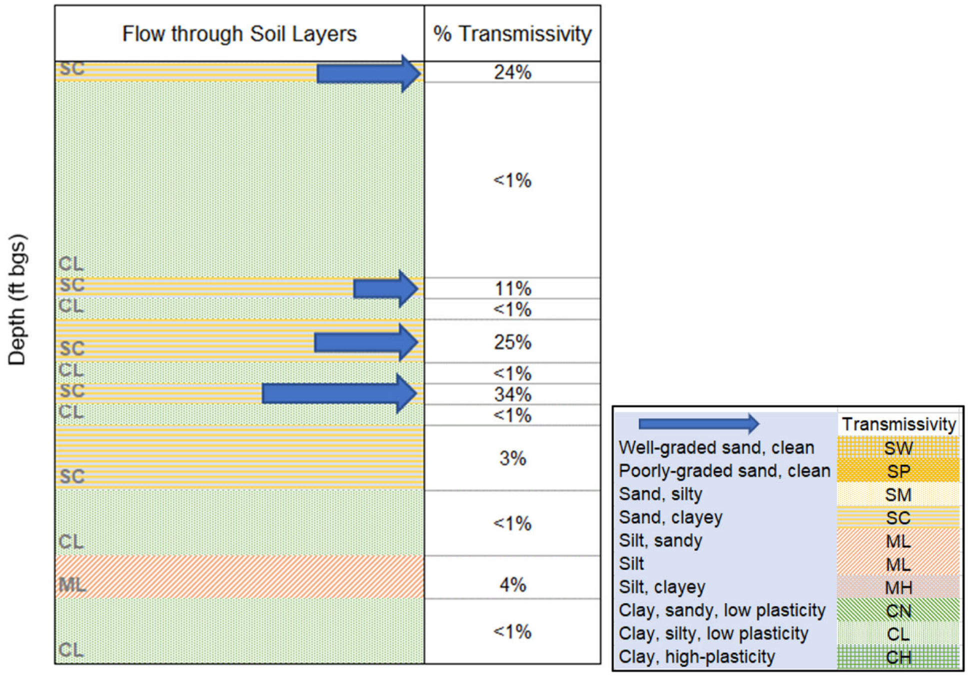


FIGURE 2 Data from example boring log, showing the Unified Soil Classification System soil types and transmissivity over a cross-section [Color figure can be viewed at wileyonlinelibrary.com]

3.4 | Final data set

Boring logs with three or more saturated soil sections were retained for further analysis. After employing these selection criteria, a total data set of 43 sites and 141 boring logs were included in the study, with an average of approximately three boring logs per site. The median saturated zone thickness of the data set evaluated was approximately 20 ft.

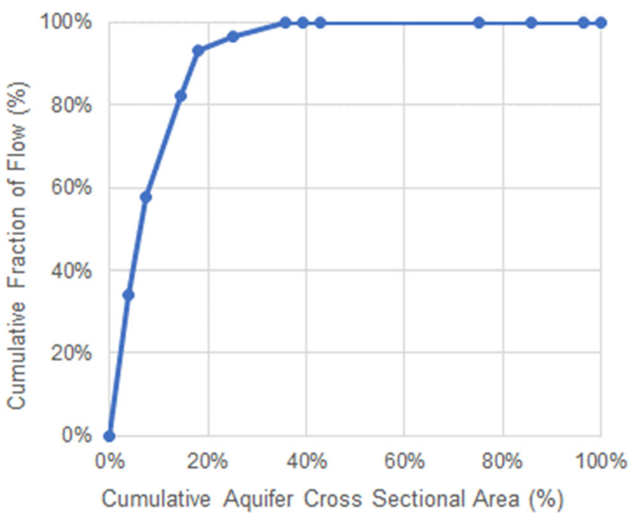


FIGURE 3 Example boring showing cumulative fraction of flow versus cumulative aquifer cross-sectional area for boring log shown in Figure 3. In this single example boring log, 90% of the flow is moving through about 16% of the aquifer cross-sectional area [Color figure can be viewed at wileyonlinelibrary.com]

4 | RESULTS

The cumulative fraction of flow versus cumulative aquifer cross-sectional area curves for all 141 boring logs are shown in Figure 4. This array of curves shows a wide distribution of geologic settings, from very heterogeneous ones as shown by lines to the left/top of the graph) to more uniform geologic settings that are closer to the 45° diagonal line. After all the boring logs at each site were averaged, a cumulative fraction of flow versus cumulative aquifer cross-sectional area curves were developed for each of the 43 sites as shown in Figure 5. Finally, the curves for each of the 43 sites were averaged to form a single curve representing all of the data in Figure 6. The empirical data from the 43 sites were then compared to Payne's theoretical curve for "most natural aquifers" as shown in Figure 7.

