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A MODELING STUDY FOR THE IMPLEMENTATION OF *IN SITU* COMETABOLIC BIOREMEDIATION OF TRICHLOROETHYLENE-CONTAMINATED GROUNDWATER

THESIS

John A. Christ, 2Lt., USAF

AFIT/GEE/ENV/97D-03

DEPARTMENT OF THE AIR FORCE
AIR UNIVERSITY
AIR FORCE INSTITUTE OF TECHNOLOGY

Wright-Patterson Air Force Base, Ohio

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THESIS

Presented to the Faculty of the Graduate School of Engineering

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Second Lieutenant, USAF

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A Modeling Study for the Implementation of *In Situ* Cometabolic Bioremediation of Trichloroethylene-Contaminated Groundwater

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John A. Christ

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ABSTRACT

The limitations of conventional groundwater remediation technologies have led to the development of innovative technologies which may achieve national hazardous waste site remediation goals. Before an innovative technology can be implemented in the field, remedial project managers, regulators and other stakeholders require adequate modeling tools to help assess the applicability of the technology at a particular site.

This modeling study investigates how an innovative technology, *in situ* cometabolic bioremediation, might be implemented to remediate a TCE-contaminated site, under different site conditions. A steady-state model is developed which couples an analytical expression to simulate the effect of flow between multiple pumping and injection wells, with an expression to calculate TCE removal as groundwater circulates through *in situ* bioreactors established around the injection wells. Varying site conditions and well configurations are investigated to determine their effect on the overall treatment efficiency of a system. A dual screen well design is found to be an effective method for contaminant capture and treatment given typical values of anisotropy. Investigation of a multiple row implementation concept proves it to be an effective configuration for site cleanup. The model is integrated into interactive software which serves as a technology screening tool.

A Modeling Study for the Implementation of *In Situ* Cometabolic Bioremediation of Trichloroethylene-Contaminated Groundwater

1.0 INTRODUCTION

1.1 MOTIVATION

The wide spread and frequent discharge of toxic chemicals to soil, surface water and groundwater can have detrimental consequences for water quality, wildlife and the ecosystem in general. In the early 1970's these harmful effects were realized and made known to the public, forcing a change in the nation's attitude toward the environment from one of indifference and exploitation to one of caring and conservation. In 1978 the nation was made aware of an elementary school and residential housing development that had been built on a former chemical waste site that was leaking hazardous substances in Love Canal, NY. This site provided many different exposure pathways to the residents and served as a call to action for the general public. A year later the discovery of a pit full of thousands of leaky and unmarked waste drums, at the "Valley of the Drums" in Kentucky, fortified the public's awareness of the problem and forced a response in the halls of Congress.

In reply, Congress swiftly passed the Comprehensive Environmental Response, Compensation and Liability Act (CERCLA) in December of 1980, which established a "Superfund" to provide the $1.6 billion required to respond to the previous improper storage and disposal of hazardous substances (Masters, 1991).

Unfortunately, the nation's leaders had greatly underestimated the magnitude, cost and time to complete the required remediation effort. The magnitude of the problem has grown from those few well publicized incidents to 1,205 sites which are now listed on the National Priorities List (NPL), a list which identifies the most hazardous sites requiring restoration in the nation. However, the NPL is not nearly an exhaustive list of sites requiring restoration. In a recent report, the National Research Council (NRC) has estimated the overall magnitude of the nation's cleanup costs at $1 trillion spent over the next thirty years to remediate between 300 and 400 thousand sites (NRC, 1994).

Of the 1,205 NPL sites, 151 sites are owned by the federal government as of November 1996 (GAO, 1997). Of that 151, the Department of Defense (DoD) is responsible for 126 (GAO, 1995). However, these NPL sites are just a small portion of the 8,336 sites (EPA, 1997) identified by the DoD as requiring remediation at an estimated $30 billion (Astin and Sanders, 1996). Of the 8,336 DoD sites, 2,231 are owned by the Air Force. The estimated cost for remediating these Air Force sites is placed at $7.4 billion (EPA, 1997).

The above discussion illustrates the rising scope and costs associated with environmental restoration. Perhaps even more disturbing is the fact that the current technology of choice for remediating contaminated groundwater, pump-and-treat, may not even be able to remediate a site and comply with the goals of Superfund (Travis and Doty, 1990). The limitations of pump-and-treat technologies, which have been traditionally used for groundwater contamination restoration, are well known (Mackay and Cherry, 1989; NRC, 1994), yet 68% of the Superfund Records of Decision (ROD) select groundwater pumping and treating as the final remedy to achieve aquifer restoration (Travis and Doty, 1990).

The limitations of conventional technologies have brought a call for innovative technologies which can make use of the state-of-the-science to meet the regulatory goals of CERCLA (Keely *et al.*, 1986). Innovative remediation technologies have been identified as methods by which cost and time to remediate can be reduced significantly (GAO, 1994). The Government Accounting Office reports that only through the implementation of innovative technologies will the remediation goals set down by the EPA and Superfund have a chance of being attained (GAO, 1994). A letter from the General Accounting Office to then-Secretary of Energy, the Honorable Hazel R. O'Leary, stated that "developing less costly and more effective cleanup technologies may be the only way the nation can afford to clean up the vast amounts of waste generated by the nation's nuclear weapons production complex" (GAO, 1994). Environmental Protection Agency (EPA) Administrator Carol Browner has made it clear that developing and deploying new technologies for environmental protection is essential. She is quoted as saying, "The technologies we have today are not adequate to solve many of today's environmental problems, let alone the challenges that lie ahead" (Browner, 1997). The Superfund Amendments and Reauthorization Act of 1986 (SARA), in fact, emphasizes the development and use of new and innovative remediation technologies (Masters, 1991).

