An evaluation of the influence of aquifer heterogeneity on permeable reactive barrier design

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[1] The influence of heterogeneity in aquifer hydraulic conductivity (K) on contaminant plume patterns and the required thickness and length of permeable reactive barriers (PRBs) used for in situ remediation is evaluated using stochastic modeling. The results provide a quantitative means for evaluating the effects of (1) the level of aquifer heterogeneity as reflected by the standard deviation of the logarithm of K, \( \sigma_{\ln K} \), (2) the aquifer correlation structure anisotropy represented by the ratio of correlation lengths, \( \lambda_x/\lambda_y \), and (3) \( D_{\text{PRB}} \) representing the distance from the contaminant source zone to the PRB. In terms of PRB thickness, a probabilistic factor of safety related to uncertainty in influent groundwater seepage velocities (FS\(_{1.90}\)) at the location of the PRB is quantified. In terms of PRB length, a probabilistic factor of safety related to uncertainty in the length of a PRB required to capture the contaminant plume, defined as the capture length ratio (CLR), is quantified. The mean and standard deviation of CLR increase with increasing \( \sigma_{\ln K} \) compare favorably with previously published values based on a different methodology. The mean and standard deviation of CLR increase with increasing \( \sigma_{\ln K} \) and with increasing \( D_{\text{PRB}} \), and decrease slightly with increasing \( \lambda_x/\lambda_y \). Finally, the ranges in CLR are correlated with strongly divergent and strongly convergent plume patterns.


1. Introduction

[2] Permeable reactive barriers (PRBs) are subsurface emplacements of reactive materials designed to intercept a contaminant plume, provide a flow path through the reactive media, and transform the contaminants into environmentally acceptable forms to achieve remediation goals down gradient of the PRB [U.S. Environmental Protection Agency (EPA), 1998]. Remediation goals typically include contaminant effluent concentrations in compliance with prescribed maximum contaminant levels (i.e., MCLs). Properly designed and constructed PRBs have minimal impact on the natural groundwater gradient (i.e., unimpeded flow), and have low operational and maintenance costs for extended periods of time (i.e., except for the costs associated with monitoring). Zero-valent iron (Fe\(^0\)) has been used as the reactive material for the majority of constructed PRBs to promote the reductive dehalogenation of volatile organic compounds (VOCs), reduce mobile and toxic oxyanions of chromium (CrO\(_2^2\)), arsenic (H\(_2\)AsO\(_4^3\)), and selenium (HSeO\(_4^2\)) into immobile precipitates, and treat radionuclide and nitrate-bearing groundwaters [e.g., U.S. EPA, 1998; O’Hannesin and Gillham, 1998; U.S. EPA, 2002]. Biochemical systems based on the decomposition of emplaced solid organic materials oriented toward the remediation of nitrate, sulfate, and heavy metals (acid mine drainage) from impacted groundwaters also have been used as PRBs [e.g., Thombre et al., 1997; Benner et al., 1997; Robertson et al., 2000; U.S. EPA, 2002; Groudev et al., 2003; Hemsi et al., 2005].

[3] In the field, aquifer heterogeneity inherently affects the performance of PRBs. Heterogeneity induces preferential pathways of flow and contaminant transport (channeling) that expose the PRB to spatially variable groundwater seepage velocities, with localized values that may be sufficiently high such that the required PRB thickness is greater than that for a homogenous aquifer. Additionally, aquifer heterogeneity may induce divergent flow patterns that require the length of the PRB to be greater than that for a homogenous aquifer. The primary objective of this study is to evaluate the influence of aquifer heterogeneity on plume patterns and on the required thickness and length of PRBs. The approach is based on numerical modeling of flow and particle tracking for 650 synthetic stochastic heterogeneous aquifers pertaining to different simulation cases. The results include (1) identification of plume pattern categories with frequencies of occurrence, (2) quantification of a probabilistic factor of safety for scaling the PRB thickness, and (3) quantification of a probabilistic factor of safety for scaling the PRB length. The evaluation is limited to PRBs consisting of a continuous trench subjected to two-dimensional horizontal flow within a heterogeneous aquifer (i.e., funnel-and-gate scenarios for PRBs and injected subsurface treatment zones are not evaluated). Also, the effects of factors that can influence PRB design and performance other than aquifer heterogeneity, such as...
2. Background

2.1. PRB Design Based on Homogenous Aquifers

[4] The most simplistic approach to PRB design is based on the assumptions of homogeneous aquifer and PRB, uniform flow perpendicular to the PRB, uniform contaminant residence time within the PRB, and the validity of relatively simple reaction mechanisms within the PRB, such as first-order kinetics in the case of VOC degradation by Fe⁰ [Gavaskar et al., 1998; U.S. EPA, 1998]. In this case, a closed-form analytical solution for the minimum PRB thickness based on steady state one-dimensional advective-dispersive transport with first-order reaction kinetics can be written as follows [e.g., Eykholt and Sivavec, 1995]:

\[ T_{PRB,Homog} = \frac{2}{v} \ln \left( \frac{C_{in}}{C_{eff}} \right) = \frac{2}{\sqrt{v^2 + 4KD}} \ln \left( \frac{C_{in}}{C_{eff}} \right) \]

