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Hydrogeologic modeling for permeable reactive barriers

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Abstract

The permeable reactive barrier technology for in situ treatment of chlorinated solvents and other groundwater contaminants is becoming increasingly popular. Field scale implementation of this and other in situ technologies requires careful design based on the site-specific hydrogeology and contaminant plume characteristics. Groundwater flow modeling is an important tool in understanding the hydraulic behavior of the site and optimizing the reactive barrier design. A combination of groundwater flow modeling and particle tracking techniques was used to illustrate the effect of hydraulic conductivity of the aquifer and reactive media on key permeable barrier design parameters, such as the capture zone width, residence time, flow velocity, and discharge. Similar techniques were used to illustrate the modeling approach for design of different configurations of reactive barriers in homogeneous and heterogeneous settings. © 1999 Elsevier Science B.V. All rights reserved.

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1. Introduction

The recent development of permeable reactive barriers technology has presented a potentially viable alternative to conventional pump-and-treat systems for remediation of chlorinated solvent-contaminated groundwater. Additionally, dissolved metals, such as

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chromium, and petroleum hydrocarbons are being targeted for treatment with permeable barriers. The overall design, implementation, and monitoring of permeable barriers are discussed in Ref. [1]. The critical issues for the design of reactive barriers include the incorporation of appropriate reaction rates and site hydraulics. The issues related to the reaction rates for degradation of chlorinated solvents with reactive iron are reasonably well-understood and are presented in other papers in this volume. However, experience at several pilot-scale and full-scale permeable barrier sites shows that significant hydrologic challenges need to be overcome for successful implementation of this technology. Computer modeling is an important tool for incorporating the site-specific hydrogeology into the design of the permeable barriers. This paper reviews the use of hydrogeologic models in the design and evaluation of permeable barriers. The discussion includes the general requirements of the modeling codes useful for permeable barrier application, a brief overview of the modeling methodology, and a review of previous modeling studies for permeable barrier design. Some review sections presented here are updated from the work published by the first author in the permeable barrier design book [1]. Although the emphasis in this paper is on funnel-and-gate reactive barriers, a similar approach applies to other barrier designs.

Hydrogeologic modeling can be used at several stages of the permeable barrier technology implementation, including the initial feasibility assessment, the site selection, design optimization, design of the performance monitoring network, and the longevity assessment. The major advantage of constructing a detailed groundwater flow model is that several design configurations, site parameters, and performance and longevity scenarios can be readily evaluated once the initial model has been set up. Thus, the combined effect of several critical parameters can be incorporated simultaneously into one model. Groundwater modeling has been used at most previous permeable barrier installations. In most cases, groundwater flow models have been used in conjunction with particle tracking codes to construct flownets showing travel paths and residence times through the reactive cell. The models are usually set up after laboratory column tests have shown the feasibility of the degradation and estimated the reaction half-lives and the resulting residence time requirements.

The two primary, interdependent parameters of concern evaluated with models when designing a permeable barrier are *hydraulic capture zone width* and *residence time*. Capture zone width refers to the width of the zone of groundwater that will pass through the reactive cell or gate (in the case of funnel-and-gate configurations) rather than pass around the ends of the barrier. Capture zone width can be maximized by maximizing the discharge (groundwater flow volume) through the reactive cell or gate. Residence time refers to the length of time contaminated groundwater is in contact with the reactive medium within the reactive cell or gate. Residence times can be maximized either by minimizing the discharge through the reactive cell or by increasing the flowthrough thickness of the reactive cell. Thus, the design of permeable barriers must balance the capture zone width and residence time requirements. Contamination that lies outside the capture zone will not flow through the reactive cell, and so will not be treated. Similarly, if the residence time in the reactive cell is too short, contaminant levels may not be reduced sufficiently to meet regulatory requirements. In addition to the capture zone and residence time, groundwater models are also used in the following ways.

(1) Determining a suitable location for the permeable barrier with respect to the plume distribution, site hydrogeology, and site-specific features such as property boundaries and underground utilities.

(2) Determining a suitable permeable barrier configuration (e.g. continuous reactive barrier or funnel-and-gate system).

(3) Determining the width of the reactive cell and, for a funnel-and-gate configuration, the width of the funnel.

(4) Evaluating the potential for underflow, overflow, or flow across aquifers.

(5) Incorporating the effects of fluctuations in groundwater flow velocity and direction into the design.

(6) Helping in media selection and long-term performance evaluation by specifying required particle size and hydraulic conductivity (K) of the reactive medium with respect to the hydraulic conductivity of the aquifer.

(7) Evaluating scenarios for future potential flow bypass due to reduced porosity resulting from precipitate formation. This gives an indication of the safety factors needed in the design.

(8) Assisting in planning appropriate monitoring well locations and monitoring frequencies.

2. The role of adequate site characterization

One of the most important prerequisites to a successful permeable barrier design and installation is adequate hydrogeologic site characterization. In many cases, the preliminary information is available from previous studies conducted at the site, such as the Remedial Investigation/Feasibility Study (RI/FS), Record of Decision (ROD) reports, and groundwater modeling reports. The preliminary site profile based on site stratigraphy, soil types, depth of water, groundwater flow direction, groundwater velocity, hydraulic conductivity, porosity, depth to confining layer, and dimensions and depth of the dissolved plume may be used to evaluate the general feasibility of permeable barrier installation. Once the decision to implement the permeable barrier technology has been taken based on a preliminary assessment of site data, more detailed information may be needed during the design phase.

The most significant data to be collected include variations in the depth, thickness, and water levels of different hydrostratigraphic units. This is achieved by drilling and sampling several locations using conventional drilling or other techniques, such as cone penetrometer testing (CPT) or the use of a Geoprobe™. However, at small sites, the traditional monitoring wells are likely to provide more reliable and higher resolution data. The data for hydraulic conductivity, porosity, and water levels are used to determine groundwater velocity at the site. The hydrostratigraphic framework developed from the site-specific geologic and hydrologic data is used to construct a conceptual understanding of groundwater flow at the site. Two of the most critical and often overlooked aspects of characterization are the aquifer heterogeneities and temporal variations in groundwater flow velocity and direction. The heterogeneities control the flow of water into the barrier at the desired rate. The temporal water level fluctuations provide an insight into the safety factor built into the design to account for unusually high or low water levels. Failure to account for temporal fluctuations may result in the plume completely bypassing the reactive barrier.

3. Requirements for reactive barrier models

The major steps involved in constructing a groundwater model are data compilation, conceptual model development, model code selection, construction, calibration, verification, and prediction. A detailed description of groundwater flow modeling and the mathematics involved is provided [2,3]. Several special features and capabilities are needed in the groundwater models used for simulation of the flow through permeable barriers. An important requirement for funnel-and-gate permeable barriers is the need to simulate the sharp hydraulic conductivity contrasts at the intersection of the aquifer and the funnel walls. The specific requirements and recommendations for the permeable barrier simulation models include the following:

(1) Two-dimensional (2D) or three-dimensional (3D) groundwater flow models may be used to simulate the flow system of a site under consideration. A 3D modeling approach is recommended so that the possibility of underflow or overflow and interactions between the adjacent aquifer can be examined for the permeable barrier and its vicinity. Vertical-flow velocities and travel times will be of critical significance in the design of systems at sites with significant vertical-flow gradients or in cases where the barriers are not keyed into the underlying confining layer (hanging barriers).