The National Research Council, in their report on alternatives to groundwater clean-up (NRC, 1994), listed a lack of adequate technical expertise as one of the barriers to implementing new and innovative technologies. Before an innovative technology can be implemented in the field, remedial project managers, regulators and other stakeholders require adequate tools to help them assess the applicability of the technology, design the implementation and optimize its use based on cost considerations. One method of providing these tools and for improving technical expertise is through the use of models and modeling studies. A properly applied model in conjunction with field evaluations and case studies can (1) assist in the problem evaluation, (2) aid in the design of the remedial strategy, (3) improve the conceptual model developed to describe the processes, (4) provide additional quantitative information for decision making, and (5) identify limitations in the data and guide collection of new data (NRC, 1990).

An innovative technology that shows great promise in helping remediate groundwater contaminated by organic compounds is *in situ* bioremediation. *In situ* bioremediation allows for (1) risk reduction as the contaminant is kept away from the surface, (2) cost savings, as water need not be pumped to the surface, (3) relief from regulatory burdens, as there is no need to permit aboveground treatment facilities or obtain permits for the disposal of treated water, and (4) permanence, as contaminants are completely mineralized rather than transferred from one environmental media to another (Semprini *et al.*, 1992).

Sturman *et al.* (1995) claim that an absence of practitioner-oriented tools that aid in decision making is one limitation to the scale-up of *in situ* remediation processes. This thesis will concentrate on the development and analysis of a model which can serve as a practitioner-oriented tool to aid in the implementation of the innovative technology, *in situ* aerobic cometabolic bioremediation. The model can be used to aid in the design, implementation and optimization of this technology, as well as providing a screening tool that can be applied to see if this technology is applicable at a particular contaminated site.

In situ aerobic cometabolic bioremediation is capable of degrading the chlorinated aliphatic hydrocarbons (CAHs) which are commonly found groundwater contaminants (Westrick *et al.*, 1984). The most common CAH, and in fact the most commonly found groundwater contaminant at U.S. hazardous waste sites, is trichloroethylene (TCE) (NRC, 1994). TCE is a solvent used for dry cleaning and metal degreasing. It is a suspected human carcinogen (Fan, 1988) and under anaerobic conditions has been shown to undergo reductive dechlorination to vinyl chloride, a known human carcinogen (Vogel and McCarty, 1985).

A recent field-scale demonstration of *in situ* aerobic cometabolic bioremediation at Edwards Air Force Base (AFB) has shown its efficacy in remediating TCE-contaminated groundwater and serves as motivation for this work (McCarty *et al.*, 1997). The model produced in this work, in conjunction with information gained from field applications like the one at Edwards AFB, has the potential to transition this technology, which may provide a solution to one of the nation's most intractable groundwater contamination problems, from the demonstration stage to full-scale implementation.

1.2 RESEARCH OBJECTIVES

(1) Develop a model which describes the important processes impacting contaminant fate and transport during the implementation of the *in situ* aerobic cometabolic bioremediation technology.

(2) Use field data obtained from the *in situ* aerobic cometabolic bioremediation demonstration at Edwards AFB to verify the model presents a relatively accurate depiction of field-scale system dynamics.

(3) Apply the model to determine how various environmental and design parameters influence the technology's operation.

(4) Using the model, conduct an informal optimization study, to see how the technology may best be applied to remediate hazardous waste sites with TCE contaminated groundwater.

1.3 DEFINITION OF TERMS

The following terminology will be used in the thesis:

<u>Abiotic</u> - Referring to processes which occur in the absence of living organisms.

<u>Aerobic Respiration</u> - The process whereby microorganisms use oxygen as the electron acceptor (NRC, 1993).

<u>Bacteria</u> - Members of a group of diverse and ubiquitous prokaryotic (i.e. cells lacking a nucleus), single-celled organisms (Atlas and Bartha, 1993).

<u>Bioremediation</u> - A managed or spontaneous process whereby microbiological interactions act on contaminant compounds, thereby remedying or eliminating environmental contamination (Madsen, 1991).

Biodegradation - The simplification of an organic compound's structure by breaking of intermolecular bonds (Madsen, 1991).

Biotic - Processes of or relating to living organisms, caused by living things.

Cometabolism - The transformation of a non growth substrate in the obligate presence of a growth substrate or another transformable compound. Cometabolism occurs by accident and the term fortuitous metabolism may be more descriptive (Arp, 1997).

Competitive Inhibition - Deleterious process which occurs when the binding of cometabolite (target contaminant) and growth supporting substrates are mutually exclusive (e.g. they bind to the same site on the enzyme). Thus, when primary substrate and target contaminant are simultaneously present, the target contaminant degradation is inhibited.

Electron Acceptor - The compound that is reduced (receives electrons) in the energy-producing oxidation-reduction reactions essential for the growth of microorganisms (NRC, 1993).

Electron Donor - The compound that is oxidized in the oxidation-reduction enzyme reactions essential for growth of microorganisms (NRC, 1993).

Enzyme - An organic catalyst which influences a reaction without becoming a reactant.

In situ Bioremediation - *In situ* is Latin for "in its original place." *In situ* bioremediation is the activation of microbial populations found in the subsurface for the destruction of contaminants in place (Madsen, 1991).

Microorganism - An organism of microscopic scale capable of reproduction and growth on primary substrates (NRC, 1993).

Methanotroph - Microorganism which utilizes methane as an energy source.

Mineralization - The conversion of an organic compound to its inorganic constituents.

Primary Substrates - The electron donor and electron acceptor that are essential to growth and reproduction of microorganisms (NRC, 1993).