where \( T_{PRB,Homog} \) is the PRB thickness, \( C_{in} \) and \( C_{eff} \) are the influent and effluent contaminant concentrations, respectively, \( C_{o} \) is the source-zone concentration, MCL is the maximum contaminant level (i.e., \( C_{in} = C_{o} \), and \( C_{eff} = MCL \)), \( k \) is the first-order degradation rate coefficient, \( D \) is the coefficient of hydrodynamic dispersion, and \( v \) is the uniform seepage velocity based on Darcy's law. Also, the analytical plug-flow solution (i.e., without considering hydrodynamic dispersion) can be written as follows [e.g., Eykholt and Sivavec, 1995; Elder et al., 2002]:

\[ T_{PRB,Homog} = \frac{v}{k} \ln \left( \frac{C_{o}}{C_{eff}} \right) = \frac{v}{k} \ln \left( \frac{C_{o}}{MCL} \right) \]

which is a classic first-order kinetic expression with \( T_{PRB,Homog}/v \) representing the reaction time. Eykholt and Sivavec (1995) used equation (2) with \( C_{in}/C_{eff} = 1000 \) for several different values of \( v \) and \( k \) resulting in PRB thicknesses ranging from 0.003048 to 3.048 m (0.01 to 10 feet).

[5] A factor of safety commonly is used in conjunction with equation (1) or (2) to account for uncertainty in flow and reactivity, due primarily to aquifer and PRB heterogeneity, hydraulic gradient variability, and temporal and spatial changes in the reactivity of the Fe⁰ [Eykholt, 1997; Elder, 2000; Elder et al., 2002]. Typical factors of safety are of the order of 2, but values as high as 10 have been reported in conjunction with higher levels of heterogeneity in aquifer K.

[6] The length of a PRB in a homogeneous aquifer is equal to the width of the source zone if the PRB is placed perpendicular to the direction of flow and centered with respect to the source zone. A factor of safety also can be used to increase the length of the PRB to account for variability in plume capture zones due to aquifer heterogeneity and variability in the direction of the hydraulic gradient. In contrast, consideration of the length of the PRB is irrelevant in cases where PRBs are laterally keyed to bedrock [e.g., Benner et al., 1997; Groudev et al., 2003].

2.2. PRB Design Based on Heterogeneous Aquifers

[7] The simple analytical solutions (e.g., equations (1) and (2)) generally are not applicable in the case where the contaminant degradation within the PRB does not follow simple (e.g., first-order) kinetics. In addition, the effects of aquifer heterogeneity on groundwater flow and contaminant transport (i.e., preferential flow and channeling) typically are taken into account through the use of numerical modeling [e.g., Poeter and Gaylord, 1990; Moreno and Tsang, 1993; Poeter and Gaylord, 1993; Elder et al., 2000; Elder et al., 2003].
Zheng and Jiao, 1998; Gavaskar et al., 1998; Elder, 2000; Bilbrey and Shafer, 2001; Elder et al., 2002; Zheng and Bennett, 2002). For example, flow channeling can be represented macroscopically by longitudinal and transverse macroscopic dispersivities that are regional properties of the heterogeneous aquifer, and proportional to $\sigma_{\ln K}$ [e.g., Gelhar et al., 1992; Gelhar, 1993; Zheng and Bennett, 2002], such that the standard deviation of the logarithm of the aquifer $K$, or $\sigma_{\ln K}$, is likely to be a major aquifer parameter affecting the design of PRBs.

Different methodologies have been used to evaluate the effect of aquifer heterogeneity on the required PRB thickness. For example, Eykholt [1997] performed a Monte Carlo analysis using equation (2) to simulate the probabilistic distribution of $C_{\text{eff}}$ as a function of $v$, $C_m$, and $K$ that were assumed to follow given probabilistic distributions. The value of the PRB thickness ($T_{\text{PRB}}$) was iterated until $C_{\text{eff}} < 0.001$ was obtained. A factor of safety (FS) was defined by dividing $T_{\text{PRB}}$ by the hypothetical PRB thickness associated with the mean values in the assumed distributions of the input variables. The process was repeated for a number of combinations of input variables, as well as for a number of standard deviations for the distributions of the input variables. The final values of FS for scaling $T_{\text{PRB}}$ ranged from about 2 to 6, with the higher values being associated with higher standard deviations of groundwater seepage velocity ($v$), as expected.

Eykhol et al. [1999] evaluated the impacts of aquifer heterogeneity and variability in the reactivity of $\text{Fe}^0$ on effluent VOC concentrations leaving a homogeneous PRB. The methodology was based on flow and particle tracking in heterogeneous aquifers considering different heterogeneity levels, i.e., $\sigma_{\ln K} = 0.5$ to 2.0, and Monte Carlo analyses considering first-order VOC degradation. A discussion of different compensating factors for reducing the vulnerability of PRBs is provided. However, the study appears to be based on a relatively small number of aquifer realizations for each case (i.e., less than five).

Elder [2000] and Elder et al. [2002] performed numerical modeling of flow and contaminant transport in three-dimensional synthetic heterogeneous aquifers generated by stacking 20 layers of spatially correlated $K$ obtained with a “turning bands” algorithm [Tompson et al., 1989]. First-order contaminant degradation kinetics within the PRB was considered, and the spatial distributions of $C_m$ and $C_{\text{eff}}$ were obtained based on contaminant transport modeling for different simulation scenarios of aquifer and PRB heterogeneity in terms of $K$ and reactivity ($\sim$10 aquifer realizations were used for each simulation case). The parameter $\sigma_{\ln K}$ was identified as having the greatest impact on the distributions of $C_m$ and $C_{\text{eff}}$ and on the performance of the PRB. Elder [2000] regressed empirical correlations relating the required FS for scaling $T_{\text{PRB}}$ to $\sigma_{\ln K}$, $K_g$ (geometric mean of $K$ in the heterogeneous aquifer), $\lambda_x$ (longitudinal correlation length), and a probability of failure. Also, varying $\sigma_{\ln K}$ affected the PRB performance more significantly than varying the PRB hydraulic conductivity ($K_{\text{PRB}}$) or reactivity, which is consistent with the observation that the contaminant residence time within the PRB is controlled by aquifer $K$ when $K_{\text{PRB}}$ is approximately 5 times greater than $K_g$ [Gavaskar et al., 1998; Elder et al., 2002]. Finally, the effects of the aquifer correlation structure and anisotropy were found to be minor [Elder et al., 2002].