(2) The codes should be able to simulate large contrasts in K at the permeable barrier and aquifer interfaces. Many permeable barrier designs include a reactive cell with K higher than that of the aquifer and flanking funnel walls with extremely low permeability. The funnels may consist of a slurry wall, which can be several feet (ft) thick, or sheet piles, which are usually less than an inch thick. Therefore, at the intersection of the aquifer with the reactive cells and funnel walls, large K contrasts are developed and many models are unable to solve these problems due to numerical instabilities. In most cases, the funnel walls are simulated by assigning a low conductivity to the model cells representing the funnel. For accurate simulations, the size of these funnel cells should be the same as that of slurry walls. This results in a very small cell size and a large number of cells in the model. The sheet piles are even thinner than the slurry walls and the required cell sizes may be even smaller. To simulate large areas with sufficient resolution near the funnels but larger cells away from the funnels, models capable of incorporating grid blocks of variable size are recommended. Some alternative approaches, such as the use of horizontal flow barrier (HFB) [4] in MODFLOW, have been devised to simulate the low-K funnel walls. The small cell sizes also result in very small head convergence criteria during numerical calculations.

(3) Many sites have significant heterogeneities, which result in the development of preferential pathways through which most of the groundwater movement occurs. The permeable barrier design itself imparts heterogeneity to the subsurface system. The simulation of these effects requires models that can handle heterogeneity. Most general-

purpose analytical models are based on the assumption of homogeneity, but most numerical models can incorporate heterogeneities.

(4) Many sites have features such as streams, drains, tunnels, or wells in the vicinity of the permeable barrier sites. For example, at some sites, pump-and-treat remediation may be active in the vicinity of the permeable barriers. These situations require the use of models that can simulate the effects of these internal sinks or sources on the permeable barrier systems.

(5) The results of the model should be amenable to use with the particle-tracking programs so that the capture zones of the permeable barriers can be evaluated. It should also be possible to calculate volumetric flow budgets for the reactive cells.

Many currently available groundwater flow modeling codes meet the above requirements [1]. A comprehensive description of nonproprietary and proprietary flow-and-transport modeling codes can be found in the U.S. Environmental Protection Agency document entitled *Compilation of Groundwater Models* [5]. Depending on the project's needs, the designer of a permeable barrier system may want to apply a contaminant transport code that can utilize the calculated hydraulic-head distribution and flow field from the flow-modeling effort. If flow and transport in the vadose zone are of concern, a coupled or uncoupled, unsaturated/saturated flow and transport model should be considered.

4. Previous modeling studies for permeable barrier applications

A review of the information available from existing sites showed that MODFLOW [6], in conjunction with particle tracking with codes such as MODPATH [7], is the code most commonly used to simulate the permeable barriers technology. One of the special options in MODFLOW is the HFB package [4]. It is especially useful in simulating the funnel-and-gate design. In normal cases, the slurry walls have to be simulated by very small cells of low K, increasing the number of cells in the model dramatically. The HFB package permits the user to assign the sides of certain cells as planes of low K, while still using a larger cell size at the funnel walls. The low-conductivity HFB planes restrict the flow of water into the cells across the faces representing slurry walls or sheet piles. Another useful addition is the ZONEBUDGET package [8], which allows the user to determine the flow budget for any section of the model. This package may be used to evaluate the volumetric flow through the cell for various design scenarios. Other programs such as FLONET [9], FRAC3DVS [10], and FLOWPATH [11], also have been used at some sites. RWLK3D, a 3D flow and transport code developed by Battelle [12], has been used in conjunction with MODFLOW to simulate the particle movement for the pilot-scale permeable cells installed at Moffett Federal Airfield [13] and Dover Air Force Base [14]. The sites that used MODFLOW include the Sunnyvale, CA site, Moffett Federal Airfield, CA [13,15], the Sommersworth Sanitary Landfill, NH, an industrial facility in Kansas, and GE Appliances, WI. FLOWPATH has been used to evaluate the design at Belfast, Northern Ireland; Fairchild Air Force Base, WA; and the DOE Kansas City site, KS.

Starr and Cherry [16] used FLONET [9] to evaluate the effects of funnel-and-gate geometry (design) and reactive cell hydraulic conductivity (K_{cell}) on the permeable barrier hydraulics. The simulated system had properties similar to those of the surficial aquifer at Canadian Forces Base Borden, Ontario, Canada. The simulated aquifer is isotropic, with a homogeneous aquifer hydraulic conductivity ($K_{aquifer}$) of 28.3 ft/day and hydraulic gradient of 0.005. The funnel walls were assumed to be 1-m (3.28-ft) thick slurry walls with K equal to 0.0028 ft/day. The K of the reactive cell was 283 ft/day, the maximum laboratory-measured value for 100% iron, in the base case. It should be noted that in several modeling studies for permeable cell installations, K_{cell} values of 142 ft/day have been used for 100% iron. The range of values for K_{cell} indicates differences in the source of granular iron, as well as variability of the K measurement itself. A porosity of 0.33 was used for all materials. The following conclusions can be drawn from Starr and Cherry's simulations:

(1) For systems with straight funnel walls, the discharge through the gate and the hydraulic capture zone width increases as the funnel width increases. However, the increase in discharge is not directly proportional to funnel width. In fact, the relative discharge through the gate decreases dramatically as the funnel width increases.

(2) For a constant funnel width, the absolute and relative discharge through the gate and the capture zone width increase with an increase in gate width. Therefore, it is desirable to have a gate as wide as practical.

(3) For a given funnel-and-gate design, the discharge through the gate increases with increase in K_{cell} relative to the $K_{aquifer}$. However, there is relatively little increase in discharge when the K_{cell} is more than 10 times higher than the $K_{aquifer}$. This implies that while cell conductivity higher than the $K_{aquifer}$ is desirable, K_{cell} does not have to be much higher than $K_{aquifer}$. This is a useful result, because the large grain sizes required for very high K_{cell} values would result in a low total surface area for reactions and lower residence times.

(4) For all orientations to the regional flow gradient, the maximum absolute discharge occurs at apex angles (the angles between the two funnel walls) of 180° (straight barrier). However, for apex angles between 127° and 233°, there is little effect on discharge. Outside this range, the discharge drops rapidly. This implies that there is no significant advantage to a slightly angled funnel-and-gate system over a straight barrier and vice versa. Sharper funnel angles may, however, reduce discharge.

(5) For all apex angles, the maximum discharge occurs when the funnel is perpendicular to the regional flow gradient.

(6) The groundwater flow models can be used effectively to design the funnel-and-gate systems at sites with special design requirements due to complex flow fields, seasonal fluctuations, or access restrictions. These may include systems with angled funnels, multiple gates, asymmetrical funnels, or U-shaped funnel and gates.

(7) A balance between maximizing the capture zone of the gate and maximizing the residence time of the contaminated water in the gate should be achieved. In general, the discharge and residence times are inversely proportional.

Shikaze [17] used FRAC3DVS code to examine 3D groundwater flow in the vicinity of a partially penetrating (hanging wall) funnel-and-gate system for 16 different combinations of parameters. All simulations were for steady-state, fully saturated groundwater flow. The 16 simulations consisted of variations in four dimensionless parameters: the ratio of K_{cell} to K_{aquifer}; the ratio of width of a single funnel wall to the depth of the funnel and gate; the ratio of total funnel wall width to the gate width; and the hydraulic gradient. The following conclusions were drawn from these simulations:

(1) Absolute discharge through the gate increases as the hydraulic gradient increases. However, there is almost no effect of hydraulic gradient on the relative discharge or on the size of the relative capture zone (ratio of hydraulic capture zone width to total width of the funnel and gate).