2.0 LITERATURE REVIEW

2.1 OVERVIEW

This chapter presents a review of the literature relevant to the conceptualization, formulation and optimization of the *in situ* aerobic cometabolic bioremediation model. Following a brief background section outlining the motivation to switch from the pump-and-treat method of aquifer reclamation to an *in situ* method for chlorinated solvents, the chapter is divided into three sections. The first section provides a chronological review of previous research concerning the aerobic cometabolic processes on which the model is based. The second section presents a review of mathematical models describing two-dimensional groundwater flow processes and provides a brief review of techniques for optimizing these models. The final section provides a review of models which combine the biodegradation processes discussed in the first section with the flow processes described in the second section.

2.1.1 Background

The Groundwater Supply Survey (GWSS) conducted in 1981 and 1982 and published in 1984 (Westrick *et al.*, 1984), provides a comprehensive analysis of the extent of the groundwater contamination problem in the United States. It is reported that in a random sample of 466 community water supplies, at least one of 29 volatile organic contaminants (VOCs) were detected 16.8 % of the time for water supply systems serving less than 10,000 persons and 28.0 % of the time for water supply systems serving more than 10,000 persons (Westrick *et al.*, 1984). These percentages were even higher for nonrandom sites selected near industrial complexes (Westrick *et al.*, 1984). The chlorinated contaminants detected most frequently were trichloroethylene (TCE), cis- and trans-dichloroethylene (cis-and trans- DCE), carbon tetrachloride (CTC), and 1,1,1-trichloroethane (1,1,1-TCA) (Westrick *et al.*, 1984). As would be expected, these contaminants are still on the list of the most frequently found groundwater contaminants (National Research Council, 1994). Barbash and Roberts (1986) give several reasons for remediating groundwater contaminated by chlorinated compounds: (1) many of these compounds show carcinogenicity, mutagenicity, or teratogenicity, (2) these compounds are quite persistent because of their relatively low biological and chemical reactivity, and (3) VOCs can be transported long distances due to their relatively weak sorption affinity and resistance to biodegradation.

The limitations of conventional treatment technologies (pump-and-treat with above ground treatment) prevent any hope of remediating most sites to regulated levels in a timely and cost-effective manner (Travis and Doty, 1990; EPA, 1996). However, the combination of traditional pump-and-treat methods with innovative treatment technologies is showing promise as an efficient method for remediating the nation's waste sites (EPA, 1996). One innovative technology that has shown promise as an efficient alternative for remediating sites contaminated with chlorinated solvents is *in situ* aerobic cometabolic bioremediation.

However, as with any treatment technology, *in situ* bioremediation has its limitations. Since these technologies are essentially an enhanced pump-and-treat system their application is still limited by site heterogeneities, biogeochemistry and compound molecular structure (McCarty, 1995). Limitations due to site heterogeneities usually center around aquifer low permeability zones. Low permeability zones present a problem for two reasons, (1) the contaminant that has diffused into these zones is slow to diffuse back into the groundwater, and (2) the substrates required for microbiological growth are slow to infiltrate these zones and induce degradation (NRC, 1994). Other mechanisms which may limit the application of *in situ* bioremediation are (1) rate limited sorption (reduced bioavailability), (2) toxicity of contaminant or environment to microorganisms, (3) lack of an essential growth substrate or nutrient, and (4) an insufficient microbial community structure (McCarty and Semprini, 1993; NRC, 1994; McCarty, 1995).

Any number of the mechanisms cited above may be responsible for the inability to degrade chlorinated compounds using *in situ* aerobic cometabolic bioremediation. To date, there is no evidence for aerobic transformation of two major chlorinated compounds, tetrachloroethylene (PCE) and Carbon tetrachloride (CTC). In addition, 1,1,1-trichloroethane (1,1,1-TCA) and 1,1-dichloroethylene (1,1-DCE) are only transformed slowly under aerobic conditions (Fogel *et al.*, 1986; Oldenhuis *et al.*, 1989; McCarty, 1993; Anderson and McCarty, 1997b). However, it has been shown that the above contaminants can dehalogenate under abiotic and anaerobic conditions (McCarty, 1993; Dolan and McCarty, 1995). One problem that has recently been realized is the toxicity effects of 1,1-DCE. If 1,1-DCE is present (typically, from the abiotic dehydrohalogenation of 1,1,1-TCA) then not only is it slow to degrade, but the transformation product is toxic, reducing the capability of microorganisms to degrade other chlorinated solvents which may be present that would normally degrade (Hopkins and McCarty, 1995; Dolan and McCarty, 1995; Anderson and McCarty, 1996). Thus, the presence of 1,1-DCE at a site indicates that aerobic cometabolic bioremediation will most likely not prove to be the most effective means of remediation.

2.2 AEROBIC COMETABOLISM

2.2.1 Background

The degradative ability of methanotrophs was realized relatively early during the experimentation on bioremediation methods. Hou *et al.* (1979) pioneered much of the work on aerobic biodegradation by researching new methane-utilizing microbes and their ability to partially degrade *n*-alkenes. Early reports include Higgins *et al.* (1980 and 1981) touting the ability of methane-utilizing bacteria to "fortuitously metabolize" multi-carbon compounds. By 1983, several more investigations had been reported concerning the ability of the monooxygenase (MMO) enzyme produced by methanotrophs to degrade compounds other than methane (Hou *et al.*, 1983). Haber *et al.* (1983) showed that this monooxygenase enzyme can oxidize and dehalogenate halogenated methane's.

Wilson and Wilson (1985) were the first to show that degradation of TCE occurred when a methane-utilizing population was provided a primary substrate (methane) and an electron acceptor (oxygen). Their report spurred an intensive investigation into the cometabolic degradation pathway of methanotrophs. The initial report by Wilson and Wilson was quickly verified by a similar study where chloroform was degraded in an aerobic column exposed to natural gas (Strand and Shippert, 1986). Fogel *et al.* (1986)

showed that this same methodology could be applied to the degradation of other chlorinated compounds such as, vinyl chloride (VC), vinylidene chloride, and *cis* and *trans*-1,2-dichloroethelyene.

