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Modeling of a permeable reactive barrier

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ABSTRACT

MODELING OF A PERMEABLE REACTIVE BARRIER

by
Gautam C Ijoor

The focus of the present study was centered on the modeling analysis to support the Permeable Reactive Barrier (PRB) design. The flow model formulated to simulate the Permeable Reactive Barrier System integrated the available geologic, hydro geologic and geo-chemical data from numerous recent installations to simulate a subsurface ground water scenario.

Different generic cases that a PRB system would fall into were identified based on its utility and aquifer conditions and then employed to produce different model adaptations. The different simulation codes and interfaces were evaluated, and the most expedient of them was used to simulate the Model.

The simulations were then used to study the sensitivity of different parameters and identify those that were critical to the design of the system. Design curves, devised to aid the design of a barrier, were verified with the residence time curves mapped for the same parameters. The results of the sensitivity analysis and the developed design curves were used to arrive at a uniform procedure for the design of a Continuous Configuration Barrier System.

The procedure were appraised by working through the design of a Permeable Reactive Barrier at a GW contaminated site located in the Piedmont Province of the Appalachian Highlands in New Jersey.

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by
Gautam C. Ijoor

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APPROVAL SHEET

DESIGN OF PERMEABLE REACTIVE BARRIERS

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This thesis is dedicated to
my parents
L. Chikkegowda and Renuka Gowda

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LIST OF SYMBOLS

C	=	Conductance
D_{trench}	=	Depth of Hanging Wall
GW vel.	=	Ground Water Velocity
h_m	=	Measured Head
h_s	=	Simulated Head
K	=	Hydraulic Conductivity
K_a /$K_{aquifer}$	=	Hydraulic Conductivity of Aquifer
K_b /$K_{barrier}$	=	Hydraulic Conductivity of Barrier
Δl	=	Nodal Spacing between Gridlines
L	=	Length of River in the Simulation
L_l	=	Depth of water applied to the top layer of a 3-dimensional finite difference model
L%	=	Percentage of loss of particles
L_{2T}	=	Length of Second Trench
$Loss_{db}$	=	Loss Through a Double Barrier
$Loss_{hw}$	=	Loss through a Hanging Wall
M	=	Thickness of a Riverbed Sediments
ME	=	Mean Error
n	=	Effective Porosity
n	=	Number of Readings for Head
N_{influx}	=	Contaminant Pathlines towards Barrier

LIST OF SYMBOLS
(continued)

$N_{influxh}$	=	Contaminant Pathlines incident to Barrier
N_{thru}	=	Influx passing through Barrier
N_{loss}	=	Influx deviating away from Barrier
N_{lossh}	=	Influx deviating below Barrier
N_{THRUb1}	=	Influx Passing through Barrier 1 in a Double Barrier
N_{THRUb2}	=	Influx Passing through Barrier 2 in a Double Barrier
N_{THRUh}	=	Influx passing through barrier
RMS	=	Root Mean Square Error
$RT_{obtained}$	=	Residence Time obtained from Design of Barrier Procedure
$RT_{required}$	=	Residence Time required for the Reduction of Contaminant or changed input
S	=	Storitivity/ Storage Coefficient
S_s	=	Specific Storage
S_y	=	Specific Yield
T	=	Time over which water is applied
vx	=	The Component of Velocity along the x-axis of the Model
vy	=	The Component of Velocity along the y-axis of the Model
vz	=	The Component of Velocity along the z-axis of the Model
W	=	Width of River in the Simulation
W_{2T}	=	Width of Second Trench
x	=	x Co-ordinate of the cell for which Velocity is Exported

LIST OF SYMBOLS
(continued)

y	=	y Co-ordinate of the center of the cell for which Velocity is Exported
z	=	z Co-ordinate of the center of the cell for which Velocity is Exported
α	=	Dispersivity
1.4e-5m/s	=	1.4×10^{-5} m/s

CHAPTER 1

INTRODUCTION, OBJECTIVES AND SCOPE

1.1 Introduction

In the past two decades considerable progress has been made to improve the quality of natural resources like the air, surface water, and soil. Among the more serious problems, groundwater (GW) contamination has proven to be an important and challenging environmental problem. Inherent heterogeneity of subsurface systems makes detection of GW contamination, not only convoluted, but also too late to apply remediation techniques of quick benefit. Almost every precedent of aquifer degradation has been detected only after a water supply well had been affected (USEPA, 1977).

In 1977, the USEPA reported that there were at least 17 million waste disposal facilities interjecting more than 6.5 million cubic meters of leachate into the subsurface streams each year, in the US alone. This resulted in the aggressive use, of the then discernible, ex-situ 'Pump-and-Treat' technology. The choice could rather be attributed to paucity of treatment technologies available, than to its preeminence. Though the immediate need for GW treatment was compensated with 'Pump-and-Treat' technique, it was received by the remediation industry with a gradually decreasing enthusiasm owing to its enormous treatment cost (Mackay and Cherry, 1989). Even after further developments, other in-situ treatment technologies proved to be less futile.

In-situ treatment technologies facilitate the treatment of groundwater without bringing it to the surface. The Permeable Reactive Barrier System is an in-situ groundwater treatment technology.

The primary focus of the present study was centered on the modeling to support the design of a Permeable Reactive Barrier system for treating chromium-contaminated groundwater. In this barrier system a reactive mixture is placed in the direction of flowing groundwater where removal of contaminant occurs passively. A PRB can thus be defined as: "an emplacement of reactive materials in the subsurface designed to intercept a contaminant plume, provide a preferential flow path through the reactive media, and transform the contaminant(s) into environmentally acceptable forms to attain remediation concentration goals at points of compliance" (USEPA, 1997; Powell and Powell, 1998; Puls and Powell, 1997).

Permeable Reactive Barriers are increasingly viewed as an excellent solution for many complex groundwater contamination problems [Korte *et al.,* 1997]. On considering a federal perspective, the USEPA recognizes this technology as having a significantly higher, contaminant attenuation to application cost ratio, than other conventional approaches in treating groundwater.

1.2 Objective and Scope

The primary objective of this study was to develop modeling procedures to support the design of a Permeable Reactive Barrier to treat contaminated groundwater economically.

This study happens to be contemporary to the geo-chemical study and design of a remediation system to attain ground water clean up levels for a chromium-contaminated site. The main objective would be the synthesis of a flow and transport model for the application of the Permeable Reactive Barrier Technology to treat hexavalent chromium contaminated groundwater, at chromium sites, associated with Chromium Ore Processing Residue (COPR), in New Jersey.

In the design of a Permeable Reactive Barrier, two parameters induced to be of prime importance are hydraulic capture zone and residence time. The former decides whether there is a potential risk of contaminant flow under or around the barrier or through the reactive media. The expected groundwater flow velocity, reactive material porosity, discharge through reactive cell and thickness of the reactive barrier or gate influence the residence time. The residence time if sufficient warrants the reduction of contaminant to meet regulatory requirements. The different critical parameters can be systematically varied to obtain the design values that ensure contaminant levels in the treated plume below the regulatory levels, for any particular case.

The procedure for modeling to support a Permeable Barrier design is expected to differ according to different modeling approaches, such as: a PRB in a relatively homogeneous aquifer; a PRB in a heterogeneous aquifer; modeling different PRB configurations and reactive material dimensions.

The Permeable Reactive Barrier is an alternative treatment technology for which routine use at Superfund and similar sites is inhibited by the lack of data on performance and cost, even though it has been accepted with monumental response in the recent years. A substantial body of relevant literature, much of which has been published mainly in the recent years, on design aspects of PRBs, chromium speciation and its behavior in soils and water and other electrochemical aspects, is available. Little literature is also available on groundwater modeling aspects. Initial objectives would include an extensive literature search of different modeling software reviews, patents, publications and dissertations of previously conducted studies.

The evaluation of the various software available in the market to model a Permeable Reactive Barrier is substantially important. An innovative technology, i.e. one that has had limited full scale application, like the PRBs is inhibited by the lack of data on ground water flow and contaminant transport/migration parameters. Many of the available packages are either not intuitive to use or do not support this technology, to the comfortable extent of answering questions on the same that could not be answered in the recent past. Generic conceptual cases should be formulated, to be used as the final evaluation criteria for the software packages recognized as suitable. These cases should be modeled to identify generic parameters that contribute a standard for remediation system design. This standard would assist us in taking productive decisions both in this study as well as in the concurrent electrochemical treatability study. The major advantage of creating a comprehensive flow model is that, once the initial case is set-up, design configurations, site parameters and performance and longevity can be readily evaluated. Intermediate results from the electrochemical study prove to be useful in establishing the generic cases, for example: the pH, between 9-9.5, found to facilitate a high reaction rate is suggestive of a double trench. Thus, periodic reviews of our findings, discussions and meetings are a secondary objective.

The objectives can thus be summarized as follows:

1. To carry out an encyclopedic literature search and posterior review of the general features of the technology and study conclusions. The study should arrive at a

conclusive definition of the PRB technology and corroborate the efficacy of developed design procedures.

2. To formulate the generic conceptual cases, taking into consideration the remotest possibility, arising out of the geo-chemical and the geological site investigation.
3. To summon periodic meetings to review parallel research outcomes, and to arrive at a consensus on their implications and the subsequent course of study.
4. To develop a flow model to help identify the critical parameters that influence the contaminant concentration in the effluent. The developed model should be validated with field data from past projects and the synchronal geo-chemical and the hydro-geological study.
5. To devise a procedure to support the design of a Permeable Reactive Barrier. A generic design convention will be developed compatible to a PRB installation.
6. To design a PRB system, to be installed at the chromium-contaminated sites in New Jersey, adopting the procedure formulated in this study.

This work will begin with a brief review of the related literature on Permeable Subsurface Barriers for contaminant removal, groundwater flow and contaminant transport (Chapter 2). This is followed by a presentation of the background of the propagation problem, i.e. the general concept, hitherto adopted design convention and a comprehensive discussion of the 'to be used' software packages used (Chapter 2). The approach to modeling, by first reviewing important aspects to be incorporated in the model i.e. conceptual generic cases, simulation code and interface selection in Chapter 3. The construction, calibration and execution of the flow model followed by a discussion on the parameters considered critical, as they influence contaminant concentration in the effluent is documented in the subsequent chapter (Chapter 4). The results of modeling a PRB promulgation, the formulation of design curves and a procedure for PRB design are also presented in the Chapter 4. The actual design of the PRB system for the chromium contaminated sites in New Jersey is then documented as a case study (Chapter 5). Finally, the study conclusions are presented along with recommendation for further study of the technology (Chapter 6).

CHAPTER 2

BACKGROUND

2.1 Reactive Barrier (General Concept)

The conventional approach to the remediation of contaminated groundwater is to *pump* the water to the ground surface, *and* subsequently *treat* the same with water treatment equipment, as required. The treated groundwater is then discharged either back into the aquifer or led away into a surface drainage source such as a stream or a river. This "*ex situ*" treatment mode, appears as the most logical approach to treat contaminated ground water, i.e. when a contaminated resource, is moved to a convenient location and then treated for the contaminants, rather than facilitating their removal in place without disturbance of site. Removing groundwater from its native aquifer on a large scale is enormously expensive [Blowes, and Ptacek, 1996]. It requires extensive energy maintenance and a continuous energy input [USEPA, 1998]. In some cases, the hydraulic conductivity of the surrounding soil is very low and the particles of the contaminant may be adsorbed onto the surface of soil particles, thus making 'Pump-and-Treat' unsuitable. If the contaminant is not degraded in the 'treat'ment phase, the disposal of the same is an additional environmental problem. The unsuitability of this conservative approach also prevails in the low permeability zones of the aquifer, during permanent aquifer restoration, owing to the difficulties posed by contaminants. Sequester liquid contaminants and precipitated and co-precipitated soluble mineral contaminants are strongly adsorbed to particle surfaces [Blowes *et al.*, 1995.]. As with any technology, advancements are being explored at different sites with the objective of alleviating these problems. These preferment, though significant, result either in the prodigal use of water resources or in increasing costs, making in-situ treatment more suitable at these sites.

2.1.1 In-Situ Treatment

The main advantage of in-situ treatments is that they facilitate the treatment of groundwater without bringing it to the surface. The resulting significant treatment and maintenance cost-savings and less energy intensive procedures have made them very popular. They are however plagued by longer time period requirements, difficulty to verify the efficacy of treatment, less uniform treatment procedures because of the complex aquifer characteristics [USEPA, 1994].

2.1.2 Permeable Reactive Barriers

One type of in-situ ground water treatment is the Permeable Reactive Barrier (PRB) technology. In the history of site remediation, no concept has evoked as much research, industrial and governmental response as has the PRBs. Permeable Reactive Barriers are increasingly viewed as the final solution for many complex groundwater contamination problems [Korte *et al.*, 1997]. The remarkable interest in PRBs by the research, industrial and governmental sectors can be attributed to the anticipated transcendental surpass of the "cost of" by the "benefits from" this technology.

The Permeable Reactive Barrier System is a patented process [U.S. Patent #5,362,394; U.S. Patent #5,514,279] developed at the University of Waterloo, Ontario, Canada. The inventors are David W. Blowes and Carol J. Ptacek both of Waterloo, Canada.

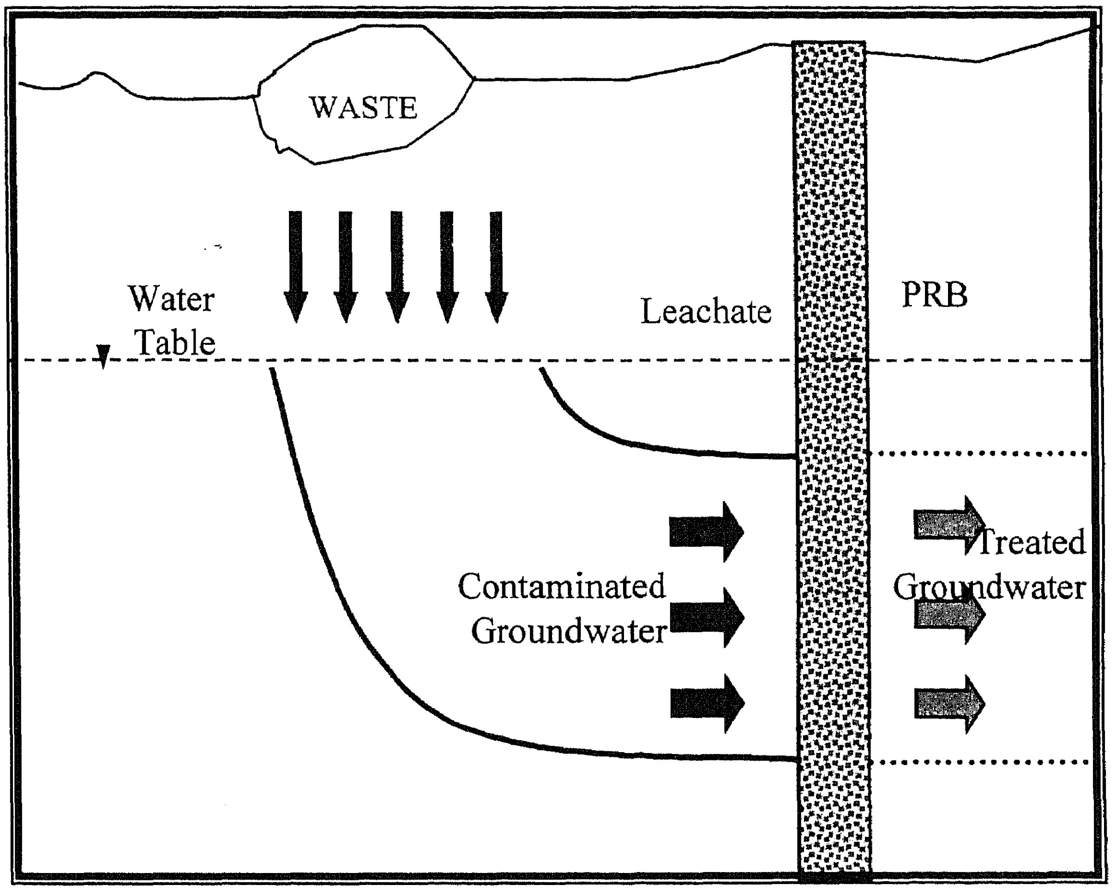


Figure 1 Treatment of Groundwater with infiltrating Leachate by Permeable Reactive Barrier

Here a biologically or chemically reactive mixture is placed in the direction of flowing groundwater where removal of contaminant occurs passively. The Aquifer, which incipiently provided the medium of transport for the contaminated groundwater, is replaced by reactive material. The contaminant contained in the groundwater reacts with the barrier material and is treated concurrent to the passage of plume (Figure 1). Figure 1 shows a Single Trench Fully Penetrating PRB transecting a contaminated plume arising at a waste site. The rate of removal of the contaminant, however, would depend on the rate of the reaction of the contaminant and reactive material. Development in emplacement procedures has spawn techniques, like slurries, hydro fracturing, and driving mantels, [Puppala, 1998] to overcome installation limitations and facilitate GW flow.

2.1.3 The Reactive Material

The reactivity of many metals with chemicals has long been known. It was however not until 1912, when Victor Grinard and Paul Sabatier shared the Nobel Prize for their preferment in organic synthesis and nickel-catalysed hydrogenation respectively, that research formally addressed metal reactions with organic and inorganic chemicals [Powell and Powell, 1998]. Until the late seventies, with the work on different metals directed toward metal corrosion, the potential of metals to degrade, subsequent degradation of solvents like 1,1,1-tricholoroethane, carbon tetrachloride, etc. [Archer, 1982; Archer and Simpson, 1977; Archer and Harter, 1978; Evans, 1960], and the remediation potential of metals went unnoticed.

In 1982 Gould studied iron as a reductant of hexavalent chromium in waste waters, and Bowers improved upon Gould's work and proposed a process for the treatment of Cr(Vl) wastewater. This procedure was made available in 1986. The use of metals for in situ remediation of subsurface contaminants was conceptualized even later after Glenn Reynolds stumbled over a hydrogenated hydrocarbon bromoform ($CHBr_3$) decline when in contact with steel and aluminum. This was hypothesized as reductive halogenation and the results were made available in 1984 [Reynolds, Hoff and Gillham, 1990]. He was working on the sorption of organic contaminants by different well casing materials. An in-depth study ensued on the use of granular iron, on account of its low cost and reactivity, for the degradation of subsurface contaminants. It was followed by a large number of conference proceedings, in the early nineties, on the use of zero-valent iron for contaminant remediation [eg. Powell, 1994; Powell *et al.*, 1995a; Powell *et al.*, 1995b; Powell *et al.*, 1994; Matheson and Tratnyek, 1994].

In the study of reactive media, *The Subsurface Restoration Conference- The Third International Conference on Groundwater Quality Research, held in Dallas, Texas*, in June 1992, is definitely worth a mention. At that time, the institutes that had been accommodating the research activity of relevance to reactive material, i.e. The University of Waterloo, Ontario, Canada, The Rice University, Houston, Texas, and The Robert S. Kerr Environmental Research Laboratory, Ada, Oklohoma, sponsored the conference under the auspices of the National Center of Groundwater Quality Research [Blowes, and Ptacek, 1992; US patent No. 5,514,279, 1996]. Researchers presented two 'posters', the first, which explicated the use of PRBs in dehalogenation, denitrification, and bioaugmentation, was presented by Robert Gillham and David Burris. David Blowes and Carol Ptacek presented the second, to divulge the reduction of Cr(VI) contaminants to a less toxic and immobile $Cr(OH)_3$ precipitate. With the publicity these posters received, the concept of subsurface reactive barriers became increasingly perceptible.

As of this writing, numerous research organizations have been testing metals, bimetal and a variety of substances, for their reactivity with different contaminants [Gillham and O' Hannesin, 1994; Powell and Powell, 1998]. Zero-valent metals have been the all time research favorites. Their endeavor to conceive the reaction mechanism of PRB material, design and emplacement of PRBs, has eventuated in a large number of proceedings, pre-reviewed research publications, and presentations on their finding which distinctly defined the invention. A basic comprehension of the invention mechanism and configuration is absolutely necessary before any study.

The barrier may be chemically or biologically active, depending on the nature of the reaction by which the reactive material promotes or participates in the breakdown or transformation of the contaminants. Alternatively, in the presence of the barrier material, the contaminant may adopt a less soluble form where by the contaminant precipitates or is adsorbed onto the material [Blowes, and Ptacek, 1996]. When the 'less soluble form' is also objectionable to water quality standards, it requires additional treatment before disposal, making the other alternative a preferred one.

The permeability of the barrier material is such that it does not adversely impede the flow of groundwater through the aquifer. The reactive mixture is usually mixed with an apropos amount of aquifer material, before it is placed in position as the barrier. This ensures that it does not provide more resistance to groundwater flow than does the aquifer material that it replaces.

The reactive material depends on the type of contaminant to be treated, and the selection of the same would be the first step in the approaches taken to optimize a PRB system. Though studies have addressed the suitability of PRBs with a large number barrier materials no consensus has been reached for the selection of the same. The types of reactive media available (Table 1) for use in a PRB can be broadly classified as follows, (Environics Directorate U. S. Air Force, 1997):

Table 1 Types of Reactive Media Available

Types	Reactive Metal Media	Comments	References
Granular Zero-Valent Metal	**Granular Iron**	**All time favorite, most common used so far in bench, pilot and full scale PRBs**	**Reduction rates were studied by Sivavec and horney, 1995;Agarwal and Tratnyek, 1996; Matheson and Tratnyek, 1994.**
	Zero-valent aluminum	**Fast reduction-rate with hydrocarbons**	**Reynolds at al., 1990; Gillham and O'Hannesin, 1992.**
	Mild Steel	**Fast reduction-rate with hydrocarbons**	**Reynolds at al., 1990; Gillham and O'Hannesin, 1992.**
	Galvanized metal	**Fast reduction-rate with hydrocarbons**	**Reynolds at al., 1990; Gillham and O'Hannesin, 1992.**
Granular Iron with amendment	**Pyrite**	**The amendment added to granular iron to moderate pH, increased during Fe^0 oxidation to Fe^{2+}**	**Burris et al., 1995; Holser et al.,1995.**
Bimetallic Media	**Fe-Cu**	**Act as galvanic couples**	**Sweeny and Fisher, 1973; Sweeny, 1983; Korte et al., 1995**
	Fe-Pd	**Enhance degradation rates**	
	Fe-Ni	**Enhance degradation rates resulting in a cost trade-off in constructing a smaller reactive wall.**	**Appleton, 1996.**
Other Innovative Reactive Media	**Cercona Iron Foam**	**Ceramic foam and aggregate products made by Cercona, inc, OH, are promising reactive materials.**	**Bostick et al., 1996.**
	Colloidal Iron	**Colloidal-size iron as a substitute to granular iron has some advantages.**	**Kaplan et al., 1996.**
	Ferrous iron-Containing Compounds	**Na_2s, FeS, FeS_2, Pyrite**	**Burris et al., 1995; Holser et al.,1995; Lipczynska-Kochany et al. (1994).**
	Reduction of Aquifer Minerals using Dithionite.	**Aquifer minerals containing ferric iron can be reduced by sodium dithionite ($Na_2S_2O_2$)**	**Amonette et al., 1994.**

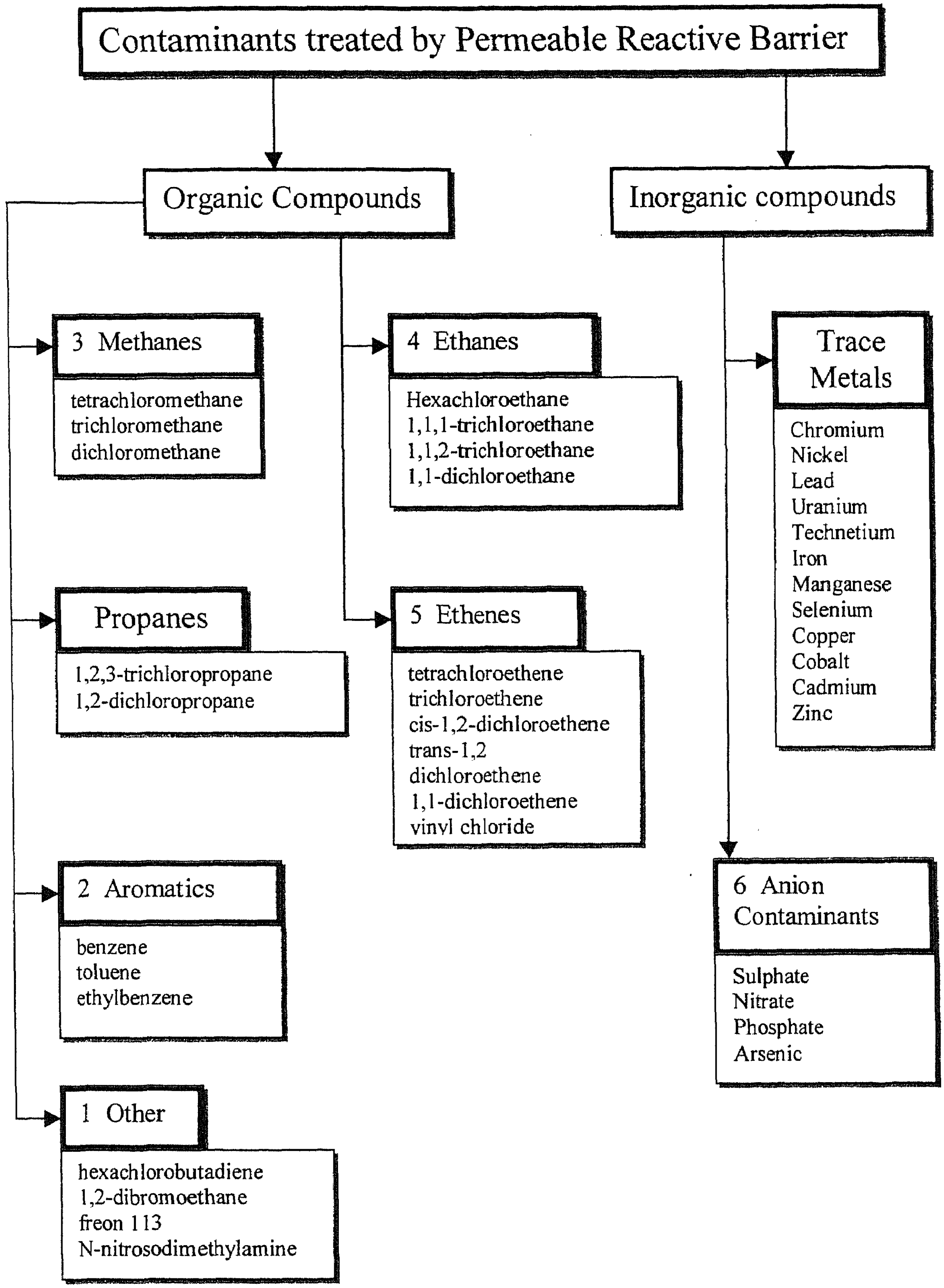


Figure 2 Organic, Inorganic Contaminants that have been Treated by PRBs

- Granular Zero-valent Metals like Granular Iron, Sn^0, Zn^0
- Granular Iron with amendments like Pyrite
- Bimetallic Media like Fe-Cu, Fe-Pd
- Other Innovative Reactive Media like Cercona Iron Foam, Colloidal Iron

Relevant references to the above applications are given in Table 1. PRBs have been shown to be effective in the remediation of groundwater contaminated by dissolved metals [Blowes and Ptacek, 1992; Blowes *et al.*, 1997], chlorinated hydrocarbons [Gillham and O'Hannesin; 1992; Gillham and O'Hannesin, 1994], dissolved nutrients [Robertson, and Cherry, 1995; Baker *et al.*, 1997], gasoline derivatives [Bianchi-Mosquera and Allen-King, 1994], acid mine drainage [Blowes *et al.*, 1997; Benner *et al.*, 1997], and landfill leachate. The USEPA has further reported the different organic and inorganic contaminants that have been successfully treated by Permeable Reactive Barriers (Figure 2).

2.1.4 Barrier Configuration

The second step to enhance treatment of the contaminant by a PRB system is the evaluation of the physical configuration of the system. This would focus on the structure of the Permeable Reactive Barrier, how the contaminated groundwater pragmatically takes the benefit of the reactive mixture, and the relative differences between the two.

The two configurations (Figure 3) most often investigated in the design of Permeable Reactive Barriers are the following [Blowes and Ptacek, 1992; Blowes *et al.*, 1997; Gillham and O'Hannesin, 1992; Gillham and O'Hannesin, 1994; Robertson, and Cherry, 1995; Baker *et al.*, 1997; Bianchi-Mosquera and Allen-King, 1994].

1. The Continuous Configuration (Figure 4).

2. The Funnel-and-Gate Configuration (Figure 5).

Conformably, the reactive material can be installed as a continuous curtain or as intermittent zones joined by impermeable walls.

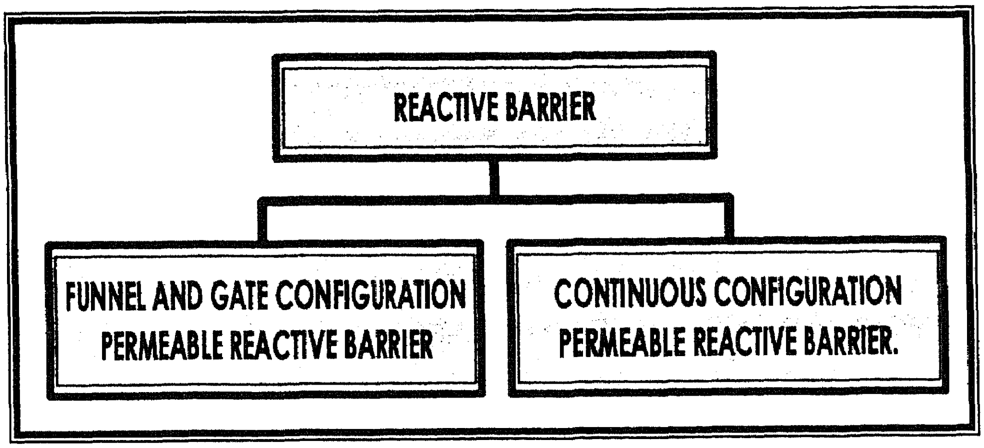


Figure 3 Barrier Configurations

2.1.4.1 The Continuous Configuration: When this configuration is adopted, the reactive material is installed in the path of the contaminated groundwater athwart the

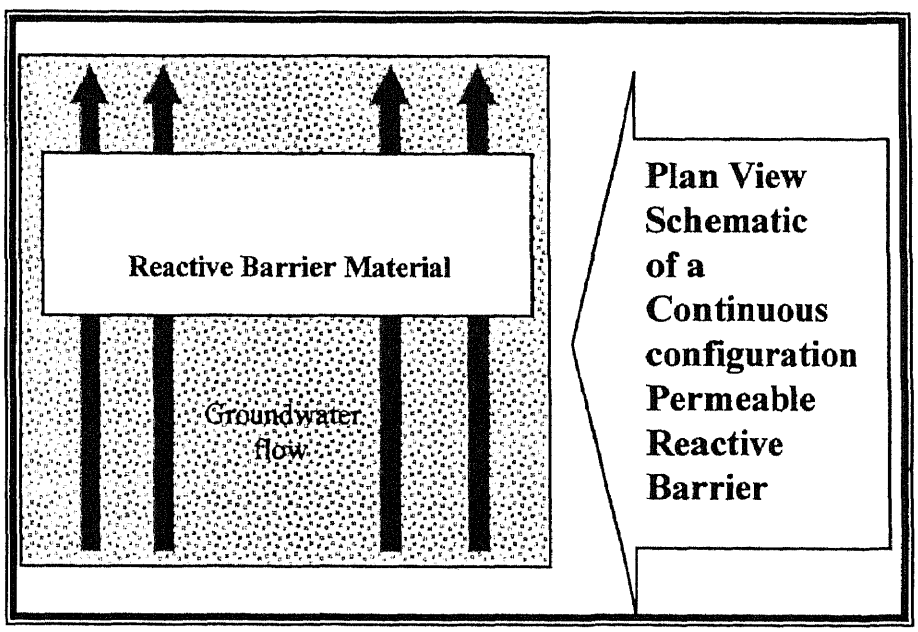


Figure 4 Continuous Configuration

direction of flow. Here the PRB completely transects the contaminated plume, without altering the direction of GW flow. Figure 4 shows a schematic of a Continuous Configuration PRB. The chief distinction from the other configuration is that, here the direction of GW flow is not altered.

2.1.4.2 The Funnel-and-Gate Configuration: This configuration consists of an alternating series of reactive material "gate(s)" and impermeable funnels. Accordingly they are called n gate funnel-and-gate configuration, where n stands for the number of reactive gates. The impermeable "funnel" directs the contaminated groundwater plume towards the "gate(s)" of reactive material. Figure 5 shows a schematic of a Funnel-and-Gate Configuration PRB. The figure also shows that chances of leakage around the barrier are greater in this configuration.

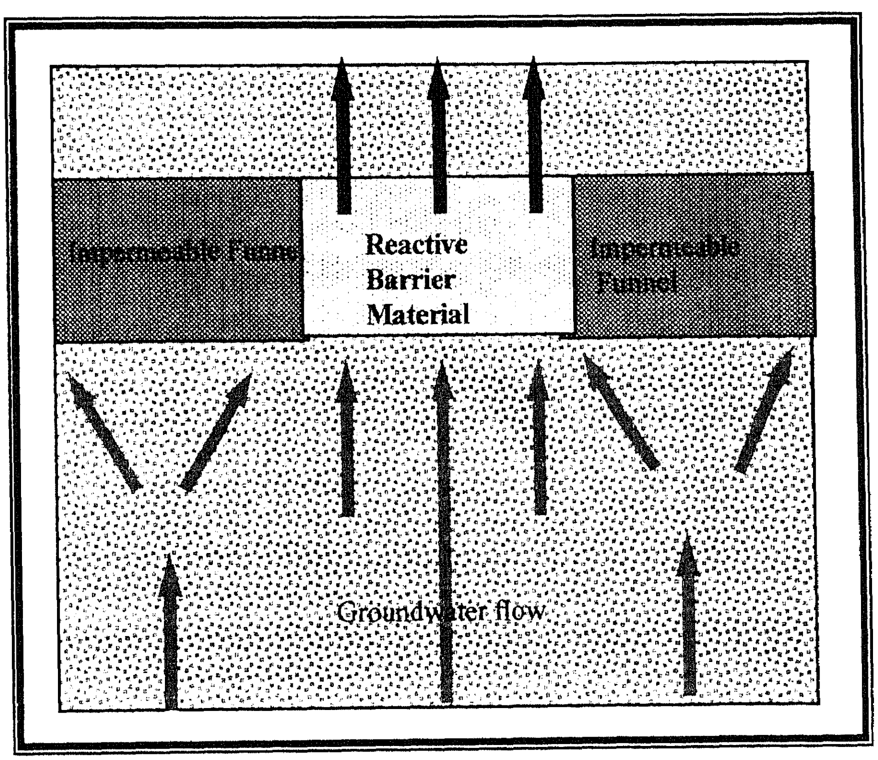


Figure 5 Funnel-and-Gate Configuration

Simulation provides an evaluation criteria, for the suitability of a barrier configuration to the project site. Though, for a similar volume of iron, the latter configuration proves to be slightly expensive, simulation results suggest that the same capture zone and residence time can be attained [Blowes *et al.*, 1997].

The degree of excavation, the transect point between the contaminated plume and the PRB, and subsequently the depth of the PRB, are independent of the configuration found suitable, and depend on the depth of the plume at the lateral point of treatment. Both, the Continuous Curtain and Funnel-and-Gate configurations are equally compatible with the new techniques to overcome the installation limitations mentioned earlier. The Funnel-and-Gate, however, has a greater influence on the ground-water flow than the continuous curtain.

2.1.5 Research Support, Regulatory Acceptance, and Application of PRB Technology

In-situ permeable reactive barriers have been placed in a number of sites, and a complete list of the same is given in Appendix A. The first, constructed at the CFB Borden in 1991 used zero-valent iron as the reactive media [Hocking et al., 1998]. The rapid increase in the number of barriers in the recent times clearly reflects the increasing inveterate maturity and acceptance of the invention. The U.S. Environmental Protection Agency has supported the development of PRBs by facilitating research collaboration. The concordance involves the National Risk Management Research Laboratory (NRMRL), the National Exposure Research Laboratory (NERL) of USEPA's Office of Research and Development (ORD), the Remediation Technologies Development Forum (RTDF) Permeable Reactive Barriers Action Team, and the USEPA's Technology Innovation

Office (TIO) [U.S.E.P.A., 1998]. Research on PRB's, supported by the Department of Defense (DOD) and the Department of Energy (DOE) has been in progress at the U.S. Department of Energy Grand Junction Office (GJO) since 1989 [U.S.D.E.G.J.O., 1998]. In addition, various institutions continue research work, funded by one or more government offices, on different aspects of PRB's.

Permeable Reactive Barriers are increasingly viewed as the final solution for many complex groundwater contamination problems [Korte *et al.,* 1997]. In fact, it is the only solution when the conventional approaches fail. An innovative technology, however, would not be a convincing remedy at a site, if it were not acceptable by the regulatory board. On considering a federal perspective, the USEPA recognizes this technology as having a significantly higher, contaminant attenuation to application cost ratio than other conventional approaches. The PRB had a significant advance when the "Chemical Treatment Wall" was identified as the preferred alternative in the Record of Decision (ROD) at a Superfund Site, the Sommersworth Municipal Landfill in Somersworth, New Hampshire. The USEPA, the Interstate Technology and Regulatory Cooperation (ITRC) Workgroup (Permeable Reactive Barrier Subgroup) and the Remediation Technologies Development Forum (RTDF) Permeable Reactive Barriers Action Team, figure actively among the institutions involved in evaluating, monitoring, providing guidance on, and defining regulatory implications associated with PRB installation and technology. The regulatory approach to the technology in many installations has been to treat PRBs as "at risk" remedies making the owner resort to conventional approaches if it failed. On a state perspective, California, with two Full-Scale-Installations (FSI) and two Pilot-Scale-Installations (PSI), Colorado, with two FSI and one PSI, Kansas, have accepted this innovative technology. New Jersey, Missouri, New York, North Carolina, Oregon, South Carolina, New Hampshire, Illinois, Florida, each with at least one installation, figure among the states that have accepted this technology (Appendix A).

This has made Permeable Reactive Barriers the most sought after innovative technology in the treatment of contaminated groundwater. In summary, the PRB technology seems to be a promising remedy for contaminant-free, potable, clean, groundwater, the installation of which would significantly increase in the future years. With the more long-term performance data becoming available, the regulatory acceptance of PRBs is expected to increase.