(2) In cases of wide but shallow funnel walls, there is an increase in the flow component that is diverted under the barrier rather than through the gate.

(3) For wider funnel walls, the increase in the relative discharge through the gate is not proportional to the increase in the funnel wall area.

5. Permeable barrier hydraulics

This section illustrates some of the hydraulic relationships for a typical funnel-and-gate configuration using numerical models. The funnel-and-gate configuration used in the discussion is based on the pilot-scale system installed at the Moffett Federal Airfield in Mountain View, CA.

5.1. Model setup

MODFLOW was used to develop a steady-state numerical approximation of the groundwater flow field and to calculate flow budgets through the gate. Particle-tracking techniques under advective flow conditions were performed using RWLK3D to delineate capture zones and travel times in the vicinity of the funnel and gate. Specific objectives included determining how changes in gate conductivity relative to aquifer conductivity affected capture zone width, retention times for groundwater moving through the gate, and flow volumes through the gate.

The simulated system consists of two 20-ft lengths of sheet piling oriented perpendicular to flow on either side of a 10 ft × 10 ft reactive cell representing the gate. The reactive cell is bounded on its sides by 10-ft lengths of sheet piling. The gate itself consists of 2 ft of 3/4 in. pea gravel located on both the upgradient and downgradient ends of the reactive cell, which has a 6-ft flowthrough thickness. The model was constructed based on the requirement that the domain should be large enough so that the boundary conditions do not affect flow in the vicinity of the permeable barrier. Further, the model cell size in the vicinity of the permeable barrier should be small enough to provide sufficient resolution for retention time calculations. For this model of a funnel-and-gate system, the domain consisted of a single layer that is 500 ft long and 300 ft wide. The grid has 98 rows and 106 columns resulting in a total of 10,388 nodes. Grid nodes are 10 ft × 10 ft at their maximum (in the general domain area) and 0.5 ft × 0.5 ft in the region of the gate itself. Specified head nodes were set along the first and last rows of the model to establish a gradient of 0.006. No flow conditions were set along the first and last columns of the model.

The funnel was simulated as an HFB having a hydraulic conductivity of 2.0×10^{-6} ft/day. For the continuous reactive barrier configuration, the funnel may be excluded from the model. The pea gravel was assigned a K of 2830 ft/day. The reactive cell consisting of granular iron was assigned a K of 283 ft/day, the maximum laboratory-measured value for 100% iron. It should be noted that in some modeling studies [18], a reactive cell with K of 142 ft/day has been used for 100% iron. In general, the K value for the reactive medium should be determined from laboratory permeability testing. Porosity was held constant at 0.30 for all materials in each of the simulations. However, recent experience at the permeable barrier installations shows that the porosity of the reactive cell may range from 0.6 to 0.75.

For this illustration, simulated K_{aquifer} was varied among 0.5, 1, 2, 5, 10, 20, 50, and 100 ft/day to represent low- and high-permeability aquifers. Once this base scenario was established, simulations were conducted to evaluate reductions in K_{cell} over time that could potentially be caused by buildup of precipitates. To determine the effects of decreased permeability of the gate over a period of operation, K_{cell} was reduced in 10% increments from the initial 283 ft/day to 28.3 ft/day for each value of K_{aquifer}. An additional set of simulations was performed with K_{cell} reduced by 95% to 14.15 ft/day, resulting in a total of 11 simulations for each value of K_{aquifer}. In addition to evaluation of effect of media properties on barrier hydraulics, these scenarios also provide insight into the impact of potential clogging of the reactive cell by precipitation. For each individual simulation, a single value for K_{aquifer} was used. The effects of geologic heterogeneities were not considered in these simulations. The results from the approximately 90 simulations were used to evaluate the impact of variations in K_{cell} and K_{aquifer} on capture zone width, flow volumes, and travel times (retention time) through the gate. A detailed presentation of the simulation results summarized below is provided elsewhere [1].

5.2. Simulation results

Capture zone width in each of the simulations was determined by tracking particles forward through the gate. Two hundred particles (one particle every 0.5 ft) were initiated along a 100-ft-long line source upgradient from the barrier. The locations of the flow divide between particles passing through the gate and those passing around the ends of the funnel were used to determine capture zone width. As anticipated for a symmetrical funnel-and-gate system in homogeneous aquifers, the capture zones extended to about half of the funnel width on each side, i.e. total capture of about 30 ft. As K_{cell} increased, the capture zone width generally increased. However, the range of variation was only about 2 ft. This shows that the capture zone width is more sensitive to the length of the funnel walls than to K of the aquifer or reactive media in homogeneous systems.

Residence time within the gate for each simulation was determined from the length of time required for the particles to pass through the reactive cell. The simulated retention time within the gate decreases as K_{aquifer} increases relative to K_{cell}. However, the residence time showed only a small increase with increase in K_{cell}, as long as K_{cell} was slightly higher than K_{aquifer}. This implies that K_{aquifer} is a key controlling parameter for residence time as long as the gate K is somewhat higher than K_{aquifer} and the hydraulic gradient is constant. Therefore, aquifers having high K may require greater gate flowthrough thickness to meet residence time requirements so that contaminant levels can be reduced to regulatory limits. It should also be noted that, there might be some variation in residence times at the edges of the reactive cell and at its center. For example, one study [19] showed that simulated residence times in a funnel-and-gate system (with caisson gates) varied from 29 h at the edges to 82 h in the center of the reactive cell.

Discharge through the gate was determined from the MODFLOW-calculated, cell-by-cell flow file using the zone budget [8]. As K_{aquifer} increases, the total discharge through the gate increases, resulting in a shorter residence time in the cell. However, the relation between the reactive media K and the discharge is not straightforward. Fig. 1 shows that relative discharge through the gate decreases in response to decreasing K_{cell} at K_{aquifer} values of 0.5, 10, and 100 ft/day. In each of the plots shown in Fig. 1, K_{cell} decreases from 283 ft/day to 14 ft/day. When K_{aquifer} is 0.5 ft/day, the K_{cell} is much