The previous studies concentrated on the use of methane as the primary substrate. In the late 1980's Nelson *et al.* (1987, 1988) published a series of papers which investigated the use of alternative primary substrates. They identified toluene monooxygenase as the enzyme responsible for the cometabolic degradation of trichloroethylene when the pure culture strain G4 was grown on toluene or phenol (Nelson *et al.*, 1987) and toluene dioxygenase as the enzyme responsible for the cometabolic degradation of trichloroethylene when *Pseudomonas putida* U was grown on toluene or phenol (Nelson *et al.*, 1988).

Since this preliminary research, several more studies have investigated the use of the toluene monooxygenase enzyme (Hopkins and McCarty, 1995; Jenal-Warner and McCarty, 1997) and the toluene dioxygenase enzyme (Wackett and Householder, 1989; Zylstra *et al.*, 1989) for TCE cometabolic degradation.

A comprehensive study was recently compiled which examines the methods for mathematically modeling the cometabolic degradation kinetics described above (Criddle, 1993).

This background section has set the stage for a discussion of several recent field investigations of aerobic cometabolic bioremediation which have been conducted in the hope of gathering data to assist in the transition of the technology to full-scale implementation.

2.2.2 Moffett Field studies

While much of the laboratory work discussed above was occurring, a team from Stanford University was building on the research of Wilson and Wilson (1985) and starting to transition the technology from the laboratory to the field. The Stanford team hoped to (1) demonstrate the efficacy of aerobic cometabolic bioremediation, (2) quantify the extent of chlorinated aliphatic hydrocarbon (CAH) degradation, (3) identify any partial transformations, (4) bracket a range of conditions under which aerobic cometabolic bioremediation is effective, (5) determine factors affecting biodegradation rates, (6) quantify the effects of sorption and (7) develop a model which can accurately simulate the *in situ* biodegradation process (Roberts, *et al.*, 1990).

Through column studies, the research team determined the shallow aquifer underlying Moffett Naval Air Station (NAS) in Mountain View, CA was an adequate test site for a pilot-scale demonstration of *in situ* aerobic cometabolic bioremediation (Lanzarone and McCarty, 1990). They determined that the aquifer had a sufficient methanotrophic bacteria population to support degradation of chlorinated solvents when degrading methane as a primary substrate (Lanzarone and McCarty, 1990). This preliminary research led to the construction of a test system which consisted of an injection and extraction well separated by a distance of 6m with intermediate monitoring wells at distances of 1, 2.2 and 4 m from the injection well (Roberts *et al.*, 1990). This configuration allowed for water to be extracted from the aquifer, where it was amended on the surface with primary substrate, oxygen and the target CAH, and then reinjected into the aquifer. This created a bioactive zone surrounding the injection well.

Tracer tests allowed measurement of the aquifer parameters. System operation with extensive monitoring allowed for evaluation of the engineering parameters and operational concepts that affected remediation efficiency. One such operational concept was the alternate pulsing of the primary substrate and electron acceptor. Pulsing the electron donor and acceptor was done for three reasons: (1) to avoid clogging at the injection well due to excessive microbial growth, (2) to achieve a uniform microbial distribution through a substantial portion of the aquifer, thereby increasing the efficiency of the system, and (3) to reduce the impact of competitive inhibition, which is a problem when both primary substrate and target CAH are simultaneously present (Roberts *et al.*, 1990).

Results were reported for degradation of VC, trans-DCE, cis-DCE and TCE using methane as a primary substrate. After demonstrating negligible losses due to abiotic processes, the researchers found the organic compounds were transformed within 2 meters of the injection well as follows: TCE, 20-30% reduction; cis-DCE, 45-55% reduction; trans-DCE, 80-90% reduction; and VC, 90-95% reduction (Semprini *et al.*, 1990). These results demonstrate that bioactive zones (BAZs) are formed within close proximity to an injection well, as had been expected (Odencrantz *et al.*, 1990; Rittmann *et al.*, 1994).

The relatively low TCE transformation that occurred under methane oxidizing conditions (20-30%) motivated the researchers to investigate other primary substrates that showed more promise in the laboratory as efficient inducers of TCE cometabolism. As discussed in section 2.2.1, phenol and toluene were found to be good primary substrates for TCE cometabolism. A second study at the Moffett site was conducted using phenol as a primary substrate. With phenol as the primary substrate over 90% removals of cis-DCE and TCE were observed in the 2-m bioactive zone near the injection well (Hopkins *et al.*, 1993a). Further study found that the remediation efficiency of higher concentrations of TCE could be maintained with increases in phenol concentration (Hopkins *et al.*, 1993b).

In a final experiment at the Moffett site *in situ* aerobic cometabolic bioremediation of TCE, cis-DCE, trans-DCE and 1,1-DCE was investigated using phenol and toluene as primary substrates and both oxygen and hydrogen peroxide as oxygen sources. The researchers found that toluene and phenol acted much the same, allowing for greater than 90% degradation of TCE, cis-DCE, and trans-DCE (Hopkins and McCarty, 1995). However, 1,1-DCE was found to degrade by only 50% and to have toxic effects on the degradation of the other compounds. These results were confirmed in the laboratory (Dolan and McCarty, 1995). Apparently a product of 1,1-DCE transformation decreases the degradation efficiency of the microorganisms (Dolan and McCarty, 1995). This result seems to suggest that this technology is not applicable at sites where the chlorinated compound 1,1-DCE is present (Hopkins and McCarty, 1995). The researchers also found that hydrogen peroxide, given the conditions present during the Moffett field studies, was an effective source of oxygen (Hopkins and McCarty, 1995).