2.2 Simulation Techniques

A model is a simplified version of the real situation (field situation) which approximately simulates an excitation-response of the real system. A model can be either physical or mathematical. A mathematical model is a numerical expression of the conceptual model. Two basic approaches can be identified in the creation of a Mathematical Model:

1. The Analytical Solution involves the solving of differential equations, which represents the conceptual model, with appropriate initial conditions and boundary conditions. This is done manually and is possible only for simple problems.
2. The Numerical Solution involves solving of a system of algebraic linear equations, which represents the conceptual model, instead of the differential equations used in the previous approach. A computer is used for the computations by converging in the solutions. This approach is possible for

complex problems and is closer to the 'often used approach' than the previous.

A physical model simulates groundwater flow directly by using a scaled reproduction of the real world, by means of a Graphic User Interface (GUI). This study uses physical models for modeling permeable subsurface barrier applications.

The U.S. Environmental Protection Agency document entitled "Compilation of Ground-Water Models gives a comprehensive description of the modeling codes found suitable for groundwater flow and contaminant transport. According to the American Society of Civil Engineers (ASCE), a total of 54 different models are used by the state respondents and 45 by consultant respondents [Reddi, 1997]. In order to find an apt modeling code that supports a reactive barrier, extensive literature has been reviewed both on modeling PRB applications and on the modeling code, and the results are compiled in the adjoining Table 2. A review of previous information denotes that the codes that meet the requirements for simulation of a PRB system are the following:

- MODFLOW and its conjunction path tracking codes.
- FLOWPATH
- FRAC3DVS
- GROWFLOW
- Funnel-and-Gate Model (FGDM)
- FLONET

Table 2 Codes Used for the Simulation of PRBs

Modeling Code	Example PRB Applications and Comments	References
MODFLOW MODPATH	Sunnyvale, California; Mofett Federal Airfield, California; the Sommersworth Sanitary Landfill, New Hampshire; an industrial facility, Kansas; GE appliances, Wisconsin.	PRC, 1996; Battelle 1996.
FLOWNET	Not readily available.	
FRAC3DVS	Not readily available.	
FLOWPATH	Belfast, Northern Ireland; Fairchild Air Force Base, Washington; Doe Kansas City, Kansas	RTDF: Permeable Reactive Barrier Installation Profiles, 1998.
GROWFLOW	Have been developed recently for the U. S. Airforce to simulate and optimize the funnel and gate configurations. As of this dissertation they have not been applied anywhere.	Everhart, 1996.
FGDM		Hartfield, 1996

The most commonly used code to simulate PRB technology is MODFLOW [McDonald and Harbaugh, 1988], in mélange with contaminant tracking codes such as MODPATH [Pollock, 1989]. MODFLOW simulates 2D and quasi or fully 3D, transient groundwater flow in anisotropic, heterogenic layered aquifer systems. It calculates piezometric head distributions, flow rates, and water balances. It incorporates modules that handle flow towards wells, towards rivers, into drains and modules that handle evapotranspiration and recharge. In the market, there are a number of software that provide a user friendly and interactive Graphic User Interface. These textural and graphical pre and post-processors advocate easy use of the simulation code and explicitly manifest simulation results, and may include one of the following:

- GMS (Groundwater Modeling System) [Brigham Young University, 1996].
- Model Cad
- Visual MODFLOW [Waterloo Hydrogeologic, Inc.,1996]
- Groundwater Vistas
- Horizontal Flow Barrier (HFB)
- ZONEBUDGET

In addition, the following particle tracking codes incorporate results obtained by MODFLOW and are usually used in conjuncture:

- MODPATH
- PATH3D
- RWLK3D

2.3 Programs Used in the Study

2.3.1 Introduction

The computer simulation groundwater modeling code used in our study is the U.S. Geological Survey Modular, three-dimensional, finite-difference, groundwater flow model abbreviated as MODFLOW.

MODFLOW simulates two-dimensional and three-dimensional, transient groundwater flow in anisotropic, heterogeneous, layered aquifer systems (McDonald and Harbaugh, 1988). It calculates piezometric head distributions, flow rates and water balances. There are different modules provided for wells, rivers, drains, evapotranspiration and recharge.

It was only after a careful review of literature available on different codes, on grounds of user friendly interfaces, it was decided that the PRB system should be simulated using MODFLOW. The review process is documented later.

Two Graphical Interfaces were found to be suitable for Permeable Reactive Barriers, namely: GMS (Groundwater Modeling System) [Brigham Young University, 1996] and Visual MODFLOW [Waterloo Hydrogeologic, Inc., 1996]. The following section discusses them.

2.3.2 Visual MODFLOW

Visual MODFLOW was developed in August 1994 by the Waterloo Hydrogeologic Incorporation. "Visual MODFLOW is a fully integrated, 3D, graphical modeling environment for professional groundwater flow and contaminant transport modeling" [Waterloo Hydrogeologic, 1996]. It is a complete, user friendly, interactive Graphic User Interface (GUI), which provides an easy to use modeling environment for all practical applications in 3D groundwater simulation. Visual MODFLOW incorporates MODFLOW, MODPATH and MT3D96 in one integrated package, and is the software that supports the powerful graphical interface.

Visual MODFLOW Graphic User Interface, is divided into three separate modules, namely: the Input Module, the Run Module, and the Output Module. The Input Module allows the user to graphically assign all of the necessary input parameters for building the groundwater and transport model. The Run Module allows the user to modify MODFLOW, MODPATH, MT3D and options that are run-specific. The Output Module allows the user to display all the modeling and calibration results for

MODFLOW, MODPATH and MT3D. The various hydrogeologic properties that have to be assigned for modeling include hydraulic conductivity, specific yield, specific storage, porosity, observation and pumping wells and boundaries (boundary conditions). The boundary conditions can be set in the model by dropdown options such as constant head cells, recharge, rivers, drains, evapotranspiration, general head boundaries and walls (horizontal flow barriers).

Visual MODFLOW has separate packages to handle the above of head-dependant boundary conditions which are as follows:

2.3.2.1 Constant Head Boundary: In transient flows, the head sometimes remains constant over a specific period of time and might change between stress periods. Such conditions can be simulated by constant head boundary option.

2.3.2.2 River Boundary: The river package is used to simulate the flow of water between an aquifer and an underlying source reservoir, which is a river or a lake. The river package simulates a surface water body separated from the groundwater system by a layer of low permeability material. The river package uses the riverbed elevation, the river stage elevations and the conductance to determine the resistance to flow between the surface water body and the groundwater. The conductance is calculated from the length of the river (L), the width of the river (W) in the cell, the thickness of a riverbed sediments (M), and the hydraulic conductivity of the river bed material (K). The conductance, C, is then calculated by: $C = \frac{KLW}{M}$

2.3.2.3 General Head Boundary (GHB): This is similar to that of the river, drain, and evapotranspiration packages, except that the G.H.B. package provides no limiting value of head.

2.3.2.4 Drain Boundary: The drain package is used to simulate the effects of features such as agricultural drains, which remove water from the aquifer and reduce some fixed head or elevation. The drain package requires the drain elevation or the drain head, which is the elevation of the free surface of water within the drain above a datum and the conductance. It is usually adjusted during model calibration.

2.3.2.5 Wall Boundary: The horizontal flow barrier (HFB) simulates the effects of a thin, vertical, low permeability feature that impedes the horizontal flow of ground water. The thickness and the hydraulic conductivity of the wall define this impedance.

2.3.2.6 Recharge Boundary: Recharge which percolates into the groundwater system as a result of precipitation can be simulated by the recharge package. Recharge is applied to the top layer of a three-dimensional finite difference model. Recharge is specified as a rate (L_1/T). The code computes the volumetric rate of water added to the model by multiplying nodal recharge rates by the area of the top of the cell.

2.3.2.7 Evapotranspiration Boundary: This package simulates the effects of plant transpiration. When the elevation of the water table is beneath the first layer of the model, evapotranspiration from the water table ceases. It is assumed that plants draw water from the top layer only.

Further hydro-geologic boundaries are presented by the following three types of conditions:

Type 1. Specified head boundary (Dirichlet conditions) for which the head is specified in the model.

Type 2. Specified flow boundary (Neumann conditions) for which the derivative of head (flux) across the boundary is given.

Type 3. Head dependent flow boundary (Cauchy or mixed boundary conditions) for which flux cross the boundary is calculated given boundary head value.

The solution methods, which solve the matrix equation by MODFLOW, are found in the Strongly Implicit Procedure (SIP), the Slice Successive Over Relaxation method (SSOR), Precondition Conjugate Gradient Package (PCG2) and the Waterloo Hydrological Solver (WHS). Of these WHS is the most stable and fast.

In 1990 the MT3D (Modular Three-Dimensional Transport Model) code, written by Dr. C. Zheng, was introduced into the Visual MODFLOW integrated package to solve the transport equation. It is a computer model for simulation of advection, dispersion and chemical reactions of the contaminants in the groundwater systems. The MT3D was designed to be used in conjunction and to interface with a Block-centered finite-difference flow model such as MODFLOW. Various input parameters for MT3D involves assigning initial concentration, dispersion, chemical reactions, observation wells, and transport boundary conditions, each of which is described as follows:

Initial Concentration: An Initial concentration for all the cells is required by the MT3D. Initial concentration can also be set to zero. This allows the transport simulation to be started from the measured or simulated plume.

Dispersion: This allows the user to enter longitudinal dispersivity, horizontal to longitudinal dispersivity ratio, vertical to longitudinal dispersivity ratio and molecular dispersion coefficient. MT3D calculates the hydrodynamic dispersion coefficient as the product of the dispersivities and the velocity plus the molecular dispersion coefficient.

Chemical Reaction: It simulates the sorption and decay (biological and radioactive) of the contaminant. This input parameter makes Visual MODFLOW compatible with PRB.

Transport Boundary Condition: The boundary condition accommodated by the MT3D are: constant concentration, recharge concentration, evapotranspiration concentration and point source concentration for a relatively long period of time, whereas point source boundary condition can be assigned to existing flow boundaries, such as rivers, drains and wells.

2.3.2 Ground Water Modeling System

Though GMS (Groundwater Modeling System) [Brigham Young University, 1996] was initially selected as an alternative interface, owing to the suitability of Visual Modflow, was less extensively used in this study. However the author recognizes its suitability to the design PRB's, and hence has dedicated this subsection to describe it briefly.

The Department of Defense Groundwater Modeling System is a powerful and comprehensive package with routines for creating and modifying input, executing, and analyzing output model finite-difference and finite-element grids, the design of the software encourages the user to generate these grids automatically from data entered in other modules. The Map module allows the user to read a tagged image format (tif) file or a drawing exchange file (dxf) and draw polygons representing hydrologic boundaries, attributes such as recharge, and material properties. The Subsurface Characterization Module can be used to construct stratigraphic interpretations from borehole or scatter data. Fence diagrams and cross sections can be displayed. Advanced scientific visualization and animation functionality can be used to investigate and display properties and processes associated with a model. GMS runs a graphical environment and executes the models in DOS protected mode.

CHAPTER 3

MODEL APPROACH

3.1 Establish Generic Design Criteria

To aid in the design of a Permeable Reactive Barrier System and to illustrate the ground water flow system at a site, a groundwater flow model was constructed using non site-specific geologic and hydrogeologic data, identified in the site characterization section. The steps involved in the construction and execution are discussed under the following headings:

3.1.1 Conceptual Model Development

The conceptual model is a three-dimensional representation of groundwater flow and contaminant transport, and thus must include all available geologic, hydro geologic, and geo-chemical data from the site. The conceptual model integrates the data with the groundwater system to be modeled and thus it becomes imperative to include geologic, topographic, and contaminant concentration and distribution maps, in-addition to chemical and physical parameters associated with aquifers.

The conceptual model in this instance was identified to fall into different basic cases depending on the available geologic, geo-chemical site data and the current applications of PRBs to contaminant plumes (Appendix A). These cases were used in the simulation model and interface selection, conceptual model construction and simulation. It was modeled to throw light on the modeling procedure and approach.

The groundwater in a site could be retained in an aquifer confined between two

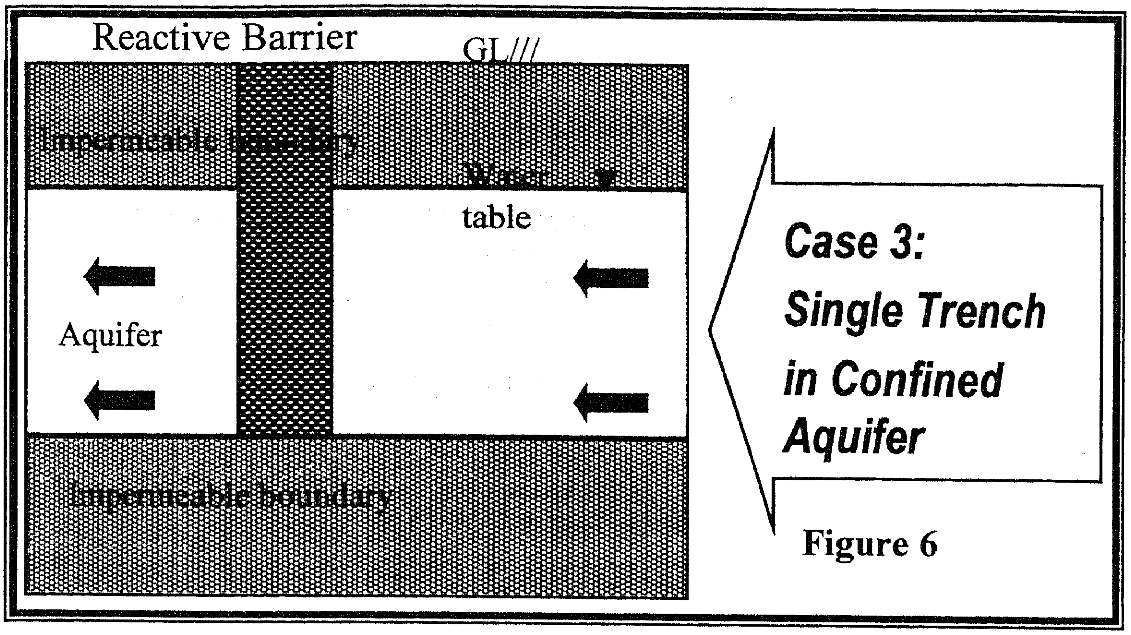


Figure 6 Single Trench in a Confined Aquifer

aquitards (Figure 6) and hence known as confined or as was the usual case, could be retained in an aquifer that had the water table as the upper boundary (Figure 7).

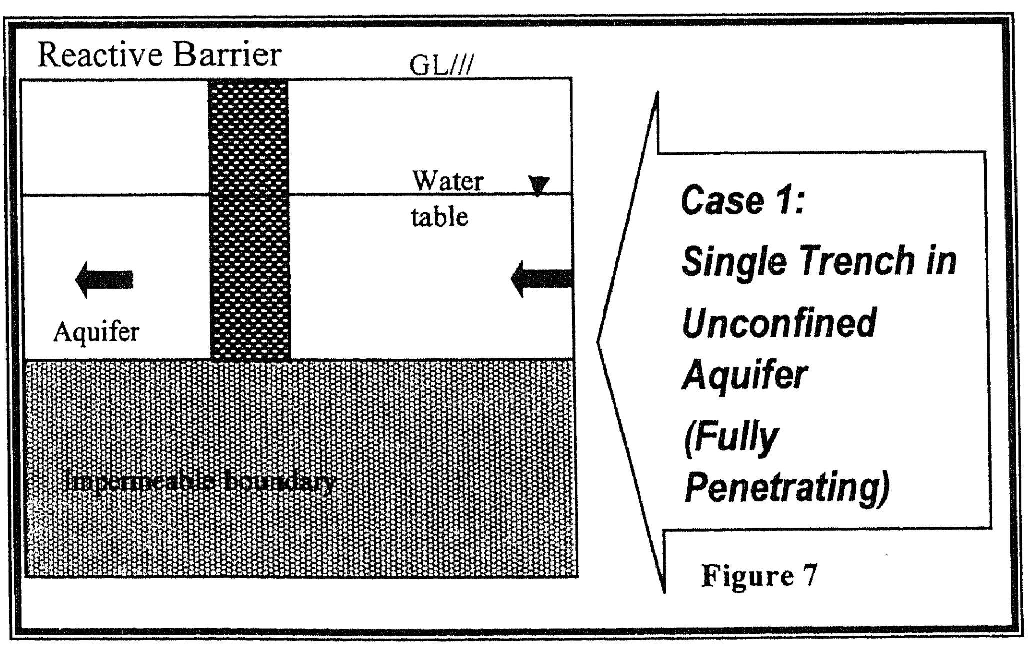


Figure 7 Single Trench in Unconfined Aquifer (Fully Penetrating)

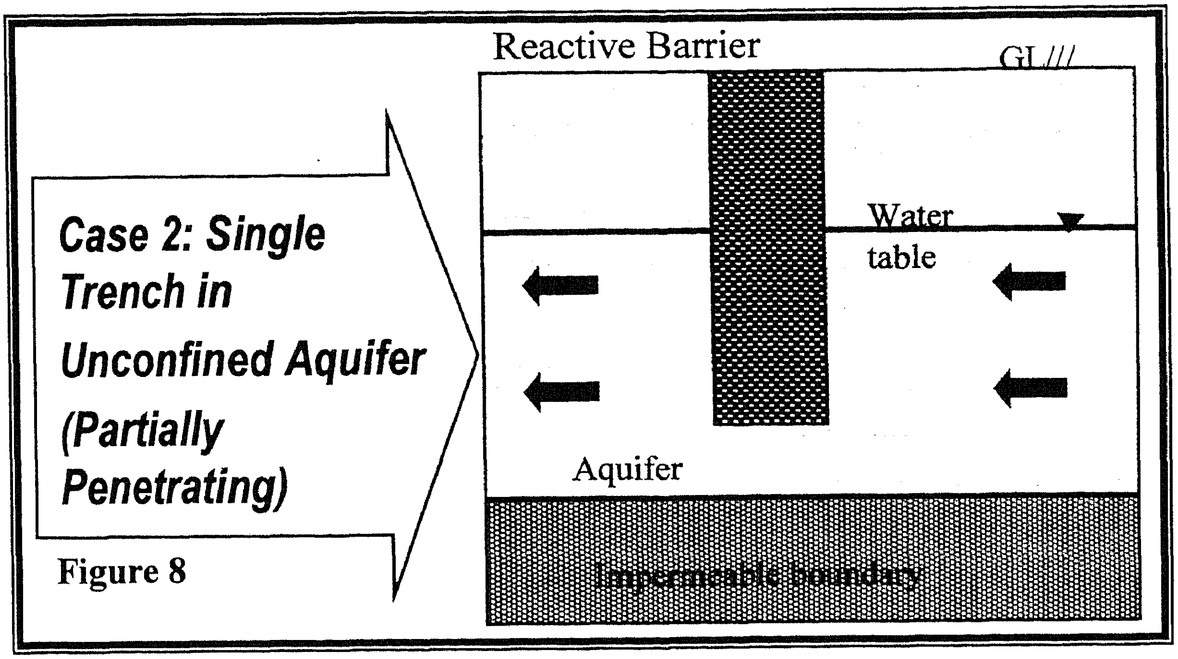


Figure 8 Single Trench in Unconfined Aquifer (Partially Penetrating)

This resulted in two cases of the PRB i.e. *Single Trench in Unconfined Aquifer and Single Trench in Unconfined Aquifer.* In an unconfined aquifer, sometimes when the

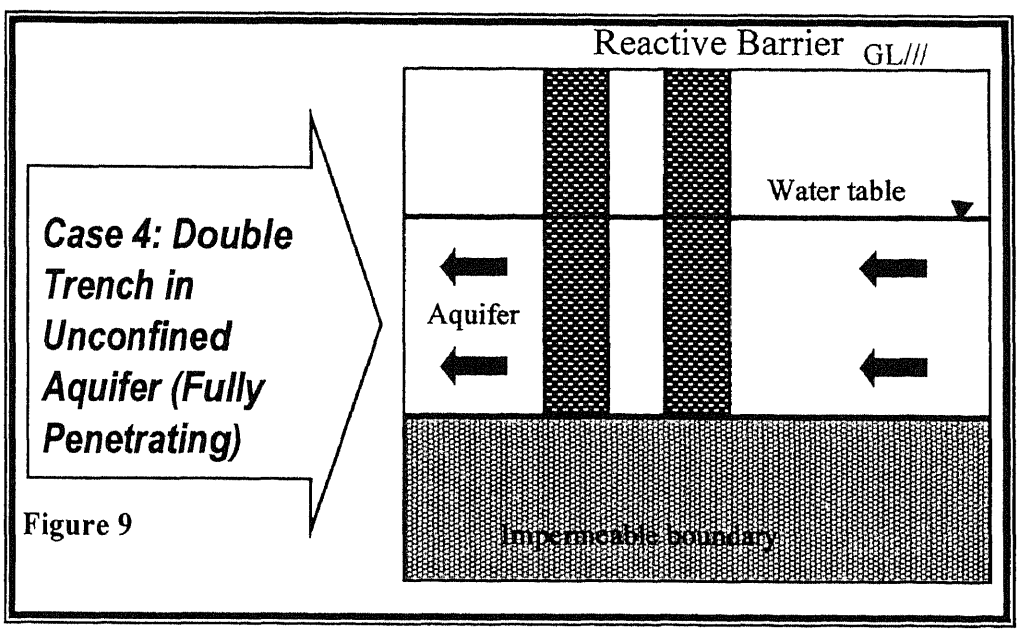


Figure 9 Double Trench in Unconfined Aquifer (Fully Penetrating)

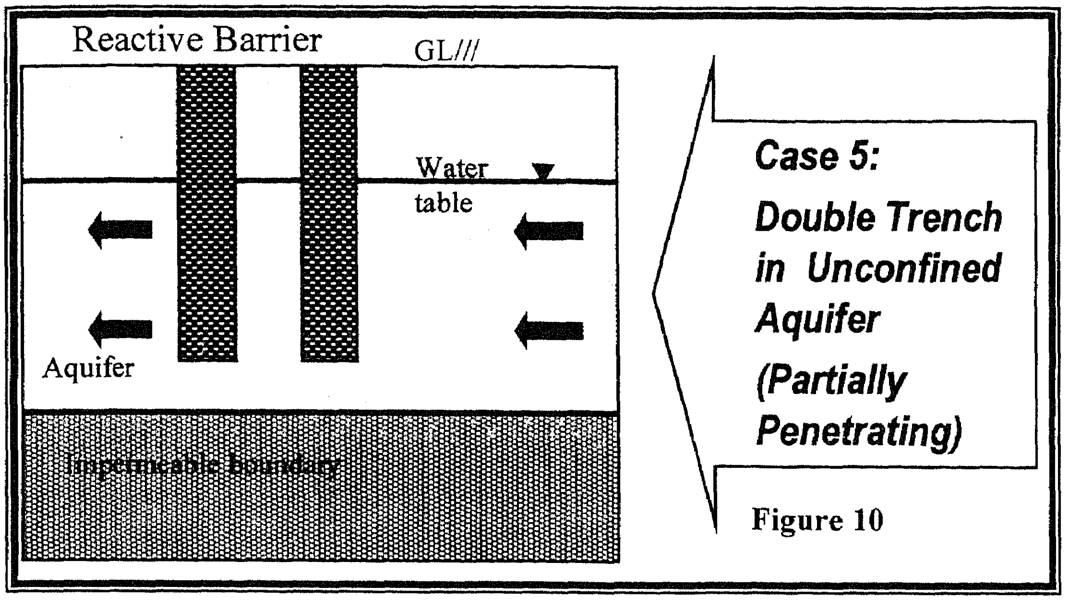


Figure 10 Double Trench in Unconfined Aquifer (Partially Penetrating)

confining bed may be very deep, or the aquifer may be vertically isotropic with the hydraulic conductivity increasing with depth, or for plain economics the PRB could be

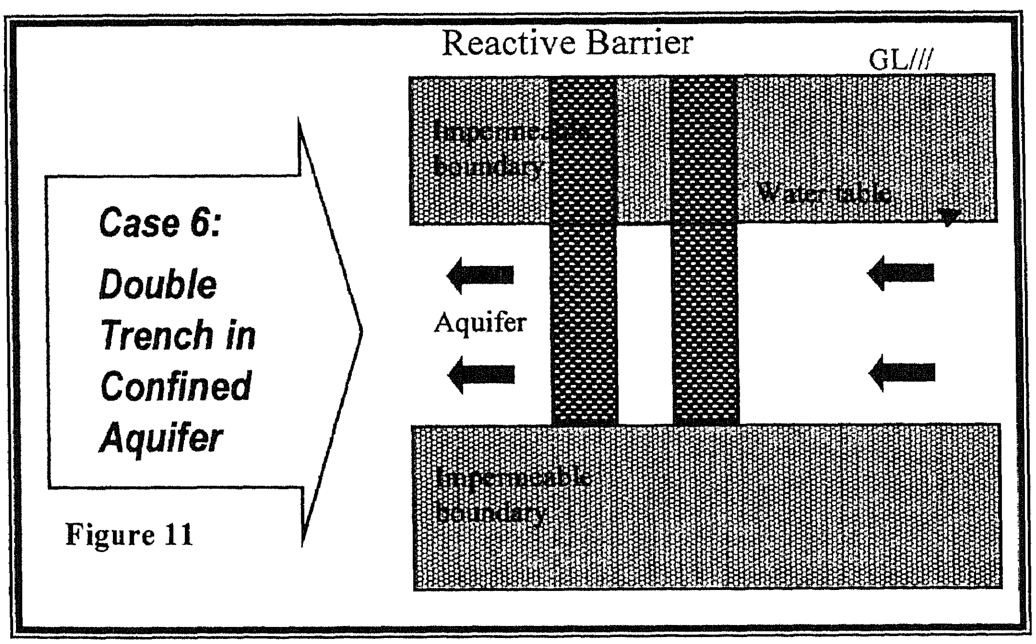


Figure 11 Double Trench in Confined Aquifer

hanging as shown in Figure 8. This resulted in a new case i.e. *Single Trench in Unconfined Aquifer (Partially Penetrating)*.

In the case study, and often in existing applications a change in the pH is necessitated. For instance in the reaction of Fe^0 and Chromium contaminants, the reduction and precipitation of Cr(VI) has been observed at pH > 10 (Blowes *et al.*, 1995; Powell *et al.*, 1995). The pH level of the New Jersey leachate samples from the site is close to 12 (Case Study). However, it is only at lower pH levels that an appreciable reaction rate can be attained. The concurrent geo-chemical study had identified that a pH between 9-9.5 facilitates a high reaction rate between Fe^0 and the chromium contaminant. This had led the research team to think in the lines of a double trench PRB against the single trench convention. This resulted in three additional cases, Figure 9, Figure10, Figure 11 corresponding to the double trench structure of the previous three cases. These cases have been modeled and documented later in this thesis.

The generic conceptual cases could be summarized as follows and are shown in

- *Case 1*: Single Trench in Unconfined Aquifer (Fully Penetrating)
- *Case 2:* Single Trench in Unconfined Aquifer (Partially Penetrating)
- *Case 3:* Single Trench in Confined Aquifer
- *Case 4:* Double Trench in Unconfined Aquifer (Fully Penetrating)
- *Case 5:* Double Trench in Unconfined Aquifer (Partially Penetrating)
- *Case 6:* Double Trench in Confined Aquifer

Figure 12 Conceptual Models

These cases are shown in Figure 13, respectively and are referred to as Conceptual Generic Cases in this study.

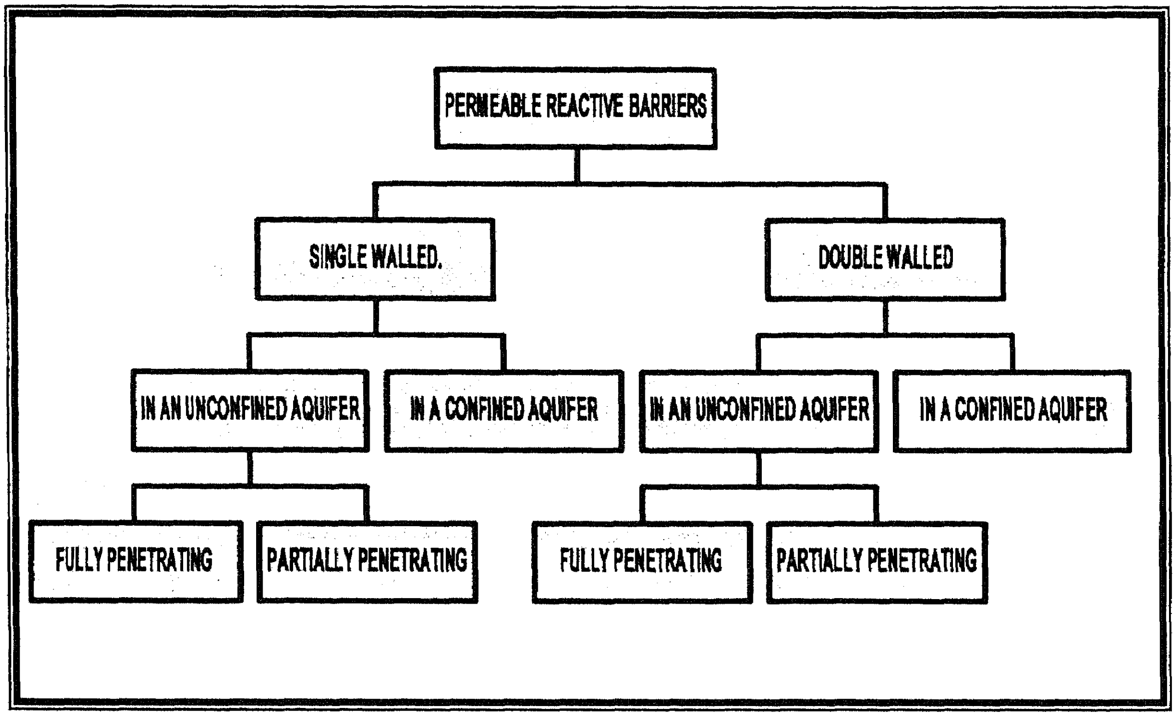


Figure 13 Conceptual Models

3.1.2 Simulation Code Interface Selection

In our study, two of the above mentioned Graphical Interfaces were used in this study, namely, GMS (Groundwater Modeling System) [Brigham Young University, 1996]; Visual MODFLOW [Waterloo Hydrogeologic, Inc., 1996].

The selection of the interfaces resulted from a two-tier review.

3.1.2.1 Selection of the Simulation Code: In addition to MODFLOW, the other codes evaluated were FLOWPATH, FRAC3DVS, GROWFLOW, Funnel-and-Gate Design

Model (FDGM) and FLOWNET were evaluated. The issues identified with these codes is shown in Table 3.

3.1.2.2 Selection of the Simulation Code Interface: Since the Simulation Code Interfaces for Modflow available were all equally user-friendly and graphically illustrative, the selection criteria was based more or less on the output presentation and their popularity in the simulation community.

Table 3 : Evaluated Simulation Codes and their Issues

CODE	ISSUES
FLOWPATH	**Could not be used to simulate a PRB when the "Partially Penetrating" case is to be simulated. In this case the groundwater flow is very complex and transient flow is to be simulated.**
FRAC3DVS	**The use of the this involves complex features that are not required to simulate simple flow through the PRB to be designed.**
GROWFLOW	**This code incompletely addresses different aspects of flow simulation. It is still under development and the use of the developed portion is a little too difficult to comprehend.**
FDGM	**This as the name states is better suited to the simulation of a Funnel-and-Gate configuration barrier. It would have been a prospective choice if this study included the configuration simulation.**
FLOWNET	**Though this code enables easy usage it is better suited for the Funnel-and-Gate configuration.**

CHAPTER 4

MODELING RESULTS

4.1 Model Construction and Calibration

As in every simulation the primary step is to establish, calibrate and develop a conceptual model. The Model Construction and Calibration was conducted after we had re-evaluated the Modflow code interfaces available in the market. This section highlights the procedure and assumptions employed in the Model Construction and Calibration.

4.1.1 Generating the Model Grid

With the generic cases in mind we established the site area to a 500m square. The first step in modeling is to choose a proper grid size. Since we were considering a 500m square, a grid interval of 10m was considered appropriate. The grid however had to be refined in parallel to the barrier to incorporate a barrier thickness of 2m (Figure 14). This could be refined further to increase and decrease thickness.

It is usually recommended that the grid be designed such that the Peclet number is less than 4 (Huyakorn and Pinder, 1983). The Peclet number is defined as:

$$P = \frac{\Delta l}{\alpha}$$ where Δl is nodal spacing and α is dispersivity

The Peclet number for the grid designed in this study area varied from 1m to 10m (Δl varied from 80m to 800m and α was 80m).

Perpendicular to the ground surface the model was divided into 5 layers. The hydraulic gradient has been reported as 0.04-0.10. The lower limit when considered produces a difference in head of 20m between the two ends of the conceptualized site. To

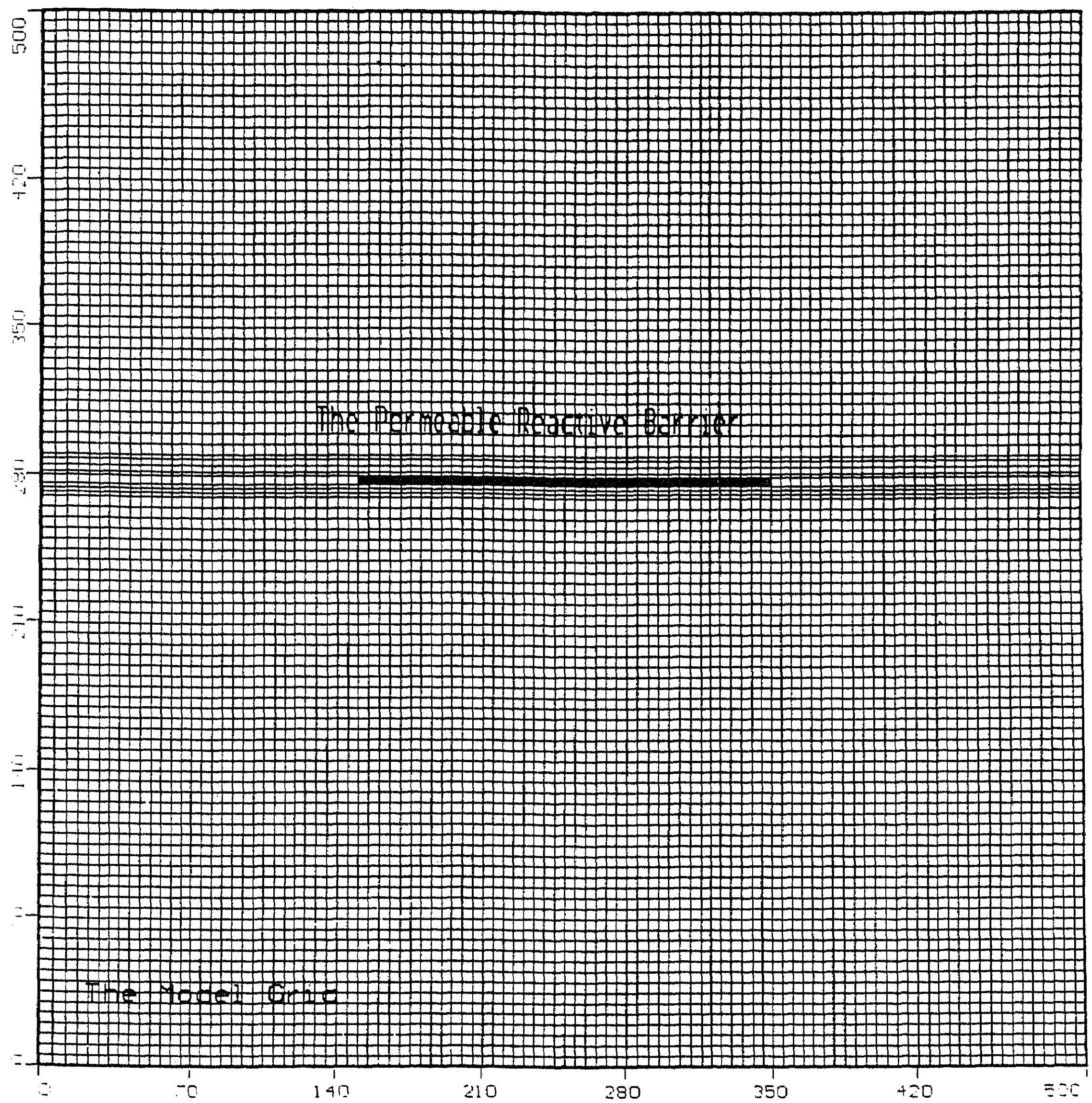


Figure 14 The Model Grid

incorporate this in the model, the depth of the aquifer is assumed to be higher than in reality. Each layer was thus integrated with a depth of 5m (Figure 15).

Elevations for the various layers were taken from the cross section drawings provided. The data was then entered into a plotting software (Surfer), and then imported to Visual Modflow. The model could thus simulate both the effects of the above mat unconfined and below mat confined aquifer systems (Figure 16).

The shallow aquifer is the unconfined aquifer since the water table forms the upper boundary. The deep aquifer between the less permeable meadow mat and aquitard, whose thickness varies greatly, is the confined aquifer. The aquitard is mostly made of less permeable clay beds.

4.1.2 Model Properties

Each cell in the model is assigned values, for hydraulic conductivity, storage, specific yield and porosity, as reported and discussed earlier. Three-dimensional isotropy has been assumed in the conceptual model to facilitate the design of the barrier.

4.1.2.1 Effective and Total Porosity: The effective porosity (n) of 0.3 is reported as a reasonable assumption by Tetra Tech NUS, Incorporation (letter dated 23rd October). It is closely related to total porosity and is almost the same (in the site under question). It is a reasonable assumption for a variety of soils.

4.1.2.2 The Hydraulic Gradient: The hydraulic gradient in the various installations reported in Appendix A ranges from 0.04-0.10. The lower limit when considered produces a difference in head of 20m between the two ends of the conceptualized site. To incorporate this in the model, the depth of the upper unconfined aquifer is considered higher than in reality.