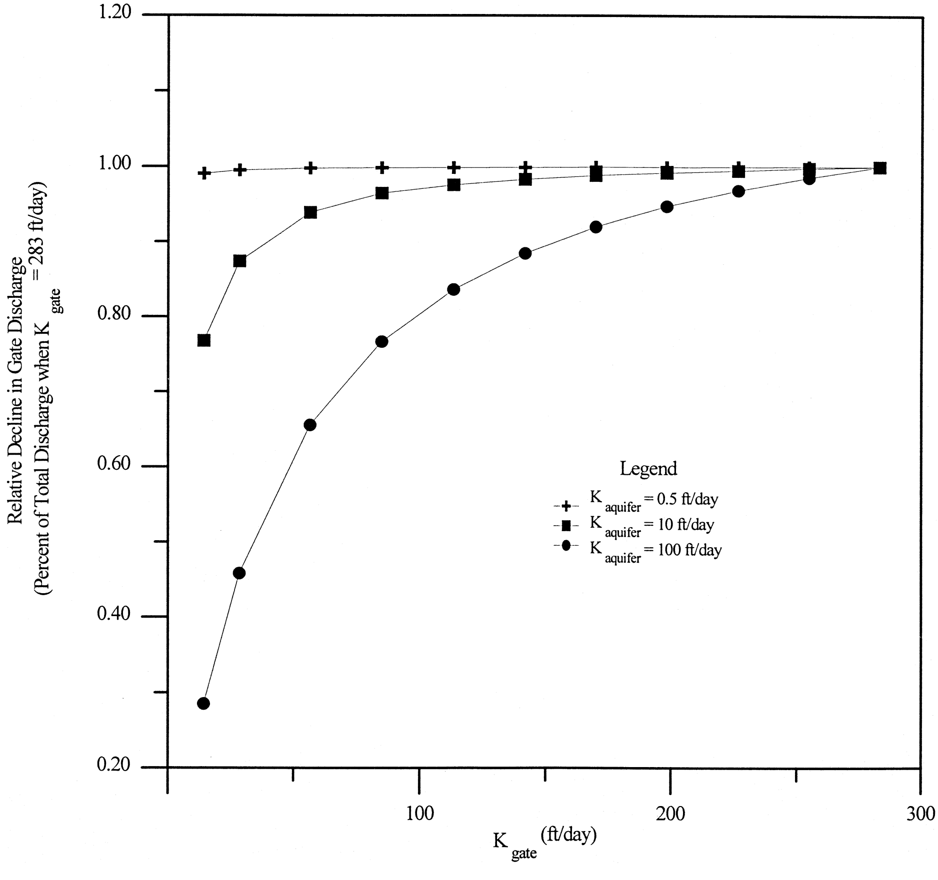

Fig. 1. Correlation between K_{cell} and relative discharge through the gate for a homogeneous, one-layer scenario (from Gavaskar et al. [1]).

greater than the K_{aquifer} for each of the 11 simulations performed, and the percent decline in discharge through the gate is very small. Decreasing K_{cell} from 283 ft/day to 14.15 ft/day resulted in only a 1% decline in the discharge through the gate. As K_{aquifer} was increased, a larger reduction in discharge through the gate occurred as the K_{cell} decreased. For K_{aquifer} of 10 and 100 ft/day, discharge through the gate decreased by roughly 27% and 71%, respectively, over the same decline in K_{gate}. In both cases, the ratio of K_{cell} to K_{aquifer} approaches or becomes less than 1 as K_{cell} decreases. Therefore, the hydraulic effects of potential precipitate buildup in the reactive cell are likely to be felt earlier in high-conductivity aquifers. However, as discussed below, there is considerable leeway before such effects are noticed.

Fig. 2 is a plot of the ratio of K_{cell} to K_{aquifer} vs. discharge through the gate for the simulations. The plot indicates that declines in reactive media K due to clogging have very little influence on the volume of groundwater passing through the gate as long as

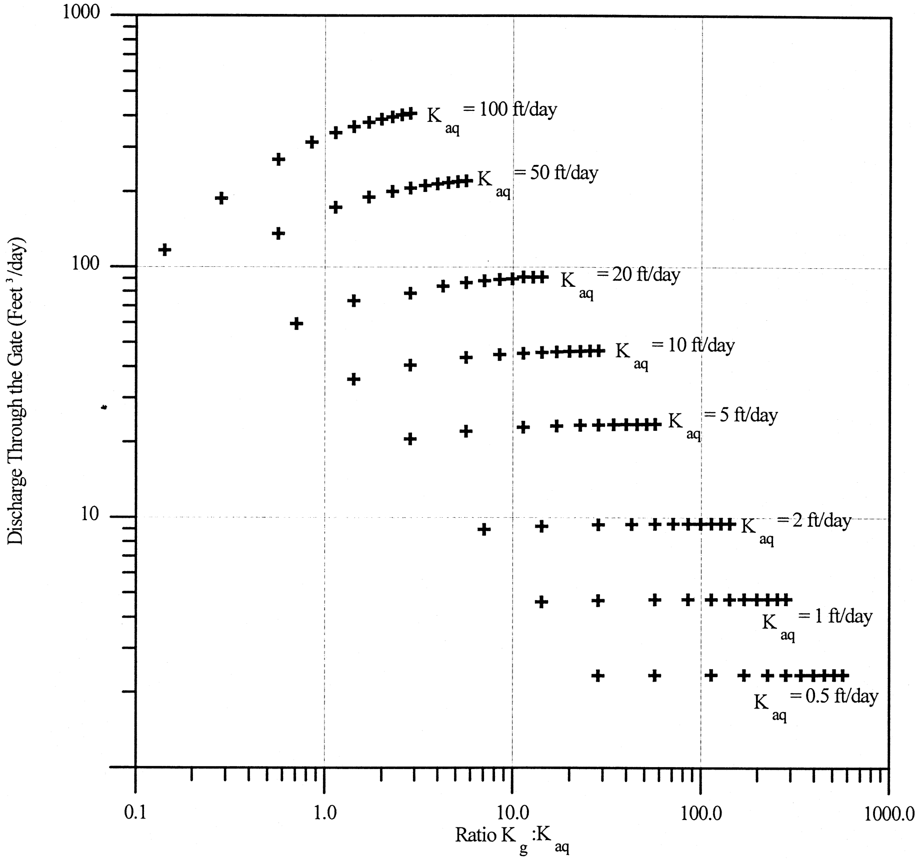

Fig. 2. Correlation between ratio of K_{cell} to K_{aquifer} vs. discharge through the gate for a homogeneous, one-layer scenario (from Gavaskar et al. [1]).

the reactive media K is roughly five times the K of the aquifer. In these instances, discharge through the gate remained at roughly 95% of the simulated discharge when the gate K was 283 ft/day. Because discharge is relatively unaffected, residence times and capture zone width will remain relatively unchanged for a given K_{aquifer}. As the ratio between K_{cell} and K_{aquifer} declines below 5, the relative decrease in discharge becomes greater and results in decreased capture zone widths and increased retention times. Thus, as long as the K of a freshly installed reactive cell is designed to be one or two orders of magnitude greater than the K_{aquifer}, there is considerable flexibility for precipitates to build up without significantly affecting the hydraulic capture zone. Finally, it should be noted that these simulations were performed at a fixed hydraulic gradient. As shown later, it is important to incorporate the seasonal variations in water levels, hydraulic gradients as well as the uncertainty in K_{aquifer} in the simulations for field installations.

6. Modeling permeable barriers in homogeneous aquifers

A relatively homogeneous aquifer can be modeled using 2D versions of flow and particle-tracking codes. This simplified approach has been used to locate and design the barrier at most existing sites. Permeable barrier features, such as the reactive cell, pea gravel, or funnel walls, can be inserted into the baseline aquifer model as heterogeneities with the appropriate hydraulic conductivity. The hydraulic conductivity of the reactive cell can be estimated based on the particle size of the reactive medium used or, for more certainty, measured through laboratory permeability testing. Design parameters, such as hydraulic capture zone width, residence time within the reactive cell, and groundwater discharge through the gate, can then be estimated for each simulation using particle tracking programs. For illustration, two example simulations of a relatively simple continuous barrier and a more complex funnel-and-dual-gate system are presented here.