2.2.3 Savannah River Site

The Savannah River Test Site (SRS) is a Department of Energy (DOE) sponsored test facility which has been used to investigate groundwater remediation strategies. At the SRS, *in situ* aerobic cometabolism was studied. Methanotrophs were stimulated by injecting natural gas (methane) and air into an aquifer using horizontal wells (see Figure 2.1).

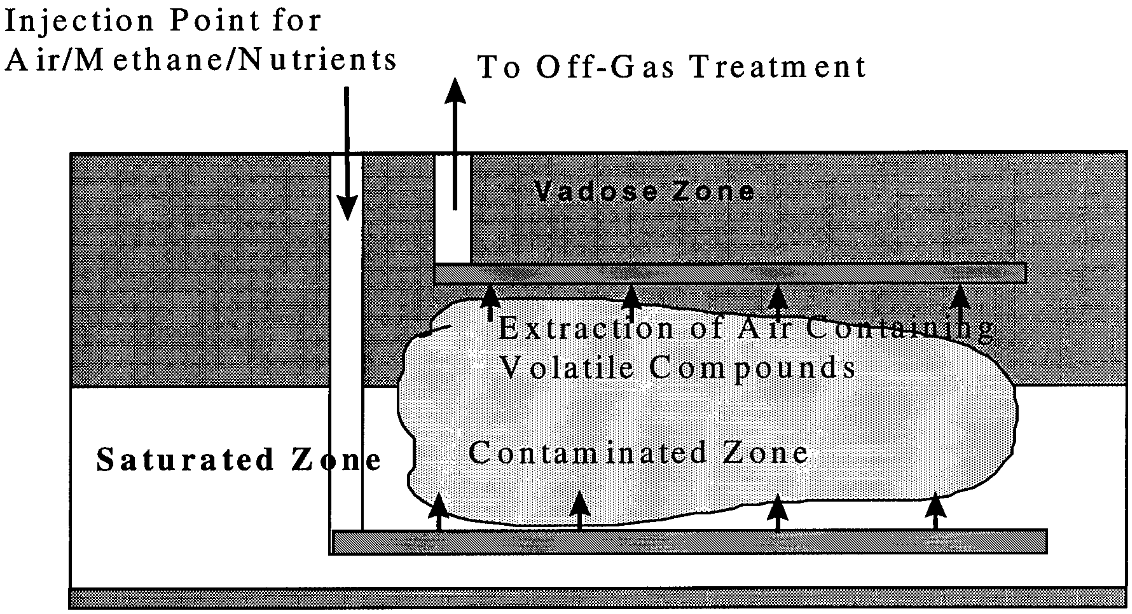


Figure 2.1: Profile view of the Savannah River Site horizontal well *in situ* bioremediation demonstration (after SRS, 1997)

One horizontal well acted as an injection well and was placed below the water table while a second horizontal well acted as an extraction well and was placed above the water table.

This well configuration allowed methanotrophs to biodegrade TCE cometabolically, while contaminants which were not biodegradable (such as PCE) were removed by air stripping (Savannah River Site (SRS), 1997).

A characterization study at the SRS showed the presence of a methanotrophic bacterial community which had the ability to degrade the TCE-contaminated groundwater (Bowman *et al.*, 1993). After methane injection in the study area, a seven order of magnitude increase in the microbial population was observed (SRS, 1997). It is reported that biostimulation was immediate and resulted in PCE/TCE dissolved concentration reductions of 95% and vapor phase PCE/TCE reductions of 99%. This is 42% more than would have been removed by air stripping alone (SRS, 1997).

Interestingly, the investigators reported that PCE was biodegraded. From the previous discussion we know that PCE has not been shown to degrade aerobically. However, the researchers speculated that anaerobic zones formed in the subsurface to allow the anaerobic reductive dechlorination of the PCE to TCE which was then aerobically cometabolized (SRS, 1997). The researchers estimated that the cometabolic treatment system reduced cleanup time by greater than 50% (SRS, 1997).

To simulate the degradation found at the site a model was developed (see section 2.4). Model simulations allowed the researchers to deduce that microbial predation had a significant impact on the TCE degradation efficiency of the remediation system (Travis and Rosenberg, 1997). Similar to the Moffett work, the model studies also showed that pulsing of nutrients could be useful in enhancing removals, by enlarging the area where the removal rates are high.

2.2.4 Lawrence Livermore National Laboratory (LLNL)

A third demonstration of aerobic cometabolism of TCE used bioaugmentation. A team of LLNL researchers injected non-indigenous microorganisms into the subsurface to form an *in situ* microbial filter. The filter degraded contaminant (TCE) as it was transported by the groundwater. The microorganism which was introduced for this study was *Methylosinus trichosporium* OB3b. This organism has the ability to effectively degrade TCE for extended periods of time without nutrient enhancement (Fox *et al.*, 1990). Modeling and bench scale studies have demonstrated its effectiveness at remediating TCE contaminated groundwater for an extended period of time (up to a month) (Taylor *et al.*, 1993). A recent trial of this technology at Chico airport, California demonstrated its effectiveness in the field (LLNL, 1997).

2.2.5 Edwards AFB Site 19 Field Scale Demonstration

Armed with the knowledge gained from the extensive investigations conducted in the laboratory and at Moffett NAS, the Stanford group was ready to implement the *in situ* aerobic cometabolic bioremediation concept at the field scale. Based on the previous studies, a site was selected which had TCE contaminated water, no 1,1-DCE present, a relatively shallow aquifer and a project manager and site regulators who were willing to implement an innovative technology (McCarty *et al.*, 1997). The selected site was Site 19 at Edwards AFB. Site 19 had two aquifers, one unconfined and one confined, both of which were contaminated, with a low permeability aquitard separating the two aquifers. The treatment system consisted of two wells, each screened at two depths in the upper and lower aquifers (see Figure 2.2). Each well injected water through one screen, and extracted water through the other. One well operated in the up flow mode while the other well operated in the down flow mode. Contaminated water was drawn into the well via the extraction screen where it was amended with nutrients and then injected into the other aquifer via the second screen.