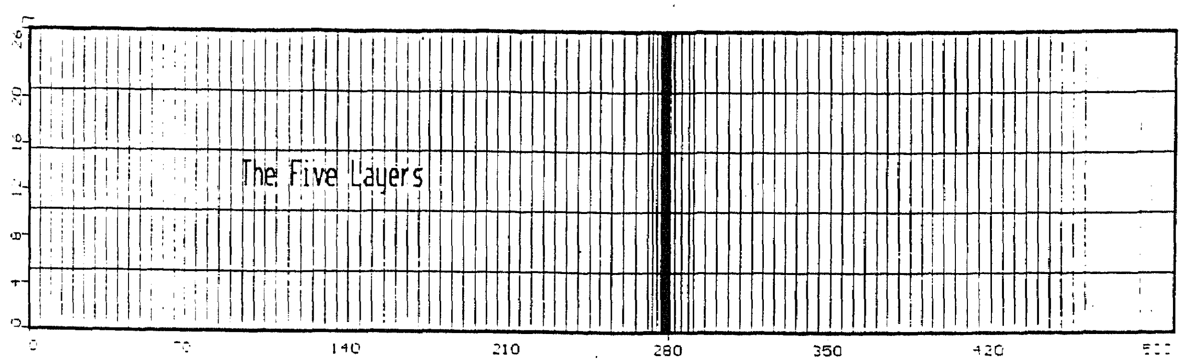


Figure 15 The Five Layers in Columnar View

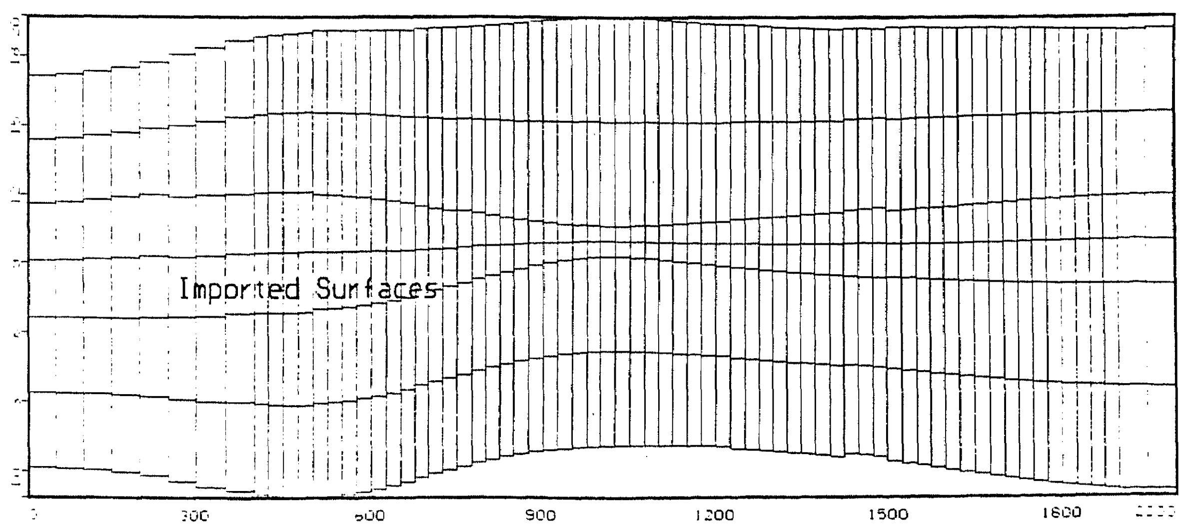


Figure 16 Imported Surfaces

4.1.2.3 Specific Storage and Storage Coefficient: Specific Storage (S_s), is used by the Visual MODFLOW interface to compute the Storage Coefficient (S) using the following equation:

$S = S_s \times b$ where S is the Storage coefficient, b is the layer thickness and S_s is the Specific Storage.

Numerous references illustrate the Storativity or Storage Coefficient (S) as the following (Powers, 1992):

1. Unconfined: S ~ 0.20
2. Confined: S ~ 0.001 (Fetter, 1991)

For an unconfined aquifer the storage term known as Specific Yield (S_y) equal to the Storativity. In the model Specific Storage and Specific Yield are taken as 1e-4 /ft and 0.2 respectively.

4.1.2.4 Hydraulic Conductivity: The hydraulic conductivity, calculated from slug tests on numerous wells in the Study Area 6 are presented in Table 19. Although a number of wells were present only 16 of them were considered as they were located in the area of interest and showed contamination. Four of these wells are deep wells and the remaining twelve are shallow wells.

In the case study, the conductivity of the unconfined aquifer was taken as 9e-6m/s, the average of the above meadow mat values of conductivity reported. The average of the below mat values is 1.4e-5m/s and was used as the hydraulic conductivity of the confined aquifer. The hydraulic conductivity (K) for the mat was taken as 6e-8m/s. The hydraulic conductivity in the X direction, Y direction and Z direction was assumed to be the same.

4.1.3 Model Boundary Conditions

Of the three boundary conditions, Dirichlet, Neumann, and Cauchy, Dirichlet conditions (constant head) were assumed. In transient flows, the head sometimes remains constant over a specific period of time and might change between stress periods. The constant head boundary option was adopted to simulate such conditions.

Since the recharge has not been reported, we assume a recharge of 100 mm/yr considered for a time period of 7300 days and assign it to every cell, when assigning model properties. To simulate a hydraulic gradient of 0.04, a constant head boundary condition of 25m and 5m is assigned to the top and bottom ends of the model. Since the area considered in the design of the barrier is a square of 500m × 500m, the sides are considered impermeable. It has been assumed that no activity had taken place at the site and the heads remain the same in the model and hence steady state simulations were performed during flow modeling.

4.1.4 Contaminant Particles

To study the sensitive parameters like hydraulic conductivity ratios, hydraulic gradient, barrier length, barrier thickness etc. the pathlines of contaminants become requisite in evaluation. Featuring an arbitrary large number of particles (50 particles) increases sensitivity of the model to slight changes in contaminant pathlines.

4.1.5 Flow Simulations

After discretizing the site and assigning the parameters to the model, flow simulations were carried out. All the flow simulations discussed in this study were performed using

Visual MODFLOW version 2.7.2 on a 400 MHz, 128 MB RAM, 15 GB hard drive, Pentium computer. All the simulations used Waterloo Hydrogeologic Solver (WHS). The convergence parameters are listed in Table 4. Details regarding the solver is not elaborated in this report but can be found in user's manual (Guiguer and Franz, 1996; Waterloo Hydrogeologic, version 2.70), however a brief explanation of the solver parameters is given in this report.

4.1.5.1 Explanation of the Solver Parameters: Nilson Guiguer and Thomas Franz have illustrated the solver parameters in the User's Manual for Visual Modflow (Guiguer and Franz, 1996; Waterloo Hydrogeologic, version 2.70). "The solver parameters illustrated the WHS solver works on a two-tier approach to a solution at one time step. Outer iterations are used to vary the factorized parameter matrix in an approach toward the solution. An outer iteration is where the hydro-geologic parameters of the flow system are updated (i.e., transmissivity, saturated thickness, storativity) in the factorized set of matrices. Different levels of factorization allow these matrices to be initialized differently to increase the efficiency of solution and model stability. Inner iterations are used to iteratively solve the matrices created in the outer iteration.

Maximum number of Outer (non-linear) Iterations: [Default = 100]

This parameter provides an upper limit on the number of outer iterations to be performed. The maximum number of iterations will only be used if a convergent solution is not reached beforehand. Fifty (50) iterations should be more than adequate for most problems. However, if the maximum number of outer iterations is reached an appropriate mass balance error is not achieved, this value should be increased.

Maximum number of Inner Iterations: [Default = 25]

This parameter provides an upper limit on the number of inner iterations to be performed. This number of iterations will only be used if a convergent solution for the current set of matrices in the "outer" iteration is not reached beforehand. 500 inner iterations should be more than adequate for most problems. However, if the maximum number of inner iterations and an appropriate mass balance error was not achieved, this value can be increased.

Head Change Criterion for Convergence: [Default = 0.05]

After every outer iteration is completed, the solver checks for the maximum change in the solution at every cell. If the maximum change in the solution is below a set of convergence tolerance (set here in the working units of feet or meters) then the solution has converged and the solver stops, otherwise a new outer iteration is started. A solution accurate to 0.01 [ft or m] will normally be sufficient for most problems unless the maximum head change throughout the modeled domain is smaller than 1 ft. or 1 m. If an appropriate mass balance is not achieved and the number of inner and outer iterations is within the maximums, this value can be decreased by an order of magnitude.

Residual Criterion For Convergence: [Default = 0.005]

While the head change criterion is used to judge the overall solver convergence, the residual criterion is used to judge the convergence of the inner iterations for the solver. If the change in successive inner iterations of the solver. If the change in successive inner iterations is less than the tolerance specified here (in working units of ft or meters), then the solver will proceed with the next outer iteration. This residual criterion for convergence of 0.001 should be appropriate for most of the problems.

However, if you notice that only a few inner iterations being performed for every outer iteration and an appropriate mass balance is not achieved, this parameter value can be decreased by one or more orders of magnitude.

Dampening Factor for the Outer Iterations: [Default = 0.5]

This factor allows the user to reduce (dampen) the head change calculated during each successive outer iteration. For most "well posed" and physically realistic groundwater flow problems, the dampening factor of one will be appropriate. This parameter can be used to make a non-convergent (oscillating or divergent) solution process more stable such that a solution will be achieved. This is done by decreasing the dampening factor to a value between 0 and 1 (only rarely < 0.6). This parameter is similar to "acceleration parameters" used in other solvers.

Relative Residual Criterion: [Default = 0]

This parameter provides another method of checking for convergence of the inner iteration. This method compares the residual from the most recent inner iteration to the residual from the initial inner iteration. Once the most recent inner iteration residual is below the initial inner iteration residual times, the relative residual criterion, the current outer iteration is completed and a new outer iteration will be started. For instance:

If most recent inner Iteration residual < initial inner iteration residual * relative residual criterion

Factorization Level: [Default = 1]

Factorization levels allows the matrices to be initialized differently to increase the efficiency of the solution and model stability".

4.1.6 Calibration

The trial-and-error calibration process was followed. In trial-and-error calibration, parameter values as reported by Tetra Tech NUS, Inc. and literature were initially

Table 4 Solver Convergence Parameters

Maximum number of outer iterations	**100**
Maximum number of outer iterations	**25**
Head change criterion for convergence	**0.05**
Residual criterion for convergence	**1**
Relative residual criterion	**0**
Factorization level	**1**

assigned to the grid. During calibration, parameter values were adjusted in sequential runs to match the simulated heads with the measured field heads.

Water levels for the year 1998 provided by Tetra Tech NUS, Inc. were used for calibrating the flow model. The parameters which were changed during calibration were the hydraulic, the vertical hydraulic conductivity, and the hydraulic conductivity of the aquifers in the X & Y direction. Other parameters like the recharge, initial and boundary conditions were not changed.

For each case, comparisons of model head and observed heads at nodes corresponding to monitoring wells were made during calibration. Comparison between the measured and simulated heads provide some idea of the spatial distribution of error in calibration. Average of the differences between the measured and simulated heads is a common way of reporting calibration results. The average difference between the observed and simulated heads can be expressed as the mean error (*ME*) and the root mean square (*RMS*) error is described as square root of the average of the squared differences in measured (h_m) and simulated heads (h_s), which is as follows:

$RMS = \left[1/n \sum_{i=1}^{n} (h_m - h_s)_i^2 \right]^{0.5}$ where h_m is the measured head and h_s the is simulated head During calibration the average difference between the simulation and observed head expressed was observed to be less than 5 %.

4.2 Model Execution

After the model has been calibrated to observed conditions, the model can be used for interpretive or predictive simulations. In the former, the parameter determined during calibration can be used to predict the response of the flow system to future events, such as the decrease in K over time or the effect of pumping in the vicinity of the PRB. A number of research papers have addressed these topics and hence this study was directed to design curves that could be used to design the barrier for different barrier and aquifer properties. This chapter discusses the execution of the model varying various parameters professed as critical.

The predictive requirements of the model determined the need for a steady-state simulation. Model output and Hydraulic heads were interpreted through the use of a Visual Modflow integrated contouring package and were applied to particle-tracking simulations to calculate and visualize ground water pathways, contaminant pathways, and fluxes through the cell. Established travel time through the cell was a key modeling result that was used to determine the thickness of the permeable cell in the case study.

Once the flow model was calibrated, the model was executed and sensitivity analysis was performed. During sensitivity analysis the effect of different parameters on the loss of a single trench fully penetrating barrier influent contaminant particles was studied. Loss of contaminant particles is calculated from the "contaminant path-lines". The loss percentage can be calculated from the following formulae:

$$N_{influx} = N_{thru} + N_{loss}$$

$$\text{Loss (\%)} = \frac{N_{loss}}{N_{influx}} \text{X } 100 \quad \text{Where}$$

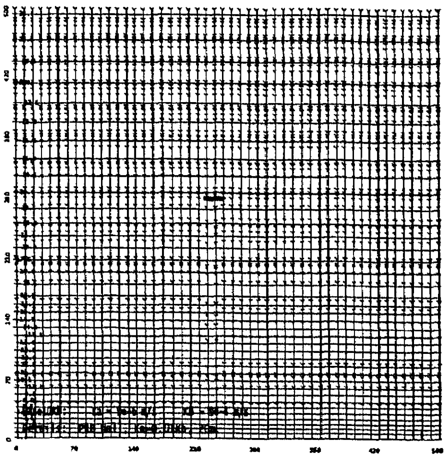
N_{influx} = Number of contaminant path-lines originating between the x-ordinates of the beginning and the end of the barrier

N_{thru} = Number of contaminant path-lines that pass through the barrier

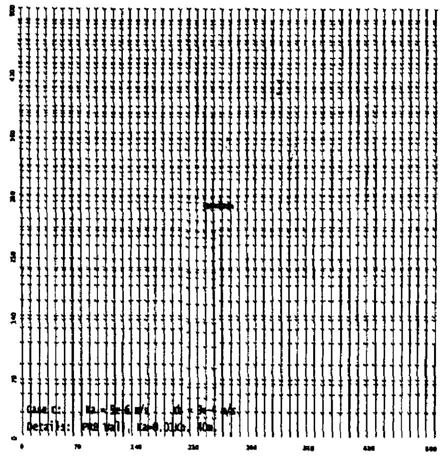
N_{loss} = Number of contaminant path-lines that originate between the x-ordinates of the beginning and the end of the barrier but do not pass through it

Figure 17, Figure 18 and Figure 19 show explicitly the execution of the model and a sample calculation of the loss % is presented in Appendix B.

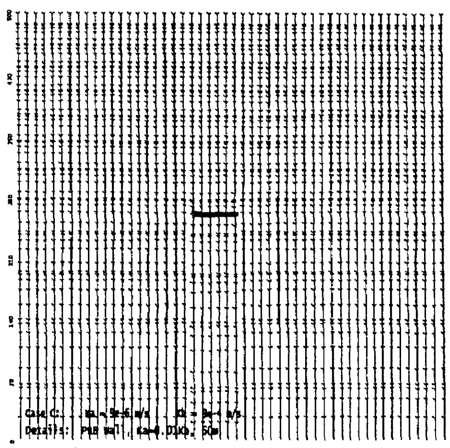
The sensitivity analysis was performed on the various generic cases identified earlier (Figure 12). This is described in Section 4.3. The design curves, which are plot of the loss % versus the different 'thought to be critical' parameters, are described in Section 4.5.



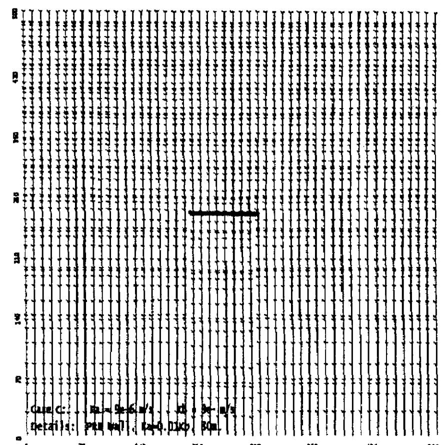
(a) Ka=0.01Kb, Length 20



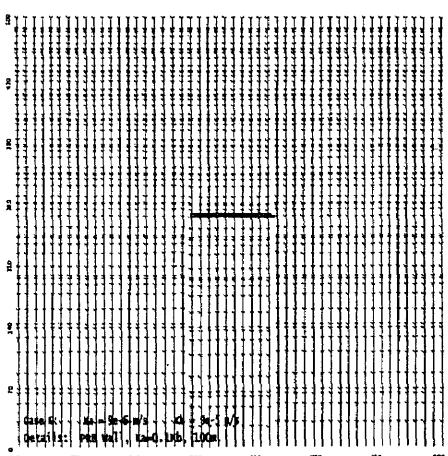
(b) Ka=0.01Kb, Length 40



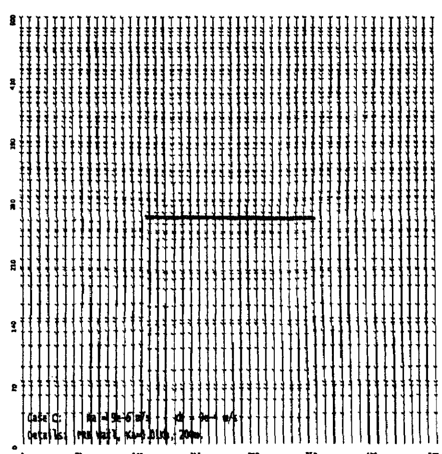
(c) Ka=0.01Kb, Length 60



(d) Ka=0.01Kb, Length 80

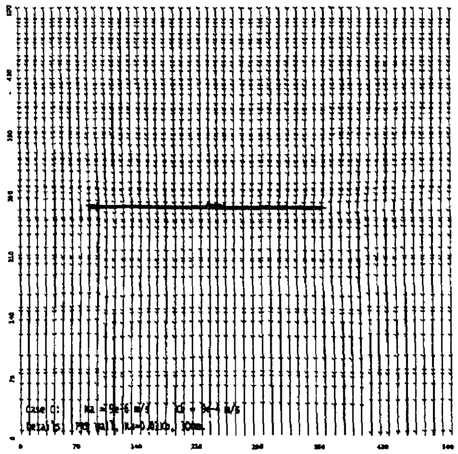


(e) Ka=0.01Kb, Length 100



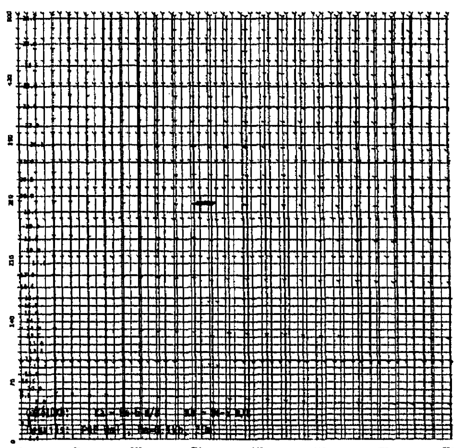
(f) Ka=0.01Kb, Length 200

Figure 17 Visual modflow Runs for Varying Lengths of Barrier at varying Aquifer to Barrier Hydraulic Conductivity Values.

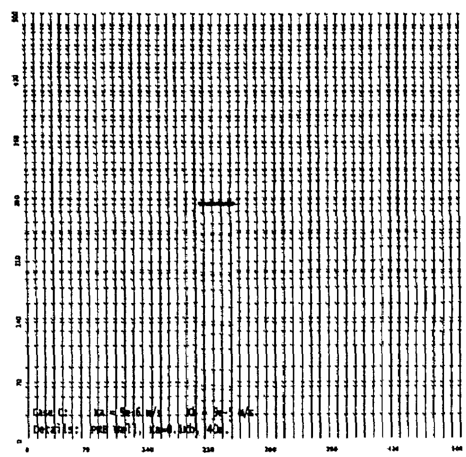


(g) Ka=0.01Kb, Length 300

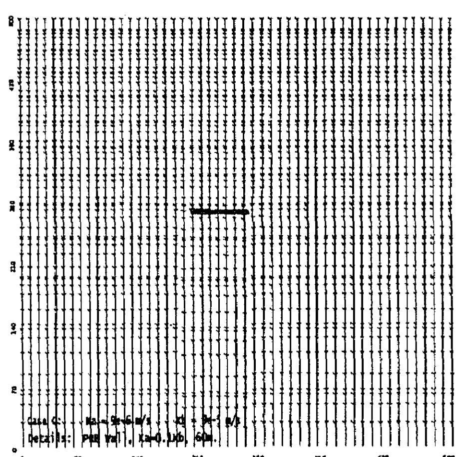
(h) Ka=0.01Kb, Length 400



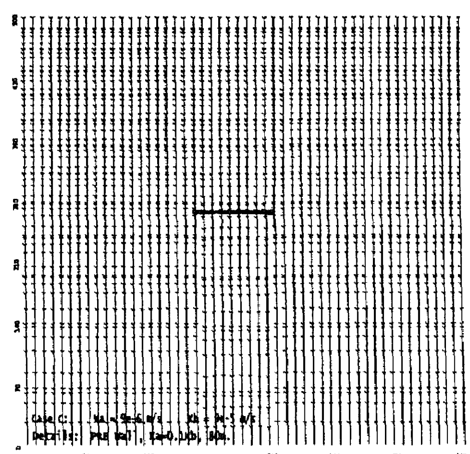
(i) Ka=0.1Kb, Length 20



(j) Ka=0.1Kb, Length 40

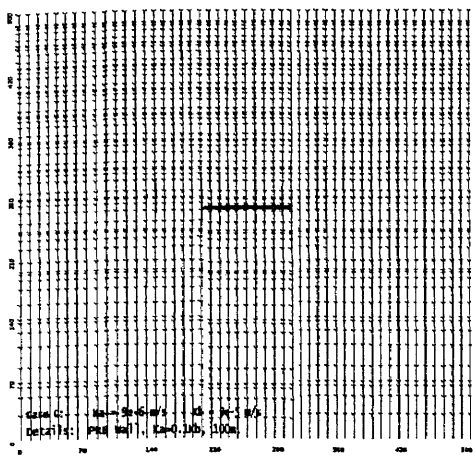


(k) Ka=0.1Kb, Length 60

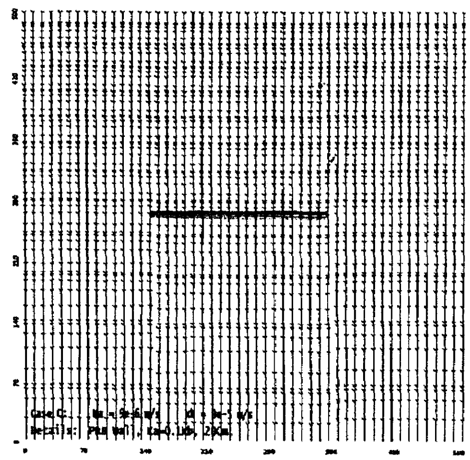


(l) Ka=0.1Kb, Length 80

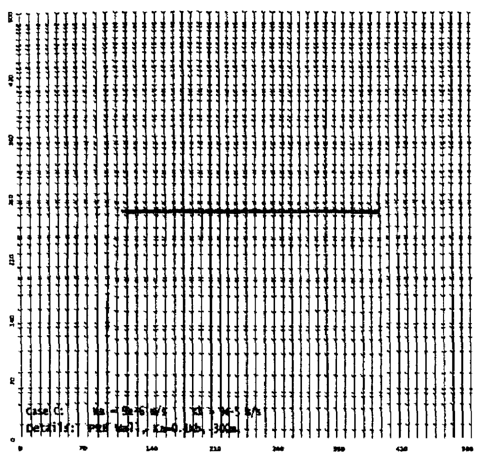
Figure 17 Visual modflow Runs for Varying Lengths of Barrier at varying Aquifer to Barrier Hydraulic Conductivity Values.



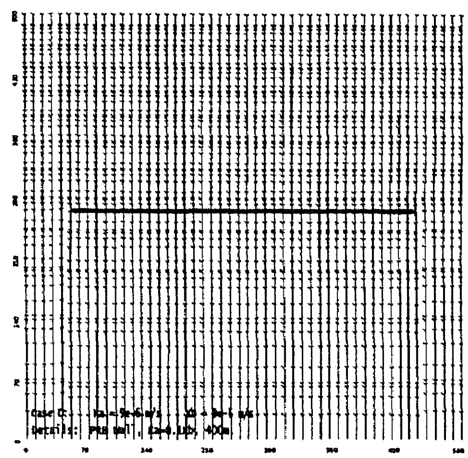
(m) Ka=0.1Kb, Length 100



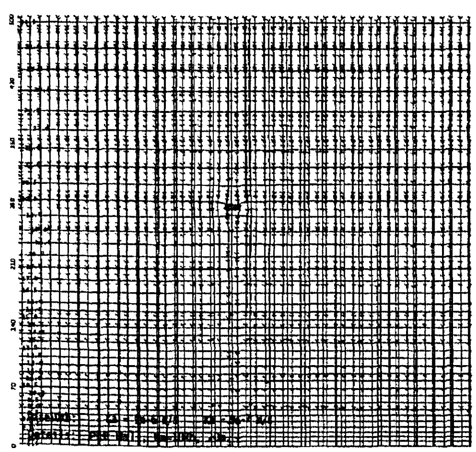
(n) Ka=0.1Kb, Length 200



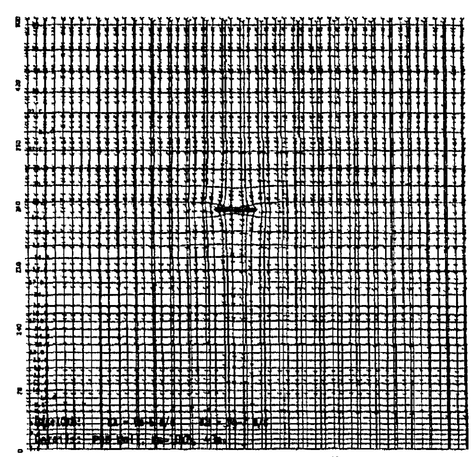
(o) Ka=0.1Kb, Length 300



(p) Ka=0.1Kb, Length 400

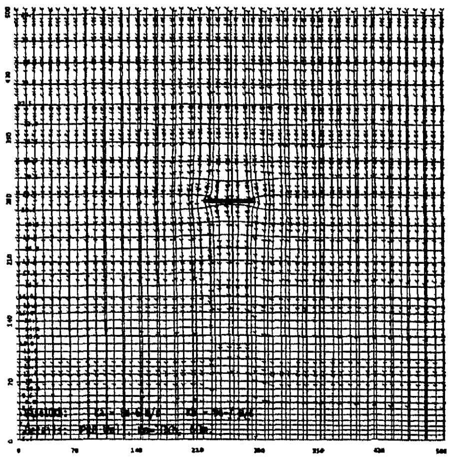


(q) Ka=10Kb, Length 20

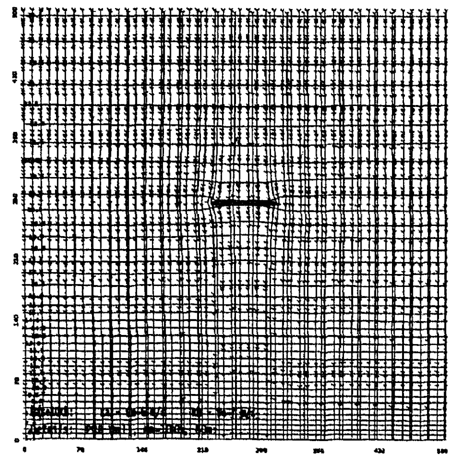


(r) Ka=10Kb, Length 40

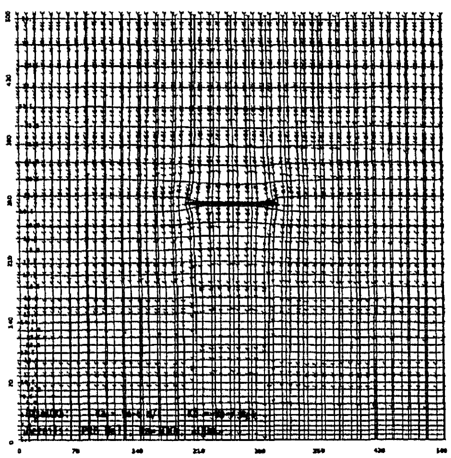
Figure 17 Visual modflow Runs for Varying Lengths of Barrier at varying Aquifer to Barrier Hydraulic Conductivity Values.



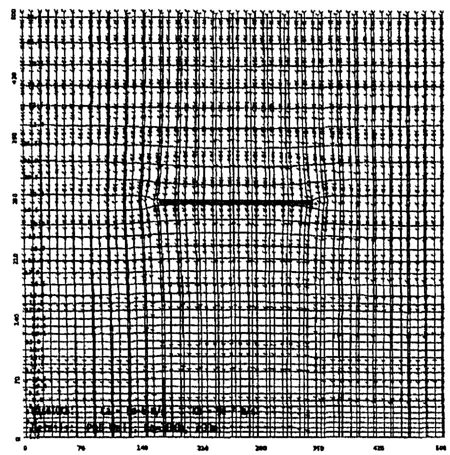
(s) Ka=10Kb, Length 60



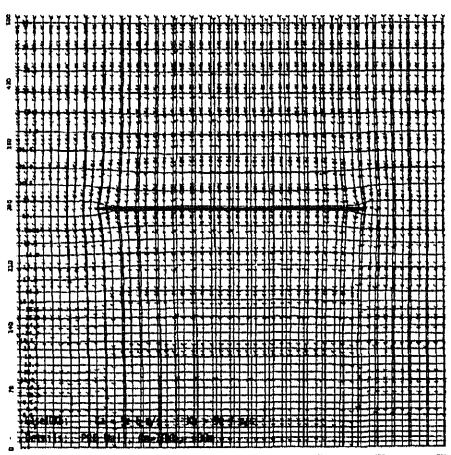
(t) Ka=10Kb, Length 80



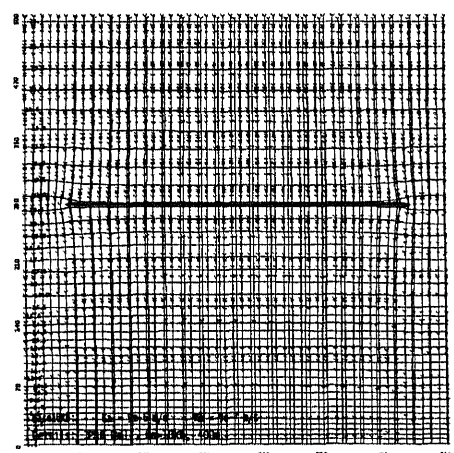
(u) Ka=10Kb, Length 100



(v) Ka=10Kb, Length 200

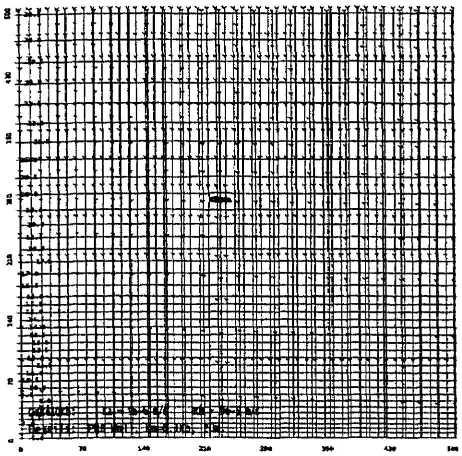


(w) Ka=10Kb, Length 300

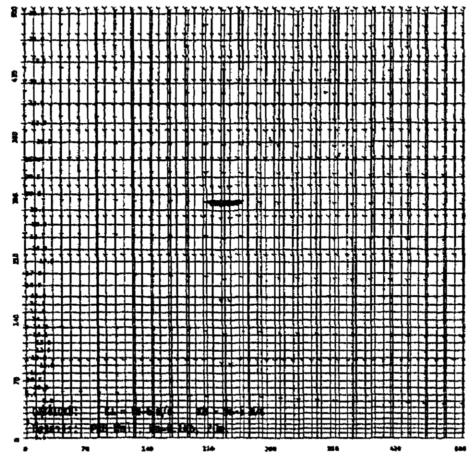


(x) Ka=10Kb, Length 400

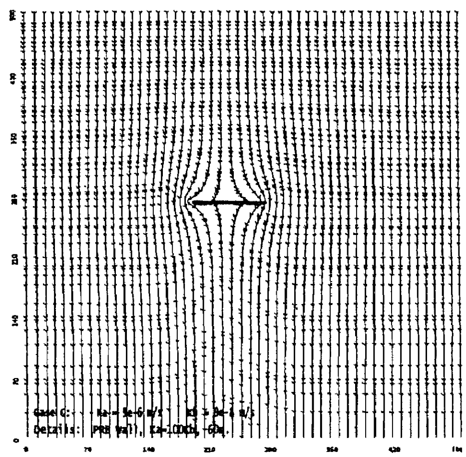
Figure 17 Visual modflow Runs for Varying Lengths of Barrier at varying Aquifer to Barrier Hydraulic Conductivity Values.



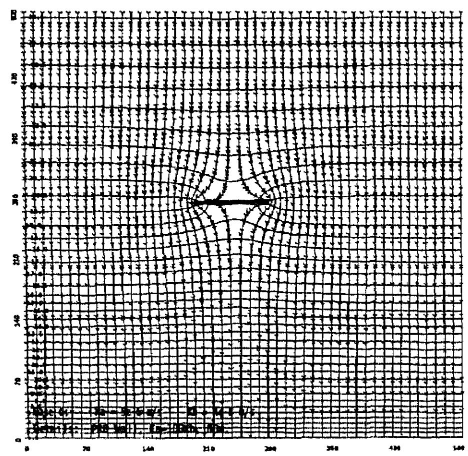
(y) Ka=100Kb, Length 20



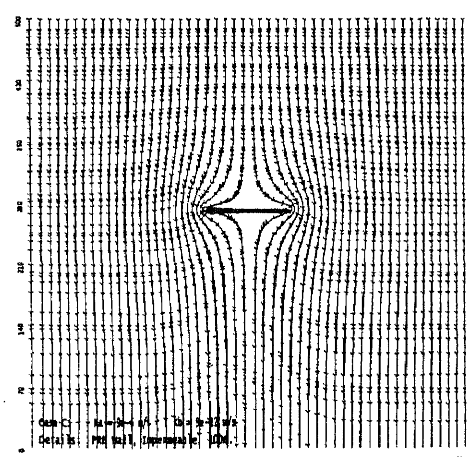
(z) Ka=100Kb, Length 40



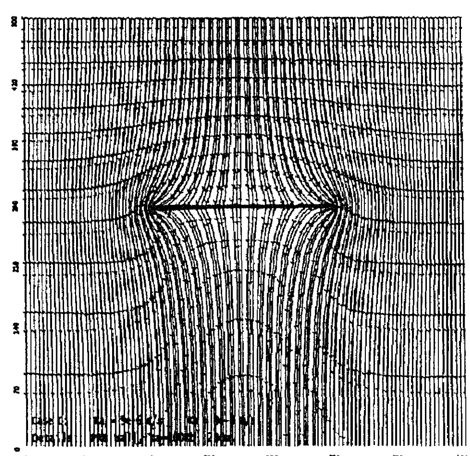
(a') Ka=100Kb, Length 60



(b') Ka=100Kb, Length 80

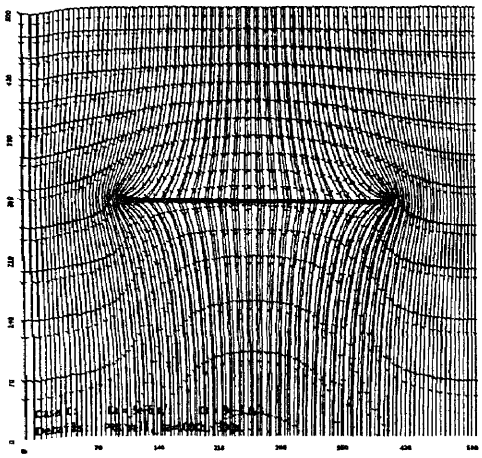


(c') Ka=100Kb, Length 100

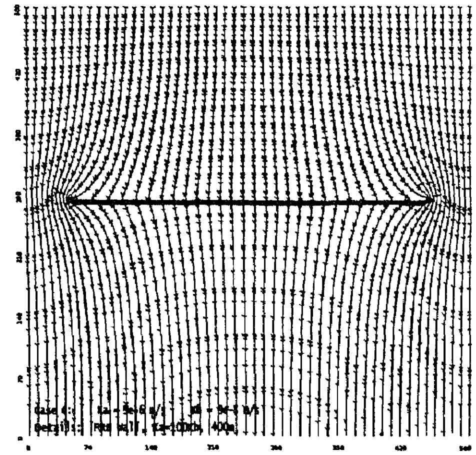


(d') Ka=100Kb, Length 200

Figure 17 Visual modflow Runs for Varying Lengths of Barrier at varying Aquifer to Barrier Hydraulic Conductivity Values.

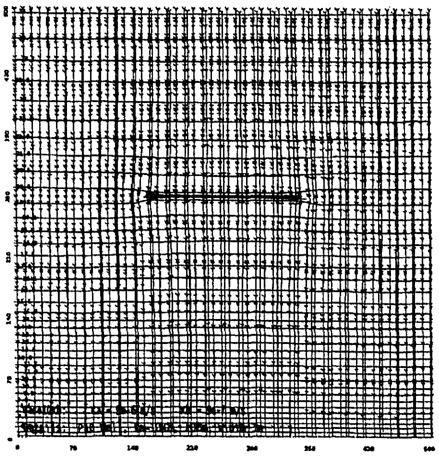


(e') Ka=100Kb, Length 300

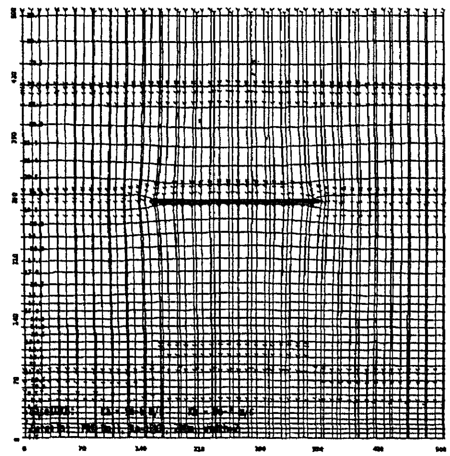


(f') Ka=100Kb, Length 400

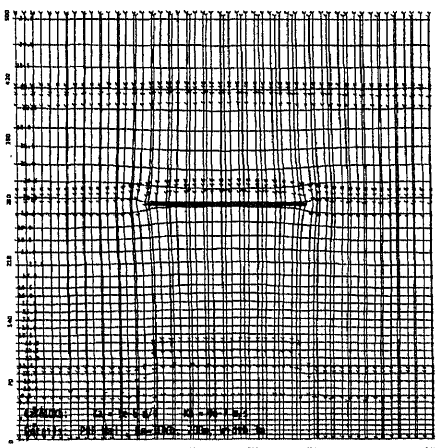
Figure 17 Visual modflow Runs for Varying Lengths of Barrier at varying Aquifer to Barrier Hydraulic Conductivity Values.