Benner et al. [2001] performed numerical modeling of flow and particle tracking in 15 moderately heterogeneous aquifers ($\sigma_{\ln K} = 1.0$) containing a funnel-and-gate system to evaluate the variability in the upstream capture width of the funnel and gate caused by aquifer heterogeneity. Predicted meandering pathlines in heterogeneous aquifers, following the paths of least resistance to flow, resulted in upstream capture widths not only varying in size, but also shifting positions within the aquifer. Bilbrey and Shafer [2001] proposed the use of a design factor of safety for increasing the funnel-and-gate dimensions due to aquifer heterogeneity.

Benner et al. [2001] performed numerical modeling of flow and particle tracking to study the spatial variability of contaminant residence time within a PRB considering layered aquifer systems, i.e., discretely heterogeneous aquifers composed of approximately four adjacent homogeneous layers with different values of $K$, and a total of 18 different simulations. The results showed the expected behavior of critical contaminant residence times occurring in conjunction with scenarios where aquifer layers with high $K$ are intercepted by the PRB.

### 3. Methodology

#### 3.1. Synthetic Aquifers

The approach adopted in this study is based on numerical modeling of steady state flow and particle tracking using MODFLOW 2000, version 1.7 [Harbaugh et al., 2000], and MODPATH, version 4.2 [Pollock, 1994], in conjunction with scenarios where aquifer layers with high $K$ are intercepted by the PRB.

### Table 1. Input Parameter Values for Different Simulation Cases

<table>
<thead>
<tr>
<th>Case</th>
<th>Purpose</th>
<th>$K_{\text{ge}}$ m/s</th>
<th>$\sigma_{\ln K}$</th>
<th>$\lambda_x$, m</th>
<th>$\lambda_y$, m</th>
<th>$\lambda_z$, m</th>
<th>$D_{\text{PRB}}$, m</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>baseline case</td>
<td>$1.0 \times 10^{-4}$</td>
<td>0.8</td>
<td>3.0</td>
<td>3.0</td>
<td>1.0</td>
<td>30</td>
</tr>
<tr>
<td>B1</td>
<td>heterogeneity in $K$</td>
<td>$1.0 \times 10^{-4}$</td>
<td>0.2</td>
<td>3.0</td>
<td>3.0</td>
<td>1.0</td>
<td>30</td>
</tr>
<tr>
<td>B2</td>
<td>$1.0 \times 10^{-4}$</td>
<td>0.4</td>
<td>3.0</td>
<td>3.0</td>
<td>1.0</td>
<td>30</td>
<td></td>
</tr>
<tr>
<td>B3</td>
<td>$1.0 \times 10^{-4}$</td>
<td>1.6</td>
<td>3.0</td>
<td>3.0</td>
<td>1.0</td>
<td>30</td>
<td></td>
</tr>
<tr>
<td>C1</td>
<td>correlation structure</td>
<td>$1.0 \times 10^{-4}$</td>
<td>0.8</td>
<td>3.0</td>
<td>3.0</td>
<td>1.0</td>
<td>30</td>
</tr>
<tr>
<td>C2</td>
<td>$1.0 \times 10^{-4}$</td>
<td>0.8</td>
<td>3.0</td>
<td>3.0</td>
<td>1.0</td>
<td>30</td>
<td></td>
</tr>
<tr>
<td>D1</td>
<td>distance from source</td>
<td>$1.0 \times 10^{-4}$</td>
<td>0.8</td>
<td>3.0</td>
<td>3.0</td>
<td>1.0</td>
<td>15</td>
</tr>
<tr>
<td>D2</td>
<td>$1.0 \times 10^{-4}$</td>
<td>0.8</td>
<td>3.0</td>
<td>3.0</td>
<td>1.0</td>
<td>45</td>
<td></td>
</tr>
</tbody>
</table>

$K_{\text{ge}}$ = geometric mean of $K$, $\sigma_{\ln K}$ = standard deviation of the logarithm of $K$, $\lambda_x$ = correlation length of $K$ along the $x$ direction, $\lambda_y$ = correlation length of $K$ along the $y$ direction, and $D_{\text{PRB}}$ = distance from the source zone to the PRB. Values in parentheses highlight parameter values that deviate from the baseline values.
conjunction with 650 synthetic stochastic heterogeneous aquifers produced using the turning bands method [Tompson et al., 1989; Elder, 2000], and different simulation cases corresponding to different sets of input parameters. Two-dimensional synthetic stochastic heterogeneous aquifers were generated as per Elder et al. [2002] using a turning bands algorithm implemented by Tompson et al. [1989] and modified by Elder [2000]. Although other methodologies for generating heterogeneous aquifers, such as the sequential Gaussian simulation (sgsim) program [Deutsch and Journel, 1998] employed by Bilbrey and Shafer [2001], could have been used in this study, the turning bands method was selected on the basis of Elder [2000] who recommended the turning bands method as a robust tool for simulating synthetic stochastic heterogeneous aquifers. Additional explanation of the turning bands method is given by Mantoglu and Wilson [1982].