6.1. Simulation of continuous reactive barrier

Fig. 3 shows the particle tracking results for 180 days in the vicinity of a continuous permeable barrier in a relatively homogeneous aquifer. This simulation consists of a 10-ft long section of reactive media having a 6-ft thickness in the direction of flow. The aquifer is simulated as a single layer having uniform hydraulic properties with a conductivity of 10 ft/day. The reactive media are simulated with a K of 283 ft/day. The flow field was simulated with a hydraulic gradient of 0.005. As indicated by the dashed lines, the capture zone has a width greater than the 10-ft length of the reactive media. The width of the capture zone will increase or decrease as the ratio of K_{cell} to the K_{aquifer} increases or decreases, respectively. Residence time through the reactive media can be estimated using particle-tracking methods to ensure sufficient time for the degradation reactions to occur. In this case, where no funnel walls are used, several short flowpaths into and out of each end of the reactive media occur. Groundwater flowing along these paths does not pass through the entire thickness of the reactive media, and

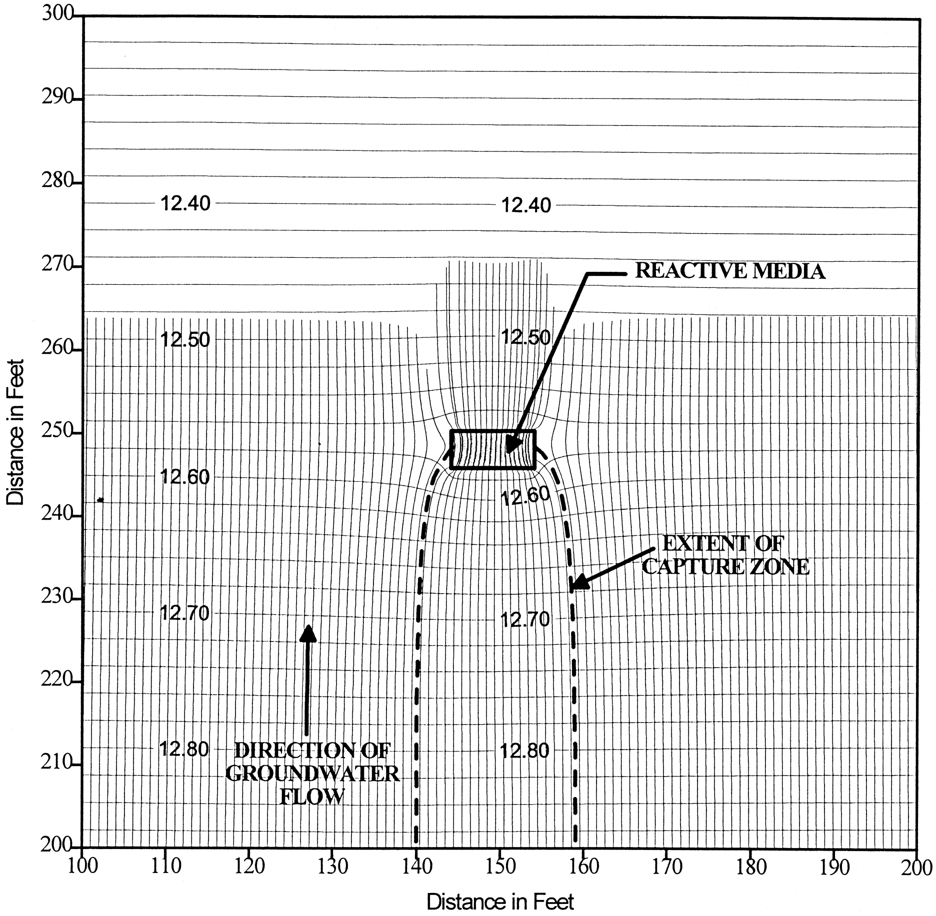

Fig. 3. Simulated capture zone for a continuous barrier scenario showing flowpaths for 180 days (from Gavaskar et al. [1]).

therefore, entrained contaminants may not be fully degraded in these instances unless appropriate safety factors are incorporated into the design.

6.2. Simulation of funnel-and-dual-gate system at Dover Air Force Base

Dover Air Force Base, located 2 miles south of Dover, DE, represents a site with relatively uniform subsurface geology in the area of interest. A permeable barrier pilot-scale demonstration has been completed in Area 5, located in the northwest portion of the Base. Groundwater beneath Area 5 is contaminated with chlorinated solvents. The permeable barrier design was determined from groundwater flow modeling.

Two geologic formations, the Columbia Formation and the Calvert Formation, are the primary geologic units of interest at the site. The Columbia Formation consists of medium to fine sand and overlies the Calvert Formation, which consists of clayey silt to silt. The Columbia Formation is 36–38 ft thick in the vicinity of the permeable barrier and contains the contaminated groundwater. The maximum concentrations encountered during detailed site characterization were 5617 ppb of perchloroethylene (PCE), 549 ppb of trichloroethylene (TCE), and 529 ppb of dichloroethylene (DCE). Water level data from three monitoring events (December 1993 low, May 1994 high, and July 1997 intermediate) were available to assess seasonal changes in groundwater flow directions and gradients. Flow directions varied between south and south-westerly (roughly 30°) between the low and high groundwater levels. Saturated thickness ranged between 19 and 24 ft between low and high groundwater levels, respectively.

Hydraulic conductivity of the Columbia Formation ranges between 1 and 150 ft/day with an expected range at the installation site of 10 to 50 ft/day. Porosity ranges between 24% to 34% with an average of 32%. Hydraulic gradients are about 0.002. Average linear flow velocities range from 0.06 to 0.3 ft/day. The hydraulic conductivity of the Calvert Formation ranges between 0.003 and 0.045 ft/day.

The permeable barrier at Area 5 was designed with the overall goal of testing two different reactive media side-by-side in a practical aquifer setting. The design objectives pertinent to modeling efforts for the installation include the following:

(1) Providing sufficient residence time for the degradation of the primary contaminants and their byproducts. To ensure that maximum contaminant levels (MCLs) are met, a residence time of 3 days (including a safety factor of 2) would be required for groundwater within the reactive cell.

(2) Capturing the more contaminated regions of the plume (concentrations greater than 1000 ppb) to test the reactive media with high concentrations.

(3) Promoting flow through the reactive cells so that the reactive media reach steady state faster.

(4) Accounting for seasonal variations in flow directions.

(5) Avoiding existing utility lines to the extent practical.

Modeling efforts were initiated with the simulation of flow fields representing conditions for the three groundwater monitoring events. A one-layer (2D) model was set up to simulate flow within the Columbia Formation. The base of the model was assumed to be the top of the Calvert Formation and was simulated as a no-flow boundary. The flow model covered an area of 1600 ft × 1800 ft and consist of 246 rows and 473 columns. Model grid cell dimensions in the vicinity of the proposed installation were 0.25 ft × 0.25 ft to permit more accurate determinations of flux through the reactive cell. Model grid cell dimensions increased to 80 ft × 80 ft away from the proposed installation.

The permeable barrier at Area 5 consists of two reactive cells or gates separated by impermeable funnel walls oriented roughly perpendicular to flow. The length of the funnel walls and the position of the reactive cells were constrained by the position of the volatile organic compound (VOC) plume and a buried water line. Because of the low hydraulic gradients, designs that maximized the funnel wall length were investigated. The total length available for the permeable barrier was about 70 ft. Three different configurations having two gates positioned along 60 ft of funnel wall were evaluated at each of the simulated water table conditions. Design 1 consisted of 20 ft of funnel wall between the gates with 20 ft on each end. Design 2 consisted of 40 ft of funnel wall between the gates with 10 ft on each end. Design 3 consisted of 30 ft of funnel wall between the gates with 15 ft on each end. Each of the designs was run at aquifer K simulated at 10 and 50 ft/day.