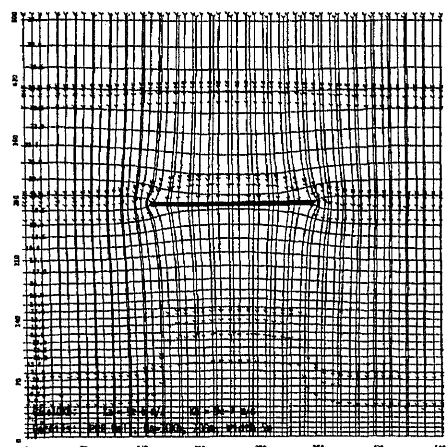
(a) Ka=10Kb, Width 1



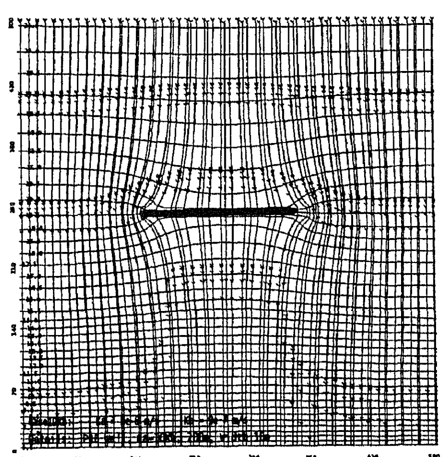
(b) Ka=10Kb, Width 2



(c) Ka=10Kb, Width 3

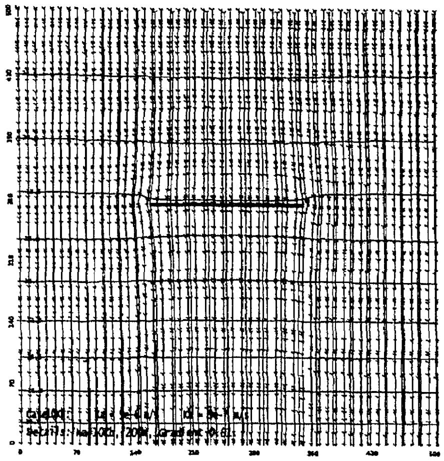


(d) Ka=10Kb, Width 5

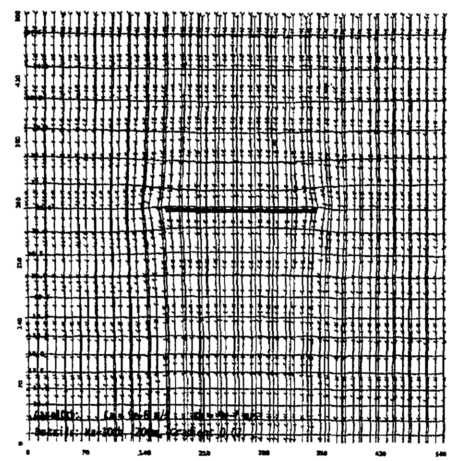


(e) Ka=10Kb, Width 10

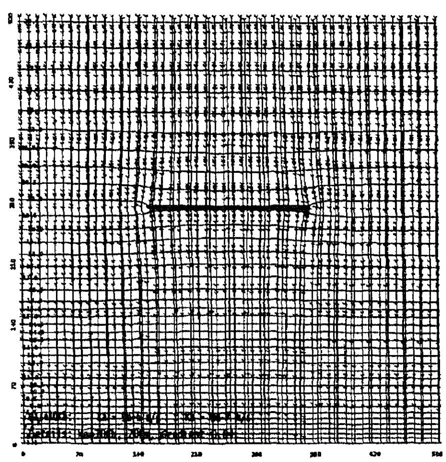
Figure 18 Visual modflow Runs for Varying Widths of Barrier



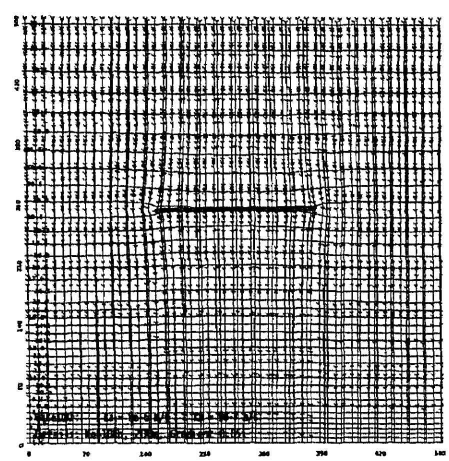
(a) Ka=10Kb, len200,grad0.01



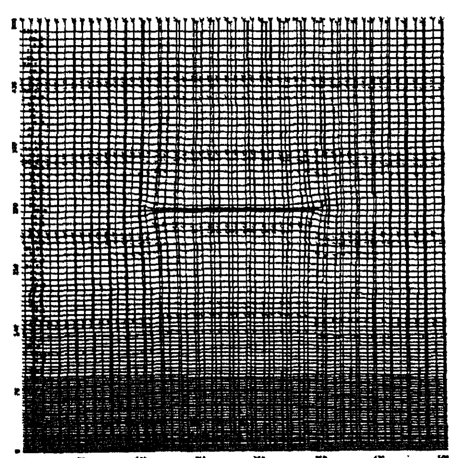
(b) Ka=10Kb, len200,grad0.02



(c)Ka= 10Kb, len200,grad0.04



(d) Ka=10Kb, len200,grad0.05



(e) Ka=10Kb, len200,grad0.1

Figure 19 Visual modflow Runs of Varying Hydraulic Gradients

4.3 Sensitivity Analysis

The calibration of the model was followed by investigation of the sensitivity of the following parameters:

4.3.1 The Barrier Length and Barrier to Aquifer Hydraulic Conductivity

The length of the barrier was varied over 20m, 40m, 60m, 80m, 100m, 200m, 300m, 400m and for each length, the model was run, adopting different aquifer to barrier hydraulic conductivity ratio. The loss % was calculated each time as explained in Appendix B. The effect of barrier length and the barrier to aquifer hydraulic conductivity (sensitivity) on the influent contaminant path-lines was thus evaluated. The change in the pathlines of the simulation output were compared with each other to identify by how much, if at all they did effect parameters barrier length and ratio of barrier to aquifer hydraulic conductivity (K_a/K_b). The values of loss % for different barrier length at different K_a/K_b ratios are tabulated in Table 6 and Table 7.

4.3.2 Barrier Width

The width of the barrier was varied over 1m, 2m, 3m, 5m, and 10m, and the model was run. The loss % was calculated each time. The change in the path-lines of the simulation output were compared with each other to identify by how much, if at all they did effect parameters barrier width. The sensitivity of barrier width on the influent contaminant path-lines was thus evaluated. The values of loss % for different barrier width are tabulated in Table 9.

4.3.3 The Hydraulic Gradient

The hydraulic gradient is a very important factor that influences the flow of groundwater in its subsurface regime. The hydraulic gradient in the aquifer was varied over range (0.01-0.1) conceptualized from the current applications (Appendix A). The loss % was calculated for these different hydraulic conditions. The results are tabulated in Table 8. The change in the path-lines of the simulation output was compared with each other to evaluate the sensitivity of the parameter. The results of the sensitivity analysis are tabulated in Table 5.

4.3.4 Loss versus Depth of Barrier (Hanging Wall)

This parameter is applicable only to a Hanging Wall Barrier. It is uneconomical, especially when the impermeable boundary lies at great depth, to construct a barrier that extends to the full depth of the aquifer. In such a case the barrier is made to hang to a fraction of the entire depth of the aquifer. The depth to which the barrier hangs should be such that it captures a large portion of the contaminants.

In the study the suitable depth of the barrier was calculated for an aquifer 25m, hence the results should be interpreted as a fraction of the entire length. The loss of contaminant path-lines is sensitive to the depth of the hanging wall. This is shown in Figure 35. Here the depth of the wall is varied over a range of 10 to 25m, i.e. 2/5 depth to full depth and the loss is calculated each time. The results are tabulated in Table 10.

The loss percentage in this case can be calculated using the following formulae:

$$Loss_{hw} = N_{influxhw} - N_{thruhw}$$

$$Loss_{hw}(\%) = \frac{N_{\inf luxhw} - N_{thruhw}}{N_{\inf luxhw}} \text{ X } 100$$ Where

$N_{influxhw}$ = Contaminant path-lines incident to barrier

N_{thruhw} = Influx passing through barrier

N_{losshw} = Loss through a hanging wall

4.3.5 Loss versus Distance between Trenches (Double Barrier)

This parameter is applicable only to a double trench barrier. Sometimes when the reduction of the contaminant takes place at a pH different from that of the groundwater two trenches are required. One to adjust the pH of the GW and the other to effect the reduction of the contaminant.

The loss of contaminant path-lines is sensitive to the distance between the two trenches. This is shown in Figure 28, where the distance between trenches is varied over the range 5 –150m and the loss of barrier 1 incident contaminants path-lines by barrier 2, is calculated each time. The results are tabulated in Table 11.

The calculation of loss percentage is a little different than in the case of single trench barrier. The loss percentage can be calculated from the following formulae:

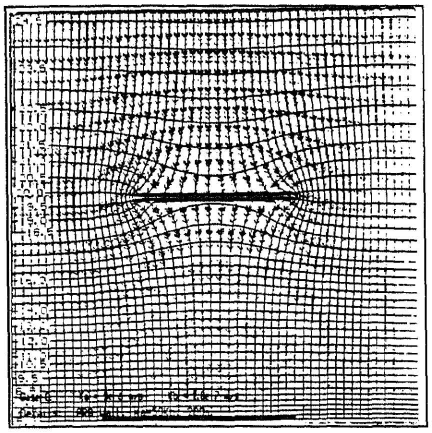
$Loss_{db} = N_{thrub1} - N_{thrub2}$

$$Loss_{db}\ (\%) = \frac{N_{thrub1} - N_{thrub2}}{N_{thrub1}} \text{ X } 100 \quad \text{Where}$$

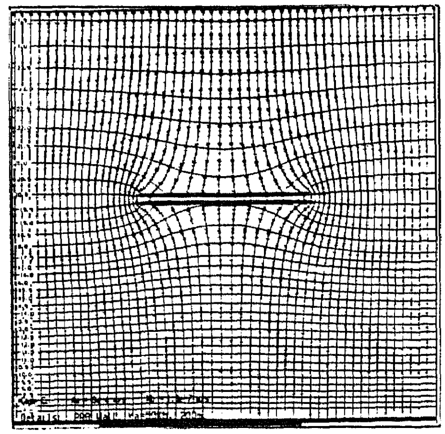
N_{thrub1} = Influx passing through barrier 1 in a double barrier

N_{thrub2} = Influx passing through barrier 2 in a double barrier

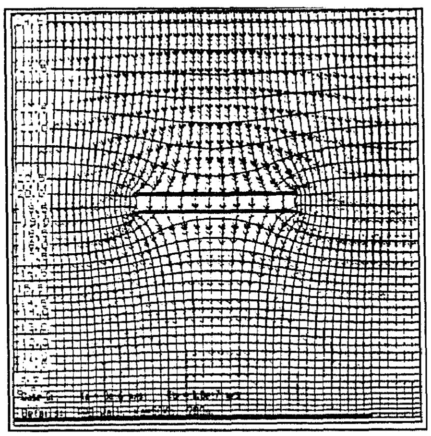
N_{lossdb} = Loss through a double barrier



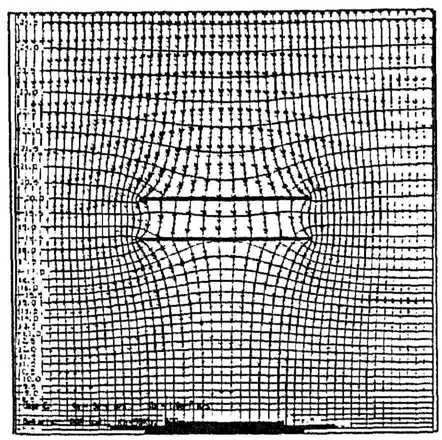
(a) Ka = 50Kb, distance 5



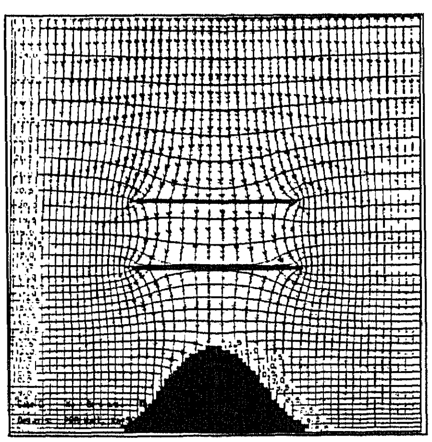
(b) Ka = 50Kb, distance 10



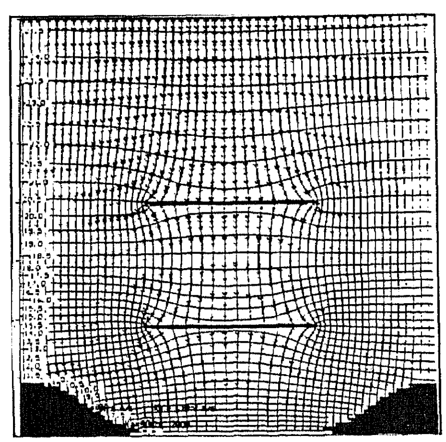
(c) Ka = 50Kb, distance 25



(d) Ka = 50Kb, distance 50

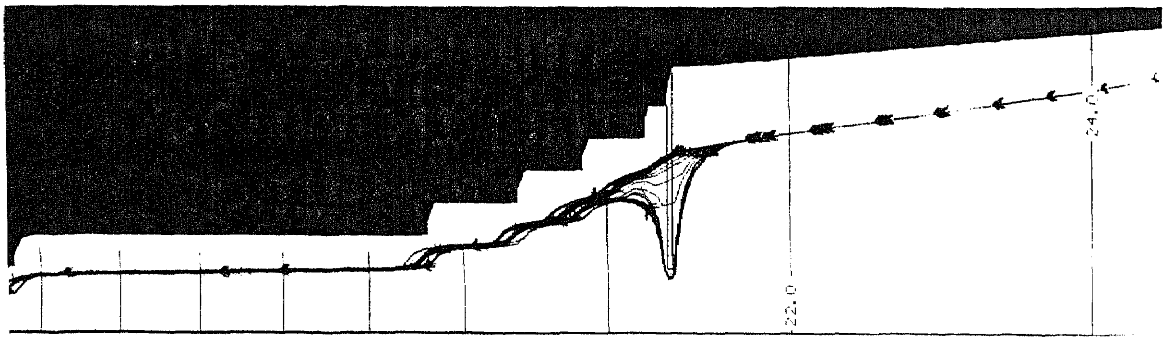


(e) Ka = 50Kb, distance 80

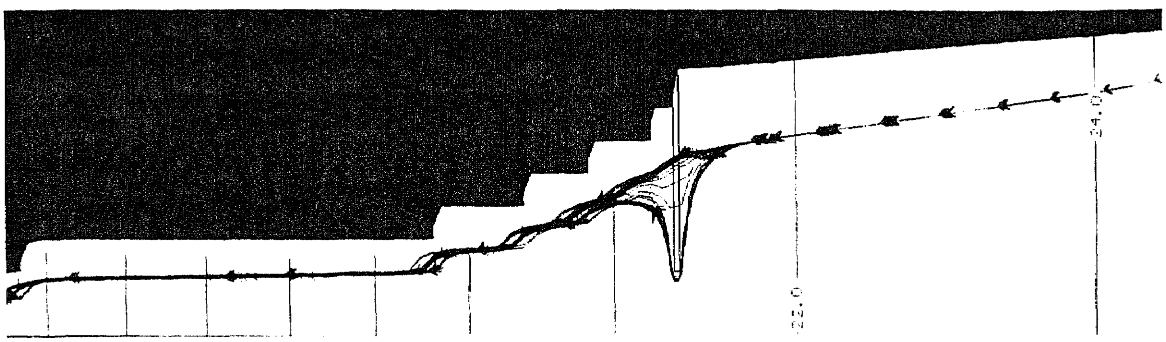


(f) Ka = 50Kb, distance 150

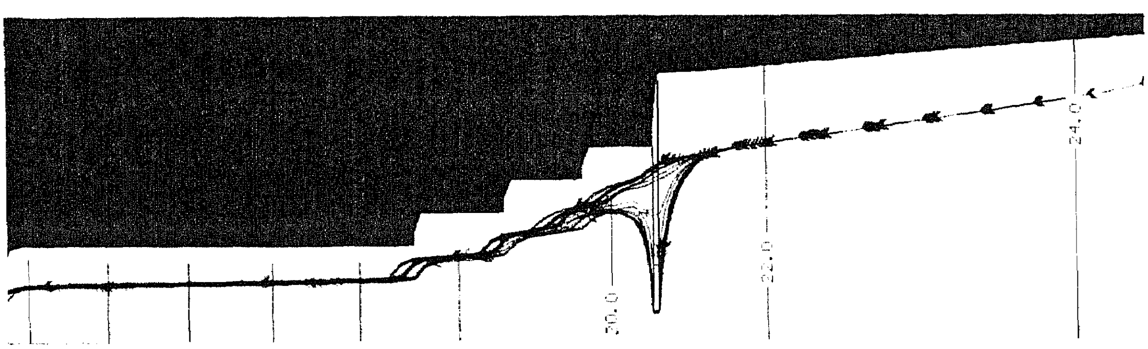
Figure 20 Visual Modflow Runs for 200m length Double Trench Barrier



Hanging Wall Depth 17.5

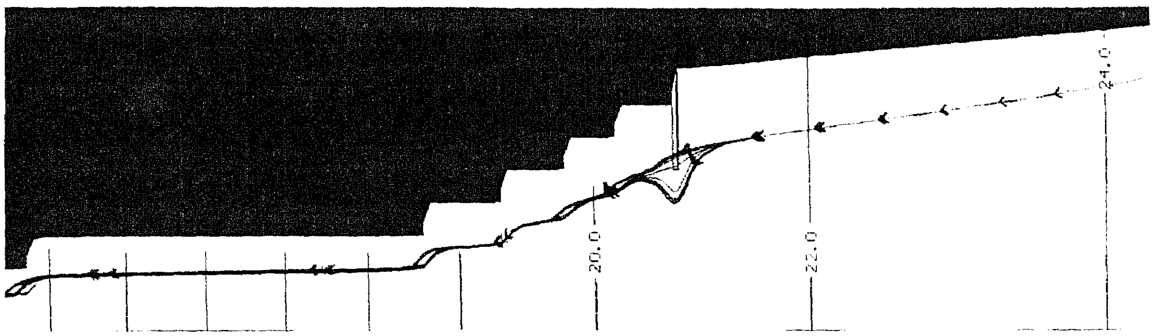


Hanging Wall Depth 20

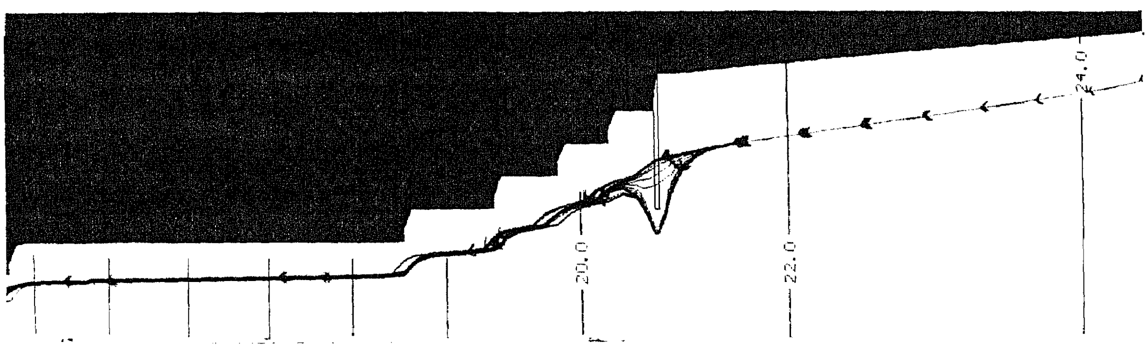


Hanging Wall Depth 22.5

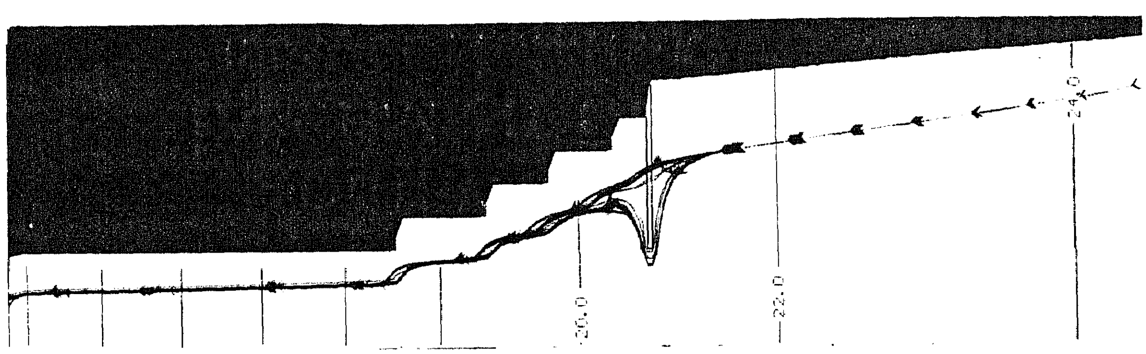
Figure 21 Visual Modflow Runs for a 200m length Hanging Wall Barrier



Hanging Wall Depth 10



Hanging Wall Depth 12.5



Hanging Wall Depth 15

Figure 21 Visual Modflow Runs for a 200m length Hanging Wall Barrier

The deviating path-lines of the simulation output was compared with each other to evaluate the sensitivity of the parameter. The results of the sensitivity analysis are tabulated in Table 5.

4.4 Calculation of the Sensitivity of a Parameter

Sensitivity analysis is conducted to determine which parameters impact the design of a barrier. Further sensitivity of a parameter can be defined as the magnitude of change in contaminant path-lines (measured by loss in this study) that unit change in a parameter provokes. It is thus calculated in this study by the following formulae:

$$\text{Sensitivity} = \frac{\text{Difference between loss \% at two values of a parameter}}{\text{Difference in the parameter}}$$

The range of values of sensitivity obtained for the various loss % calculations for a parameter is reported in the Table 5. The different values of loss % calculated are reported in the following Tables:

Table 6: Ratio of the Hydraulic Conductivity of the Aquifer to that of the Barrier.

Table 7: Barrier Length,

Table 8: Aquifer Hydraulic Gradient

Table 9: Barrier Width,

Table 10: Depth of Hanging Wall.

Table 11: Distance between the Trenches of a Double Walled Barrier.

The sensitivity of a parameter can also be determined by calculating the average slope of the design curve i.e. plot of the loss % versus the parameter. This is closely equal to that calculated from the tables in this study. The range of the parameter over which it is sensitive is also important and is discussed in the following chapter on design curves.

Table 5: Results of the Sensitivity Analysis

Property	Generic Case	Aquifer or Barrier Property	Sensitivity
Barrier Length	Case1	Barrier	Loss decreases with increase. Sensitivity = 0.1 - 1
Ratio of the Aquifer to the Barrier Hydraulic Conductivity (Ka/Kb)	Case1	Both	Loss increases with increase in ratio. Sensitivity = 0.1 - 0.4
Barrier Width	Case1	Barrier	Loss increases with increase in width Sensitivity = 3 - 8
Hydraulic Gradient		Aquifer	Sensitivity = 0
Barrier Depth	Case 2	Barrier	Not truly sensitive Sensitivity = 0.5 - 6
Distance between the Barrier Walls (Double Walled)	Case4.	Barrier	Loss approaches a constant when distance is greater than 80 m. Sensitivity = 0

4.5 Design Curves

Design curve can be defined as a graphical plot of critical and non-critical parameters against a factor (loss %) that governs the efficiency of the design entity and forms the basis of the design of the same (Permeable Reactive Barrier). The use of design curves in the design of PRBs is presented in Chapter 5. This section discusses the construction and the interpretive use of design curves.

4.5.1 Construction of Design Curves

The models for the various conceptual cases are executed by varying the different parameters perceived as critical. Sensitivity analysis is performed by calculating the loss of contaminant path-lines from model outputs. The values of loss %, calculated for different values of a parameter, are tabulated in Table 7, Table 9, Table 8, Table 6, Table 10 and Table 11. A graph is plotted, of the parameter versus Loss %. These constitute the design curves. The slope of the corresponding design curve alternatively denotes the sensitivity of a parameter.

4.5.1.1 Loss versus Barrier Length: The plot of loss % versus barrier length is shown in Figure 24. It can be seen from the graph that loss % decreases as barrier length increases approaching an asymptote (approaches a constant value), however notable contaminant path-line is only seen when the aquifer to barrier hydraulic conductivity is greater than 1. It is also shown that length of barrier of 150-200m for a contaminated plume per 500m lateral extent would prove to be economical. For greater lengths the efficiency of the barrier decreases. The parameter is very sensitive to loss between 20-150m. The sensitivity of this parameter is low at lengths > 200m.

4.5.1.2 Loss versus Aquifer to Barrier Hydraulic Conductivity: Figure 23 shows the variation of loss with aquifer to barrier hydraulic conductivity. As the barrier becomes increasingly impermeable the loss percentage increases. Interestingly, with a more or less linear decrease there is a dip in the curve that could be conveniently used in the design of the wall. A barrier hydraulic conductivity proves to be efficient. The parameter is more or less equally sensitive over a range of values (slope is constant).

4.5.1.3 Barrier Width: The plot of loss % versus barrier width is shown in Figure 26. It can be seen from the graph that loss % increases with barrier width. However the loss remains more or less constant when the barrier width is between 0.5-3.0m. The width is very important to achieve the residence time required for the chemical reduction of contaminant to take place. The width of the PRB should be designed to ensure the residence time is met. The cost to efficiency of the barrier increases with greater widths. The parameter is very sensitive at widths >3m. The sensitivity of this parameter is low at widths between 0.5-3m.

4.5.1.4 Loss versus Hydraulic Gradient: The plot of loss versus the hydraulic gradient of the ground water is presented in Figure 25. Though hydraulic gradient of the ground water is the driving force that causes ground water flow, between values of 0.01-0.1, it does not noticeably affect the contaminant path-lines. Most sites have the hydraulic gradients of aquifer lying in this range.

4.5.1.5 Loss versus Depth of Hanging Wall: In this configuration the barrier wall does not extend to the permeable boundary. The plot of $loss_{hw}$ % versus the depth of the barrier is shown in Figure 27. It can be seen from the graph that $loss_{hw}$ % increases with the decrease in barrier depth.

This design curve can be thought of being used to arrive at a relationship between the depth of contaminant determination and the depth of the barrier below, for a distance of the barrier from the source. The flow of water towards a barrier, having a higher hydraulic conductivity, results in the temporary mounding of the water table at the aquifer-barrier interface (Figure 22). The mounding of water instigates a force on the downward and then below the barrier movement of the contaminated water. This design curve thus would prove to be less expedient to establish the depth of the hanging wall to intercept contaminant detected at a certain depth in the aquifer.

Due to this mounding, the incorporation of the hanging wall should be avoided as far as possible. The evaluation of the same should be conducted by executing a specific model of and for each site rather than trying to arrive at general design curves. This corresponds to Case 2 of the generic cases i.e. Single Trench in an Unconfined Aquifer (Partially Penetrating). This study strongly recommends that this mounding effect of water at the barrier-aquifer interface and below barrier flow drive should be studied in detail to facilitate the design of an economical barrier when the impermeable boundary is deep below.

4.5.1.5 Loss versus Distance between the Trenches of a Double Wall Configuration: In this configuration the barrier consists of two walls. This corresponds to Case 4 of the generic cases i.e. Double Trench in an Unconfined Aquifer. The plot of $loss_{db}$ % versus the depth of the barrier is shown in Figure 28. There is an initial surge in loss at distances between 10m-80m. This simulation had been informally executed for other ratios of hydraulic conductivity, to evaluate the initial surge. The initial increase in the loss increases in magnitude with the increase in the aquifer to barrier hydraulic conductivity ratio. Owing to the inadequate level of accuracy with which these runs were performed, it has not been documented. It can be seen from the graph (Figure 28) that $loss_{db}$ % remains constant with the increase in distance between the trenches when such a distance is greater than 80m.

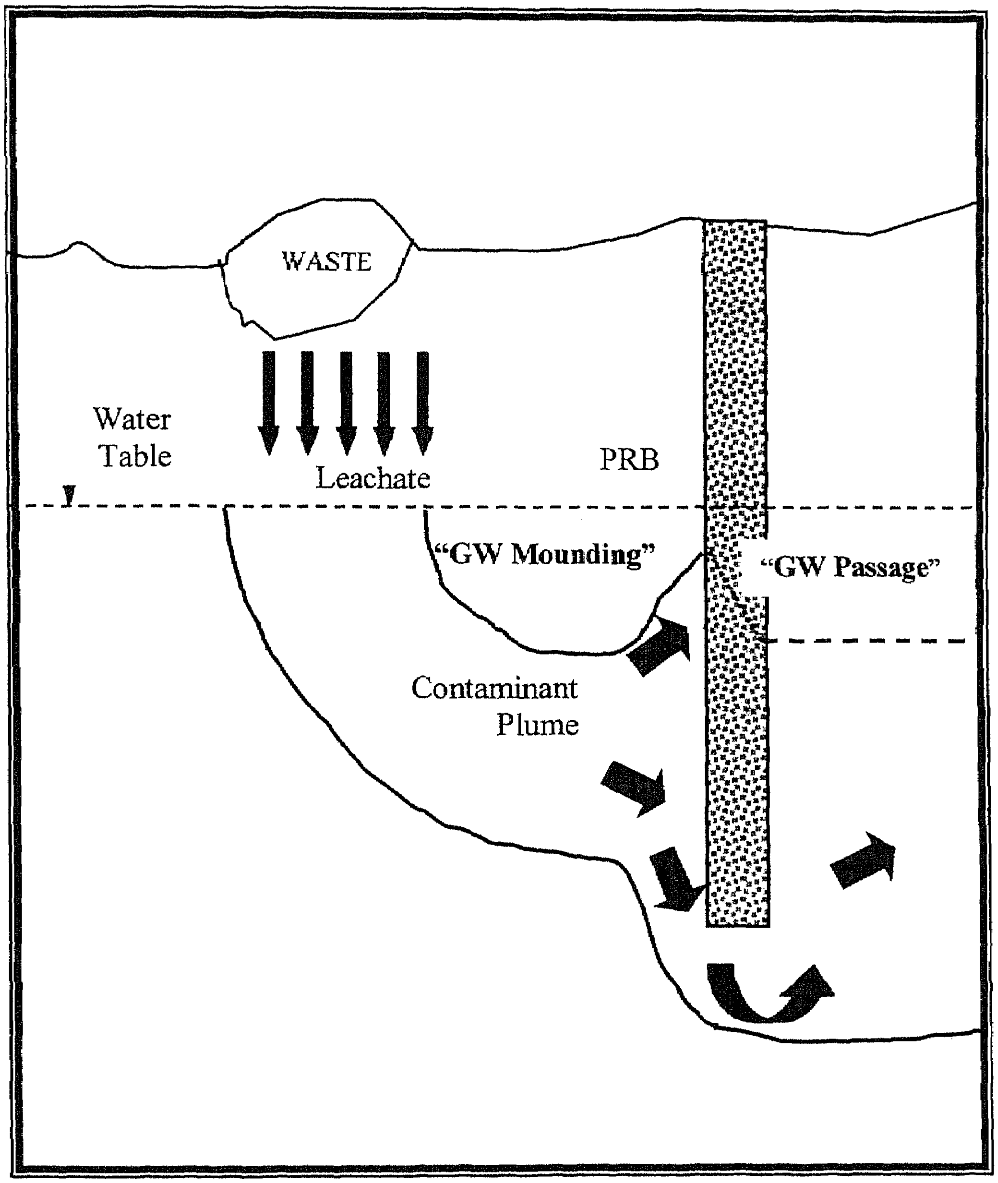


Figure 22 Water-table Mounding at Barrier Aquifer Interface and Inclined Passage Through it

Table 6 Loss versus Aquifer to Barrier Hydraulic Conductivity

B.L. = Barrier Length in meters

Ka/Kb	*225*	*100*	*75*	*50*	*10*	*1*	*0.1*	*0.01*
B.L.400	48.33	30	33.33	17.07	3.39	0	0	0
B.L. 300	69.05	41.38	44.19	32.43	8.89	0	0	0
B.L. 200	73	58.33	52.66	42.86	6.9	0	0	0
B.L. 100	79.16	62.5	55.88	42.86	20	0	0	0
B.L. 80	86.67	62.5	61.54	67	25	0	0	0
B.L. 60	100	66.67	71.43	72.38	22.23	0	0	0
B.L. 40	100	100	90	75	33.34	0	0	0
B.L. 20	100	100	100	90	33.34	0	0	0

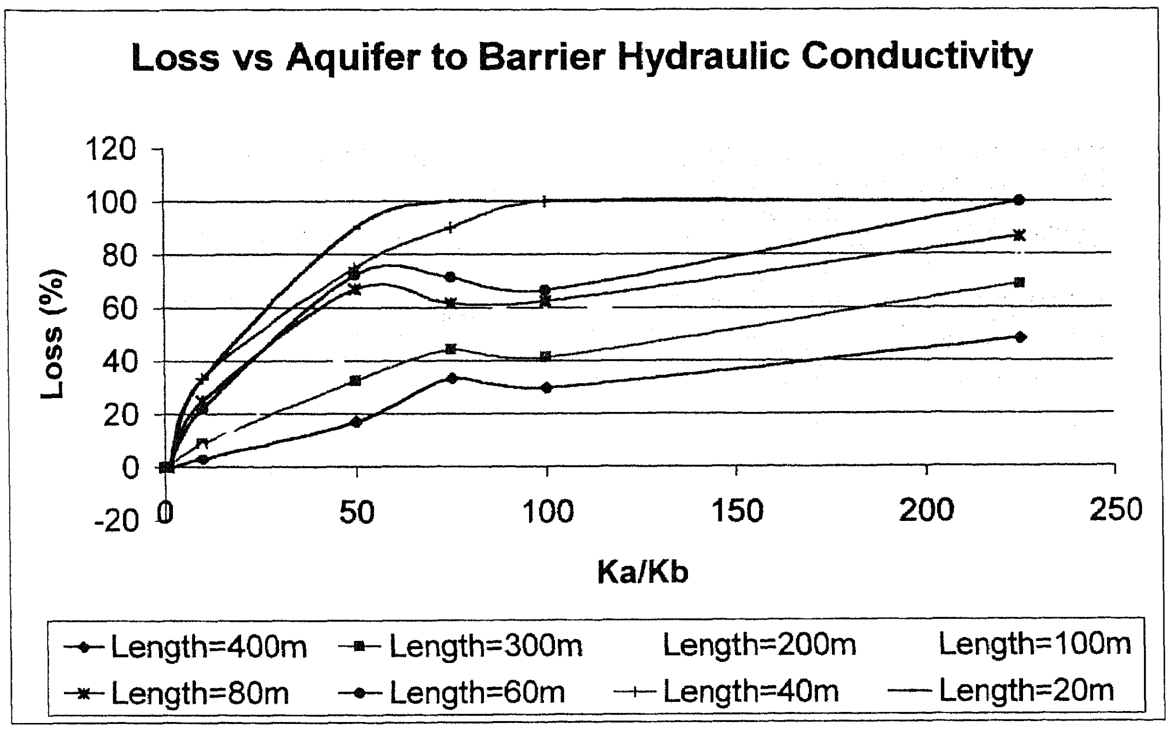


Figure 23 Graph showing Loss versus Aquifer to Barrier Hydraulic Conductivity

Table 7 Loss versus Barrier Length

*Ka/Kb
B.L. = Barrier Length in meters

Barrier Length	*400*	*300*	*200*	*100*	*80*	*60*	*40*	*20*
225*	48.33	69.05	73	79.16	86.67	100	100	100
100*	30	41.38	58.33	62.5	62.5	66.67	100	100
75*	33.33	44.19	52.63	55.88	61.54	71.43	75	100
50*	17.07	32.43	42.86	42.86	72.72	75	75	100
10*	3.39	8.89	6.9	20	25	22.23	33.34	33.34
1*	0	0	0	0	0	0	0	0
0.1*	0	0	0	0	0	0	0	0
0.01*	0	0	0	0	0	0	0	0