Each cell in the discretized domain is assigned an outcome of the random variable K assuming that the probability density function of K is log normal [e.g., Freeze and Cherry, 1979], and that K values are spatially correlated along the two domain directions (i.e., x- and y-directions). In this case, the logarithm of K is described by a mean ($\mu_{\ln K}$) and a standard deviation ($\sigma_{\ln K}$) [Aitchison and Brown, 1957]. Also, $K_0$ can be defined as $e^{\mu_{\ln K}}$, such that 95.2% of all K values fall within the interval $K_0/\exp(2\sigma_{\ln K}) < K < K_0 \times \exp(2\sigma_{\ln K})$. The spatial autocorrelation between values of K at different domain cells is based on the assumption of an exponential autocorrelation function along each domain direction. On the basis of exponential autocorrelation functions, values of K in different cells become practically uncorrelated (autocorrelation < 0.05) when the separation distance between the cells is greater than ~3$\lambda$.

Statistically meaningful aquifer realizations using the turning bands method require the domain length along each direction to be greater than 25 times the value of $\lambda$ along that direction, and the grid-discretization size along each direction to be less than 0.2 times $\lambda$ for that direction [Ababou et al., 1989]. These requirements are more stringent than those of Tompson et al. [1989], who recommend a domain length >20$\lambda$ and grid-discretization size <0.5$\lambda$. Random seed numbers for the turning bands algorithm were selected following the guidelines provided with the turning bands algorithm; i.e., odd integer seed numbers that are less than $2^{20}$.

Representative values for correlation lengths ($\lambda$) for different types of aquifer materials are given by Elder et al. [2002]. On the basis of values for $\lambda$ reported by Elder et al. [2002] and the aforementioned considerations, the longitudinal correlation length $\lambda_x$ was assumed in this study to be equal to 3.0 m, whereas the transverse correlation length $\lambda_y$ was considered to vary to provide correlation structure anisotropy ratios ($\lambda_x/\lambda_y$) of 1.0, 1.5, and 3.0 (i.e., $\lambda_y = 3.0, 2.0, \text{and} 1.0 \text{m, respectively}$). Two examples of heterogeneous aquifers are illustrated in Figure 1, one isotropic (left) and one anisotropic with $\lambda_x/\lambda_y = 3.0$ (right). Since two-dimensional synthetic heterogeneous aquifers were employed, the correlation structure in the flow domains was considered fixed along the vertical direction; i.e., perfect correlation in a vertical column of

![Divergent and Convergent Patterns](image-url)
cells with the vertical correlation length equal to the cell thickness.

3.2. Modeling Flow and Particle Tracking

[17] A cross-sectional schematic of the physical scenario being considered is shown in Figure 2, and an isometric view of the aquifer model domain is shown in Figure 3. Three-dimensional aquifer domains consisted of a top, unconfined heterogeneous layer with dimensions 80 m × 70 m and comprising 800 rows (parallel to the x direction) and 700 columns (Figure 3). The grid size of 0.1 m along both domain directions was within the range of grid sizes (0.05 to 0.40 m) used by Elder et al. [2002]. Constant-head boundary conditions were applied to the first and last columns in the domain, resulting in an imposed hydraulic gradient parallel to the x direction of 0.01. Locally, the hydraulic gradient is heterogeneously distributed throughout the aquifer due to heterogeneity in aquifer K [e.g., Zheng and Jiao, 1998]. A centered, 15-m-long source zone was defined near the up-gradient side of the domain, parallel to the y direction, and consisting of 76 adjacent tracking particles (Figure 3). This number of particles was chosen after verifying that particle tracking results were the same for either 76 or 151 particles. The use of 76 particles resulted in smaller MODPATH output files and a concomitant reduction in computational memory requirements.

[18] The influent side of the PRB was assumed to be located at a variable distance $D_{\text{PRB}} = 15, 30, \text{ or } 45 \text{ m}$ down gradient of the source zone. The distance between the source zone and the PRB was significantly greater than the minimum of $\sim 2\lambda_x$ recommended for more realistic simulations subject to flow channeling [Elder, 2000].

[19] For all flow simulations, the maximum acceptable value for the volumetric budget discrepancy was 0.1 %. The preconditioned conjugate gradient (PCG) algorithm [Hill, 1990] was employed as the MODFLOW 2000 solver (PCG package [Harbaugh et al., 2000]), and proved capable of solving flow in heterogeneous aquifers within the volumetric budget discrepancy of usually $\sim 0.05 \%$. In some cases, particularly in the cases with higher values of $\sigma_{\text{lnK}}$, the input PCG parameters, including the prescribed maximum numbers of inner and outer iterations and the damping and relaxation parameters, were varied slightly to ensure the required accuracy of the solution. Since MODPATH was used in conjunction with steady state results for flow, the input of a transport time step discretization was not required, as described by Pollock [1994].

[20] The number of aquifers used for each simulation case was a compromise between having a sufficient number of aquifers to provide adequate probabilistic distributions of the results while limiting the number of aquifers due to the practical constraints of time and computational memory. The number of aquifers for each simulation case was defined incrementally until the level of variation in the results (i.e., in the parameters of the resulting probabilistic distributions) detected upon addition of new aquifer realizations was considered to be insignificant. The required number of aquifer realizations and simulations for each simulation case varied with the level of aquifer heterogeneity (i.e., $\sigma_{\text{lnK}}$). The total number of aquifers utilized in this study was 650, with 45 aquifers for $\sigma_{\text{lnK}} = 0.2$, 50 aquifers for $\sigma_{\text{lnK}} = 0.4$, 120 aquifers for $\sigma_{\text{lnK}} = 0.8$ (including different simulation cases), and 200 aquifers for $\sigma_{\text{lnK}} = 1.6$.