Model results for the three designs are summarized in Table 1. The table lists the funnel-and-gate configuration, aquifer and gate parameters, the flux through the gate, gate velocity, pore volumes passing through the gate each month, total capture zone width at the funnel wall, and travel time (residence time) through the reactive cell. The flux through the gate area was calculated from the MODFLOW results. Travel time through the gate was calculated from particle tracking results using RWLK3D [12]. The travel time was then used to calculate the groundwater velocity and residence times through the gate. The particle paths and travel time calculations through the funnel-and-gate design simulated in this study are shown in Fig. 4. Variations in travel time through the gates were small, generally less than 5%, along different flow paths through the gates for each simulation. The number of pore volumes passing through the gate each month was calculated by dividing the travel time for groundwater passing through the

Table 1
Summary of scenarios simulated for the design of Dover Air Force Base funnel-and-gate system

Scenario	Funnel type	$K_{aquifer}$ (ft/day)	K_{cell} (ft/day)	Flux through gate (ft^3/day)	Velocity through gate (ft/day)	Pore volume per month	Total capture zone width at gate	Residence time (days)
Base case	None	10	NA	1.8	0.067	0.50	NA	60.0
December 1993	None	50	NA	8.4	0.323	2.42	NA	12.4
Base case	None	10	NA	2.1	0.056	0.42	NA	71.0
May 1994	None	50	NA	9.9	0.258	1.94	NA	15.5
Base case	None	10	NA	2.5	0.074	0.55	NA	54.2
July 1997	None	50	NA	11.4	0.345	2.59	NA	11.6
Design 1	20-20-20	10	283	9.3	0.174	1.30	50.4	23.0
December 1993	20-20-20	50	283	38.7	0.750	5.63	51.0	5.3
Design 1	20-20-20	10	283	9.6	0.149	1.12	50.4	26.9
May 1994	20-20-20	50	283	39.2	0.625	4.69	49.0	6.4
Design 1	20-20-20	10	283	11.8	0.198	1.49	50.8	20.2
July 1997	20-20-20	50	283	49.5	0.851	6.38	47.4	4.7
Design 2	10-40-10	10	283	9.8	0.181	1.36	61.6	22.1
December 1993	10-40-10	50	283	39.4	0.755	5.66	59.6	5.3
Design 2	10-40-10	10	283	10.2	0.160	1.20	57.6	25.0
May 1994	10-40-10	50	283	40.9	0.645	4.84	57.2	6.2
Design 2	10-40-10	10	283	12.5	0.207	1.55	59.7	19.3
July 1997	10-40-10	50	283	50.6	0.870	6.52	57.6	4.6
Design 3	15-30-15	10	283	9.6	0.179	1.34	54.0	22.4
December 1993	15-30-15	50	283	39.7	0.769	5.77	52.0	5.2
Design 3	15-30-15	10	283	10.0	0.155	1.16	53.6	25.8
May 1994	15-30-15	50	283	40.3	0.645	4.84	53.6	6.2
Design 3	15-30-15	10	283	12.2	0.203	1.52	53.8	19.7
July 1997	15-30-15	50	283	50.5	0.851	6.38	52.4	4.7

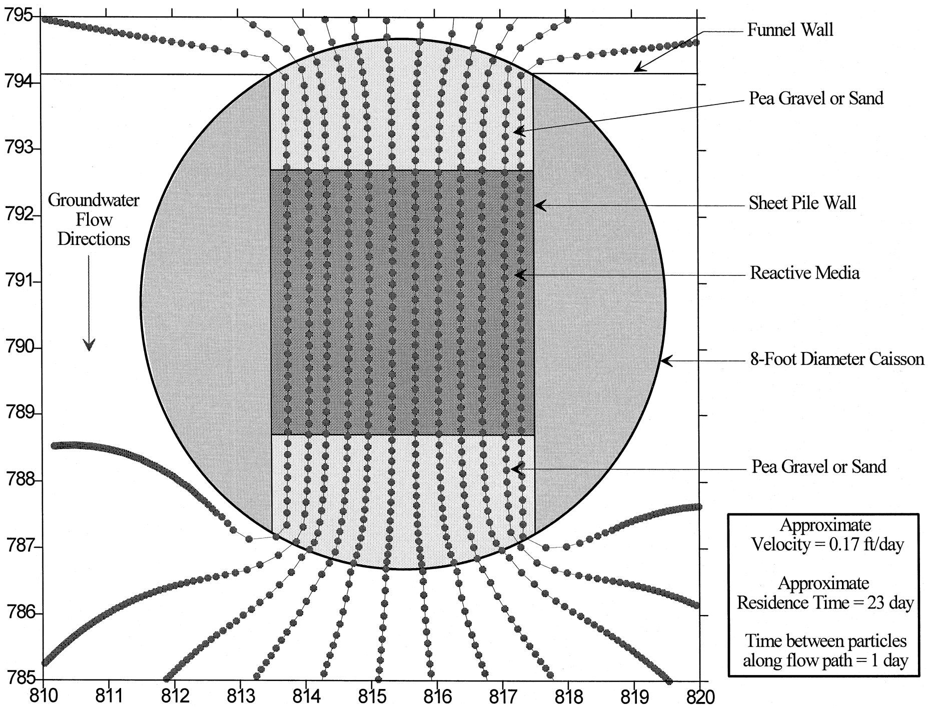

Fig. 4. Simulated flowpaths and travel times through a funnel-and-gate system in a homogeneous aquifer.

gate into 30 days/month. Forward particle tracking techniques were used to determine capture zone widths by evenly spacing particles upgradient of the funnel and gate and then determining the positions of the flow divides separating groundwater that passes through the gates from groundwater that passes around the ends of the funnel walls.

The simulated water levels and flow paths for Design 3 in the immediate vicinity of the proposed funnel and gate based on December 1993 flow conditions are shown in Fig. 5. Fig. 5A illustrates the Design 3 model results for aquifer *K* at 10 ft/day. Fig. 5B illustrates the Design 3 model results for aquifer *K* at 50 ft/day. In each case, groundwater flow directions are nearly perpendicular to the funnel and gate. Water levels are roughly 0.7 ft lower for the simulation with aquifer *K* equal to 50 ft/day. Particles were placed along a line upgradient of the funnel and gate and tracked forward over a period of 3 years to delineate the flow paths and capture zones for the system. Table 1 and Fig. 5 illustrate the system's sensitivity to aquifer *K*. Based on the December 1993 conditions, the flow velocities through the gate range from 0.18 to 0.77 ft/day and the travel times in the gate vary from 5 to 22 days over the range of *K* expected at the site. The actual travel times and velocities will depend on the exact *K* and porosity values for the aquifer and the media and on the hydraulic gradients prevalent at a given time.