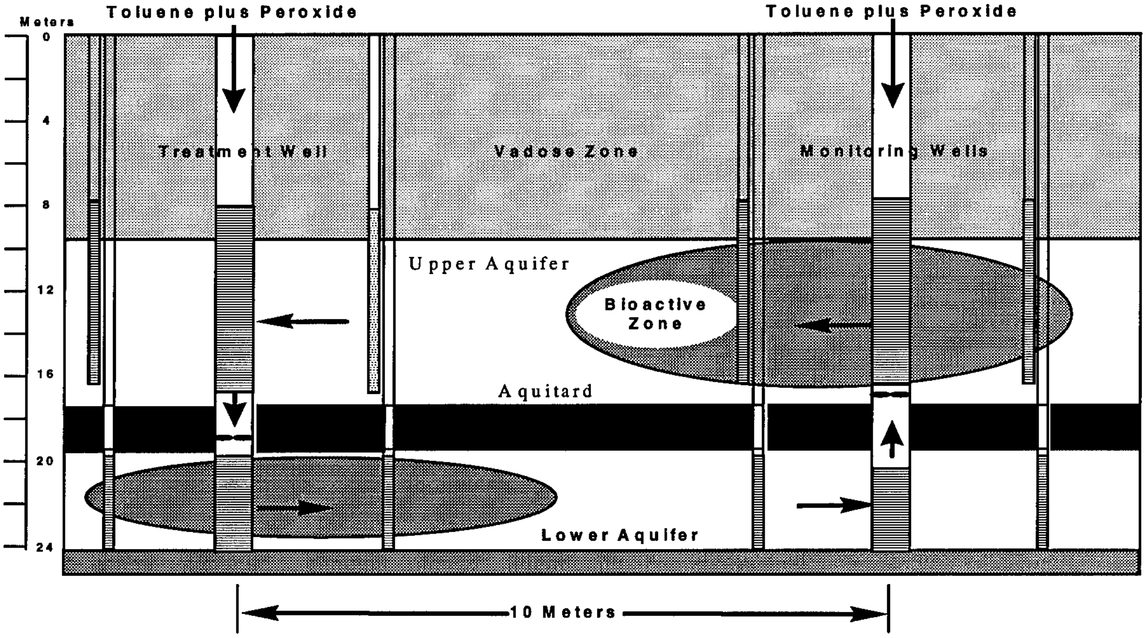


Figure 2.2: Edwards *in situ* bioremediation demonstration (after McCarty *et al.*, 1997)

This system set up a recirculation pattern between the two wells allowing for increased degradation efficiency due to multiple passes through the bioactive zones (McCarty *et al.*, 1997).

The primary substrate selected for the demonstration was toluene due to the fact that toluene has an established maximum contaminant level goal (MCLG), does not create taste and odor problems below 24 μg/L, and is not a precursor to probable carcinogens (McCarty *et al.*, 1997). A combination of hydrogen peroxide and molecular oxygen were used as the source of electron acceptor (McCarty *et al.*, 1997). Molecular oxygen was used initially to establish the microbial community. This was followed by the addition of hydrogen peroxide due to its ability to introduce more oxygen into the subsurface and its bactericidal effects which reduce bioclogging near the injection screen (Pardieck *et al.*, 1992; Morgan and Watkinson, 1992; McCarty *et al.*, 1997).

The results of the demonstration are promising. The treatment efficiency for a single pass through the treatment zone was 83 and 87 percent in the lower and upper aquifers, respectively (McCarty *et al.*, 1997). However, recirculation provided multiple passes through the treatment zone increasing the overall treatment efficiency of the system to between 97 and 98 percent. Toluene was found to be degraded by 99.98 percent to approximately 1.1 μg/L. This concentration was well below the 20 μg/L maximum concentration for toluene established by the regulators, thus, calming fears about injecting a hazardous substance (McCarty *et al.*, 1997). In a related laboratory study, the TCE degradative capacity and rates of the microorganisms extracted from the Edwards AFB aquifer were found to be similar to field conditions (Jenal-Wanner and McCarty, 1997). It is interesting to note, however, that in the laboratory the percent degradation was a function of the depth at which the microorganisms were harvested (Jenal-Wanner and McCarty, 1997). Also, unlike previous studies where biodegradation rates decreased with time (Munakata-Marr *et al.*, 1997), the steady-state TCE removal rates varied little over the year long study (Jenal-Wanner and McCarty, 1997).

2.3 FLOW MODELING

2.3.1 Recirculation System Design

Remediation of a contaminant plume using *in situ* aerobic cometabolic bioremediation requires contact between four key ingredients - primary substrate, electron acceptor, target contaminant, and microorganisms (McCarty and Semprini, 1993; Lang, 1995). Injecting water amended with the primary substrate and electron acceptor may not accomplish mixing because of the displacement of contaminated water.

In this case, only a small bioactive zone is formed in the mixing region at the interface between the injected pulse and the contaminated water (see Figure 2.3). Over time dispersion and diffusion may more completely mix the injected and indigenous waters, however, the majority of the introduced substrates will have been utilized, rendering the method ineffective (Lang, 1995).