[21] Graphical visualizations of aquifers and flow solutions were obtained with the three-dimensional software ModelViewer, version 1.0 (U.S. Geological Survey, March 2002), described by Hsieh and Winston [2002]. MATLAB® version 6.5 (The MathWorks, Inc., Natick, Massachusetts) was employed to develop algorithms for handling data and performing calculations.

3.3. Simulation Cases

[22] The primary objectives of the study were to evaluate the effects of (1) the level of aquifer heterogeneity ($\sigma_{\text{lnK}}$), (2) the aquifer correlation structure anisotropy ($\lambda_x/\lambda_y$), and (3) the distance between the source zone and the PRB ($D_{\text{PRB}}$) on the PRB design. The simulation cases performed to achieve these objectives are summarized in Table 1.

[23] Simulation case A represents the baseline case against which the other simulation cases are compared. Aquifers pertaining to case A are characterized by $\mu_{\text{lnK}} = -9.2$ corresponding to $K_x = 1.0 \times 10^{-4} \text{ m/s}$, which is consistent with medium-to-coarse sands, isotropic K with $\lambda_x = \lambda_y = 3.0 \text{ m}$, and a moderate level of aquifer heterogeneity with $\sigma_{\text{lnK}} = 0.8$. Also, $D_{\text{PRB}}$ in this case was 30 m.

[24] Simulation cases B1, B2, and B3 were performed to evaluate the effect of the level of aquifer heterogeneity on PRB design. Values for all input parameters were identical.
Figure 6. Examples of strongly divergent plumes resulting from the highest level of aquifer heterogeneity considered in this study (i.e., $\sigma_{\ln K} = 1.6$, case B3).

Figure 7. Examples of strongly convergent plumes resulting from the highest level of aquifer heterogeneity considered in this study (i.e., $\sigma_{\ln K} = 1.6$, case B3).
to those for baseline case A, except that $\sigma_{lnk}$ was changed from 0.8 for case A to 0.2, 0.4, and 1.6 for cases B1, B2, and B3, respectively. Aquifers with $\sigma_{lnk} > 1.6$ were not considered in this study because (1) the results of Elder [2000] indicated that increasing $\sigma_{lnk}$ from 2.0 to 4.0 had a comparatively smaller effect on the PRB design than increasing $\sigma_{lnk}$ from 1.0 to 2.0, (2) values of $\sigma_{lnk}$ typically are <1.44 for sands and <2.1 for sands and gravels [Elder et al., 2002], and (3) the fact that (as shown later) scaling factors for the PRB thickness in aquifers with $\sigma_{lnk} = 1.6$ were found to be sufficiently high such that the use of PRBs in aquifers with $\sigma_{lnk} > 1.6$ likely is not a practical solution for in situ remediation.

Simulation cases C1 and C2 were performed to evaluate the effect of the aquifer correlation structure on the PRB design via the magnitude of the correlation structure anisotropy ratio $\lambda_x/\lambda_y$. The values for all parameters in cases C1 and C2 were identical to those for baseline case A, except that $\lambda_y$ was changed from 3.0 m in case A to 2.0 m for case C1 and 1.0 m for case C2 resulting in correlation structure anisotropy ratios, $\lambda_x/\lambda_y$, of 1.5 and 3.0, respectively.

[26] Simulation cases D1 and D2 were performed to evaluate the effect of the distance between the source zone and the PRB on the PRB design. The values for all parameters in cases D1 and D2 were identical to those for baseline case A, except that $D_{PRB}$ was changed to 15 m for case D1 and 45 m for case D2.

3.4. Factor of Safety Approach

[27] Probabilistic factors of safety for PRB design are defined as scaling factors by which a PRB thickness or length associated with a simplified scenario (i.e., homogeneous aquifer with $K = K_g$, negligible variability in hydraulic gradient, negligible PRB fouling, etc.) can be multiplied in order to take into account uncertainty associated with more realistic scenarios, such as those taking into account aquifer heterogeneity. In general, a global or overall factor of safety can be defined as follows:

$$FS = \prod_{i=1}^{n} FS_i = FS_1 \times FS_2 \times FS_3 \times \ldots \times FS_n,$$

where $FS$ is the global factor of safety for scaling the PRB thickness or extension in length, and $FS_i$ are partial factors of safety related to the uncertainty associated with different factors. A partial factor of safety is considered in this study with respect to the effect of aquifer heterogeneity on the thickness of a PRB, namely, a partial factor of safety associated with variability in influent groundwater seepage velocities ($FS_1$). Thus the global factor of safety with respect to PRB thickness, $FS_1$, is simply represented in this study by $FS_1$. The global factor of safety with respect to PRB length, $FS_L$, is represented in this study by the partial factor of safety associated with the variability in required capture zone length, which is referred to hereinafter as the capture length ratio, CLR, such that $FS_L = CLR$. Other possible partial factors of safety (e.g., related to PRB reactivity or the hydraulic gradient) are not evaluated in this study.