At the most homogeneous site, 90% of the groundwater flow was transmitted through about 67% of the aquifer cross-section, while at the most heterogeneous site 90% of the groundwater flow was transmitted through only 13% of the aquifer cross-section. Using the median value from the 43 sites indicated that 90% of the groundwater flow was carried by only 30% of the aquifer cross-section (Figure 7). About 50% of the flow was conducted by the most permeable 15% of the aquifer cross-section at these sites. Overall, these data support the conclusion that groundwater flow in unconsolidated sand/silt/clay aquifers is extremely heterogeneous with most of the flow (and most of the mass flux) going through a small, highly permeable portion of the aquifer. This flow-only result corroborates the "90% of mass flux" rule of thumb because mass flux combines flow heterogeneity and concentration heterogeneity. This flow-only analysis also provides moderate (but not confirmatory) support for the "mobile porosity" because 30% of the cross-sectional area

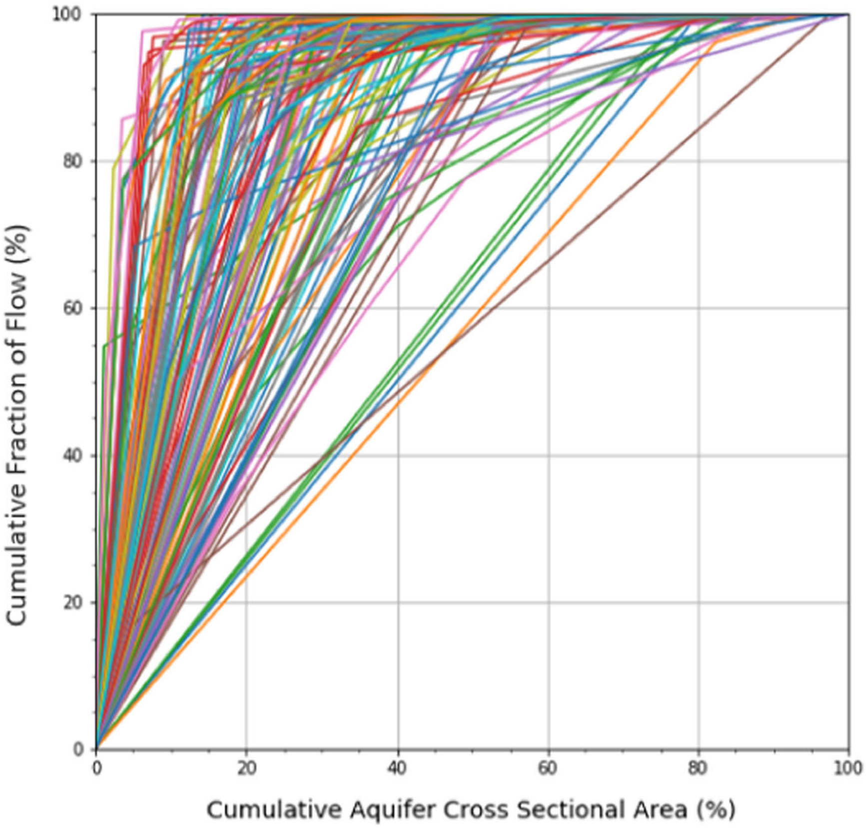


FIGURE 4 Cumulative fraction of flow versus cumulative aquifer cross-sectional area for 141 boring logs. The curves that are clustered to the top/left represent high heterogeneity settings with more low-permeability material in the logs, while the few points near the diagonal line represent logs with more uniform settings [Color figure can be viewed at wileyonlinelibrary.com]