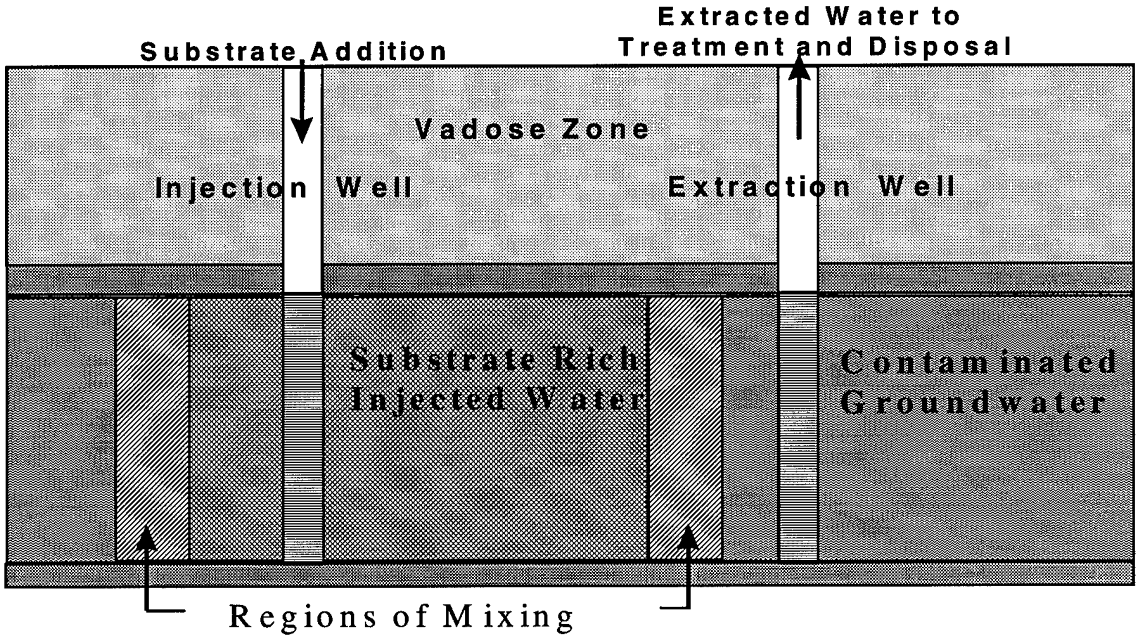


Figure 2.3: Substrate injection without recirculation from mixing (after Lang, 1995).

An underground recirculation system is one method which has been proposed as a way of increasing the contact between the contaminant and the introduced substrates and transporting the mixture to indigenous microorganisms (McCarty and Semprini, 1993). Several well designs have been proposed to accomplish this goal.

One well design which has already been discussed, was employed at the Edwards demonstration (see section 2.2.5). This design draws contaminated water into the well where the nutrients (primary substrate and electron acceptor) are added and then injects this mixture back into the aquifer through a second well screen (McCarty *et al.*, 1997). This creates a bioactive zone surrounding the injection screen of the well. Two dual screened wells placed near each other provide recirculation of contaminated groundwater, thereby bringing the contaminated water in contact with the bioactive zone. Thomas and

Ward (1989) proposed a remediation design similar to the one used at the Edwards demonstration. However, they proposed the use of single screened wells (one injection and one pumping) with recirculation and mixing accomplished above ground (see Figure 2.4).

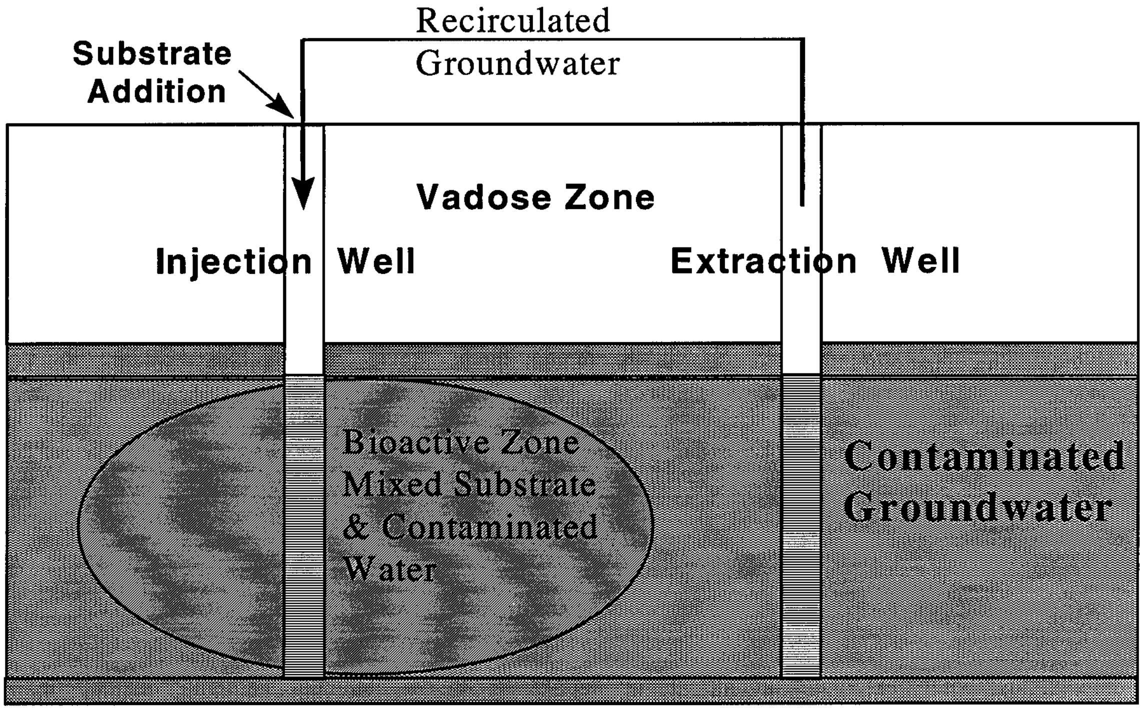


Figure 2.4: Substrate injection with above ground recirculation for mixing (after Lang, 1995)

A third design that increases mixing between the key ingredients is a groundwater circulation well (GCW). A groundwater circulation well is basically one of the two wells used at the Edwards demonstration without the presence of an aquitard. It consists of a well screened at two depths which takes in water at one depth to either treat it in-well (Herrling *et al.*, 1991a; Gvirtzman and Gorelick, 1993; Gvirtzman and Gonen, 1995) or amend it with nutrients (Herrling *et al.*, 1991b; Parsons Engineering Inc., 1997) before injecting it back into the aquifer.