4. Results and Discussion

4.1. Plume Patterns

[28] As shown in Figure 4, plume patterns are influenced by the level of aquifer heterogeneity (i.e., magnitude of $\sigma_{lnk}$), with distinct plume patterns developed as a function of $\sigma_{lnk}$. Distinct contrasts between divergent and convergent plume patterns occur for the simulation cases with higher $\sigma_{lnk}$ (i.e., cases A and B3), whereas the contrast attenuates for lower values of $\sigma_{lnk}$ (cases B1 and B2). As illustrated by the plume patterns shown in Figure 5 resulting from considering the highest level of aquifer heterogeneity evaluated in this study (i.e., case B3 with $\sigma_{lnk} = 1.6$), plume patterns can be categorized qualitatively as strongly divergent, divergent, hybrid, convergent, and strongly convergent. Examples of strongly divergent and strongly convergent plumes occurring for case B3 are shown in Figures 6 and 7, respectively, for the purpose of illustrating the variability in plume morphology observed in this study. Finally, frequencies of occurrence for the different plume pattern categories are summarized in Figure 8 for cases A and B3. For case B3 with $\sigma_{lnk}$ of 1.6, 24% of all heterogeneous aquifers produced either strongly divergent or strongly convergent plumes, each with approx-

![Figure 8. Frequency of occurrence of plume pattern categories for cases A ($\sigma_{lnk} = 0.8$) and B3 ($\sigma_{lnk} = 1.6$).](image-url)
Figure 9. Distributions of particle seepage velocities $v_x$ and $v_y$ for particles arriving at the location of the PRB: (a) $\sigma_{\ln K} = 0.2$ (case B1), (b) $\sigma_{\ln K} = 0.4$ (case B2), (c) $\sigma_{\ln K} = 0.8$ (case A), and (d) $\sigma_{\ln K} = 1.6$ (case B3).

Figure 10. Distributions of factor of safety $FS_1$ for particles arriving at the location of the PRB: (a) $\sigma_{\ln K} = 0.2$ (case B1), (b) $\sigma_{\ln K} = 0.4$ (case B2), (c) $\sigma_{\ln K} = 0.8$ (case A), and (d) $\sigma_{\ln K} = 1.6$ (case B3).
approximately a 12% frequency of occurrence. Also, for case A with \( \sigma_{lnK} \) of 0.8, divergent and convergent plumes with approximately equal frequencies of occurrence (i.e., 52 and 48%) were observed.

4.2. Thickness of a PRB

The factor of safety associated with the variability in influent seepage velocities due to aquifer heterogeneity, \( FS_1 \), is evaluated on the basis of probabilistic distributions of longitudinal groundwater seepage velocities (\( v_x \)) arriving at the location of the PRB normalized with respect to the uniform velocity that would be associated with the homogeneous aquifer with \( K = K_g \), i.e.:

\[
FS_1 = \frac{T_{PRB}}{T_{PRB, Homog}} = \frac{v_x}{v_{x, Homog}}.
\]

where \( T_{PRB, Homog} \), \( T_{PRB} \), \( v_{x, Homog} \), and \( v_x \) are the PRB thicknesses and seepage velocities associated with homogeneous and heterogeneous aquifers, respectively. The purpose of \( FS_1 \) is to ensure an adequate residence time for the PRB located within the heterogeneous aquifer (by definition, \( FS_1 = 1 \) for a homogeneous aquifer). The variable \( v_x \) is probabilistic and characterized by a frequency distribution for each heterogeneous aquifer since each tracked particle in the aquifer arrives at the location of the PRB with a different \( v_x \). The ninetieth-percentile value of

Figure 11. Particle tracking results considering 76 versus 151 particles.

Figure 12. Frequency distributions of \( FS_{1,90} \) for scaling the PRB thickness (refer to Table 1 for parameter sets used for simulation cases).
FS₁, referred to herein as FS₁₉₀, for each heterogeneous aquifer is adopted as a representative value, which is similar to the approach used by Elder [2000] for the variable Cₑₚ. The probabilistic distributions of FS₁₉₀ can be developed based on the ensemble of all heterogeneous aquifers belonging to a given simulation case or category.

The distributions of seepage velocities \( v_x \) and \( v_y \) for particles arriving at the location of the PRB are shown in Figure 9 for cases B1 (\( \sigma_{lnK} = 0.2 \)), B2 (\( \sigma_{lnK} = 0.4 \)), A (\( \sigma_{lnK} = 0.8 \)), and B3 (\( \sigma_{lnK} = 1.6 \)), as \( \sigma_{lnK} \) is the parameter that most significantly affects the distributions of \( v_x \) and \( v_y \). The results for cases C1, C2, D1, and D2 with \( \sigma_{lnK} = 0.8 \) are similar to those for case A and therefore are not shown.

Each line in a plot in Figure 9 represents the distribution for the 76 particles in one heterogeneous aquifer, and each plot represents the results for the ensemble of all heterogeneous aquifers for a simulation case. The distributions of \( v_x \) and \( v_y \) in the plots spread more significantly as the magnitude of \( \sigma_{lnK} \) increases from 0.2 to 1.6. This spreading is inherently related to the magnitude of \( \sigma_{lnK} \) as opposed to the number of aquifer realizations (e.g., compare Figures 9a and 9b, both of which are based on approximately the same number of aquifer realizations). As shown in Figure 9, because of preferential flow, the longitudinal seepage velocities, \( v_x \), for the heterogeneous aquifers are often significantly higher than the \( v_x \) of \( 3 \times 10^{-6} \) m/s (and \( v_y = 0 \)) that would be associated with the homogeneous aquifer with \( K = K_g \) for the same hydraulic gradient and porosity.