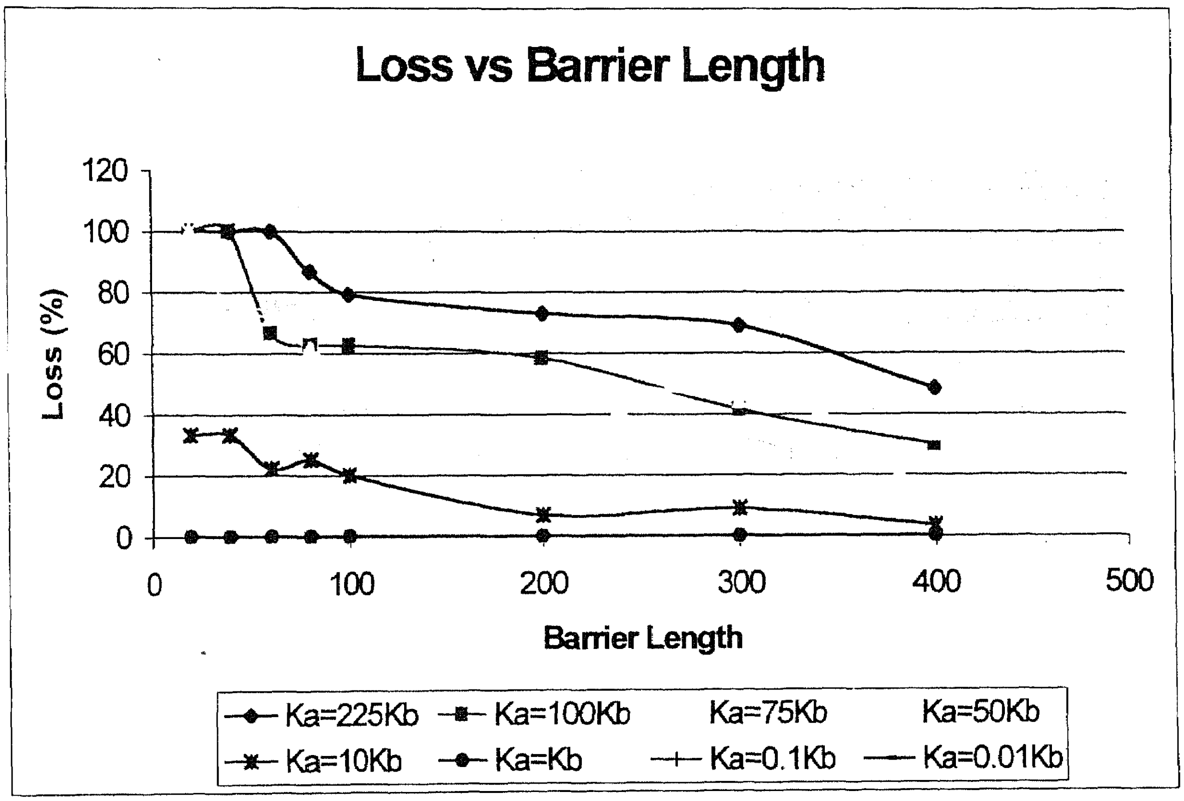


Figure 24 Graph showing Loss versus Barrier Length

Table 8 Loss versus Gradient

Gradient	*0.01*	*0.02*	*0.04*	*0.05*	*0.1*
Loss	6.9	6.9	6.9	6.9	6.9

Barrier Length = 200m
Ka = 10 Kb

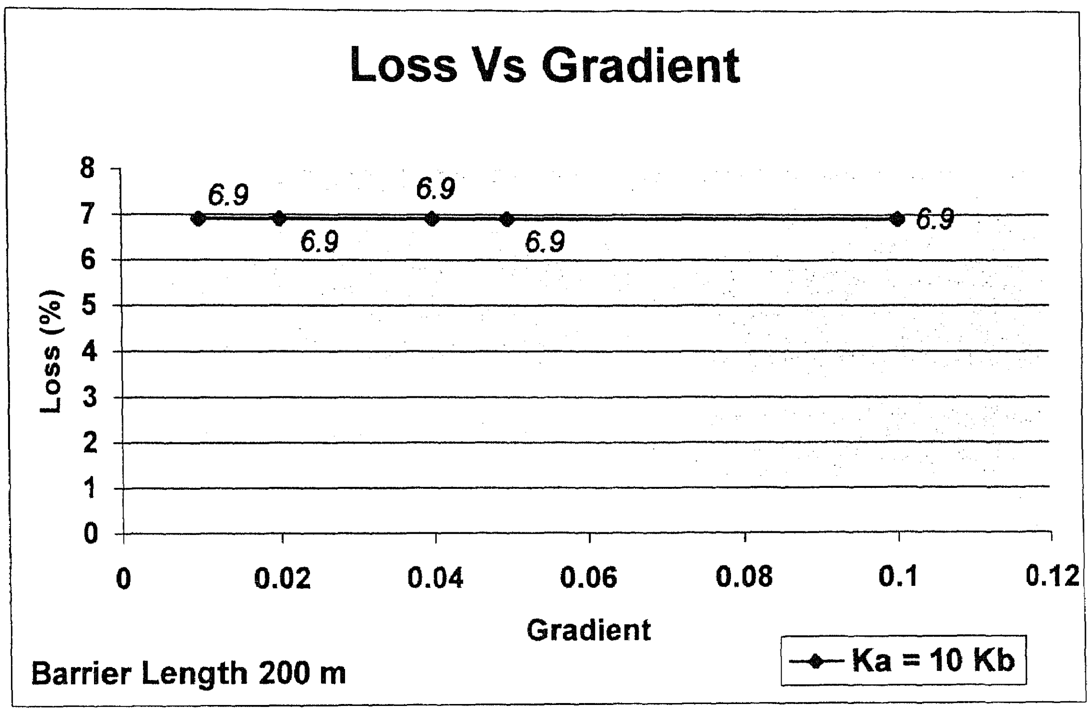


Figure 25 Graph showing Loss versus Gradient

Table 9 Loss versus Width

Width (m)	*1*	*2*	*3*	*5*	*10*
Loss	6.9	6.9	8	20.69	34.48

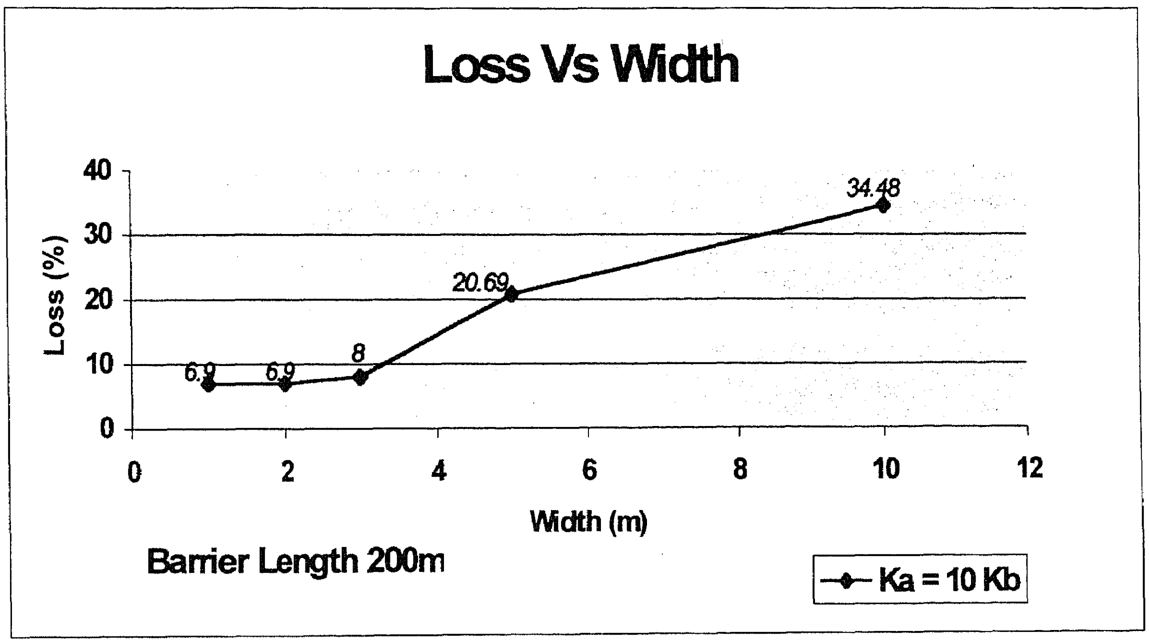


Figure 26 Graph showing Loss versus Width

Table 10 Loss versus Barrier Depth

Barrier Depth (m)	*25*	*22.5*	*20*	*17.5*	*15*	*12.5*	*10*
$Loss_{hw}$	0	45	60	76.92	87.5	90	92

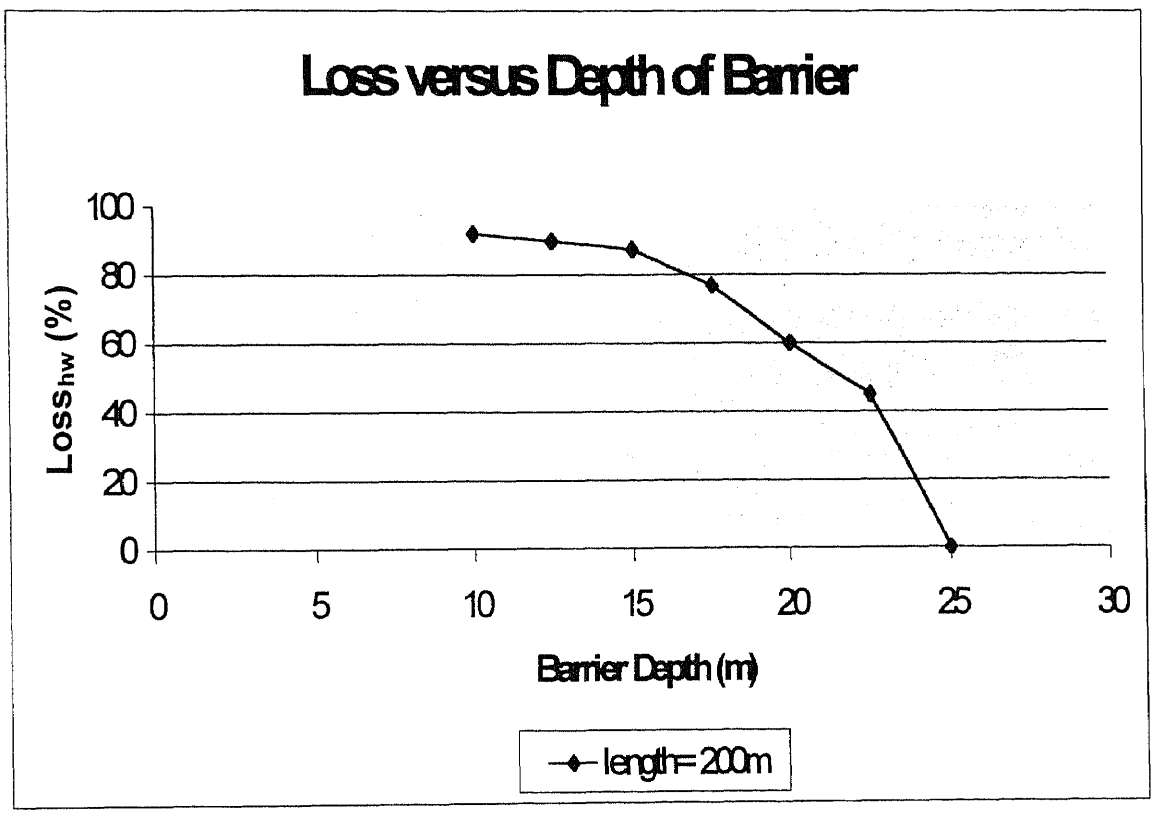


Figure 27 Graph Showing Loss versus Barrier Depth

Table 11 Loss versus Distance between Trenches (Double Barrier)

*Distance Between Trenches in meters
B.L. = Barrier Length in meters

Barrier Length (m)	*5*	*10*	*25*	*50*	*80*	*150*
***50**	0	0	0	14	9.1	8.04
***75**	0	0	0	20	10	10
***100**	0	0	25	25	11.11	11.11

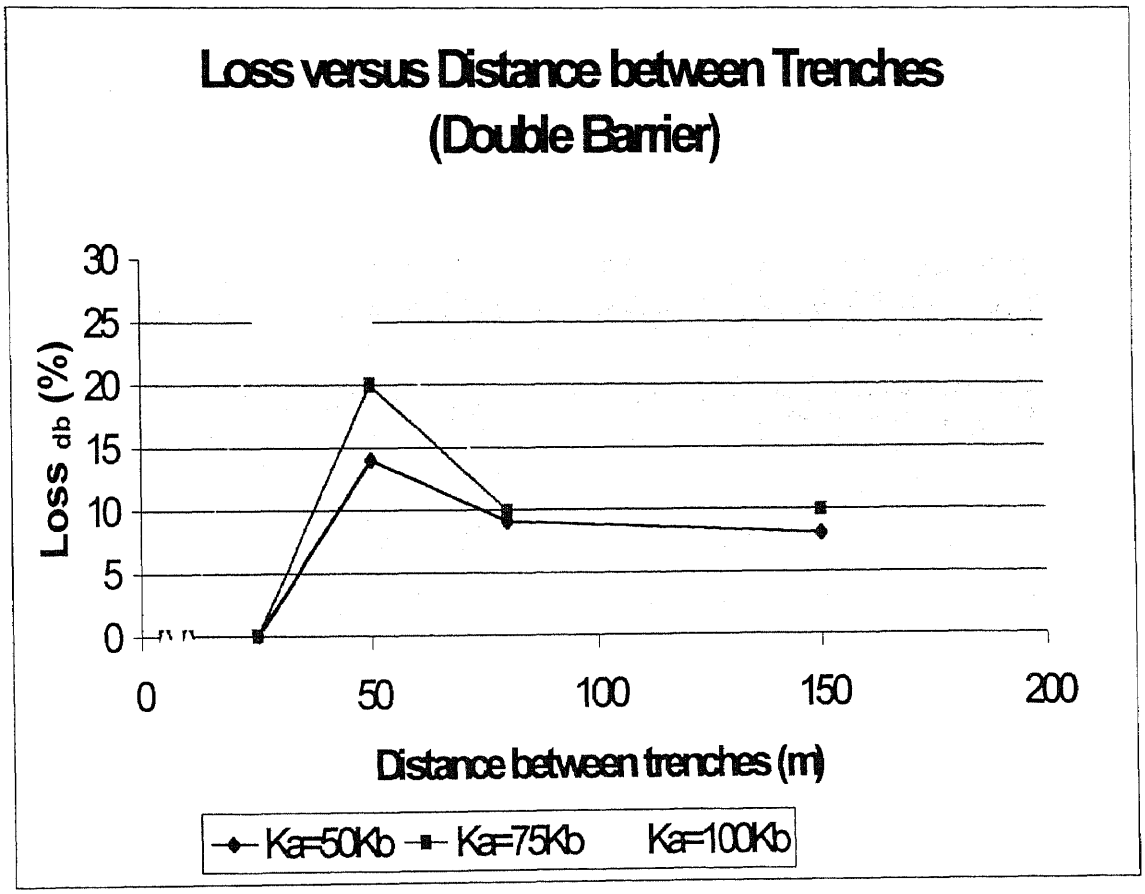


Figure 28 Graph showing Loss versus Distance between Trenches (Double Barrier)

4.6 Residence Time

Residence time is the time taken by water (GW in this case) to flow through a reactor (a PRB in this case), expressed in days, minutes, or seconds depending on its magnitude. The determination of residence time forms the basis of any modeling evaluation to support a PRB application. The residence time that a PRB configuration can create should be at least equal to the time required by the reactive material of the barrier to completely reduce the contaminant.

4.6.1 Determination of the Residence Time

Simulations used to replicate site conditions can be used to determine the residence time. Models created and executed have numeric engines to estimate the velocity of the ground water at the midpoints of each cell in the fabricated model grid. These velocities are exported out in the ASCII format and can be used in the calculation of residence time.

4.6.1.1 The Velocity Export: The export option in the velocity menu of Visual Modflow allows the user to export the current three-dimensional output data set to an ASCII file. The exported velocity data consists of 6 columns, x, y, z, vx, vy, and vz that should be interpreted as follows:

Column 1: x co-ordinate of the center of the cell for which velocity is exported (x)

Column 2: y co-ordinate of the center of the cell for which velocity is exported (y)

Column 3: z co-ordinate of the center of the cell for which velocity is exported (z)

Column 4: The component of velocity along the x-axis of the model (vx)

Column 5: The component of velocity along the y-axis of the model (vy)

Column 6: The component of velocity along the z-axis of the model (vz)

A partial sample of the velocity export, (the entire would run into at least 700 pages) showing the velocities at the center of the barrier cells in the model, is presented in Appendix C. The interpretation of the partial export is presented in Table 12 and is considered in determination of the residence time.

4.6.1.2 The Calculation of Residence Time: The partial list of exported velocity in Table 12 predicts the velocity, in the principle directions, at the center of the barrier cells. The resultant velocity can be calculated for each set. The resultant of the three components is calculated, per set, using the following formulae:

$$V = \sqrt{vx^2 + vy^2 + vz^2}$$

where V = The resultant velocity through the barrier grid cell

vx = The component of velocity, through one barrier grid cell, along the x-axis of the model

vy = The component of velocity, through one barrier grid cell, along the y-axis of the model

vz = The component of velocity, through one barrier grid cell, along the z-axis of the model

The maximum of the resultant velocities indicates the shortest period that the contaminated water would remain in the barrier. Residence time calculations are hence based on the maximum resultant, of the velocities along the principle directions, at the center of barrier cells of the model.

The residence time is calculated using the following formulae:

$$R = \frac{1}{86400(V_m)}$$

where R = The residence time in days/m

V_m = The maximum resultant velocity

Maximum resultant velocity and residence time calculations, for each model executed, are presented in Table 13. Sample resultant velocity and residence time calculations are discussed in Appendix C. The residence time thus determined for varying length, width, hydraulic gradient and ratio of aquifer to barrier hydraulic conductivity is summarized in Table 14. These values are used in the 3-step Procedure for Barrier Design explained in the next section.

Details of Table 12 are presented below

Details: $K_{aquifer}$ = $10K_{barrier}$	**Gradient = 0.02**
Length = 200m	**Width = 2.0m**
Maximum Average Velocity = 7.72×10^{-7} m/s	
Residence Time = 1/ v x 60 x 60 x 24 days	
= 15 days	

Table 12 Velocities Exported to an ASCII Format

x coordinate	y coordinate	z coordinate	Velocity along x axis m/s	Velocity along y axis m/s	Velocity along z axis m/s	Resultant Velocity $v=\sqrt{V_x^2+V_y^2+V_z^2}$ m/s
152.5	279	7.8	1.280178e-010	-5.027534e-007	-4.764703e-010	5.027534e-007
157.5	279	7.8	3.662109e-011	-6.044709e-007	-4.819723e-010	6.044709e-007
162.5	279	7.8	3.376007e-011	-6.565355e-007	-4.858237e-010	6.565355e-007
167.5	279	7.8	2.803802e-011	-6.880154e-007	-4.885747e-010	6.880154e-007
172.5	279	7.8	2.403259e-011	-7.089039e-007	-4.907755e-010	7.089039e-007
177.5	279	7.8	1.945496e-011	-7.236513e-007	-4.924261e-010	7.236513e-007
182.5	279	7.8	1.544952e-011	-7.344908e-007	-4.940766e-010	7.344908e-007
187.5	279	7.8	1.144409e-011	-7.427171e-007	-4.95177e-010	7.427171e-007
192.5	279	7.8	8.010864e-012	-7.490864e-007	-4.968276e-010	7.490864e-007
197.5	279	7.8	5.722046e-012	-7.541281e-007	-4.97928e-010	7.541281e-007
202.5	279	7.8	4.005432e-012	-7.581786e-007	-4.995786e-010	7.581786e-007
207.5	279	7.8	4.005432e-012	-7.614345e-007	-5.00679e-010	7.614345e-007
212.5	279	7.8	4.577637e-012	-7.640939e-007	-5.023296e-010	7.640939e-007
217.5	279	7.8	5.722046e-012	-7.662359e-007	-5.0343e-010	7.662359e-007
222.5	279	7.8	6.866455e-012	-7.679728e-007	-5.039802e-010	7.679728e-007
227.5	279	7.8	8.010864e-012	-7.693321e-007	-5.039802e-010	7.693321e-007
232.5	279	7.8	9.155273e-012	-7.703774e-007	-5.045304e-010	7.703774e-007
237.5	279	7.8	9.155273e-012	-7.711403e-007	-5.045304e-010	7.711403e-007
242.5	279	7.8	9.155273e-012	-7.716286e-007	-5.045304e-010	7.716286e-007
247.5	279	7.8	8.010864e-012	-7.718688e-007	-5.045304e-010	7.718688e-007
252.5	279	7.8	6.866455e-012	-7.718542e-007	-5.045304e-010	7.718542e-007
257.5	279	7.8	6.866455e-012	-7.716088e-007	-5.045304e-010	7.716088e-007
262.5	279	7.8	6.29425e-012	-7.711033e-007	-5.045304e-010	7.711033e-007
267.5	279	7.8	6.29425e-012	-7.703404e-007	-5.045304e-010	7.703404e-007
272.5	279	7.8	8.010864e-012	-7.692806e-007	-5.045304e-010	7.692806e-007
277.5	279	7.8	9.727478e-012	-7.679067e-007	-5.0343e-010	7.679067e-007
282.5	279	7.8	1.144409e-012	-7.661818e-007	-5.0343e-010	7.661818e-007
287.5	279	7.8	1.25885e-012	-7.640398e-007	-5.017794e-010	7.640398e-007
292.5	279	7.8	1.25885e-012	-7.613804e-007	-5.012292e-010	7.613804e-007
297.5	279	7.8	1.20163e-012	-7.581245e-007	-4.990284e-010	7.581245e-007
302.5	279	7.8	9.727478e-011	-7.540885e-007	-4.97928e-010	7.540885e-007
307.5	279	7.8	6.866455e-011	-7.490323e-007	-4.962774e-010	7.490323e-007
312.5	279	7.8	3.433228e-011	-7.426313e-007	-4.95177e-010	7.426313e-007
317.5	279	7.8	-1.144409e-011	-7.34405e-007	-4.935264e-010	7.34405e-007
322.5	279	7.8	-5.722046e-011	-7.23584e-007	-4.913257e-010	7.23584e-007
327.5	279	7.8	-9.727478e-011	-7.087811e-007	-4.896751e-010	7.087811e-007
332.5	279	7.8	-1.430511e-011	-6.878729e-007	-4.87473e-010	6.878729e-007
337.5	279	7.8	-2.059937e-011	-6.563785e-007	-4.836229e-010	6.563785e-007
342.5	279	7.8	-2.288818e-011	-6.043128e-007	-4.797715e-010	6.043128e-007
347.5	279	7.8	-1.097072e-011	-5.026281e-007	-4.748198e-010	5.026281e-007

Table 13 Velocity and Residence Time Calculations

Filename	x coordinate	y coordinate	z coordinate	vx velocity along x axis m/s	vy velocity along y axis m/s	vz velocity along z axis m/s	v= $\sqrt{vx^2+vy^2+vz^2}$ Velocity m/s	Residence Time $\frac{1}{vx 60 x 60 x 24}$ days/m
Kb0.01len20	220-240	279	7.8	1.2e-008	5.1e-007	1.6e-007	5.34e-007	21.67
Kb0.01len40	200-240	279	7.8	1.5e-008	5.1e-007	1.4e-007	5.29e-007	21.9
Kb0.01len60	190-250	279	7.8	1.0e-009	7.8e-007	1.2e-008	7.8e-007	14.84
Kb0.01len80	200-280	279	7.8	7.7e-009	5.1e-007	1.4e-007	5.28e-007	21.9
Kb0.01len100	200-300	279	7.8	1.8e-008	5.1e-007	1.4e-007	5.29e-007	21.9
Kb0.01len200	150-350	279	7.8	9.4e-008	4.9e-007	1.4e-007	5.18e-007	22.34
Kb0.01len300	100-400	279	7.8	1.4e-007	4.8e-007	1.6e-007	5.25e-007	22.04
Kb0.01len400	50-450	279	7.8	1.2e-008	4.8e-007	2.0e-007	5.2e-007	22.25
Kb0.1len20	220-240	279	7.8	6.7e-009	5.4e-007	9.1e-008	5.5e-007	21.04
Kb0.1len40	200-240	279	7.8	1.0e-008	5.4e-007	8.9e-008	5.5e-007	21.04
Kb0.1len60	190-250	279	7.8	5.7e-009	5.3e-007	8.8e-008	5.37e-007	21.55
Kb0.1len80	200-280	279	7.8	4.9e-009	5.0e-007	8.2e-008	5.1e-007	22.69
Kb0.1len100	200-300	279	7.8	8.2e-009	5.3e-007	8.9e-008	5.37e-007	21.55
Kb0.1len200	150-350	279	7.8	1.0e-009	5.3e-007	8.8e-008	5.37e-007	21.55
Kb0.1len300	100-400	279	7.8	6.8e-009	5.5e-007	8.8e-008	5.6e-007	20.66
Kb0.1len400	50-450	279	7.8	7.0e-009	5.3e-007	8.7e-008	5.37e-007	21.55
Kb10len20	225-245	279	7.8	6.0e-011	1.4e-006	1.7e-009	1.4e-006	8.26
Kb10len40	220-260	279	7.8	9.2e-012	1.8e-006	2.1e-009	1.8e-006	6.43
Kb10len60	220-280	279	7.8	5.7e-012	2.0e-006	2.3e-009	2.0e-006	5.78

Table 13 continued

Kb10len80	220-300	279	7.8	2.8e-011	2.1e-006	2.4e-009	2.1e-006	5.51
Kb10len100	200-300	279	7.8	5.2e-011	2.1e-006	2.4e-009	2.1e-006	5.51
Kb10len200	150-350	279	7.8	5.0e-011	2.2e-006	2.8e-009	2.2e-006	5.2
Kb10len300	100-400	279	7.8	1.2e-010	2.3e-006	3.4e-009	2.3e-006	5.03
Kb10len400	50-450	279	7.8	5.7e-010	2.4e-006	3.5e-009	2.4e-006	4.8
Kb50len20	200-220	279	7.8	1.3e-011	8.0e-007	3.7e-010	8.0e-007	14.46
Kb50len40	200-240	279	7.8	2.3e-011	1.2e-006	4.6e-010	1.2e-006	9.64
Kb50len60	190-250	279	7.8	2.2e-011	1.6e-006	6.9e-010	1.6e-006	7.2
Kb50len80	200-280	279	7.8	4.7e-011	1.8e-006	1.1e-009	1.8e-006	6.43
Kb50len100	200-300	279	7.8	7.8e-011	2.2e-006	2.5e-009	2.2e-006	5.2
Kb50len200	150-350	279	7.8	9.9e-012	3.0e-006	3.5e-009	3.0e-006	3.85
Kb50len300	100-400	279	7.8	6.4e-012	3.4e-006	4.0e-009	3.4e-006	3.4
Kb50len400	50-450	279	7.8	1.9e-012	3.7e-006	3.1e-010	3.7e-006	3.73
Kb75len20	200-220	279	7.8	1.3e-011	5.9e-007	2.4e-010	5.9e-007	19.61
Kb75len40	200-240	279	7.8	9.1e-007	9.5e-007	3.2e-008	9.5e-007	12.18
Kb75len60	190-250	279	7.8	2.4e-011	1.2e-006	5.0e-010	1.2e-006	9.64
Kb75len80	200-280	279	7.8	7.2e-011	1.6e-006	1.5e-009	1.6e-006	7.2
Kb75len100	200-300	279	7.8	5.8e-009	2.2e-006	5.7e-008	2.2e-006	5.2
Kb75len200	150-350	279	7.8	1.3e-011	2.8e-006	2.6e-009	2.8e-006	4.13
Kb75len300	100-400	279	7.8	3.2e-012	3.2e-006	3.0e-009	3.2e-006	36
Kb75len400	50-450	279	7.8	6.1e-012	3.4e-006	3.2e-009	3.4e-006	3.4

Table 13 continued

Kb100len20	220-240	279	7.8	6.0e-011	1.4e-006	1.7e-009	1.4e-006	20.27
Kb100len40	220-260	279	7.8	1.8e-014	2.5e-006	9.5e-013	2.5e-006	14.63
Kb100len60	220-280	279	7.8	8.8e-010	1.6e-006	7.6e-009	1.6e-006	11.2
Kb100len80	220-300	279	7.8	7.2e-009	2.4e-006	6.8e-008	2.4e-006	8.4
Kb100len100	200-300	279	7.8	5.9e-015	2.5e-006	9.5e-013	2.5e-006	7.63
Kb100len200	150-350	279	7.8	6.9e-010	2.6e-006	4.7e-009	2.6e-006	5.1
Kb100len300	100-400	279	7.8	7.3e012	2.9e-006	3.4e-009	2.9e-006	4.5
Kb100len400	50-450	279	7.8	7.2e-012	3.2e-006	2.7e-009	3.2e-006	4.2
Kb255len20	200-220	279	7.8	6.6e-008	5.0e-006	4.3e-008	5.0e-006	23.4
Kb255len40	200-240	279	7.8	1.5e-008	5.1e-007	1.4e-007	5.1e-007	22.7
Kb255len60	190-250	279	7.8	4.0e-011	5.8e-007	4.3e-010	5.8e-007	19.9
Kb255len80	200-280	279	7.8	7.7e-009	5.1e-007	1.4e-007	5.1e-007	22.7
Kb255len100	200-300	279	7.8	5.0e009	7.5e-007	4.4e-007	7.5e-007	15.4
Kb255len200	150-350	279	7.8	8.8e-011	1.07e-006	5.0e-007	1.07e-006	10.8
Kb255len300	100-400	279	7.8	9.8e-010	1.3e-006	7.7e-007	1.3e-006	8.3
Kb255len400	50-450	279	7.8	1.0e-011	2.4e-006	4.3e-008	2.4e-006	4.8
Kb10len200width1	150-350	279.5	7.8	3.4e-012	7.9e-007	2.4e-009	7.9e-007	14.65
Kb10len200width2	150-350	278	7.8	2.9e-011	7.7e-006	6.0e-009	7.7e-006	15.0
Kb10len200width3	150-350	279.5	7.8	3.4e-011	7.3e-007	3.1e-009	7.3e-007	15.85
Kb10len200width5	150-350	279.5	7.8	3.2e-010	6.9e-007	7.9e-009	6.9e-007	16.8
Kb10len200width10	150-350	279.5	7.8	1.0e-009	5.8e-007	1.4e-008	5.8e-007	19.9

Table 13 continued

Kb10len200grad0.01	150-350	279	7.8	1.5e-007	5.0e-007	4.7e-009	5.2e-007	22.25
Kb10len200grad0.02	150-350	279	7.8	1.5e-011	1.4e-006	1.1e-009	1.4e-006	8.26
Kb10len200grad0.04	150-350	279	7.8	9.1e-012	2.3e-006	3.4e-009	2.3e-006	5.03
Kb10len200grad0.05	150-350	279	7.8	9.1e-012	2.3e-006	3.4e-009	2.3e-006	5.03
Kb10len200grad0.1	150-350	279	7.8	9.4e-011	5.9e-006	3.3e-010	5.9e-006	1.96

Table 14 Residence Time Determined for Different Model Simulations (Described in previous Section)

Length	Width	K_a/K_b	Hydraulic Gradient	Residence Time (days)
LENGTH				
20	2.0	0.01	0.04	43.34
40	2.0	0.01	0.04	43.8
60	2.0	0.01	0.04	29.68
80	2.0	0.01	0.04	43.8
100	2.0	0.01	0.04	43.8
200	2.0	0.01	0.04	44.68
300	2.0	0.01	0.04	44.08
400	2.0	0.01	0.04	44.5
20	2.0	0.1	0.04	42.08
40	2.0	0.1	0.04	42.08
60	2.0	0.1	0.04	43.1
80	2.0	0.1	0.04	45.38
100	2.0	0.1	0.04	43.1
200	2.0	0.1	0.04	43.1
300	2.0	0.1	0.04	41.32
400	2.0	0.1	0.04	43.1
20	2.0	10	0.04	16.52
40	2.0	10	0.04	12.86
60	2.0	10	0.04	11.56
80	2.0	10	0.04	11.02
100	2.0	10	0.04	11.02
200	2.0	10	0.04	10.4
300	2.0	10	0.04	10.06
400	2.0	10	0.04	9.6
20	2.0	50	0.04	28.92
40	2.0	50	0.04	19.28
60	2.0	50	0.04	14.4
80	2.0	50	0.04	12.86
100	2.0	50	0.04	10.4
200	2.0	50	0.04	7.7
300	2.0	50	0.04	6.8
400	2.0	50	0.04	7.46
20	2.0	75	0.04	39.22
40	2.0	75	0.04	24.36
60	2.0	75	0.04	19.28
80	2.0	75	0.04	14.4
100	2.0	75	0.04	10.4
200	2.0	75	0.04	8.26

Table 14 continued

300	**2.0**	**75**	0.04	**7.2**
400	**2.0**	**75**	0.04	**6.8**
20	**2.0**	**100**	0.04	**40.54**
40	**2.0**	**100**	0.04	**29.26**
60	**2.0**	**100**	0.04	**22.4**
80	**2.0**	**100**	0.04	**16.8**
100	**2.0**	**100**	0.04	**15.26**
200	**2.0**	**100**	0.04	**10.2**
300	**2.0**	**100**	0.04	**9.0**
400	**2.0**	**100**	0.04	**8.4**
20	**2.0**	**225**	0.04	**46.8**
40	**2.0**	**225**	0.04	**45.4**
60	**2.0**	**225**	0.04	**39.8**
80	**2.0**	**225**	0.04	**45.4**
100	**2.0**	**225**	0.04	**30.8**
200	**2.0**	**225**	0.04	**21.6**
300	**2.0**	**225**	0.04	**16.6**
400	**2.0**	**225**	0.04	**9.6**
WIDTH				
200	**1.0**	**10**	0.04	**29.3**
200	**2.0**	**10**	0.04	**30.0**
200	**3.0**	**10**	0.04	**47.55**
200	**5.0**	**10**	0.04	**84.0**
200	**10.0**	**10**	0.04	**199.0**
GRADIENT				
200	**2.0**	**10**	0.01	**44.5**
200	**2.0**	**10**	0.02	**16.52**
200	**2.0**	**10**	0.04	**10.06**
200	**2.0**	**10**	0.05	**10.06**
200	**2.0**	**10**	0.1	**3.92**

4.6.2 The Residence Time Curves

The residence time calculated for the different model runs summarized in Table 14 is used to plot the variation of residence time for different barrier lengths, barrier widths, hydraulic gradients and ratios of aquifer to barrier hydraulic conductivity. The graphs prepared are discussed in this section.

4.6.2.1 Residence Time versus Ratio of Aquifer to Barrier Hydraulic Conductivity: Residence time calculated is plot against the ratio of aquifer to barrier hydraulic conductivity. From the resulting curve (Figure 29) it can be seen that for a barrier of any length, the residence time increases with the increase in the K_a/K_b ratio. However a slight decrease in the residence time can be observed for barrier lengths greater then 100m.

When the length of the barrier is small the potential for the escape of water around the sides is great and hence the net velocity through a section of a barrier is low. Barriers of greater length cause a low 'around barrier leakage' potential, instigate the through barrier water flow, at a greater velocity and hence slightly decrease the residence time. The barrier designed should possess a length that shows a slight initial decrease in residence time.

4.6.2.2 Residence Time versus Barrier Length: The residence time decreases with the increase in barrier length approaching a constant (Figure 30). However small barrier lengths have been seen to effect a high loss of contaminant and hence should be avoided even though they produce greater residence times.

4.6.2.3 Residence Time versus Hydraulic Gradient: Residence time decreases with an increase in hydraulic gradient, changing exponentially for smaller values and barely changing for larger values.