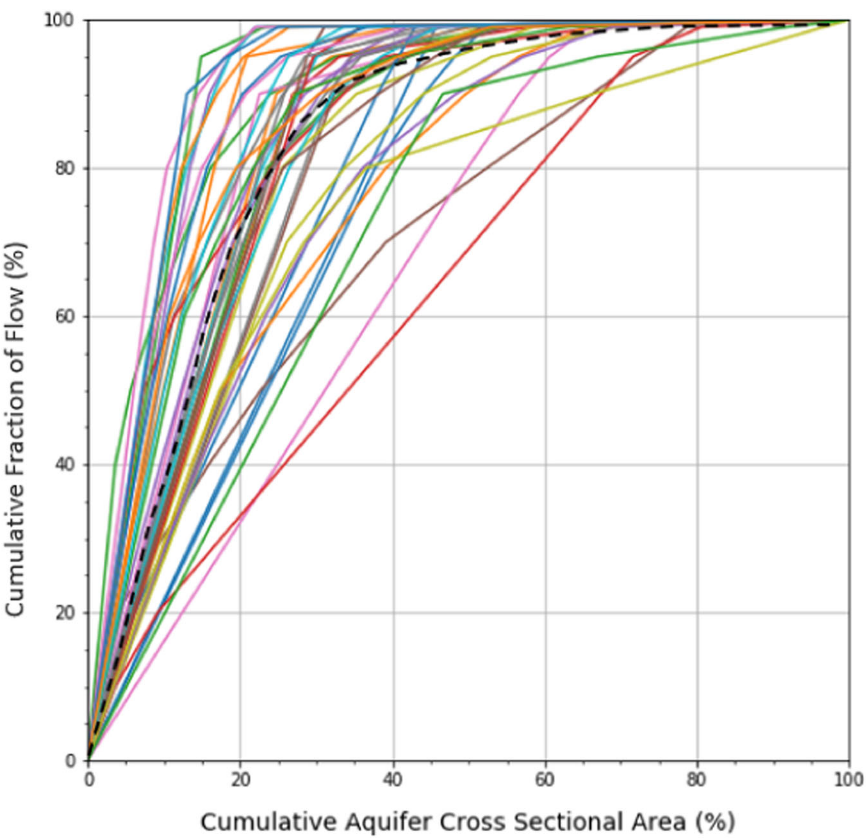
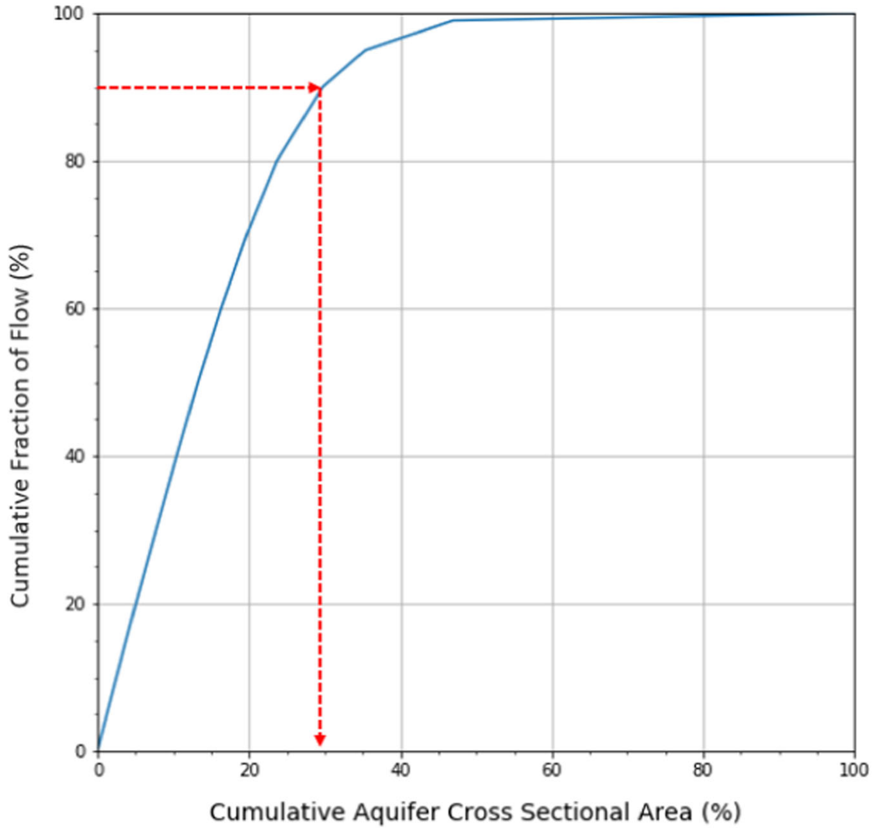


FIGURE 5 Average cumulative fraction of flow versus cumulative aquifer cross-sectional area for each of the 43 sites. At the most homogeneous site, 90% of the groundwater flow was transmitted through about 67% of the aquifer cross-section, while at the most heterogeneous site 90% of the groundwater flow was transmitted through only 13% of the aquifer cross-section. The average site showed about 90% of the groundwater being conducted through about 30% of the cross-sectional area [Color figure can be viewed at wileyonlinelibrary.com]

FIGURE 6 Average cumulative fraction of flow versus cumulative aquifer cross-sectional area for all 43 sites and all 141 boring logs analyzed. At these sites, approximately 90% of the groundwater flow was flowing through about 30% of the aquifer cross-section [Color figure can be viewed at wileyonlinelibrary.com]