The distributions of FS₁ for particles arriving at the location of the PRB are shown in Figure 10 for simulation cases A and B1 to B3, each plot representing the collection of FS₁ distributions for all heterogeneous aquifers in the simulation case (plots for cases C1, C2, D1, and D2 are similar and therefore are not shown). The distributions of FS₁ spread more significantly as the magnitude of \( \sigma_{lnK} \) increases from 0.2 to 1.6 in a manner similar to that for \( v_x \). As shown in Figure 10a, the range for the ninetieth-percentile values of FS₁ (i.e., FS₁₉₀) can be established for each simulation case on the basis of the results for all aquifers in the case.

Particle tracking results (\( v_x \) distributions) considering either 76 or 151 tracked particles for two examples of heterogeneous aquifers (cases A and B3) are shown for comparison in Figure 11. As previously noted, the use of 76 particles was preferred in this study since the results using 76 particles are virtually identical to those using 151 particles.

Probabilistic incremental and cumulative distributions of FS₁₉₀ are shown in Figure 12 for all cases. The mean, standard deviation, and skewness of the FS₁₉₀ distributions determined from the data increase as the level in aquifer heterogeneity (i.e., \( \sigma_{lnK} \)), correlation structure anisotropy, and distance from source to PRB increase. Table 2 provides a summary of results for scaling the PRB thickness (refer to Table 1 for parameter sets used for simulation cases).

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**Table 2. Summary of Results**

<table>
<thead>
<tr>
<th>Case</th>
<th>Factor of Safety, FS₁₉₀</th>
<th>Capture Length Ratio, CLR</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>2.71 ± 0.75</td>
<td>1.24 ± 0.32</td>
</tr>
<tr>
<td>B1</td>
<td>1.60 ± 0.10</td>
<td>1.09 ± 0.08</td>
</tr>
<tr>
<td>B2</td>
<td>1.91 ± 0.23</td>
<td>1.14 ± 0.15</td>
</tr>
<tr>
<td>B3</td>
<td>5.14 ± 2.54</td>
<td>1.54 ± 0.60</td>
</tr>
<tr>
<td>C1</td>
<td>2.87 ± 0.71</td>
<td>1.20 ± 0.26</td>
</tr>
<tr>
<td>C2</td>
<td>3.74 ± 0.80</td>
<td>1.16 ± 0.24</td>
</tr>
<tr>
<td>D1</td>
<td>2.64 ± 0.72</td>
<td>1.13 ± 0.22</td>
</tr>
<tr>
<td>D2</td>
<td>2.74 ± 0.86</td>
<td>1.33 ± 0.35</td>
</tr>
</tbody>
</table>

---

**Figure 13.** Effects of level of aquifer heterogeneity (\( \sigma_{lnK} \)), correlation structure anisotropy, and distance from source to PRB on the factor of safety FS₁₉₀ for scaling the PRB thickness (refer to Table 1 for parameter sets used for simulation cases).
The trends in $FS_{1,90}$ as a function of the level of aquifer heterogeneity, the correlation structure anisotropy ratio, and the distance from the source zone to the PRB are shown in Figure 13. On the basis of results shown in Figure 13, $\sigma_{\ln K}$ appears to have a greater effect on $FS_{1,90}$ than either $\lambda_x/\lambda_y$ or $D_{PRB}$, i.e., for the ranges of values for $\sigma_{\ln K}$, $\lambda_x/\lambda_y$, and $D_{PRB}$ considered in this study. For the highest level of aquifer heterogeneity evaluated in this study (i.e., $\sigma_{\ln K} = 1.6$), $FS_{1,90}$ (Figure 13a) is of the order of 5.0 (mean) to 10 (mean plus two standard deviations), comparing favorably with values given by an empirical correlation of Elder [2000] that relates the factor of safety for scaling the PRB thickness to $\sigma_{\ln K}$, $m_{\ln K}$, $\lambda_x$, and $\lambda_y$, and to an input probability of failure, although the methodology employed in the present study is significantly different than that used by Elder [2000].

### 4.3. Length of a PRB

The capture length ratio (CLR) is evaluated on the basis of probabilistic distributions of the required capture zone lengths at the location of the PRB normalized with respect to the width of the source zone (i.e., direction parallel to the length of the PRB), i.e.,

$$CLR = \frac{L_{PRB}}{W_S},$$

where $L_{PRB,Homog}$ and $L_{PRB}$ are the required PRB lengths associated with homogeneous and heterogeneous aquifers, respectively, and $W_S$ is the width of the source zone. By definition, CLR = 1 in a homogenous aquifer. The length $L_{PRB}$ is a probabilistic variable characterized by a frequency distribution for each ensemble of aquifers in a given simulation case. The definition of a required $L_{PRB}$ assumes the PRB to be placed perpendicular to the general hydraulic gradient direction for the entire aquifer, and centered and parallel with respect to the source zone. The PRB is assumed symmetrical with respect to a centerline such that the longer required half of $L_{PRB}$ dictates the total $L_{PRB}$ (i.e., the required $L_{PRB}$ equals twice the longer half).

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**Figure 14.** Frequency distributions for capture length ratio for scaling the PRB length (refer to Table 1 for parameter sets used for simulation cases).
Probabilistic incremental and cumulative distributions of CLR are shown in Figure 14 for all cases. The mean and standard deviation of the CLR distributions obtained from the data increase with increasing level of aquifer heterogeneity (i.e., $\sigma_{\ln K}$), with mean values for CLR of 1.09, 1.14, 1.24, and 1.54 corresponding to $\sigma_{\ln K}$ values of 0.2 (cases B1), 0.4 (case B2), 0.8 (case A), and 1.6 (case B3), respectively. Additionally, CLR distributions are positively skewed for all heterogeneity levels, with skewness generally decreasing with increasing $\sigma_{\ln K}$. The trend of decreasing skewness with increasing $\sigma_{\ln K}$ can be explained on the basis of the convergent and strongly convergent plume patterns that result in some values of CLR < 1.0 for cases A and B3.