4.6.2.4 Residence Time versus Width: As expected the residence time increases with an increase in width however the rate of increase is very low. Evidently, increasing width

Table 15 Residence Time versus Aquifer to Barrier Hydraulic Conductivity

B.L. = Barrier Length in meters
Residence Time is in days

Ka/Kb	*225*	*100*	*75*	*50*	*10*	*0.1*	*0.01*
B.L.400	8.4	8.4	6.8	7.46	9.6	43.1	44.5
B.L. 300	16.6	9.0	7.2	6.8	10.06	41.32	44.08
B.L. 200	21.6	10.2	8.26	7.7	10.4	43.1	44.68
B.L. 100	30.8	15.26	10.4	10.4	11.02	43.1	43.8
B.L. 80	45.5	16.8	14.4	12.86	11.02	45.38	43.8
B.L. 60	39.8	22.4	19.28	14.4	11.56	43.1	29.68
B.L. 40	45.4	29.26	24.36	19.28	12.86	42.08	43.8
B.L. 20	46.8	40.54	39.22	28.92	16.52	42.08	43.34

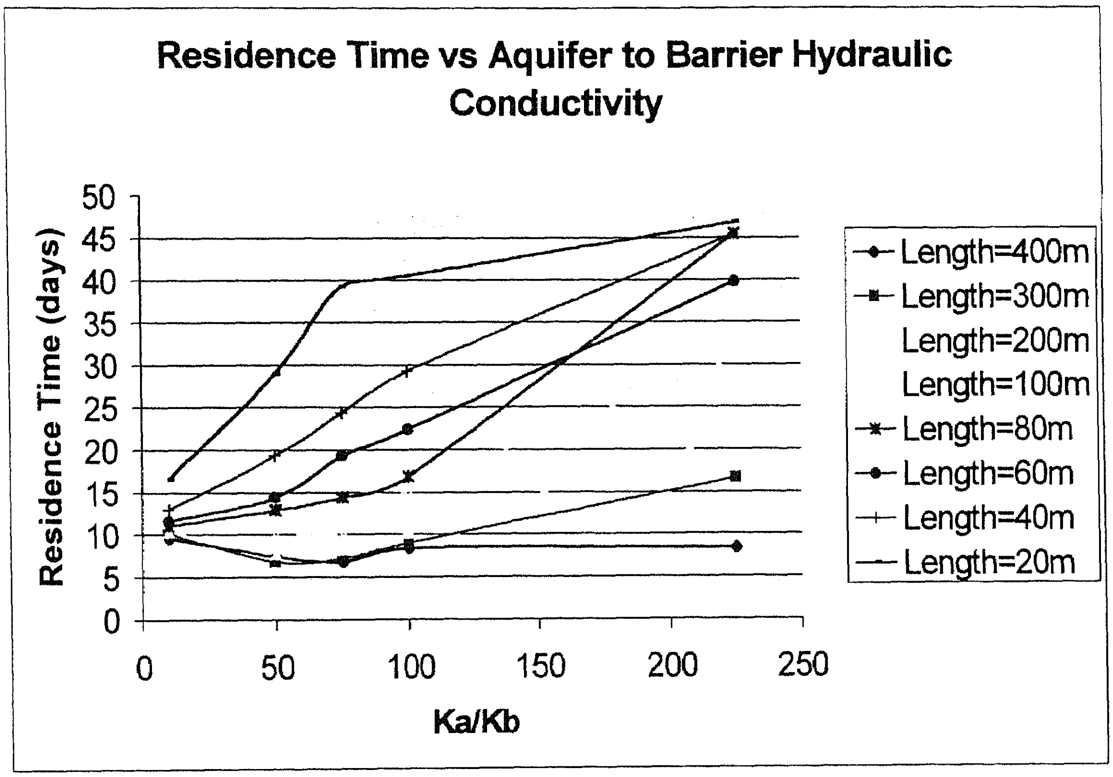


Figure 29 Graph showing Residence Time versus Aquifer to Barrier Hydraulic Conductivity

Table 16 Residence Time versus Barrier Length

*Ka/Kb
Residence Time is in days
Barrier length is in meters

Barrier Length	*400*	*300*	*200*	*100*	*80*	*60*	*40*	*20*
225*	8.4	16.6	21.6	30.8	45.4	39.8	45.4	46.8
100*	8.4	9.0	10.2	15.26	16.8	22.4	29.26	40.54
75*	6.8	7.2	8.26	10.4	14.4	19.28	24.36	39.22
50*	7.46	6.8	7.7	10.4	12.86	14.4	19.28	28.92
10*	9.6	10.06	10.4	11.02	11.02	11.56	12.86	16.52
0.1*	43.1	41.32	43.1	43.1	45.38	43.1	42.08	42.08
0.01*	44.5	44.08	44.68	43.8	43.8	29.68	43.8	43.34

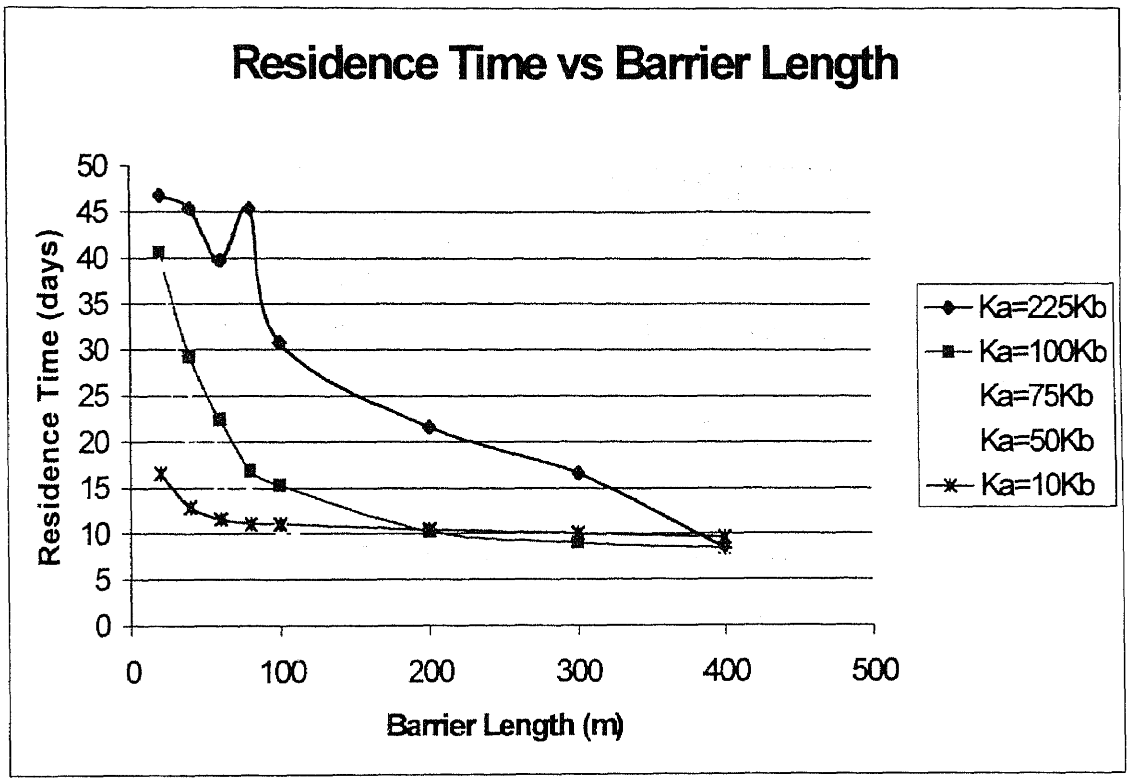


Figure 30 Graph showing Residence Time versus Barrier Length

Table 17 Residence Time versus Gradient

Gradient	*0.01*	*0.02*	*0.04*	*0.05*	*0.1*
Residence Time (days)	44.5	16.52	10.06	10.06	3.92

Residence Time is in days
Barrier Length = 200m
Ka = 10 Kb

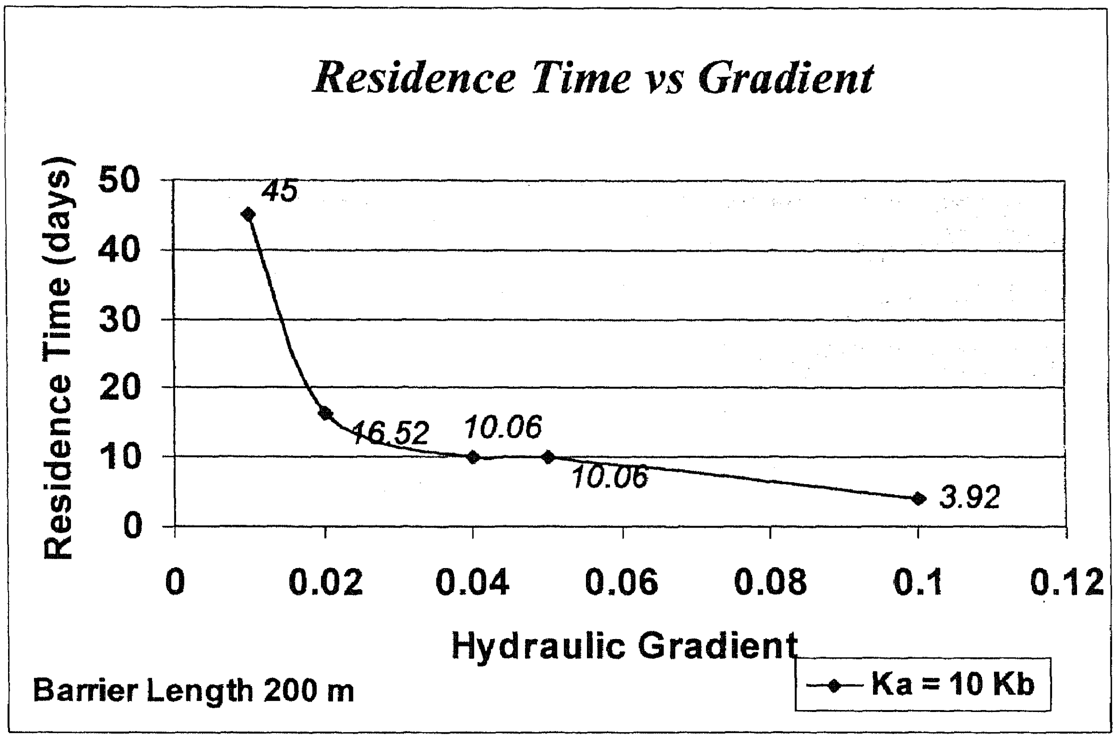


Figure 31 Graph showing Residence Time versus Gradient

Table 18 Residence Time versus Width

Width (m)	*1*	*2*	*3*	*5*	*10*
Residence Time (Days/m)	14.65	30	47.55	84	199

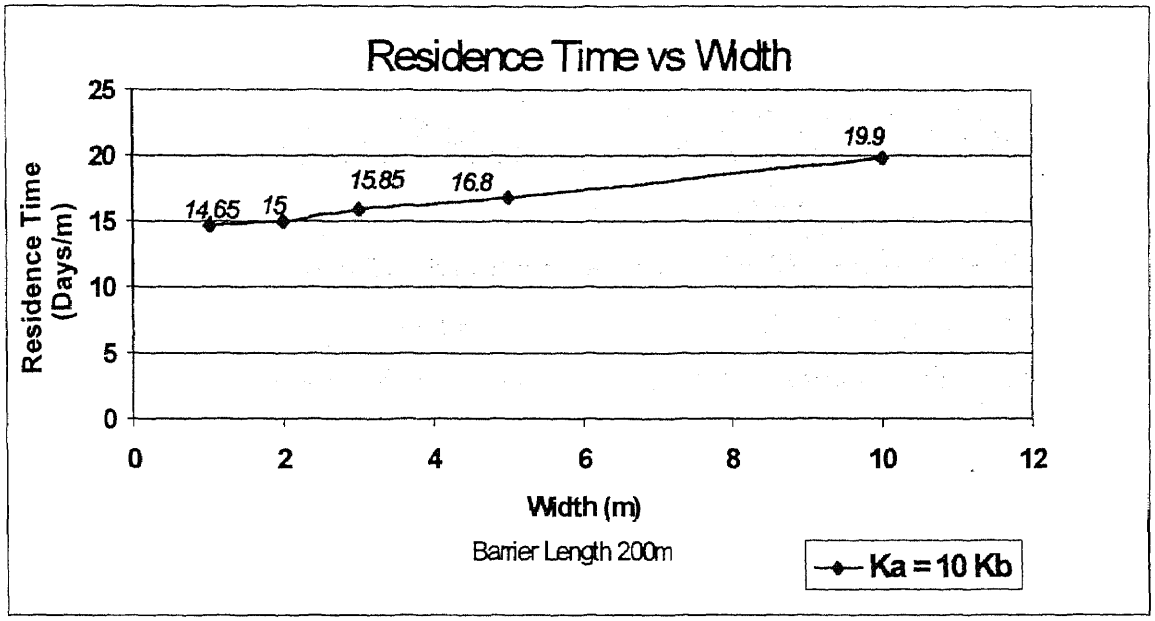


Figure 32 Graph showing Residence Time versus Width

cannot be used to increase residence time, as the incorporation of the barrier would prove uneconomical.

These graphs help validate the results of the loss of contaminant analysis and the design procedure.

4.7 The Three Step Procedure for the Design of a Permeable Reactive Barrier System

Based on the design curves, this study encompassed a procedure for the design of a barrier. The three steps in this procedure are illustrated in Figure 33 and discussed below:

Step1: The length of the barrier should be kept between 150-300m

From the design curve in Figure 24 it is lucid that, for a particular range of K_a/K_b ratio the loss of contaminant path-lines is more or less constant when a length ranging from 150m-300m is incorporated.

Step2: The ratio of the hydraulic conductivity of the aquifer to that of the barrier should be less than 50-100.

The amenities of having a barrier with a great hydraulic conductivity seem to be constrained from a residence time achievement point of view. However the cross sections of the simulations in the study show that there is a "water-table mounding" at the aquifer barrier interface. This interface is responsible for a transverse flow through the barrier (Figure 22). This transverse path is longer than the straight path the flow would have followed in the absence of this 'water-table mounding'. The actual residence time (transverse path) is a little greater than the residence time (straight path) in the absence of the 'water-table mounding'. It appears that the ratio of the aquifer to barrier hydraulic conductivity, up to a certain limit, does not or to a very small extent affects the residence time. This is in keeping with the results of the sensitivity analysis reported in Table 10 that shows that loss is not very sensitive (0.1-0.4) to changes in K_a/K_b ratios. It is primarily necessary to achieve the residence time in the barrier to ensure high contaminant removal. However this cannot be achieved at a high contaminant loss. Hence, the barrier K_a/K_b ratio should be kept less than 50-100.

Step 3: The barrier width should be kept between 1-3m.

This is to ensure low contaminant loss, and is a direct deduction from the design curve in Figure 22. Keeping the barrier width between 1-3m does not only help reduce contaminant loss but also to reduce the barrier cost.

These three steps are evaluated for accuracy, and redone for refinement based on the deviation of the residence time for the obtained design (read from the Table 14) from the residence time required for contaminant removal (from the geo-chemical study).

Design of different barrier arrangements are centered on similar design steps with additional alterations, based on the curves in Figure 27 and Figure 28, specific to the configuration. The steps are illustrated in Figure 33.

If the barrier is double walled, the second wall is designed similar to the first. The distance between the walls is kept less than 15m or greater than 80m to prevent high contaminant loss. If the barrier is hanging create and execute a site specific model on the same lines as described in this study.

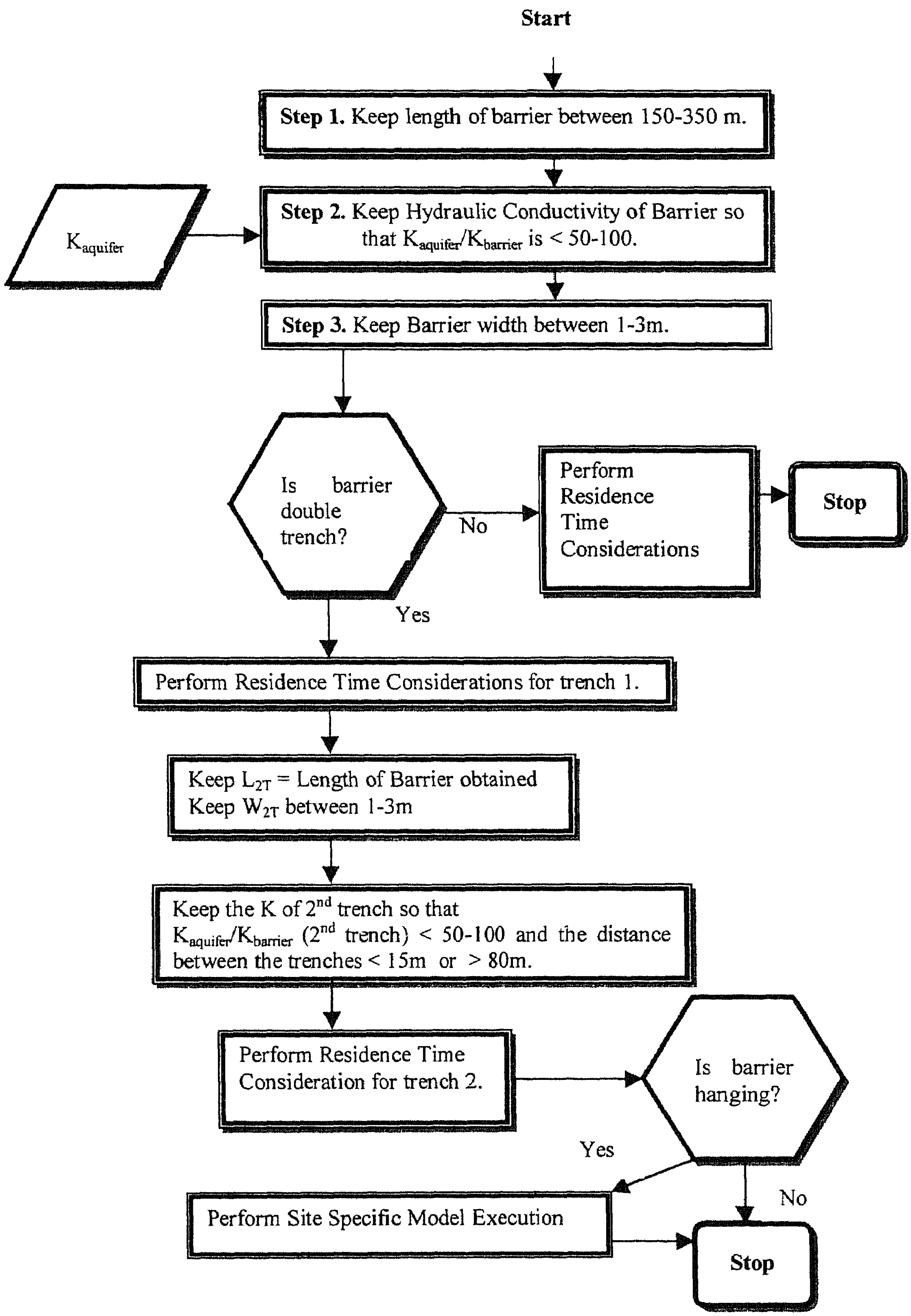


Figure 33: A Three Step Procedure for the Design of Barrier

Where:

$RT_{obtained}$ = Residence Time Obtained from Design Of Barrier Procedure

$RT_{required}$ = Residence time required for the reduction of contaminant or change in ptt

L_{2T} = Length of 2nd trench

$K_{aquifer}$ = Hydraulic Conductivity of Aquifer

$K_{barrier}$ = Hydraulic Conductivity of Barrier

D_{trench} = Distance between trenches of a double trench PRB

$D_{ptrench}$ = Depth of hanging Wall

W_{2T} = Width of 2nd trench

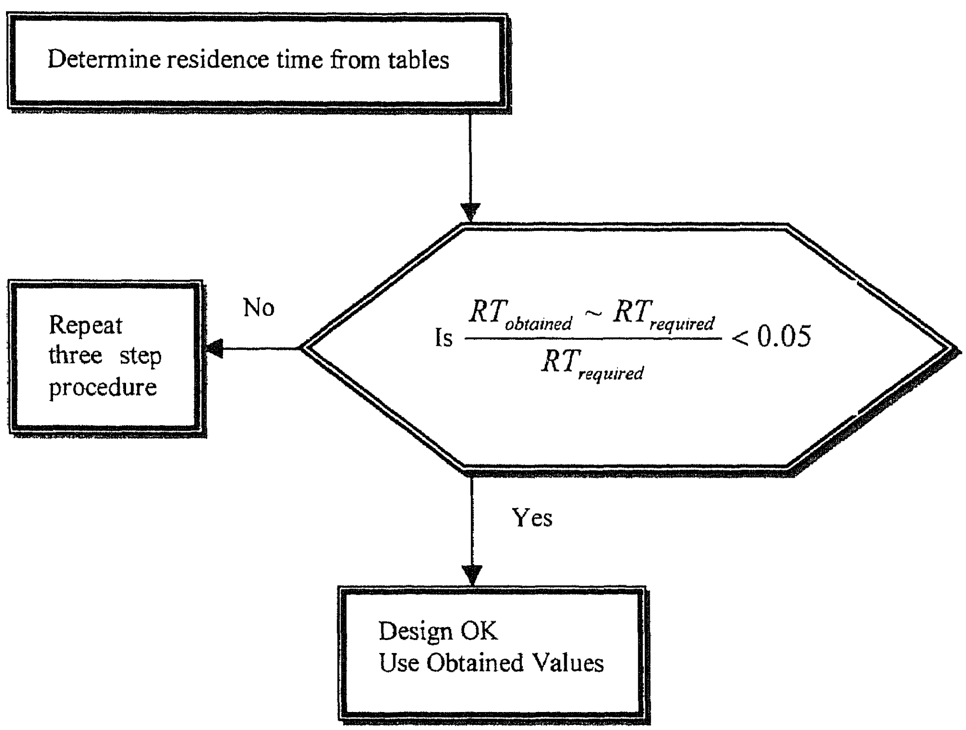


Figure 34: Residence Time Considerations

CHAPTER 5

CASE STUDY

5.1 Typical Site Characteristics

The first step in any modeling assignment is the development of a conceptual model. The conceptual model is a 3D representation of the ground water flow and transport system based on all geologic, hydrogeologic, and geo-chemical data for the site. This makes a brief discussion of the project site indispensable.

The various parameters required for modeling the flow and transport were obtained by the reports and drawings provided by the Tetra Tech inc. located at Pittsburgh in Pennsylvania (www.tetratech.com).

The site under consideration in this study, which is located in the Piedmont Province of the Appalachian Highlands, is shown in the Figure 35a. These are the sites contaminated with chromium and are to be remediated using the PRB technology. They are located at Hudson County in New Jersey.

The soil texture above the meadow mat shown in the cross-section is mostly fill and can be classified as silty sand (SM) with some rock fragments, wood, glass, residue and trace clay. The soil below the meadow mat consists of gray to brown sand and grades into a red brown sandy silt (ML/SM) which grades into a silty sand (till) with a trace of gravel and rock fragments.

To obtain the ground water parameters of the site under consideration, a number of shallow and deep wells have been sunk at locations shown in the Figures. The

Tetra Tech NUS, Inc., are tabulated in Table 19. The slug tests were conducted on the shallow and the deep wells. The site plan and two geologic cross-sections for the study area are shown in the Figure 35a, 35b, 35c.

The objective of the study conducted on Permeable Reactive Barriers was formulated in early months of 1997. Parallel geo-chemical and hydro geological studies had been proposed necessary. The geo-chemical study has been successfully documented in the master's thesis of my colleague Hemant S. Desai. The hydro geologic study, that is the primary subject of this dissertation, was conducted under the able advice of Dr. John Schuring. The overview of the PRB study process is shown in the flowchart in (Figure 36).

5.2 The Design of the Barrier using the Three Step Procedure

- **Step 1: Keep the length of the barrier between 150-350m.**

Arbitrarily a barrier length of 200m is selected for every 500m length of contaminant plume.

- **Step 2: Keep the hydraulic conductivity so that $K_{aquifer}/K_{barrier}$ is < 50-100**

The hydraulic conductivity of the aquifer is 9 x 10^{-6}m/s. The barrier hydraulic conductivity is set to 9 x 10^{-7}m/s to keep $K_{aquifer}/K_{barrier} = 10$.

- **Step 3: Keep the barrier width between 1-3m**

The barrier width is fixed at 2m.

The geo-chemical study has proposed a barrier system consisting of two walls. One to increase the pH and the other to reduce the contaminant. The residence times for the first and the second walls have been determined to be 7 days and 12 days respectively.

- **Residence Time Considerations for First Trench**

From Table 14 the residence time is read to be 10.4 days. $RT_{required} - RT_{obtained}$ is –3.4 The design is satisfactory. We incorporate obtained values.

- **Design of Second Wall**

The distance between the two walls is fixed at 2m. The length width and hydraulic conductivity is kept identical to the first wall.

- **Residence Time Considerations for Second Trench**

From Table 14 the residence time is read to be 10.4 days. $RT_{required} - RT_{obtained}$ is 1.6 days The design is not acceptable. We do not incorporate obtained values instead we fix the width of wall to 2.2 m. from the residence time graphs the residence time is found to be 15.2 days. When the tree step procedure is re-run $RT_{required} - RT_{obtained}$ is found to be 3.2. The design is satisfactory. We do now incorporate obtained values.

- **Result of Design Procedure**

The barrier system at the site consists of two trenches 2m apart. Each trench is 200m long designed to a hydraulic conductivity to 9 x 10^{-7}m/s. The width of the first and the second trench is 2m and 2.2m respectively.

Table 19 Shallow and Deep Wells and Corresponding Calculated Hydraulic Conductivity at Site

Shallow wells

Well Number	Hydraulic Conductivity (ft/day)
073-MW-BB11	1.72
087-MW-A26	4.57
087-MW-019	3.11
087-MW-029	2.19
088-MW-G19	1.20
115-MW-E8	19.10
115-MW-E14	1.85
115-MW-O13	1.57
115-MW-AA15	3.14
125-MW-L3	0.78
134-MW-Q8	5.14
163-MW-R5	18.26

Deep wells

Well Number	Hydraulic Conductivity (ft/day)
087-MW-019D	40.90
115-MW-E8D	5.82
115-MW-E14D	2.79
115-MW-O13D	3.41

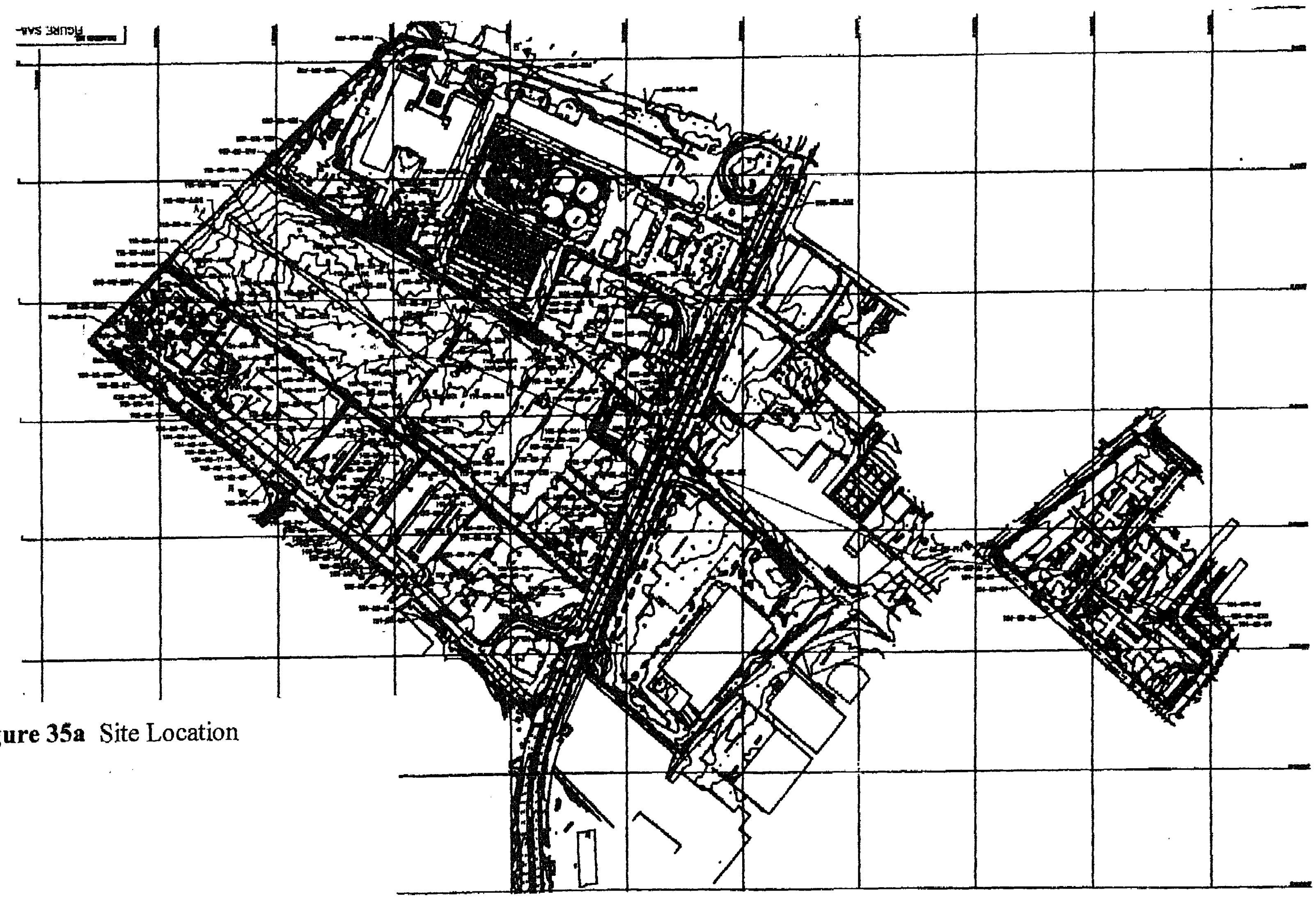


Figure 35a Site Location

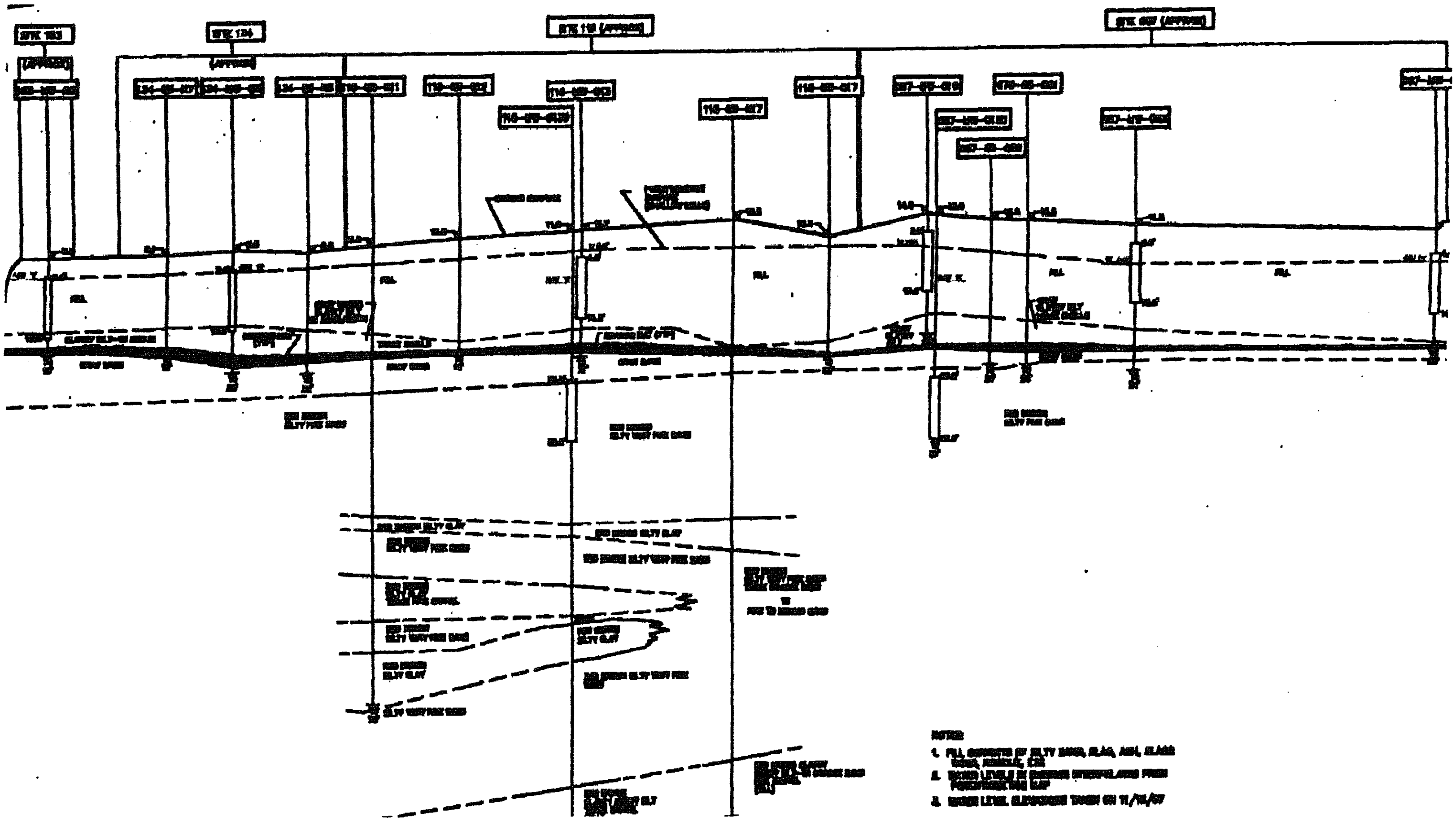


Figure 35b Cross Section A-A'

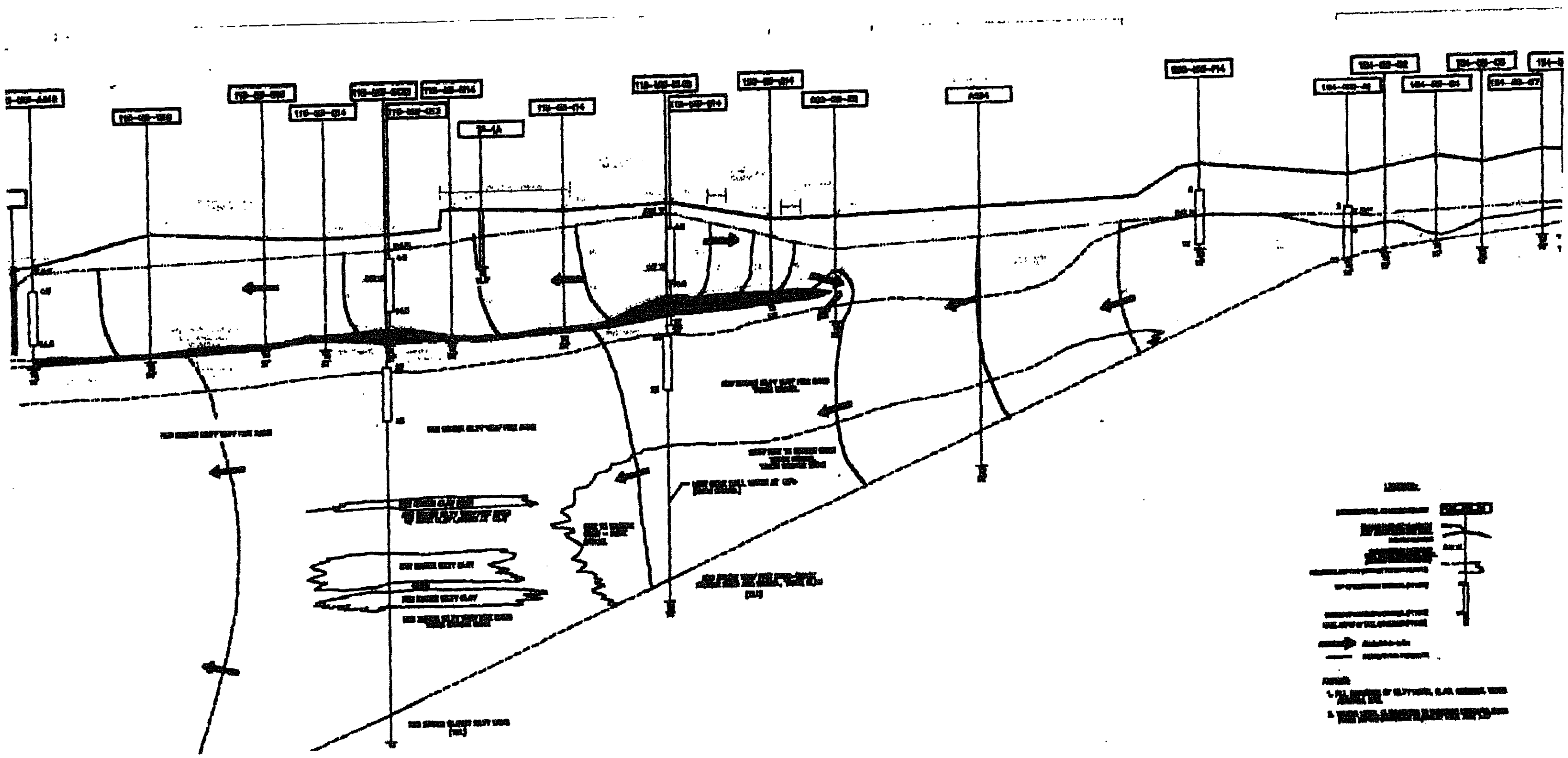


Figure 35c Cross Section B-B'

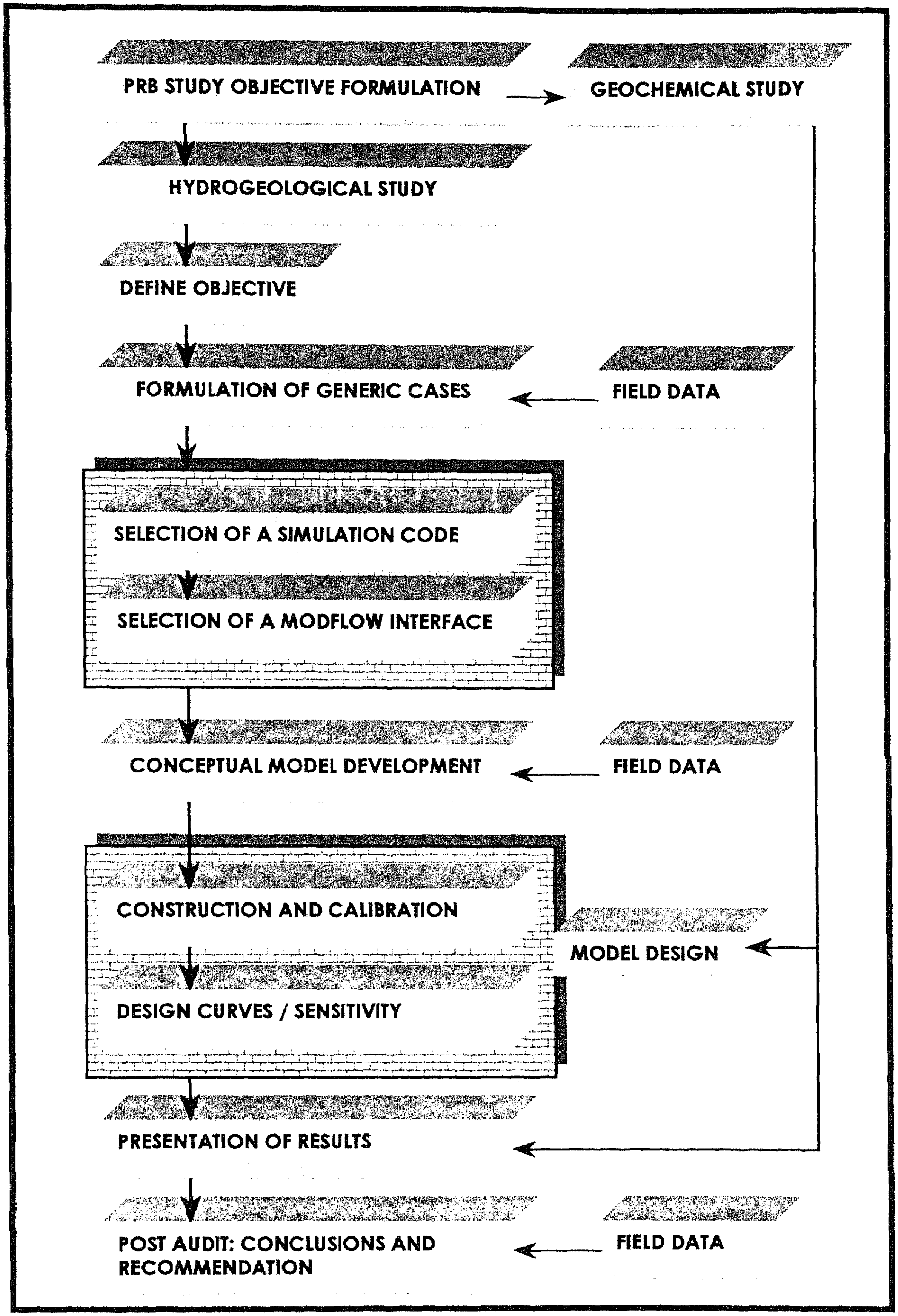


Figure 36 Overview of the PRB design study

CHAPTER 6

RECCOMENDATIONS AND CONCLUSIONS

6.1 Conclusions

Permeable Reactive Barrier System is an in-situ technology to treat contaminated groundwater by placing reactive material in the path of the GW. The reactive material intercepts the ground water and transforms the contaminant to a less environmentally harmful form, thereby reducing the contaminant concentration to below the permissible.

The focus of the present study was centered on the modeling analysis to support the PRB design. Prediction of the geometry and evaluation of different configurations is important in the design of a Permeable Reactive Barrier. While considerable modeling study had addressed the Funnel-and-Gate Configuration, limited modeling attention had been given to the Continuous Configuration. Studies on the continuous configuration were directed towards geo-chemical aspects of the configuration and the modeling support was directed towards prediction of the flow system in response to future events like the decrease in hydraulic conductivity over time or the effect of pumping in the vicinity of a PRB. No consensus had been reached on a uniform procedure to design a Continuous Configuration PRB. Therefore the overall objective of this study was to concoct modeling procedures and to formulate design curves to support the design of a Permeable Reactive Barrier to treat contaminated ground water economically. The study has arrived at the following conclusions:

1. Comparison of the different simulation codes and interfaces resolved that Modflow with either of the two Graphic User Interfaces used in this study, namely, Visual Modflow and Ground Water Modeling System provide a versatile, user-friendly environment for GW simulations.
2. A conceptual model of a contaminated aquifer in association with the PRB system can be broadly considered to fall into six generic cases. These cases arise from having confined and unconfined aquifers, single and double trench barriers, and fully and partially penetrating configurations. In this PRB system design study all these cases have been addressed. Models of each case have been calibrated and executed.
3. The model was calibrated using the data ranges from available PRB installation sites and the specific case addressed in this study. This enabled the model to simulate as closely as possible the subsurface actualities. The basic set of assumptions was established prior to the model calibration to reflect as closely as possible the GW flow regime. The unconfined aquifer was considered to be deeper than reality to accommodate the ranges in hydraulic gradient at the different PRB installations and to vary the same. Models with impermeable boundaries at great depths were assumed to simulate within a reasonable range of error confined, unconfined and deep aquifer conditions. The number of barrier incident particles that the model incorporated were decided so as to reflect true contaminant concentrations.
4. The sensitivity analysis showed that the most critical parameter was barrier width followed by the length of 'less than aquifer' permeable barriers. The length of 'more than aquifer' permeable barrier is not sensitive. An important result of the sensitivity analysis is that the loss is not or only slightly sensitive to K_a/K_b ratio. This can be

attributed to the 'water table mounding and subsequent inclined path' phenomenon. The hydraulic gradient does not affect the loss of contaminant.