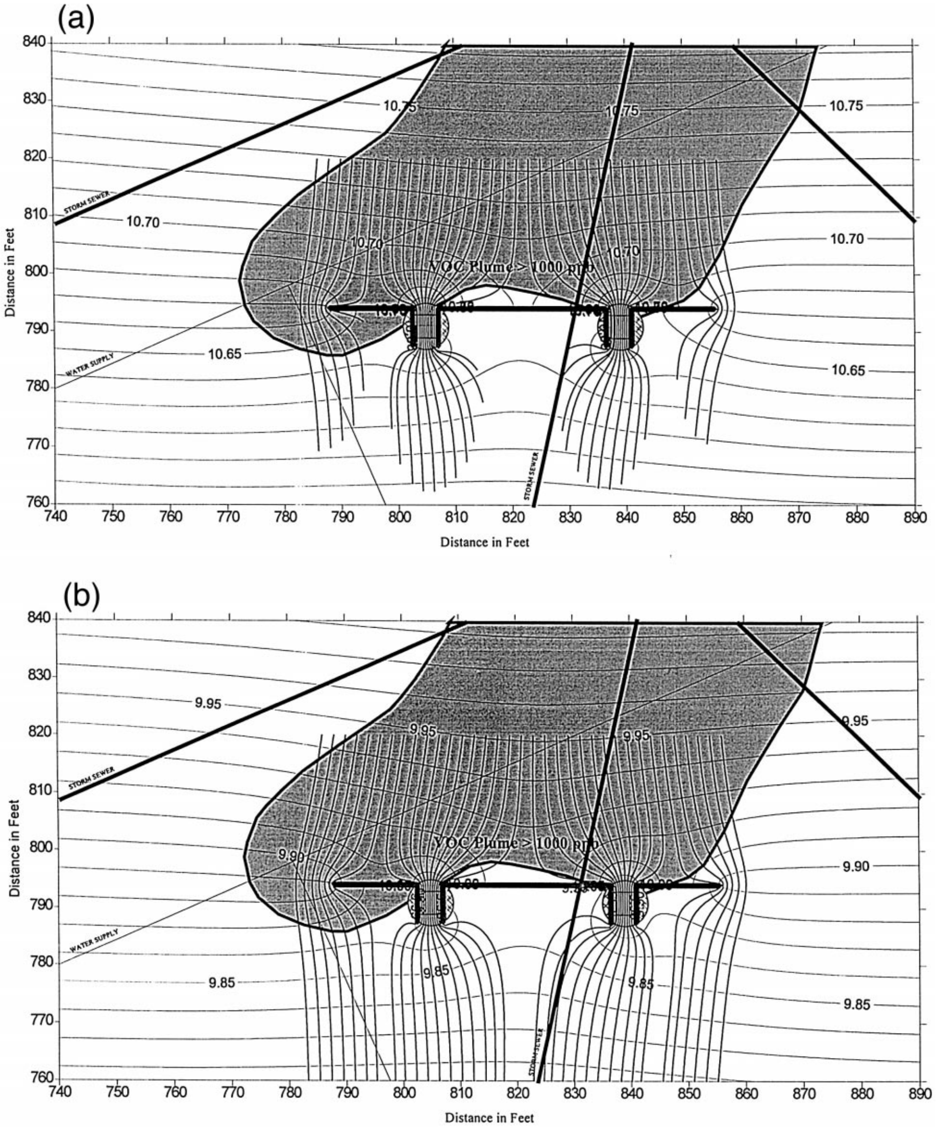

Fig. 5. Simulated flow patterns for Design 3 at Dover Air Force Base funnel-and-gate system showing effect of aquifer conductivity variability. (A) $K_{\mathrm{aquifer}} = 10$ ft/day. (B) $K_{\mathrm{aquifer}} = 50$ ft/day.

Fig. 6A and B illustrate the ability of Design 3 to accommodate the seasonal variations in flow directions based on May 1994 and July 1997 flow conditions, respectively. As seen in this figure and in Table 1, there is no major change in flow velocities and residence times with changes in flow directions. The shift in flow directions results in different portions of the groundwater flow entering the gate. Under all conditions simulated here, based upon the known range in flow directions, the

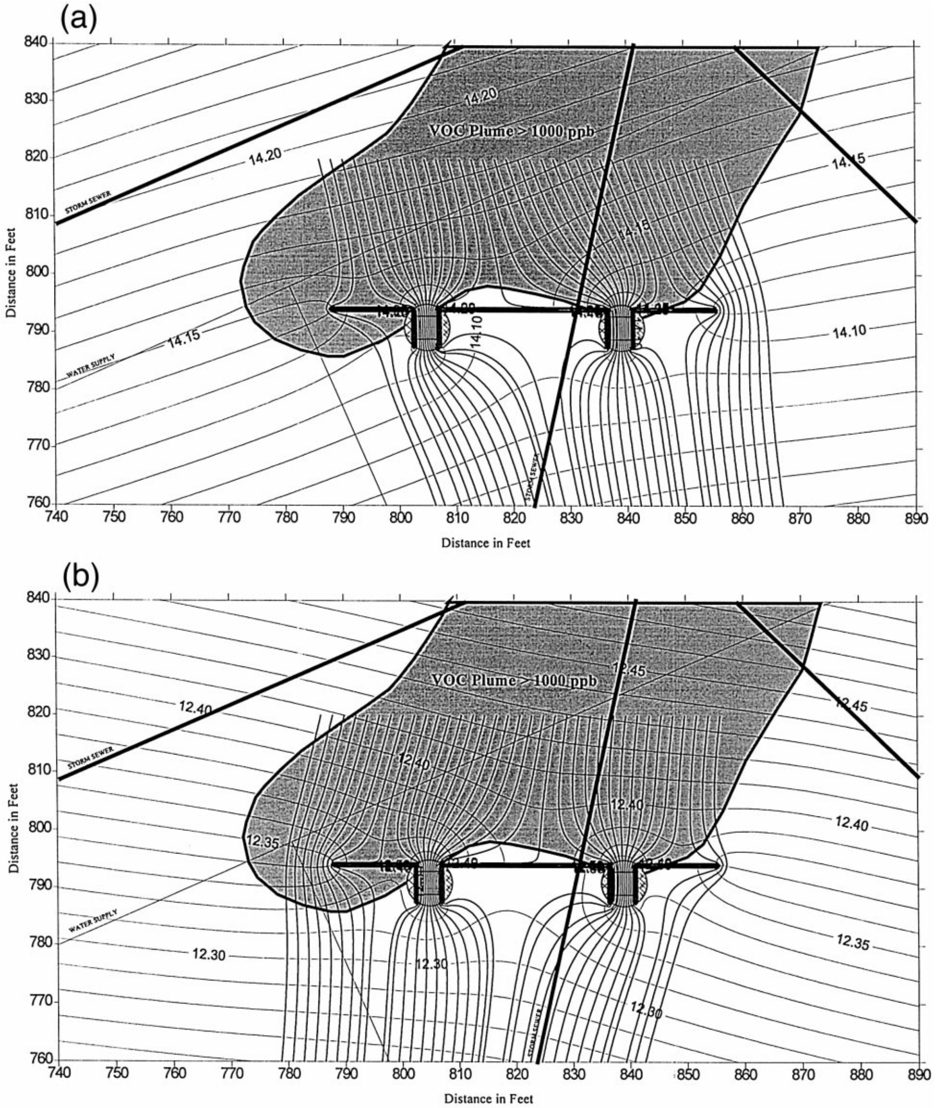

Fig. 6. Simulated flow patterns for Design 3 at Dover Air Force Base funnel-and-gate system showing effect of seasonal water level fluctuations on plume capture. (A) May 1994 water levels. (B) July 1997 water levels.

funnel-and-gate configuration of Design 3 continues to capture the targeted partial portion of the plume for this demonstration site. However, if capture of the entire plume is the remediation goal, care should be exercised in designing funnel-and-gate widths that capture the entire plume under extremes of flow direction change.

Based upon the modeling results, Design 3 was selected for the permeable barrier installation at this site. The target residence time in the reactive cell was 3 days; model results for Design 3 indicate a range in residence time between 4 and 26 days for the conditions simulated. The target residence time in the pretreatment zone was 2 days; model-simulated results indicate a residence time of 2 to 13 days. The simulated capture zone width ranged from 50 to 55 ft and consistently captured the targeted portion of the plume. The targeted time for 30 pore volumes to pass through the reactive cell (and achieve steady state) was 10 months; the predicted time for passing 30 pore volumes ranged from 5 to 26 months.