The mean and standard deviation of the CLR distributions slightly decrease with increasing correlation structure anisotropy ratio, $\lambda_x/\lambda_y$, with mean values for CLR of 1.24, 1.20, and 1.16 corresponding to $\lambda_x/\lambda_y$ values of 1.0 (case A), 1.5 (case C1), and 3.0 (case C2), respectively. These results are consistent with the fact that as $\lambda_y$ decreases, particle trajectories become less meandering (intuitively, there is less transverse macroscopic dispersion), resulting in shorter capture zone lengths at the PRB location. In this case, no clear trend for skewness was obtained with respect to increasing $\lambda_x/\lambda_y$.

Finally, the mean and standard deviation of the CLR distributions increase with increasing distance from the source zone to the PRB, $D_{PRB}$, with mean values of 1.13, 1.24, and 1.33 corresponding to $D_{PRB}$ values of 15 m (case D1), 30 m (case A), and 45 m (case D2), respectively. These results are consistent with the expected behavior since locating the PRB further down-gradient with respect to the source zone results in a broader plume to be encompassed by the PRB. Also, no clear trend for skewness with respect to increasing $D_{PRB}$ was obtained. A summary of the results is provided in Table 2.

Values of CLR corresponding to the mean and mean plus one and two standard deviations are plotted as a function of the level of aquifer heterogeneity (i.e., $\sigma_{\ln K}$), the correlation structure anisotropy ratio ($\lambda_x/\lambda_y$), and the distance from the source zone to the PRB ($D_{PRB}$) in Figure 15. As shown in Figure 15, CLR is affected significantly by the level of aquifer heterogeneity (i.e., $\sigma_{\ln K}$), and both $\lambda_x/\lambda_y$ and $D_{PRB}$ also have noticeable effects on CLR. For example, considering the values of CLR corresponding to the mean plus two standard deviations, a CLR value of ~2.7 results for case B3 with $\sigma_{\ln K}$ of 1.6, whereas a CLR value of ~2.0 results for case A with $\sigma_{\ln K}$ of 0.8. Finally, CLR also can provide a quantitative means for categorizing plume patterns as shown in Figures 6 and 7. For example, CLR ranges from ~2 to ~3 when strongly divergent plumes occur with case B3, whereas CLR ranges from only ~0.3 to ~0.5 when strongly convergent plumes occur with case B3. Thus CLR values <1 imply convergent plume patterns, whereas CLR values >1 imply divergent plume patterns.

5. Conclusions

The influence of heterogeneity in aquifer hydraulic conductivity (K) on plume patterns and the required thickness and length of PRBs was evaluated using stochastic modeling. In terms of PRB thickness, a probabilistic factor of safety related to uncertainty in influent groundwater seepage velocities ($FS_s$) was quantified, and in terms of PRB length, a factor of safety defined as the capture length ratio (CLR) was quantified. The influences of the level of aquifer heterogeneity (i.e., magnitude of $\sigma_{\ln K}$), the correlation structure anisotropy ratio ($\lambda_x/\lambda_y$), and the distance from the source zone to the PRB ($D_{PRB}$) on CLR were evaluated. For the ranges in values of $\sigma_{\ln K}$, $\lambda_x/\lambda_y$, and $D_{PRB}$ considered in this study, the level of aquifer heterogeneity (i.e., $\sigma_{\ln K}$) had the greatest effect on the factors of safety. However, the effects of $\lambda_x/\lambda_y$ and $D_{PRB}$ on the required length of PRBs were noticeable and greater than the relatively minor effects of $\lambda_x/\lambda_y$ and $D_{PRB}$ on the required thickness of PRBs.

The main implications of the present study are that quantified factors of safety for scaling the thickness and length of PRBs in heterogeneous aquifers significantly affect the PRB design. Considering the highest level of aquifer heterogeneity evaluated in this study ($\sigma_{\ln K} = 1.6$), the factor of safety for PRB thickness, $FS_1$ ($0.5$), was of the order of 5.0 for mean partial factor of safety, and 10 for
mean plus two standard deviation partial factor of safety. The trends versus $\sigma_{\ln K}$ showed relatively good correlation with previously published values based on a different methodology. Also, for $\sigma_{\ln K} = 1.6$, the global factor of safety for PRB length, $FS_l = (CLR)$, corresponding to the mean plus two standard deviations in CLR was of the order of 2.7.

[42] On the basis of magnitudes of scaling factors obtained in this study, the required thickness and length of a PRB located in a heterogeneous aquifer can be expected to significantly differ from values evaluated on the basis of a homogeneous aquifer (i.e., $K = K_0$). Thus in situ characterization of the aquifer in which the PRB is to be constructed is extremely important. In cases where aquifer heterogeneity is significant (e.g., $\sigma_{\ln K} > 1.6$), the effect of the aquifer heterogeneity may be to the extent that the use of PRBs for in situ remediation is rendered impractical, requiring the consideration of other remediation technologies. In addition, other possible sources of uncertainty not evaluated in this study, such as variability in PRB reactivity and fouling, may affect the design and performance of PRBs.

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