5. During calibration of the model the average difference between the simulation and observed head expressed as mean error and the root mean square error was less than 5 %. Thus it can be concluded that the model was consistent with the ground water regime not only of the site considered in the case study but also with other instillation sites.
6. The most important result of this study is that the design curves were used to conceive a procedure for the design of a continuous barrier. The design procedure has been validated to include both barrier and aquifer properties and is with respect to all but one conceptual case. The mounding effect of the water table motivates the design rationale for a partially penetrating barrier (hanging wall) to include a site specific model execution.
7. When it is required to pre-treat the ground water a double trench barrier installation becomes necessary. Though the individual trenches can be designed similar to the single trench the loss of contaminant is sensitive to the distance between the barrier. In the case of the double trench barrier configuration the design agendum was hypothesized to include the distance between the trenches as a key parameter.
8. Residence time is sensitive to aquifer to barrier hydraulic conductivity, barrier length, barrier width and hydraulic gradient of the water table at the site. A barrier can be thus designed for minimum contaminant loss and then the mentioned critical parameters can be worked with to achieve the desired residence time.

The three-step design procedure formulated in this study was used to design a Permeable Reactive Barrier at the site. The barrier system thus designed consists of two trenches 2m apart. Each trench is 200m long designed to a hydraulic conductivity to 9 x 10^{-7}m/s. The width of the first and the second trench is 2m and 2.2m respectively.

6.2 Recommendations for Further Study

Modeling studies to support the design of a Permeable Reactive Barrier is encyclopedic and certain aspects of the predictive GW flow have been identified to be beyond the scope of this study and is recommended for further study.

1. A large amount of literature has addressed the Superfund favorite Funnel-and-Gate Configuration Barriers. However this study has informally modeled the same, but with different modifications. Owing to the extensive literature focus and the inadequate level of accuracy with which these simulations were conducted it has not been documented. However this study identifies that this configuration facilitates modular design for capacity add-ons. The design of the barrier systems in modules or blocks that can function independently and can be increased to meet future increases in load would prove useful in increasing the life of the instillation. A correlation of contaminant load to PRB modules is an interesting objective of a formal investigation. It is strongly recommended that this point of view be considered for further study.
2. The design of the hanging wall PRB has not been comprehensively addressed in this study. It was concluded that a site-specific simulation be resorted to when the

incorporation of the same is unavoidable. This study recommends that this conceptual case be evaluated to arrive at a general design procedure.

3. The mounding effect of the water table incident on a less conductive (than aquifer) barrier propels a below barrier evasion of contaminated ground water. It also causes the inclination of the contaminant through the barrier, increasing the contaminant residence time. This phenomenon, identified but not evaluated in this study, can be harnessed to accommodate lower conductivity barriers in the PRB system and to incorporate this technology when high contaminant-reducing agent reaction time is required. However this hypothesis requires further study.

4. The design curves have been adopted to formulate a design procedure. The sensitivity analysis has evaluated the degree to which a parameter is critical. A correlation of loss of the contaminant to properties of the barrier and aquifer is required to deem this study complete. This study urges the evaluation of a relationship of the following form:

   Influx loss = f (length of barrier, width of barrier, hydraulic conductivity ratio)

   A correlation of residence time to different parameters is perceptible from the residence time graphs. This would prove an interesting subject for technical study.

5. The conceptual cases were all investigated from a design perspective using a model that to a certain level of uncertainty simulates cases other than the basic 'single wall in confine aquifer case'. Further studies should investigate other conceptual cases using case specific model simulations.

6. Different barrier configurations, which are combinations of the discussed generic cases, may be plausible. In fact recent installations have been known to incorporate

the discussed case combinations. These barriers may prove to be more effectual at a specific site, and should be investigated. The design of a barrier should therefore have an additional step to investigate conceptual configurations and verify if it is possible for a specific site.

APPENDIX A

CURRENT APPLICATIONS OF REACTIVE BARRIERS TO CONTAMINANT PLUMES

As of this dissertation work, 7 full scale reactive barriers and 11 pilot scale plants have been installed in the field and have been documented here (EPA/600/f-67, 1998, Puls & Powell, 1998, Compilation of Permeable reactive Barrier Action Team, 1999).

1. **Site location: Intersil Semiconducter site in Sunnyvale, California**

Site Hydrogeology: The site consists of an aquifer confined on the top by a clayey to silty-clay layer, and on the bottom by a silty-clay to clayey aquitard. The aquifer, characterized by an irregular geometry with clay lenses, is constituted by interfingering zones of silt, sand and gravel.

Installation Date: January 1995

Contaminants and their Concentration: The contaminants are trichloroethelene (TCE)-50-200μg/L, cis-1,2 dichloroethelene (cDCE)- 450-1000μg/L, Vinyl Chloride (VC)- 100-500μg/L, and Freon 113® - 20-60μg/L

Barrier Configuration: Funnel-and-Gate with up gradient and down gradient permeability zones.

Funnel Material: Slurry walls

Funnel Length: NA

Reactive Gates Provided: 1 no.

Reactive Material: NA

Reactive Zone Height/Length/Thickness: 11ft/36ft/4ft

Mass Of Reactant: NA

Permeable Reactive Barrier Depth: 20ft

Dissertation Conceptual Model: Case 3

Total System Length: NA

Cost: $ 41,000,000

Special Features:

- The cleanup goal is to reduce contaminant concentration to below the MCL (Maximum Contaminant Level) set by the State of California and the Primary Drinking Water Standards.
- VOC concentrations below cleanup goals have been reported since installation.

2. **Site location (full-scale field test)**: Industrial site, Belfast, Northern Ireland

Site Hydrogeology: It consists of an aquifer composed of a hydraulically conductive mixture of sand, silt, gravel lenses in glacial till. The discrete clay or clayey silt lenses constrain GW flow. The aquifer extends to 40ft, and the water table is intercepted at a depth of 20ft from ground surface.

Installation Date: December 1995

Contaminants and their Concentration: The contaminants at the site were Trichloroethylene (TCE)-390 mg/l, 1,2- cis dichloroethelene, and other breakdown products.

Barrier Configuration: Circular reaction Vessel

Funnel Material: Bentonite Cement Slurry Walls

Funnel Length: 100ft +100ft.

Reactive Gates Provided: NA

Reactive Material: Zero-valent Iron

Reactive Zone Height/Length/Thickness: 33ft/16ft/4ft dia.

Mass Of Reactant: 15 tons

Permeable Reactive Barrier Depth: 33ft

Dissertation Conceptual Model: Case 2

Total System Length: 200ft

Cost: $ 375,000

Special Features:

- Manhole to facilitate periodic stratification.
- Design residence time of 5 days.
- Varied flow rates through the reactor were observed.
- 99.7% reduction in TCE and cDCE accomplished.

3. Site location: periphery of an industrial property, Coffeyville, Kansas

Site Hydrogeology: The site is made up of a hydrologically and geochemically complex aquifer, vastly composed of basal sand and gravel over the confining shale bedrock.

Installation Date: January 1996

Contaminants and their Concentration: The contaminants are trichlorethelene(TCE)- 400 μg/l, and 1,1,1- trichloethane (TCA)- 100 μg/l.

Barrier Configuration: Funnel-and-Gate.

Funnel Material: Soil-bentonite slurry walls.

Funnel Length: 490ft x 2 (on either side)

Reactive Gates Provided: 1 no.

Reactive Material: Zero-valent Iron

Reactive Zone Height/Length/Thickness: 11ft/20ft/3ft

Mass Of Reactant: 70 tons

Permeable Reactive Barrier Depth: 15ft-30ft

Dissertation Conceptual Model: Case 1

Total System Length: 1000ft

Cost: $ 400,000

Special Features:

- The lateral extent of the contaminant plume is 875 yds.
- A high funnel/gate ratio accommodates the low GW flow velocity (0.2 ft/day).
- Contaminant concentration below the MCL is achieved in the effluent GW.

4. Site location (PRB installation): Government Facility, Lakewood, Colorado

Site Hydrogeology: The site consists of an 15-25ft thick unconfined aquifer, made up of a hydraulically connected mass of unconsolidated gravelly sand overlying fractured claystone, confined at the lower end by unfractured claystone. The aquifer is characterized by irregular geometry, clay lenses in the sand and sandstone lenses in the claystone, lateral geologic heterogeneity and varying contaminant concentrations.

Installation Date: October 1996

Contaminants and their Concentration: The contaminants at the site include 1,1,1-trichloroethane (TCA)-700μgL^{-1}, 1,1-dichloroethylene (1,1,DCE) -700μgL^{-1}, trichloroethylene (TCE) -700μgL^{-1}, and cis dichloroethylene (cDCE), and VC-15μgL^{-1}.

Barrier Configuration: Funnel-and-Multiple Gate

Funnel Material: Sealable joint sheet piles

Funnel Length: 1,040-ft funnel section

Reactive Gates Provided: 4 nos.

Reactive Material: Zero-valent Iron

Reactive Zone Height/Length/Thickness: 10-15ft/4x40=160/2-6ft (gates differed in thickness).

Mass Of Reactant: No information

Permeable Reactive Barrier Depth: 15 to 25ft.

Dissertation Conceptual Model: Case 1

Total System Length: 1200ft.

Cost: $1,000,000

Special Features:

- 1^{st} multiple gate system.
- Expected GW velocity range: 1ft/day to 10ft/day depending on hydrogeologic conditions in the vicinity of the wall.
- A decrease in porosity of 0.5% a year was estimated, attributed to the precipitation of calcite and siderite corresponding to the decrease in calcium and inorganic carbon respectively in the treated groundwater.
- Increase in upgradient hydraulic head and the ensuing head difference is accountable for the contaminated water moving around the barrier, espied recently at the site.

5. **Site location:** former plating industrial facility, Central New York

Site Hydrogeology: The site consists of a gravel and sand water table aquifer that extends to a depth of 21ft, confined at the lower end by an impermeable clay layer . The water table can be intercepted at a depth of 4-5ft from the surface. The aquifer material has been reported to exhibit a hydraulic conductivity ranging from 16-230 ft/day.

Installation Date: December 1997

Contaminants and their Concentration: The contaminants of concern encountered in the untreated GW are trichloroethelene, cis 1,2-dichloroethylene (cDCE), and Vinyl Chloride (VC). The total volatile organic compounds (VOC) concentrations range from 300μg/l to 900μg/l

Barrier Configuration: Double Trench Continuous Wall

Funnel Material: NA

Funnel Length: NA

Reactive Gates provided: NA

Reactive Material: Granular Zero-valent Iron

Reactive Zone Height/Length/Thickness:

- 1st trench: 18-21ft/plume width/1ft
- 2nd trench: (10ft upgradient of the 1st) 18-21ft/plume width/1ft

Mass Of Reactant: NA

Permeable Reactive Barrier Depth: 21 ft

Dissertation Conceptual Model: Case 4

Total System Length: 50ft.

Cost: $797,000

Special Features:

- The concept of double trench was introduced to increase residence time in reactive media. The Double trench considered in our study how ever has a different objective.
- The continuous configuration barriers were identified as more feasible on account of their lower cost & no scope for leakage around barrier.
- Down gradient samples at the time of implementation were found to still contain some VOC's.

6. **Site location:** U.S. Department of Energy's City Plant, Kansas City, Missouri

Site Hydrogeology: The site consists of semi-confined aquifer consisting of alluvial sediments characterized by low plasticity clays (K= 0.75 ft/day) that overlie basal gravel (K= 34 ft/day). The bottom-confining layer is made up of basal shales.

Installation Date: April 1998

Contaminants and their Concentration: The contaminants are 1,2-dichloroethylene (1,2-DCE)-1377 μg/L and vinylchloride (VC)-291 μg/L.

Barrier Configuration: Differing thickness continuous curtain permeable reactive barrier.

Funnel Material: NA

Funnel Length: NA

Reactive Gates Provided: NA

Reactive Material: Zero-valent Iron (Fe^0)

Reactive Zone Height/Length/Thickness: First 6 ft. depth: 6 ft./full length/6 ft., next 2 ft. depth: 2 ft./full length/6 ft., next 4 ft. depth: 4 ft./full length/6 ft. of sand.

Mass Of Reactant: NA

Permeable Reactive Barrier Depth: NA

Dissertation Conceptual Model: not conceptualized

Total System Length: NA

Cost: $ 1.5 million

Special Features:

- This differing thickness configuration was used for the first time to compensate for different flow velocities in the clay and basal gravel.
- The contaminant level achieved is not below the MCL but it is expected to fall below the same soon.

Hydrogeologic concerns: NA

7. **Site location (Demonstration Project):** Lowry Air Force Base, Colorado

Site Hydrogeology: The site consists of an unconfined aquifer consisting of alluvial deposits and an artificial fill overlying a combination silty claystones and sandy siltstones. The upper 10 ft. of the confining bedrock is fractured and serves as a part of the aquifer.

Installation Date: October 1996

Contaminants and their Concentration: Primarily consists of trichloroethylene (TCE)-1400 μg/L.

Barrier Configuration: Funnel-and-Gate System

Funnel Material: Sheet piles

Funnel Length: 14 ft. to a depth of 17 ft.

Reactive Gates Provided: 1 no.

Reactive Material: Zero-valent Iron (Fe^0)

Reactive Zone Height/Length/Thickness: about 20 ft./ 10 ft./ 5 ft.

Mass Of Reactant: NA

Permeable Reactive Barrier Depth: NA

Dissertation Conceptual Model: Case 2

Total System Length: NA

Cost: $ 530,000

Special Features:

- The PRB was designed and built as a short term solution.
- The new remediation system consists of and PRB upgradient containment slurry wall.

Hydrogeologic concerns: NA

8. **Site location (full-scale demonstration):** U.S. Coast Guard Support Center in Elizabeth City, North Carolina

Site Hydrogeology: The site consists of an unconfined aquifer made up of highly conductive mass of fine gravel to coarse sand, 2-6 ft. deep. Highest concentrations of chromium and chlorinated organic compounds have been reported in this layer. The aquifer is confined at the base by a low conductivity aquitard made up of clayey, fine sand to silty clay. The groundwater starts at a depth of 6 ft. though the aquifer is intercepted at a depth of 16-20 ft. below the ground surface.

Installation Date: June 1995

Contaminants and their Concentration: The contaminants are hexavalent chromium (Cr^{+6})- greater than 3430 μg/L and trichloroethylene (TCE)- greater than 4320 μg/L.

Barrier Configuration: Continuous Barrier Configuration

Funnel Material: NA

Funnel Length: NA

Reactive Gates Provided: NA

Reactive Material: Zero-valent Iron (Fe^0)

Reactive Zone Height/Length/Thickness: 21 ft./150ft./2ft. The wall starts at a depth of 3 ft.

Mass Of Reactant: 450 tons of Granular Iron

Permeable Reactive Barrier Depth: 3-26 ft

Dissertation Conceptual Model: Case 1

Total System Length: 150 ft.

Cost: $ 500,000 (total installation cost)

Special Features:

- The cleanup goal set was 0.05 mg/L for Cr^{+6} and 5 μg/L for TCE.
- As expected all chromium is devoid within the first 6 inches of barrier.
- Chromium and chlorinated contaminant concentration down gradient the barrier is below the clean up goal.
- Cores collected at the site are being studied to evaluate the formation of secondary precipitates that may affect the barrier performance over time.
- Two contaminants were treated.

9. **Site location (pilot-scale field demonstration):** Atlantic Coastal Plain Physiographic Province at Dover Air Force Base, Delaware. The demonstration was funded by the Strategic Environmental Research and Development Program (SERDP).

Site Hydrogeology: The site consists of an unconfined aquifer (K= 10-50 ft./day), made up of cretaceous to recent sedimentary deposits of gravel, sand, silt, clay, limestone, marl, chalk, overlying clay aquitard located at 40-45 ft. below the surface. The water table is intercepted at 5-15 ft.

Installation Date: January 1998

Contaminants and their Concentration: The contaminants at the site are perchloroethylene (PCE)-5617 μg/L, trichloroethylene (TCE)-541 μg/L, dichloroethylene (DCE)-529 μg/L.

Barrier Configuration: Funnel-and-Gate

Funnel Material: Sheet piles

Funnel Length: NA

Reactive Gates Provided: 2 nos

Reactive Material: NA

1. Gate1: Zero-valent Iron (Fe^0) with 10% iron/sand pretreatment zone to stabilize flow and remove D.O.
2. Gate2: Zero-valent Iron (Fe^0) with 10% pyrite/sand pretreatment zone to moderate the pH of reactive bed and to decrease the precipitates formed.

Reactive Zone Height/Length/Thickness: 45ft./gate length/8 ft.

Mass Of Reactant: NA

Permeable Reactive Barrier Depth: 45 ft.

Dissertation Conceptual Model: Case 1

Total System Length: NA

Cost: $800,000

Special Features:

- Major objective of the demonstration include comparison of two reactive media schemes and examining innovative emplacement techniques to reduce the cost of construction for a PRB system.
- The demonstration is being used to update the U.S. Army Corps of Engineers', "Design Guidance for Application of Permeable Barriers to remediate Dissolved Chlorinated Solvents", February 1997.

10. Site location (pilot-scale field demonstration): Canadian Forces Base in Borden, Ontario, Canada

Site Hydrogeology: The site consists of a 'superficial' unconfined aquifer (K=20.5 ft./day), made up of medium to fine sand, overlying a thick clay deposit. The aquifer, water table, contaminant plume and impermeable clay extend 6.5 ft.-10 ft., 9.7 ft., about 13 ft. and 30 ft. respectively from the ground surface.

Installation Date: 1991

Contaminants and their Concentration: The contaminants are trichloroethylene (TCE)- 250,000 μg/L and perchloroethylene (PCE)- 43,000 μg/L.

Barrier Configuration: Continuous Barrier Configuration

Funnel Material: NA

Funnel Length: NA

Reactive Gates Provided: NA

Reactive Material: It consists of a mixture (K=124 ft./day) of zero-valent granular iron (Fe^0) and coarse sand in the ratio 11:39.

Reactive Zone Height/Length/Thickness: (each rectangular cell) 32 ft./18 ft./5 ft.

Mass Of Reactant: NA

Permeable Reactive Barrier Depth: 32 ft.

Dissertation Conceptual Model: Case 1

Total System Length: NA

Cost: Installation cost, exclusive of the cost of reactive material and labor, $ 30,000.

Special Features:

- Individual joint sheet piles, sealed with bentonite sealant were interlocked to create rectangular cells for emplacement of reactive mixture.
- The system reduced TCE and PCE concentrations by 90% and 86% respectively.
- The concentration distribution monitoring detected small amount of calcium carbonate precipitates at the end of five years. This data is suggestive that the barrier has a minimum life of ten years.
- The residual source was remediated using permanganate flushing.
- The primary purpose of this implementation was to evaluate the suitability of the following techniques to remediate PCE,CCl_4 and toluene: abiotic reductive dechlorination using zero-valent iron (Fe^0), followed by oxygen releasing compound (ORC^{TM}) to promote aerobic biodegradation; natural attenuation; and a permeable nutrient injection wall, using benzoate to promote anaerobic biodegradation, followed by an aerobic (oxygen) biosparge gate for aerobic biodegradation.

11. Site location (second part of the previous pilot scale demonstration): Formerly U.S. Naval Air Station in Alameda, California

Site Hydrogeology: The site consists of a sandy fill aquifer (K=0.057 ft./day) with an underlying confining layer composed of silts and clay 15-20 ft. thick. The ground water is intercepted at 4-7 ft. below the ground surface.

Installation Date: December 1996

Contaminants and their Concentration: The contaminants are trichloroethylene (TCE), cis-1,2-dichloroethylene (cDCE), vinyl chloride (VC), and toluene, benzene, ethyl benzene, and xylene (BTEX). The upgradient concentration of chlorinated VOCs exceed 100 mg/L and toluene up to 10 mg/L.

Barrier Configuration: Funnel-and-Gate System

Funnel Material: NA

Funnel Length: 10 ft. on either side

Reactive Gates Provided: 1 no.

Reactive Material: Zero-valent Iron (Fe^0), followed by oxygen biosparging. The media is made up of coarse sand mixed with 5% Fe^0, five feet of Fe^0, a 3 ft. pea gravel transition zone, a 3 ft. biosparge zone and a 2 ft. pea gravel zone.

Reactive Zone Height/Length/Thickness: /15 ft./10 ft.

Mass Of Reactant: NA

Permeable Reactive Barrier Depth: 24-40 ft.

Dissertation Conceptual Model: Case 1

Total System Length: NA

Cost: $ 400,000

Special Features:

- The remedial objectives of the project generally were met, except with respect to cDCE and VC, with typical effluent concentrations of about 136 μg/L and 217 μg/L respectively.
- results obtained to date suggest sparging rates in the biosparge zone should be minimized to reduce volatilization of contaminants from the water column.

12. Site location (2 no. pilot-scale demonstrations): The industrial area of Cape Canaveral Air Station, Florida

Site Hydrogeology: The water table is 5 ft. below the ground surface.

Installation Date: October-November 1997

Contaminants and their Concentration: The contaminants are trichloroethylene (TCE)-90 mg/L, vinyl chloride (VC)-7 mg/L and dichloroethylene (DCE)-170 mg/L.

Barrier Configuration: Triple trench continuous curtain configuration

Funnel Material: NA

Funnel Length: NA

Reactive Gates Provided: NA

Reactive Material: 100% Zero-valent Iron (Fe^0) for the first and a mixture of Fe^0 with guar gum and a binder for the second.

Reactive Zone Height/Length/Thickness: 45 ft./32"/4" for each panel

Mass Of Reactant: 98 tons and 107 tons for the two emplacements.

Permeable Reactive Barrier Depth: 45 ft.

Dissertation Conceptual Model: Not conceptualized in this study. Both wall systems consist of a 50 ft. main wall placed centrally with two 10 ft. walls placed 4 ft. upstream and 4 ft. downstream, giving a total reactive length of 70 linear ft. to ground water flow. The panels overlap.

Total System Length: 70 linear ft. for each technique.

Cost: The total installation costs for the two barriers was $809,000

Special Features:

- Evaluation of two emplacement techniques for PRBs.
- Results of the demonstrations and quarterly monitoring to continue until November 1998 is expected to be published by February 1999.

13. Site location (pilot-scale installations): Industrial facility, New York

Site Hydrogeology: The site consists of a 15 ft. shallow sand aquifer (K=1.6 in/sec) that overlies dense clay confining layer, located 20 ft. below ground surface. The water table is intercepted at 4-5 ft. depth.

Installation Date: May 1995

Contaminants and their Concentration: The primary contaminant is trichloroethylene (TCE)-300 μg/L. The reductive dehalogenation of TCE has resulted in cis 1,2-dichloroethylene (cDCE)-100-500 μg/L and vinyl chloride (VC)-80 μg/L.

Barrier Configuration: Funnel-and-Gate Configuration

Funnel Material: Joint sheet piles

Funnel Length: 15 ft.

Reactive Gates Provided: 1 no.

Reactive Material: Zero-valent Iron (Fe^0)

Reactive Zone Height/Length/Thickness: 15 ft./12 ft./3.5 ft.

Mass Of Reactant: NA

Permeable Reactive Barrier Depth: 18 ft.

Dissertation Conceptual Model: Case 1

Total System Length: NA

Cost: $250,000 and reactive material cost $0.12/gal treated.

Special Features:

- Chlorinated VOCs were reduced to the MCLs.
- Microbial analysis on ground water samples indicate no significant increase in microbial population.
- Approximately, 2,098,800 gal of ground water was treated during an operation of pilot scale system.
- PRB system to be replaced by full scale installation in 1997.
- The ground water velocity through the zone is equal to 1 ft./day.

14. Site location (pilot-scale installations): Large Experimental Aquifer Program (LEAP) at Oregon Graduate Institute of Science and Technology near Portland, Oregon

Site Hydrogeology: The site consists of shallow unconfined sand aquifer (K=56.7 ft./day).

Installation Date: October 1997

Contaminants and their Concentration: The contaminants are chromate (Cr^{+6})-12 mg/L and perchloroethylene (PCE)-2 mg/L.

Barrier Configuration: A hanging wall continuous curtain with a perforated metal frame, consisting of three modules each about 6.5 ft. long.

Funnel Material: NA

Funnel Length: NA

Reactive Gates Provided: NA

Reactive Material: Surface modified Zeolite (SMZ)

Reactive Zone Height/Length/Thickness: 6.5 ft./20 ft./3 ft.

Mass Of Reactant: NA

Permeable Reactive Barrier Depth: 6.5 ft., 3 ft. above the impermeable base.

Dissertation Conceptual Model: Case 4

Total System Length: 20 ft.

Cost: $ 100,000

Special Features:

- The main purpose of the demonstration is to evaluate a surface modified zeolite (SMZ) PRB system.
- Full scale implementation is anticipated.
- Two results of this demonstration are: the performance of the PRB is very sensitive to its interface with the aquifer material; it is difficult to locate low conductivity zones.

15. Site location (pilot-scale installations): Former NAS Moffett Field in Mountain View, California

Site Hydrogeology: The aquifer at the site is made up of mixture of sands and gravels present as lens-shaped, inter braided channeled deposits incised into clay and silt layers. There are two aquifer zones separated by a discontinuous semi confining clay layer which serves as the aquitard ($K=10^{-5}-10^{-3}$ ft./min.). Soil porosity value in the silts and the sand strange from 30%-45%.

Installation Date: April 1996

Contaminants and their Concentration: The contaminants are trichloroethylene (TCE)-2990 μg/L, dichloroethylene (1,2-DCE)-280 μg/L, perchloroethylene (PCE)-26 μg/L.

Barrier Configuration: Funnel and gate configuration with upgradient and downgradient 2 ft. pea gravel sections.

Funnel Material: Steel sheet piles

Funnel Length: 20 ft. on either side

Reactive Gates Provided: 1 no.

Reactive Material: Granular Zero-valent Iron (Fe^0)

Reactive Zone Height/Length/Thickness: /6ft./10ft.

Mass Of Reactant: NA

Permeable Reactive Barrier Depth: 5-65 ft.

Dissertation Conceptual Model: Case 1

Total System Length: NA

Cost: $ 375,000

Special Features:

- The US Department of Defense Environmental Security Technology Certification Program (ESTCP) sponsored a project at Moffett Field for the Naval Facilities Engineering Service Center to collect performance monitoring and cost data for eventual technology certification and validation. A final technology evaluation report is planned for the public release in about August 1998.
- Principal contaminant concentrations had been reduced to below MCLs.
- The flow velocity through the cell is about ½ ft./day.

16. **Site location (pilot-scale demonstration):** SGL Printed Circuits site in Passaic County, New Jersey.

Site Hydrogeology: NA

Installation Date: November 1994

Contaminants and their Concentration: The contaminants are trichloroethylene (TCE)-54-549 μg/L, perchloroethylene (PCE)-4100-13000 μg/L and cis-1,2-dichloroethylene (cDCE)-35-1600 μg/L.

Barrier Configuration: Above ground treatment reaction vessel

Funnel Material: NA

Funnel Length: NA

Reactive Gates Provided: NA

Reactive Material: Reactive iron medium

Reactive Zone Height/Length/Thickness: NA

Mass Of Reactant: 39,000 lbs

Permeable Reactive Barrier Depth: NA

Dissertation Conceptual Model: This technology employs the Pump-and-treat technology for evaluating the reaction.

Total System Length: NA

Cost: Process cost estimated to be $91/1000 gal treated. Installation cost for system $ 48,000. Annual operation and maintenance cost ~ $10,000.

Special Features:

- The system was a close resemblance of the PRB system primarily for the purpose of evaluation of metal-enhanced dechlorination process for destroying CVOCs.
- During demonstration 61,000 gal of contaminated ground water was treated.
- Removal efficiencies greater than 99.9% and clean up level of 1 μg/L for all three contaminants was achieved.

17. **Site location (pilot-scale installation):** Somersworth Sanitary Landfill Superfund Site, New Hampshire

Site Hydrogeology: The site is made up of a sand and gravel aquifer (K=14-28 ft./day), about 40 ft. thick, in which the water table varies from a depth of less than 2-20 ft. below ground surface. The hydraulic gradient varies from 0.01-0.004.

Installation Date: The objective of the pilot scale installation is to obtain data for the implementation of a full scale design by February 1999.

Contaminants and their Concentration: The contaminants are trichloroethylene (TCE)-as high as 370 μg/L and vinyl chloride (VC)-as high as1900 μg/L.

Barrier Configuration: Funnel-and-Gate

Funnel Material: Slurry walls

Funnel Length: 4.5 ft.

Reactive Gates Provided: 1 no.

Reactive Material: Zero-valent Iron (Fe^0)

Reactive Zone Height/Length/Thickness: 8 ft. diameter

Mass Of Reactant: NA

Permeable Reactive Barrier Depth: NA

Dissertation Conceptual Model: Case 1

Total System Length: NA

Cost: Installation cost is to be determined.

Special Features:

- The pilot scale implementation is of special interest in verifying whether unacceptable biofouling or precipitation is occurring in the reactive media.

18. **Site location (full-scale demonstration):** Aircraft Maintenance Facility in southern Oregon

Site Hydrogeology: The site is made up of aquifer (K=3 ft./day) consisting of heterogeneous alluvial deposits ranging from sandy silts to silty gravel overlying a fine grained aquitard. The water table is intercepted at a depth of 4-8 ft.

Installation Date: March 1998

Contaminants and their Concentration: The contaminants are trichloroethylene (TCE) and its degradation compounds. The total VOC concentration is ~ 500μg/L.

Barrier Configuration: Funnel-and-Gate System

Funnel Material: 2 ft. thick soil-bentonite wall ($K=10^{-4}$ ft./day).

Funnel Length: 650 ft.

Reactive Gates Provided: 2 nos.

Reactive Material: First gate: 100% zero-valent iron (Fe^0), second gate: mixture of sand and iron filings.

Reactive Zone Height/Length/Thickness: First gate: 2 layers each 16-20 ft./50 ft./9 in.; second gate: 16-20 ft./50 ft./3 ft.

Mass Of Reactant: NA

Permeable Reactive Barrier Depth: 20-34 ft. below ground surface

Dissertation Conceptual Model: Case 1

Total System Length: NA

Cost: $ 600,000

Special Features:

- For each gate four monitoring wells, two up gradient and two down gradient have been installed.

19. Site location (full-scale implementation): Operating unit of the Caldwell Trucking Superfund Site in northern New Jersey

Site Hydrogeology: The site consists of a 25 ft. deep sand and gravel aquifer (K~ 0.1 in/sec) overlying impermeable clay or fractured basal floors. The sand and gravel are characteristics of glacial deposition. The water table is intercepted at a depth of 5-15 ft. below the ground surface.

Installation Date: March 1998

Contaminants and their Concentration: The contaminants are trichloroethylene (TCE)- 6000-10,000 μg/L.

Barrier Configuration: The system consists of two 3-in walls

Funnel Material: NA

Funnel Length: NA

Reactive Gates Provided: NA

Reactive Material: Zero-valent Iron (Fe^0)

Reactive Zone Height/Length/Thickness: NA

Mass Of Reactant: NA

Permeable Reactive Barrier Depth: The PRB extends from a depth of 25ft. to a depth of 40 ft.

Dissertation Conceptual Model: This case has not been conceptualized in this study.

Total System Length: The first hydrofracing wall is 90 ft. in length; the second permeation infilling wall is 150 ft. in length.

Cost: $ 1,120,000

Special Features:

- The clean up standard, at the site, for TCE is 50 μg/L.
- It is at this site that the PRB system would replace the Pump and Treat system in the site's Record of Decision (ROD), if the performance data for one year of operation shows that the PRB system is achieving remedial objectives.
- The PRB system was installed in the glacial deposits and a fractured basal zone using a combination of hydraulic fracturing of the upper sand and gravel zone and permeation infilling of the lower sedimentary zone.

20. Site location (pilot-scale field test): X-625 Ground water Treatment Facility at the U.S. Department of Energy's (DOE) Portsmouth Gaseous Diffusion Plant in Piketon, Ohio

Site Hydrogeology: The site consists of a silty gravel aquifer (K~ 20 ft./day), confined on the top by 30 ft. of silt and on the bottom by bedrock, 32-40 ft. below ground surface.

Installation Date: March 1996

Contaminants and their Concentration: The contaminants are trichloroethylene (TCE)- 72-150 μg/L.

Barrier Configuration: Horizontal Well Configuration

Funnel Material: NA

Funnel Length: NA

Reactive Gates Provided: NA

Reactive Material: Zero-valent Iron (Fe^0)

Reactive Zone Height/Length/Thickness: 500 ft. horizontal well collects contaminated ground water from the aquifer.

Mass Of Reactant: NA

Permeable Reactive Barrier Depth: located at a depth of 30 ft. below ground surface.

Dissertation Conceptual Model: This case has not been conceptualized.

Total System Length: 500 ft.

Cost: $ 4,000,000

Special Features:

- The ground water fed into a building constructed at an elevation of 3-5 ft. below the bedrock ids distributed through a series of canisters filled with reactive media.
- The electrochemical enhancement of the iron media is being considered in the upgrade.
- Though the TCE concentration brought below 5 μg/L mineral precipitation was observed.

21. Site location(full-scale implementation): down gradient inactive mine tailings impoundment at the Nickel Rim mine site at Sudbury, Ontario, Canada

Site Hydrogeology: The site consists of 10-20 ft. contaminated aquifer (GW vel.=49 ft./year) confined to a valley and thus bounded on both sides and below by bedrock. The ground water emanating from the tailings is discharged into a nearby lake.

Installation Date: August 1995

Contaminants and their Concentration: The contaminants are Nickel (Ni)- up to 10 mg/L, iron (Fe)- 740-1000 mg/L and sulphate- 2400-3800 mg/L.

Barrier Configuration: Continuous 'Valley-Bounded' Configuration

Funnel Material: NA

Funnel Length: NA

Reactive Gates Provided: NA

Reactive Material: It is a mixture composed of municipal compost, leaf compost, wood chips and pea gravel. Coarse sand buffer zones were installed on up gradient and down gradient of reactive material.

Reactive Zone Height/Length/Thickness: 14 ft./12 ft./50 ft.

Mass Of Reactant: NA

Permeable Reactive Barrier Depth: 14 ft.

Dissertation Conceptual Model: Case 1

Total System Length: 50 ft.

Cost: $ 30,000

Special Features:

- A 12 in clay cap was placed on the PRB to minimize entry of surface water and oxygen.

- This an example of organic reduction of sulphate and metal sulphide precipitation.
- Monitoring shows that sulphate, iron, nickel concentrations was reduced to 110-1900 mg/L, < 1-91 mg/L and < 0.1 mg/L respectively in the effluent.

22. Site location (large-scale treatability test): 100D Area of U.S. Department of Energy (DOE) Hanford site in Washington

Site Hydrogeology: The aquifer (K=100 ft./day) at the site composed of glacial fluvial sediments dominantly sands and gravels. The upper surface of the 15 ft. thick contaminated aquifer, is 85 ft. below ground surface, and is confined on the lower end by an aquitard.

Installation Date: September 1997

Contaminants and their Concentration: The contaminants are chromate (Cr^{+6})- 2 mg/L.

Barrier Configuration: In this method a chemical reducing agent, is injected down gradient the contaminant source area to alter the chemical redox potential of the aquifer fluid and sediments, thus immobilizing the metals.

Funnel Material: NA

Funnel Length: NA

Reactive Gates Provided: NA

Reactive Material: Sodium dithionite

Reactive Zone Height/Length/Thickness: sodium dithionite is injected into series of five existing wells, to a depth of 100 ft. bgs, the treated zone for each of which overlap creating a 150 ft barrier approximately 50 ft. wide.

Mass Of Reactant: NA

Permeable Reactive Barrier Depth: up to 100 ft.

Dissertation Conceptual Model: Unconceptualized

Total System Length: 150 ft.

Cost: $ 480,000

- This is a In Situ Redox Manipulation (ISRM) method.

- At this site sodium dithionite is the redox potential altering chemical reducing agent that immobilizes redox sensitive chromium migration.
- The aqueous chromate concentrations have been reduced to less than 8 μg/L.

23. Site location (full-scale 2 different PRB systems): Y-12 Site at U.S. Department of Energy's (DOE) Oak Ridge National Laboratory, Tennessee

Site Hydrogeology: The aquifer at the site is composed of weathered bedrock (K~ $4x10^{-4}$ in./sec) confined on top by unconsolidated clay and regolith (K~ $4x10^{-7}$ in./sec). The water table is intercepted at 10-15 ft. and the PRBs focus on remediating the ground water in the shallow unconsolidated zone.

Installation Date: November-December, 1997

Contaminants and their Concentration: The contaminants are Uranium (U), Nitric acid (HNO_3) and technetium (Tc).

Barrier Configuration: System1: Continuous trench system; System 2: Funnel and gate system.

Funnel Material: In system 2, the natural ground water gradient and permeability contrast between the gravel back fill in the trench and surrounding native silt and clay, is designated to generate flow through the iron treatment zone.

Funnel Depth: 25 ft. (in system 2)

Reactive Gates Provided: 1 no. (in system 2)

Reactive Material: System 1: mixture of gravel and zero-valent (Fe^0); System 2: iron treatment zone.

Reactive Zone Height/Length/Thickness: System 1 is of length 225 ft. parallel to direction of ground water. System 2 is 250 ft. long.

Mass Of Reactant: 80 tons Zero-valent Iron (in system 1)

Permeable Reactive Barrier Depth: NA

Dissertation Conceptual Model: Case 2 (both)

Total System Length: System 1: 225 ft.; System 2: 250 ft.

Cost: The total installation cost for both the walls is $ 1,000,000.

Special Features:

- Monthly monitoring indicates that Fe^0 is an efficient and cost effective method to simultaneously remove radionuclides.

24. **Site location (pilot-scale demonstration):** The grounds of a public school in Langton, Ontario, Canada

Site Hydrogeology: The site consists of an unconfined aquifer composed of medium sand (72 ft./day). The water table is intercepted at a depth of 10 ft. (GW vel. = 330 ft./yr).

Installation Date: August 1993

Contaminants and their Concentration: The contaminants are phosphate (PO_4^{3-}) and nitrate (NO_3^-).

Barrier Configuration: Funnel-and-Gate Configuration

Funnel Material: NA

Funnel Length: The funnel walls extend 5 ft. below the water table.