7. Modeling permeable barriers in heterogeneous aquifers

Modeling studies and barrier design at most existing permeable barrier sites so far have been primarily based on the assumption that the aquifer sediments in the vicinity of the permeable barrier are homogeneous. However, at many sites, there is strong heterogeneity in the sediments. This heterogeneity is mainly due to the variations in depositional environments of the sediments. The general implications of heterogeneity are that more detailed site characterization is required and more complex models are needed.

Examples of the effect of heterogeneity on the flowpaths and capture zones can be seen from the modeling work conducted in support of the design and performance monitoring for the Moffett Federal Airfield site [13,15]. Geologically, this site consists of a series of high conductivity sand channels separated by lower conductivity silty and clayey zones. A seven-layer MODFLOW model with heterogeneous layering was constructed. Modeling results show that the presence of heterogeneities due to multiple subsurface channels causes the capture zones to be substantially asymmetrical. Fig. 7 is a simulated flowpath diagram showing the result of backward particle tracking for 25 days with particles starting from the funnel area in model Layers 1 through 4 at the funnel location. The reactive cell is present in Layers 2, 3, and 4 of the model.

The most striking observation from Fig. 7 is that the capture zone for a permeable barrier at a heterogeneous site is highly asymmetrical and there is a significant difference in the residence time at different depth levels. For example, there is almost no movement of particles in 25 days in Layers 1 and 2. In Layer 3, the particle movement is very fast directly upgradient of the gate, but very slow upgradient of the funnel walls. In Layer 4, the particle movement is very fast upgradient of the gate in the west funnel wall but still very slow upgradient of the east funnel. The modeling conclusions about the flow system at this site were later verified by the authors with a tracer test conducted at the site.

These differences in particle velocities and resulting irregularities in the capture zones are because the lower part of the reactive cell is located in a high-permeability sand channel, whereas the funnel walls and the upper portion of the reactive cell are located in the lower conductivity interchannel deposits. The location of sand channels at the site was determined based on the preexisting Base-wide site characterization maps and from site-specific CPT data. The irregularities in flow may result in vastly different residence times in the reactive cell. Pea gravel sections along the upgradient and downgradient

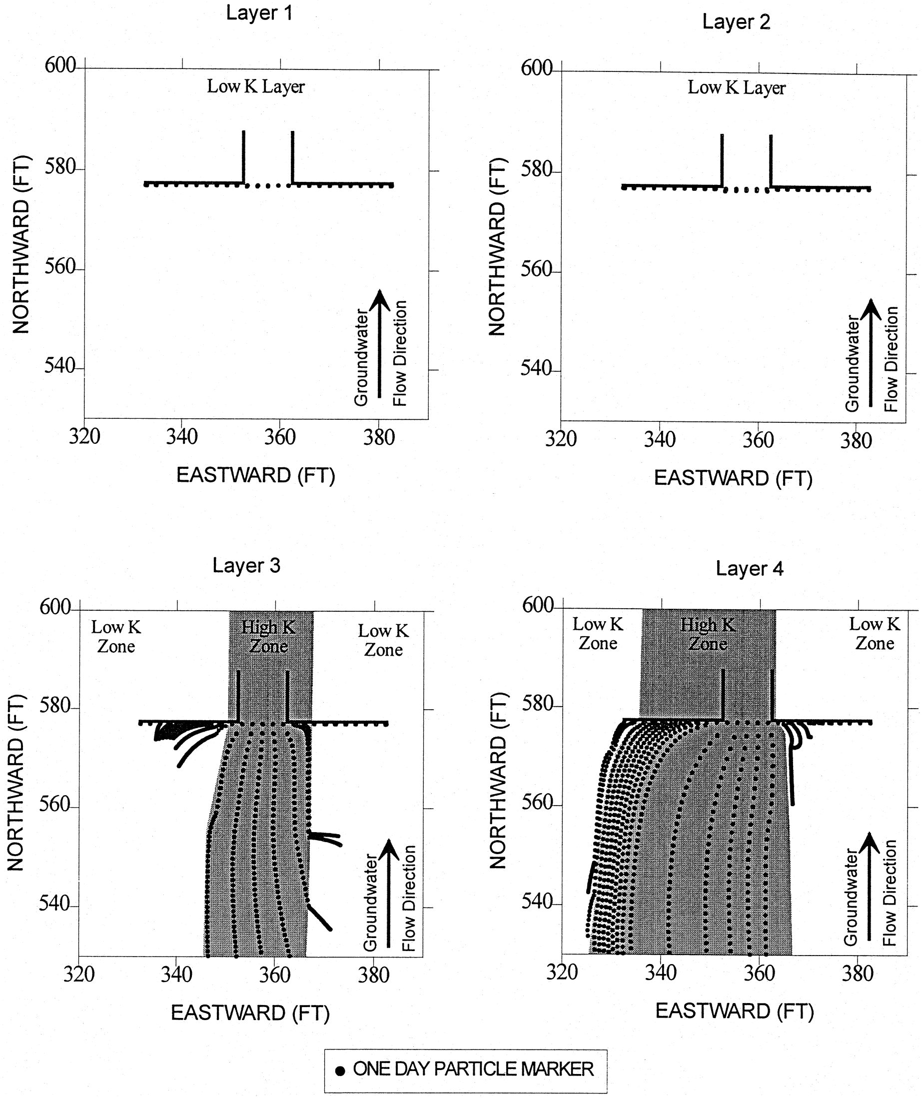

Fig. 7. Backward particle tracking showing the effect of heterogeneity on capture zones (from Gavaskar et al. [1]).

edges of the reactive cell help homogenize the flow vertically and horizontally to some extent. This example illustrates the need for placing the reactive cell in a zone of high conductivity that forms a preferential pathway for most of the flow and contaminant transport through the aquifer. Additionally, the dependence of capture zones on aquifer heterogeneities illustrates the need for detailed site characterization and adequate hydrogeologic modeling prior to permeable barrier design and emplacement.

8. Summary

Hydrogeologic modeling provides an efficient and cost-effective means for feasibility evaluation, design optimization, and performance assessment for permeable reactive barrier technology. The use of hydrogeologic models is becoming more common with wider application of the technology at complex, full-scale field sites. This becomes more critical when the sites in question have hydrogeologic heterogeneities and fluctuating flow systems. The most common approach for design optimization involves a flow model using MODFLOW with flow budget calculations and particle-tracking codes for flow field visualization. The major optimization parameters determined from modeling include discharge through the reactive cell, residence times, and capture zone width. In addition, modeling has also been used to evaluate the impact of decreasing hydraulic conductivity in response to potential precipitation, and to incorporate appropriate safety factors in the design.

Some general observations regarding reactive barrier hydraulics can be made from the simulations presented in this paper. As discharge through the reactive cell increases, capture zone width increases, and travel time through the reactive cell (residence time) decreases. The particle tracking estimates of residence times can be used to optimize the flowthrough thickness of the reactive cell for achieving the desired reduction in contaminant levels. When designing a reactive cell, it is important to note that aquifer hydraulic conductivity is the sensitive parameter for discharge and residence time through the reactive cell, as long as the reactive cell hydraulic conductivity is about half an order of magnitude greater than the aquifer conductivity. As the reactive media conductivity approaches the cell aquifer conductivity, the reactive media conductivity becomes a more important parameter and the capture efficiency of the cell decreases. For funnel-and-gate configurations, hydraulic capture zone width appears to be most sensitive to funnel length and aquifer heterogeneity. Finally, adequate site characterization is critical to successful implementation of the technology at the field scale.

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