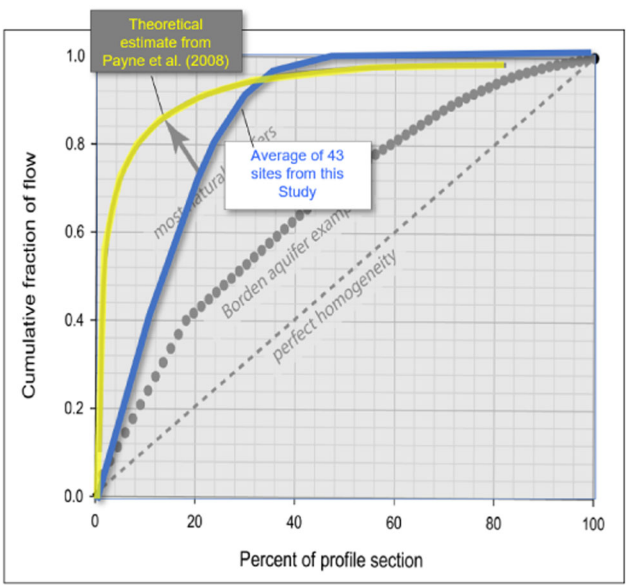


FIGURE 7 Cumulative fraction of flow versus cumulative aquifer cross-sectional area from Payne et al. (2008) theoretical analysis (yellow line) compared with the empirical analysis of 43 sites and 141 boring logs (blue line). The empirical data show slightly less heterogeneity than Payne et al.'s theoretical analysis. Underlying graph from Payne et al. (2008, see fig. 2) [Color figure can be viewed at wileyonlinelibrary.com]

multiplied by a typical value for total porosity of 0.35 yields about 0.11 “mobile porosity” of an aquifer on a cross-sectional basis compared with the Payne et al. (2008) range of 0.02–0.11.

5 | CONCLUSIONS

First, there has been increasing interest in understanding the heterogeneity of groundwater flow through aquifer cross-sections as indicated by these cumulative flow/cross-sectional area relationships:

(1) Payne et al. (2008) estimated that 90% of the flow in “most natural aquifers” flowed through only 20% of the aquifer cross-section.
(2) A sequence stratigraphy training course suggested that 90% of the mass flux (which considers both heterogeneity in flow and concentration) moved through only 10% of the aquifer material (Cramer et al. 2018).

While the authors of the two references above are well-known in the field, and these types of values have been widely circulated in the remediation field, no references to any underlying data are provided. Data mining of 141 geologic boring logs at 43 randomly selected unconsolidated geology sites in California was used to develop a quantitative empirical relationship between cumulative groundwater flow and cumulative aquifer cross-sectional area for each of the 43 sites. The groundwater flow through each soil type segment in each geologic log (e.g., well-sorted sands [SW] and silts [ML]) was estimated using representative hydraulic conductivities for each soil type. The cumulative flow was then plotted versus the cumulative aquifer cross-section. This analysis showed that on average at these 43 sites 90% of the groundwater flow was carried by about 30% of the most permeable portion of the aquifer cross-section, with 90% of the flow carried by 67% of the cross-section area at the most homogeneous site and 16% at the most heterogeneous site.

Second, a 2008 conceptual model for analyzing contaminant transport in groundwater suggested that the "effective porosity" (with a commonly used value of 0.25) should be replaced with a much smaller "mobile porosity" ranging from 0.02 to 0.10 (Payne et al., 2008) The data from the 141 boring logs suggested that a representative "mobile porosity" of these sites is about 0.11, much less than the commonly used effective porosity of 0.25 but just above the "normal range of "0.10 or less" presented by the Payne et al. (2008).

To our knowledge, this study provides the largest quantitative analysis of cumulative groundwater flow/cross-sectional area relationships for a database of this size (141 borings and 43 sites). The results can help anchor the commonly used metric about aquifer heterogeneity to the one supported by data from 43 sites: "on average about 90% of flow occurs through 30% of the aquifer cross-section." In addition, the analysis supports that a true effective porosity of about 0.10 may be more representative than a more commonly used effective porosity of 0.25. This value of 0.11 is on the upper end of the reported values in Payne et al.'s "mobile porosity" concept.

Overall these data provide a quantitative depiction of the log-normal, heterogeneous nature of groundwater flow, with most of the flow (and most of the mass flux in the case of groundwater plumes) going through a small, highly permeable portion of the aquifer cross-section. Site characterization should focus on high-resolution sampling to quantify mass flux/mass discharge, and remediation should focus on the sources of high mass flux zones that are flowing through a small fraction of the aquifer cross-section.

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