Reactive Gates Provided: NA

Reactive Material: The gate contains two distinct treatment zones:

1. The PO_4^{3-} treatment zone, which is 2 ft. thick, contains a reactive mixture of 6% iron and calcium oxides (Fe/Ca oxides), 9% high-Ca limestone, and 85% local aquifer sand.
2. The 2 ft. thick NO_3^- treatment zone contains wood chips that removes nitrate by bacterial denitrification.

Reactive Zone Height/Length/Thickness: Central gate is 6 ft. wide, 6 ft. long and 6 ft. below the water table.

Mass Of Reactant:

Permeable Reactive Barrier Depth: 16 ft. from central gate

Dissertation Conceptual Model: Case 1

Total System Length:

Cost: $ 5000

Special Features:

- In case of funnel and gate configurations, if the funnel material is not firmly keyed into underlying impermeable material, underflow must be carefully considered.

- A decrease in concentration of PO_4^{3-} and NO_3^-, from 1.0-1.3 mg/L to 0.3 mg/L and from 23-82 mg/L to 2 mg/L respectively, has been reported.

25. Site location (field-scale demonstration): Abandoned Uranium upgrader site in Fry Canyon, Utah

Site Hydrogeology: The underlying aquifer, made up of poorly sorted fine to medium grained sand alluvial deposits, and the water table are located 1-6 ft. deep and 8-9 ft deep respectively (GW vel.=1.5 ft./day)

Installation Date: August 1997

Contaminants and their Concentration: Uranium (U)- 60 μg/L in background well to 20700 μg/L beneath the tailings.

Barrier Configuration: Funnel-and-Gate Configuration

Funnel Material: NA

Funnel Length: NA

Reactive Gates Provided: NA

Reactive Material: The system consists of three barriers each constructed of different reactive materials i.e. char phosphate (PO_4); foamed zero-valent iron (Fe^0) pellets; amorphous ferric oxide (AFO).

Reactive Zone Height/Length/Thickness: Each barrier is 4 ft./ 7 ft./ 3 ft.

Mass Of Reactant: NA

Permeable Reactive Barrier Depth:

Dissertation Conceptual Model: Case 1

Total System Length: 7 ft. (each)

Cost: $ 140,000 excluding the cost of design.

Special Features:

- Steady-state modeling results report that the GW vel.= 4.5 ft./day.
- This demonstration shows that the Fe^0 barrier is the most efficient in removing uranium from ground water, though the removal efficiency of the other two is also significant.

- The Fe^0 barrier is however associated with clogging and iron release problems, in contrast to the AFO barrier which is less subjected to these problems.

APPENDIX B

SAMPLE MODEL RUNS AND LOSS CALCULATIONS USING DIFFERENT BARRIER LENGTHS FOR CASE Ka = 100Kb

Loss of contaminant particles is calculated from the "contaminant path-lines". The loss percentage can be calculated from the following formulae:

$N_{influx} = N_{thru} + N_{loss}$

$$\text{Loss (\%)} = \frac{N_{loss}}{N_{influx}} \text{X } 100$$ Where

N_{influx} = Number of contaminant path-lines originating between the x-ordinates of the beginning and the end of the barrier.

N_{thru} = Number of contaminant path-lines that pass through the barrier.

N_{loss} = Number of contaminant path-lines that originate between the x-ordinates of the beginning and the end of the barrier but do not pass through the it.

Model Execution

The number of particles incident on the barrier is 50. Higher number of particles leads to high model run time and difficulty to calculate loss percentage. Varying the criterion specific to the run, the loss percentage is calculated using the above formulae. The location of the barrier has been overlaid on the model run printouts and view zoomed in on the barrier to aid in calculating the loss percentage.

Sample Calculations

Kb100len100 i.e. Ka = 100 Kb and length of barrier = 100m.

$N_{influx} = N_{thru} + N_{loss}$

$= 6 + 10$

$= 16$

$$\text{Loss (\%)} = \frac{N_{loss}}{N_{influx}} \text{X } 100$$

$= 10/16 \times 100$

$$= \frac{10}{16} \quad X\ 100$$

$$= 62.5$$

Using this procedure with different criterion the plots of loss versus barrier length, versus width, versus gradient, versus hydraulic conductivity ratios are formulated.

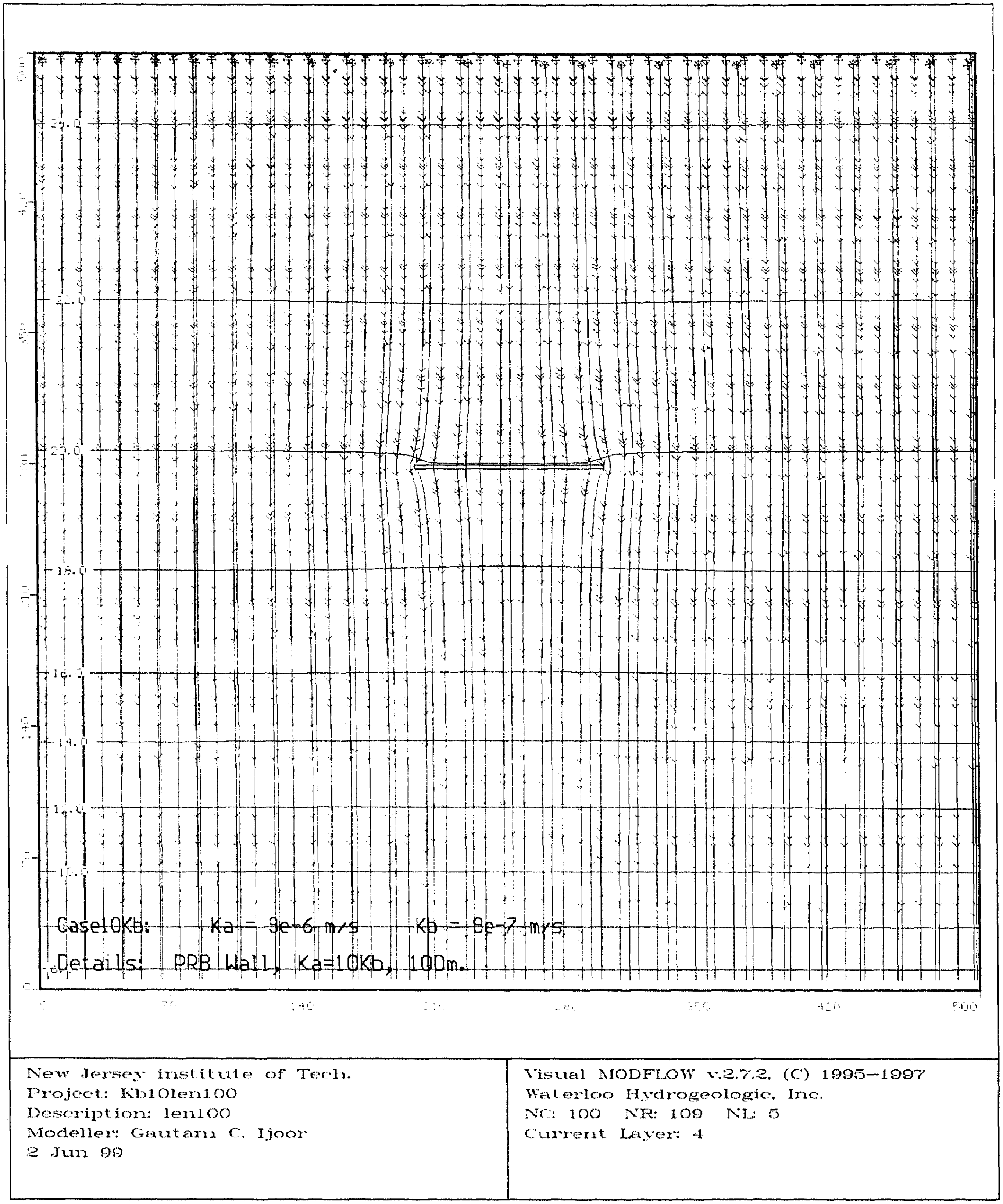


Figure 37: Model Output

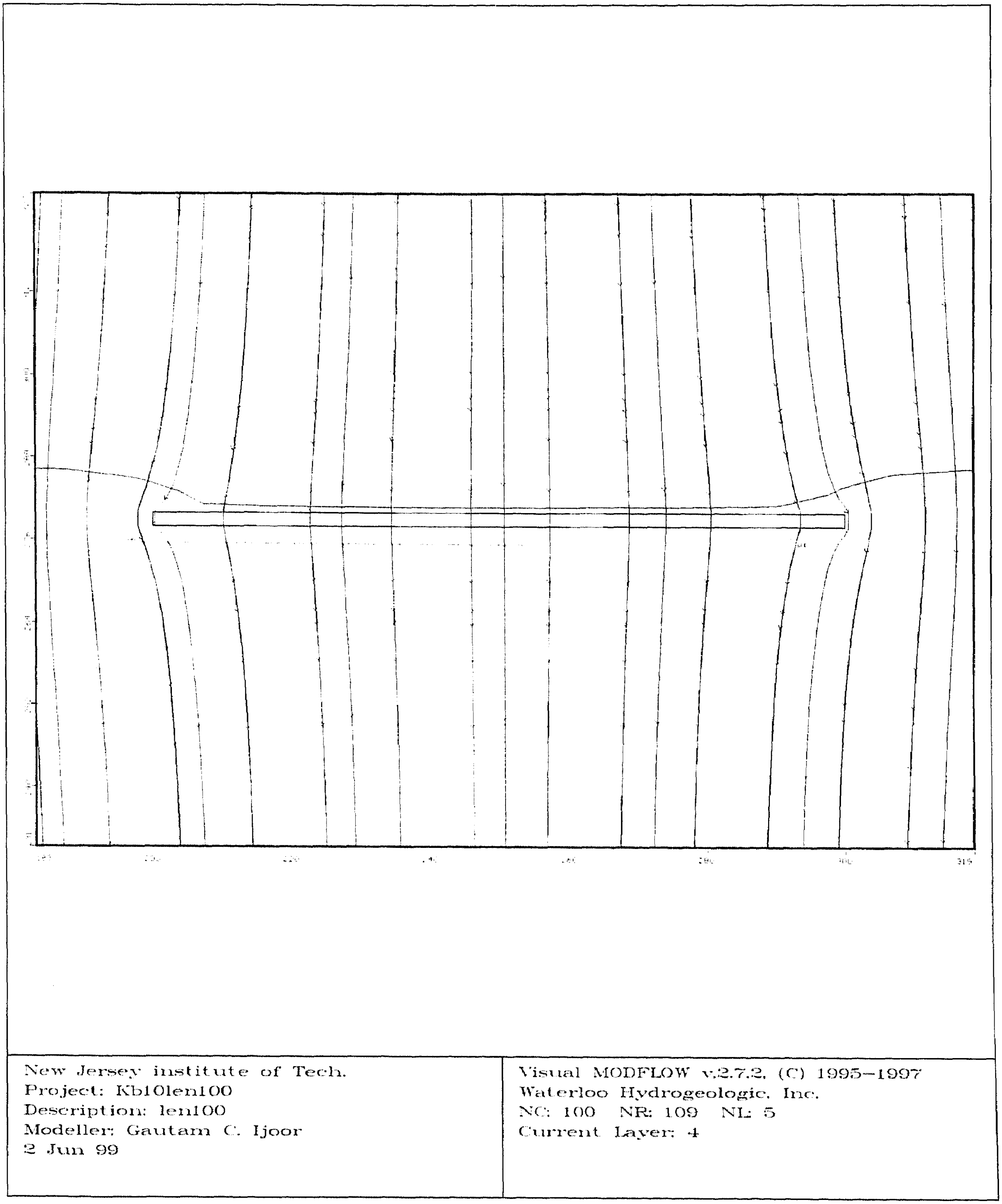


Figure 38: Model Output Zoom-in

APPENDIX C

SAMPLE PLOT OF LOSS VERSUS BARRIER LENGTH

The loss of contaminant particles are calculated from "contaminant pathlines" according to procedure in Appendix B.

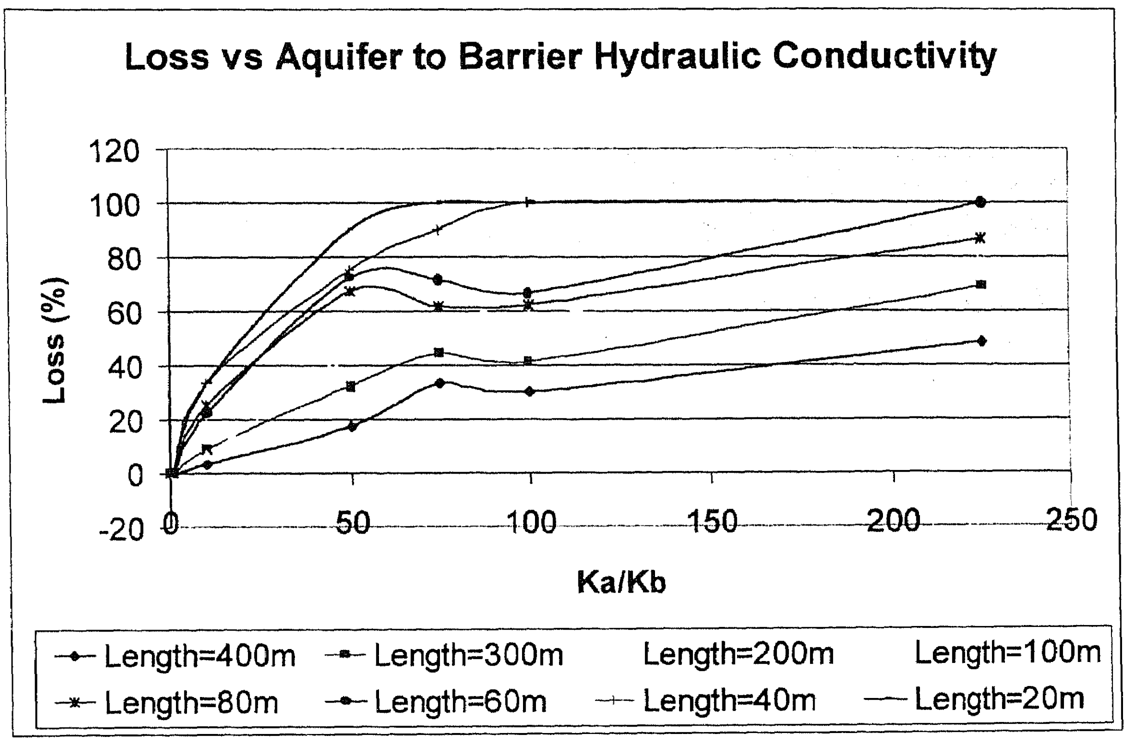
Model Execution

The length of the barrier is varied over the following values: 20, 40, 60, 80, 100, 200, 300,400. The number of particles incident is retained to 50. The ratio of hydraulic conductivities of the aquifer to the barrier is varied over 0.01, 0.1, 1, 10, 25, 50, 75, 100, 225 and the loss percentage is calculated as mentioned. The plot is then created, using the obtained data, for the loss versus the barrier length and for the loss versus the hydraulic conductivity ratio.

The data obtained can be tabulated as follows:

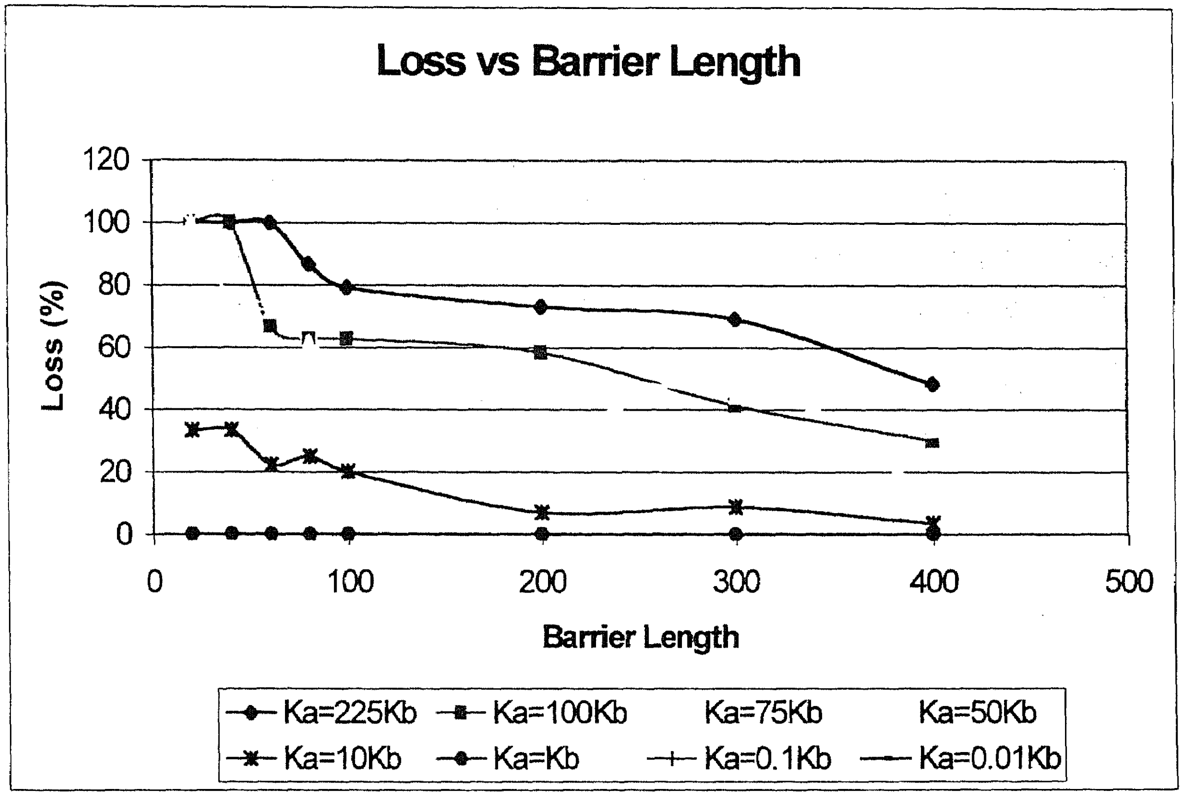
B.L. = Barrier Length

Ka/Kb	225	100	75	50	10	1	0.1	0.01
B.L.400	48.33	30	33.33	17.07	3.39	0	0	0
B.L. 300	69.05	41.38	44.19	32.43	8.89	0	0	0
B.L. 200	73	58.33	52.66	42.86	6.9	0	0	0
B.L. 100	79.16	62.5	55.88	42.86	20	0	0	0
B.L. 80	86.67	62.5	61.54	67	25	0	0	0
B.L. 60	100	66.67	71.43	72.38	22.23	0	0	0
B.L. 40	100	100	90	75	33.34	0	0	0
B.L. 20	100	100	100	90	33.34	0	0	0



*Ka/Kb

Barrier Length	*400*	*300*	*200*	*100*	*80*	*60*	*40*	*20*
225*	48.33	69.05	73	79.16	86.67	100	100	100
100*	30	41.38	58.33	62.5	62.5	66.67	100	100
75*	33.33	44.19	52.63	55.88	61.54	71.43	75	100
50*	17.07	32.43	42.86	42.86	72.72	75	75	100
10*	3.39	8.89	6.9	20	25	22.23	33.34	33.34
1*	0	0	0	0	0	0	0	0
0.1*	0	0	0	0	0	0	0	0
0.01*	0	0	0	0	0	0	0	0



APPENDIX D

SAMPLE VELOCITY EXPORT AND THE CALCULATION OF RESULTANT VELOCITY, ITS MAXIMUM AND THE RESIDENCE TIME

The export option in the velocity menu of Visual Modflow allows the user to export the current three-dimensional output data set to an ASCII file. The exported velocity data consists of 6 columns x, y, z, vx, vy, and vz being the x coordinate, y coordinate, z coordinate, velocity component along the x axis, velocity component along the y axis and velocity component along the z axis respectively. The coordinates and the velocities refer to the center of the barrier cells of the model grid. A partial sample export is presented below as file Kb10len200grad0.01.asc

Kb10len200grad0.01

152.5	280.0965	7.8	-1.517143e-007	-5.058824e-007	-4.797715e-009
157.5	280.0965	7.8	-5.023384e-008	-6.049624e-007	-4.863739e-009
162.5	280.0965	7.8	-2.714539e-008	-6.566656e-007	-4.907755e-009
167.5	280.0965	7.8	-1.69487e-008	-6.879972e-007	-4.940766e-009
172.5	280.0965	7.8	-1.148415e-008	-7.088596e-007	-4.962774e-009
177.5	280.0965	7.8	-8.22258e-009	-7.235525e-007	-4.97928e-009
182.5	280.0965	7.8	-6.116867e-009	-7.343685e-007	-4.990284e-009
187.5	280.0965	7.8	-4.686356e-009	-7.425714e-007	-5.00679e-009
192.5	280.0965	7.8	-3.673553e-009	-7.48959e-007	-5.017794e-009
197.5	280.0965	7.8	-2.93541e-009	-7.54011e-007	-5.023296e-009
202.5	280.0965	7.8	2.363205e-009	-7.580329e-007	-5.039802e-009
207.5	280.0965	7.8	-1.905441e-009	-7.612992e-007	-5.050806e-009
212.5	280.0965	7.8	-1.533508e-009	-7.63956e-007	-5.06181e-009
217.5	280.0965	7.8	-1.218796e-009	-7.660902e-007	-5.072814e-009
222.5	280.0965	7.8	-9.498596e-010	-7.678323e-007	-5.078316e-009
227.5	280.0965	7.8	-7.095337e-010	-7.691683e-007	-5.083818e-009

232.5	280.0965	7.8	-5.0354e-010	-7.702421e-007	-5.083818e-009
237.5	280.0965	7.8	-3.204346e-010	-7.709686e-007	-5.083818e-009
242.5	280.0965	7.8	-1.487732e-010	-7.714621e-007	-5.083818e-009
247.5	280.0965	7.8	5.722046e-012	-7.717232e-007	-5.083818e-009
252.5	280.0965	7.8	1.544952e-010	-7.717086e-007	-5.083818e-009
257.5	280.0965	7.8	3.147125e-010	-7.714475e-007	-5.083818e-009
262.5	280.0965	7.8	4.806519e-010	-7.709681e-007	-5.083818e-009
267.5	280.0965	7.8	6.637573e-010	-7.701844e-007	-5.083818e-009
272.5	280.0965	7.8	8.811951e-010	-7.691246e-007	-5.083818e-009
277.5	280.0965	7.8	1.115799e-009	-7.677741e-007	-5.078316e-009
282.5	280.0965	7.8	1.384735e-009	-7.660465e-007	-5.072814e-009
287.5	280.0965	7.8	1.70517e-009	-7.638837e-007	-5.06181e-009
292.5	280.0965	7.8	2.071381e-009	-7.612555e-007	-5.050806e-009
297.5	280.0965	7.8	2.5177e-009	-7.579892e-007	-5.039802e-009
302.5	280.0965	7.8	3.089905e-009	-7.539533e-007	-5.028798e-009
307.5	280.0965	7.8	3.839493e-009	-7.488867e-007	-5.017794e-009
312.5	280.0965	7.8	4.846573e-009	-7.425273e-007	-5.00679e-009
317.5	280.0965	7.8	6.26564e-009	-7.342671e-007	-4.995786e-009
322.5	280.0965	7.8	8.371353e-009	-7.234365e-007	-4.973778e-009
327.5	280.0965	7.8	1.163864e-008	-7.087291e-007	-4.957272e-009
332.5	280.0965	7.8	1.709747e-008	-6.878807e-007	-4.929763e-009
337.5	280.0965	7.8	2.728271e-008	-6.565059e-007	-4.896751e-009
342.5	280.0965	7.8	5.035973e-008	-6.048314e-007	-4.847233e-009
347.5	280.0965	7.8	1.518059e-007	-5.057518e-007	-4.786711e-009

In the model that is exported to give the file above the barrier is located between the x coordinates 150m-350m, and between the y coordinates 280m-278m. The barrier an alteration in the water table, which causes the contaminated water to pass the barrier at layer 4 (z coordinate 7.8). At higher levels the barrier cells are dry. The negative signs preceding the velocities indicate that the contaminated water flows against the increase in the respective coordinate.

The resultant of the three components is calculated, per set, using the following formulae:

$$V = \sqrt{vx^2 + vy^2 + vz^2}$$

where V = The resultant velocity through the barrier grid cell

vx = The component of velocity, through one barrier grid cell, along the x-axis of the model

vy = The component of velocity, through one barrier grid cell, along the y-axis of the model

vz = The component of velocity, through one barrier grid cell, along the z-axis of the model

The residence time per meter corresponds to the maximum velocity. The residence time is calculated using the following formulae:

$$R = \frac{1}{86400(V_m)}$$

where R = The residence time in days/m

V_m = The maximum resultant velocity

The resultant velocities are presented below.

Details: $K_{aquifer} = 10K_{barrier}$ **Gradient = 0.02**
Length = 200m **Width = 2.0m**

x coordi-nate	y coordi-nate	z coordi-nate	Velocity along x axis m/s	Velocity along y axis m/s	Velocity along z axis m/s	Resultant Velocity v= $\sqrt{Vx^2+Vy^2+Vz^2}$ m/s
152.5	279	7.8	1.280178e-010	-5.027534e-007	-4.764703e-010	5.027534e-007
157.5	279	7.8	3.662109e-011	-6.044709e-007	-4.819723e-010	6.044709e-007
162.5	279	7.8	3.376007e-011	-6.565355e-007	-4.858237e-010	6.565355e-007
167.5	279	7.8	2.803802e-011	-6.880154e-007	-4.885747e-010	6.880154e-007
172.5	279	7.8	2.403259e-011	-7.089039e-007	-4.907755e-010	7.089039e-007
177.5	279	7.8	1.945496e-011	-7.236513e-007	-4.924261e-010	7.236513e-007
182.5	279	7.8	1.544952e-011	-7.344908e-007	-4.940766e-010	7.344908e-007
187.5	279	7.8	1.144409e-011	-7.427171e-007	-4.95177e-010	7.427171e-007
192.5	279	7.8	8.010864e-012	-7.490864e-007	-4.968276e-010	7.490864e-007
197.5	279	7.8	5.722046e-012	-7.541281e-007	-4.97928e-010	7.541281e-007
202.5	279	7.8	4.005432e-012	-7.581786e-007	-4.995786e-010	7.581786e-007

207.5	279	7.8	4.005432e-012	-7.614345e-007	-5.00679e-010	7.614345e-007
212.5	279	7.8	4.577637e-012	-7.640939e-007	-5.023296e-010	7.640939e-007
217.5	279	7.8	5.722046e-012	-7.662359e-007	-5.0343e-010	7.662359e-007
222.5	279	7.8	6.866455e-012	-7.679728e-007	-5.039802e-010	7.679728e-007
227.5	279	7.8	8.010864e-012	-7.693321e-007	-5.039802e-010	7.693321e-007
232.5	279	7.8	9.155273e-012	-7.703774e-007	-5.045304e-010	7.703774e-007
237.5	279	7.8	9.155273e-012	-7.711403e-007	-5.045304e-010	7.711403e-007
242.5	279	7.8	9.155273e-012	-7.716286e-007	-5.045304e-010	7.716286e-007
247.5	279	7.8	8.010864e-012	-7.718688e-007	-5.045304e-010	7.718688e-007
252.5	279	7.8	6.866455e-012	-7.718542e-007	-5.045304e-010	7.718542e-007
257.5	279	7.8	6.866455e-012	-7.716088e-007	-5.045304e-010	7.716088e-007
262.5	279	7.8	6.29425e-012	-7.711033e-007	-5.045304e-010	7.711033e-007
267.5	279	7.8	6.29425e-012	-7.703404e-007	-5.045304e-010	7.703404e-007
272.5	279	7.8	8.010864e-012	-7.692806e-007	-5.045304e-010	7.692806e-007
277.5	279	7.8	9.727478e-012	-7.679067e-007	-5.0343e-010	7.679067e-007
282.5	279	7.8	1.144409e-012	-7.661818e-007	-5.0343e-010	7.661818e-007
287.5	279	7.8	1.25885e-012	-7.640398e-007	-5.017794e-010	7.640398e-007
292.5	279	7.8	1.25885e-012	-7.613804e-007	-5.012292e-010	7.613804e-007
297.5	279	7.8	1.20163e-012	-7.581245e-007	-4.990284e-010	7.581245e-007
302.5	279	7.8	9.727478e-011	-7.540885e-007	-4.97928e-010	7.540885e-007
307.5	279	7.8	6.866455e-011	-7.490323e-007	-4.962774e-010	7.490323e-007
312.5	279	7.8	3.433228e-011	-7.426313e-007	-4.95177e-010	7.426313e-007
317.5	279	7.8	-1.144409e-011	-7.34405e-007	-4.935264e-010	7.34405e-007
322.5	279	7.8	-5.722046e-011	-7.23584e-007	-4.913257e-010	7.23584e-007
327.5	279	7.8	-9.727478e-011	-7.087811e-007	-4.896751e-010	7.087811e-007
332.5	279	7.8	-1.430511e-011	-6.878729e-007	-4.87473e-010	6.878729e-007
337.5	279	7.8	-2.059937e-011	-6.563785e-007	-4.836229e-010	6.563785e-007
342.5	279	7.8	-2.288818e-011	-6.043128e-007	-4.797715e-010	6.043128e-007
347.5	279	7.8	-1.097072e-011	-5.026281e-007	-4.748198e-010	5.026281e-007

Maximum Average Velocity = 7.72 x 10^{-7} m/s
Residence Time = 1/ v x 60 x 60 x 24 days
= 15 days

Sample Calculations

$$V = \sqrt{vx^2 + vy^2 + vz^2}$$

$$= \sqrt{(1.28x10^{-10})^2 + (5.027x10^{-7})^2 + (4.76x10^{-10})^2}$$

$$= \sqrt{1.63x10^{-20} + 2.52x10^{-13} + 2.26x10^{-19}}$$

$$= 5.02 \text{ x } 10^{-7} \text{ m/s}$$

from the table above V_m = 7.7 x 10^{-7} m/s

$$R = \frac{1}{86400(V_m)}$$

$$= \frac{1}{86400(7.7x10^{-7})}$$

$$= 15.03 \text{ days}$$

Using this criterion the residence time per meter is calculated for different model runs and tabulated. The residence time per meter thus calculated is then multiplied by the width to get the residence time. The resultant time calculations are presented in Table 13 in section 4.6. The values are then used to plot the variation of residence time for different barrier lengths, barrier widths, hydraulic gradients and ratios of aquifer to barrier hydraulic conductivity.

Filename	x coordinate	y coordinate	z coordinate	vx velocity along x axis m/s	vy velocity along y axis m/s	vz velocity along z axis m/s	v= $\sqrt{vx^2+vy^2+vz^2}$ Velocity m/s	Residence Time $\frac{1}{vx60x60x24}$ days/m
Kb0.01len20	220-240	279	7.8	1.2e-008	5.1e-007	1.6e-007	5.34e-007	21.67
Kb0.01len40	200-240	279	7.8	1.5e-008	5.1e-007	1.4e-007	5.29e-007	21.9
Kb0.01len60	190-250	279	7.8	1.0e-009	7.8e-007	1.2e-008	7.8e-007	14.84
Kb0.01len80	200-280	279	7.8	7.7e-009	5.1e-007	1.4e-007	5.28e-007	21.9
Kb0.01len100	200-300	279	7.8	1.8e-008	5.1e-007	1.4e-007	5.29e-007	21.9
Kb0.01len200	150-350	279	7.8	9.4e-008	4.9e-007	1.4e-007	5.18e-007	22.34
Kb0.01len300	100-400	279	7.8	1.4e-007	4.8e-007	1.6e-007	5.25e-007	22.04
Kb0.01len400	50-450	279	7.8	1.2e-008	4.8e-007	2.0e-007	5.2e-007	22.25
Kb0.1len20	220-240	279	7.8	6.7e-009	5.4e-007	9.1e-008	5.5e-007	21.04
Kb0.1len40	200-240	279	7.8	1.0e-008	5.4e-007	8.9e-008	5.5e-007	21.04
Kb0.1len60	190-250	279	7.8	5.7e-009	5.3e-007	8.8e-008	5.37e-007	21.55
Kb0.1len80	200-280	279	7.8	4.9e-009	5.0e-007	8.2e-008	5.1e-007	22.69
Kb0.1len100	200-300	279	7.8	8.2e-009	5.3e-007	8.9e-008	5.37e-007	21.55
Kb0.1len200	150-350	279	7.8	1.0e-009	5.3e-007	8.8e-008	5.37e-007	21.55
Kb0.1len300	100-400	279	7.8	6.8e-009	5.5e-007	8.8e-008	5.6e-007	20.66
Kb0.1len400	50-450	279	7.8	7.0e-009	5.3e-007	8.7e-008	5.37e-007	21.55
Kb10len20	225-245	279	7.8	6.0e-011	1.4e-006	1.7e-009	1.4e-006	8.26
Kb10len40	220-260	279	7.8	9.2e-012	1.8e-006	2.1e-009	1.8e-006	6.43
Kb10len60	220-280	279	7.8	5.7e-012	2.0e-006	2.3e-009	2.0e-006	5.78

Kb10len80	220-300	279	7.8	2.8e-011	2.1e-006	2.4e-009	2.1e-006	5.51
Kb10len100	200-300	279	7.8	5.2e-011	2.1e-006	2.4e-009	2.1e-006	5.51
Kb10len200	150-350	279	7.8	5.0e-011	2.2e-006	2.8e-009	2.2e-006	5.2
Kb10len300	100-400	279	7.8	1.2e-010	2.3e-006	3.4e-009	2.3e-006	5.03
Kb10len400	50-450	279	7.8	5.7e-010	2.4e-006	3.5e-009	2.4e-006	4.8
Kb50len20	200-220	279	7.8	1.3e-011	8.0e-007	3.7e-010	8.0e-007	14.46
Kb50len40	200-240	279	7.8	2.3e-011	1.2e-006	4.6e-010	1.2e-006	9.64
Kb50len60	190-250	279	7.8	2.2e-011	1.6e-006	6.9e-010	1.6e-006	7.2
Kb50len80	200-280	279	7.8	4.7e-011	1.8e-006	1.1e-009	1.8e-006	6.43
Kb50len100	200-300	279	7.8	7.8e-011	2.2e-006	2.5e-009	2.2e-006	5.2
Kb50len200	150-350	279	7.8	9.9e-012	3.0e-006	3.5e-009	3.0e-006	3.85
Kb50len300	100-400	279	7.8	6.4e-012	3.4e-006	4.0e-009	3.4e-006	3.4
Kb50len400	50-450	279	7.8	1.9e-012	3.7e-006	3.1e-010	3.7e-006	3.73
Kb75len20	200-220	279	7.8	1.3e-011	5.9e-007	2.4e-010	5.9e-007	19.61
Kb75len40	200-240	279	7.8	9.1e-007	9.5e-007	3.2e-008	9.5e-007	12.18
Kb75len60	190-250	279	7.8	2.4e-011	1.2e-006	5.0e-010	1.2e-006	9.64
Kb75len80	200-280	279	7.8	7.2e-011	1.6e-006	1.5e-009	1.6e-006	7.2
Kb75len100	200-300	279	7.8	5.8e-009	2.2e-006	5.7e-008	2.2e-006	5.2
Kb75len200	150-350	279	7.8	1.3e-011	2.8e-006	2.6e-009	2.8e-006	4.13
Kb75len300	100-400	279	7.8	3.2e-012	3.2e-006	3.0e-009	3.2e-006	36
Kb75len400	50-450	279	7.8	6.1e-012	3.4e-006	3.2e-009	3.4e-006	3.4

Kb100len20	220-240	279	7.8	6.0e-011	1.4e-006	1.7e-009	1.4e-006	20.27
Kb100len40	220-260	279	7.8	1.8e-014	2.5e-006	9.5e-013	2.5e-006	14.63
Kb100len60	220-280	279	7.8	8.8e-010	1.6e-006	7.6e-009	1.6e-006	11.2
Kb100len80	220-300	279	7.8	7.2e-009	2.4e-006	6.8e-008	2.4e-006	8.4
Kb100len100	200-300	279	7.8	5.9e-015	2.5e-006	9.5e-013	2.5e-006	7.63
Kb100len200	150-350	279	7.8	6.9e-010	2.6e-006	4.7e-009	2.6e-006	5.1
Kb100len300	100-400	279	7.8	7.3e012	2.9e-006	3.4e-009	2.9e-006	4.5
Kb100len400	50-450	279	7.8	7.2e-012	3.2e-006	2.7e-009	3.2e-006	4.2
Kb255len20	200-220	279	7.8	6.6e-008	5.0e-006	4.3e-008	5.0e-006	23.4
Kb255len40	200-240	279	7.8	1.5e-008	5.1e-007	1.4e-007	5.1e-007	22.7
Kb255len60	190-250	279	7.8	4.0e-011	5.8e-007	4.3e-010	5.8e-007	19.9
Kb255len80	200-280	279	7.8	7.7e-009	5.1e-007	1.4e-007	5.1e-007	22.7
Kb255len100	200-300	279	7.8	5.0e009	7.5e-007	4.4e-007	7.5e-007	15.4
Kb255len200	150-350	279	7.8	8.8e-011	1.07e-006	5.0e-007	1.07e-006	10.8
Kb255len300	100-400	279	7.8	9.8e-010	1.3e-006	7.7e-007	1.3e-006	8.3
Kb255len400	50-450	279	7.8	1.0e-011	2.4e-006	4.3e-008	2.4e-006	4.8
Kb10len200width1	150-350	279.5	7.8	3.4e-012	7.9e-007	2.4e-009	7.9e-007	14.65
Kb10len200width2	150-350	278	7.8	2.9e-011	7.7e-006	6.0e-009	7.7e-006	15.0
Kb10len200width3	150-350	279.5	7.8	3.4e-011	7.3e-007	3.1e-009	7.3e-007	15.85
Kb10len200width5	150-350	279.5	7.8	3.2e-010	6.9e-007	7.9e-009	6.9e-007	16.8
Kb10len200width10	150-350	279.5	7.8	1.0e-009	5.8e-007	1.4e-008	5.8e-007	19.9

Kb10len200grad0.01	150-350	279	7.8	1.5e-007	5.0e-007	4.7e-009	5.2e-007	22.25
Kb10len200grad0.02	150-350	279	7.8	1.5e-011	1.4e-006	1.1e-009	1.4e-006	8.26
Kb10len200grad0.04	150-350	279	7.8	9.1e-012	2.3e-006	3.4e-009	2.3e-006	5.03
Kb10len200grad0.05	150-350	279	7.8	9.1e-012	2.3e-006	3.4e-009	2.3e-006	5.03
Kb10len200grad0.1	150-350	279	7.8	9.4e-011	5.9e-006	3.3e-010	5.9e-006	1.96

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