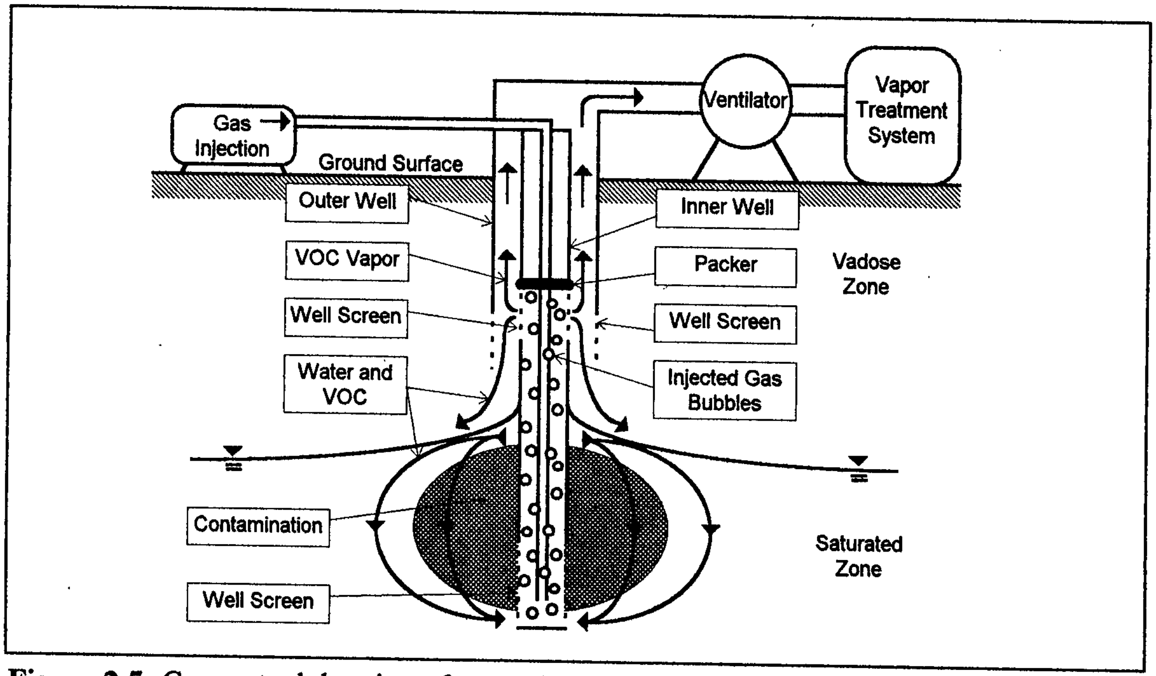


Figure 2.5: Conceptual drawing of groundwater circulation well (in-well air stripping depicted) (after Stanford, 1997)

Others have investigated the flow regime surrounding a dual-screened groundwater circulation well (Herrling and Stamm, 1992; Philip and Walter, 1992; MacDonald and Kitanidis, 1993).

2.3.2 Numerical versus Analytical Methods

There are three modeling methods which can be used to simulate the groundwater flow field around an injection or extraction well: (1) numerical, (2) semi-analytical, and (3) analytical (Javandel *et al.*, 1984). A numerical model is required to handle many transient problems, most stratified three-dimensional problems (Huyakorn *et al.*, 1986a, 1986b; Guven *et al.*, 1986; Harmsen *et al.*, 1991; Matagna, 1993; Yeh *et al.*, 1995; Schafer, 1996) and the effects of partially penetrating pumping wells in confined and unconfined aquifers (Faybishenko, 1995; Bair and Lahm, 1996). Numerical modeling is used primarily due to its ability to adapt to complex governing equations and boundary conditions. Several authors have presented semi-analytical methods for flow field delineation (Javandel *et al.*, 1984; Pollock, 1988; Chrysikopoulos *et al.*, 1990; Lu, 1994) that can be used if simplifying assumptions can be made. Analytical models are usually the easiest to use and provide simplified one and two dimensional depiction's of groundwater flow.

Several recent papers have compared numerical, semi-analytical and analytical models. These papers point out that numerical techniques are much better at describing aquifer systems than either of the other two methods (Bair and Roadcap, 1992; Springer and Bair, 1992). However, it is important to recognize the difference in data required to run each of the models. Numerical models usually require an extensive amount of knowledge about a site. In contrast, analytical models require a smaller number of parameters for analysis, and serve as excellent screening tools to determine qualitative aspects of a site before a full numerical analysis is performed. Also, analytical models are relatively simple tools that can be applied to quickly gain insight into relevant processes at a site. This research will focus on analytical modeling.

Analytical models require simplifying assumptions. Typically, these models assume steady-state conditions, in a homogeneous, isotropic, confined aquifer of constant thickness. These assumptions may seem quite limiting. However, when considering the goals of the modeling study (screening, gain insight into processes) the assumptions may be justified. In addition, a lack of the field data required to utilize the complex models is often the case.

2.3.3 2-D Analytical Models

Dacosta and Bennett (1960) presented a solution to an injection well and an extraction well placed in a steady uniform flow field. They were concerned with the air conditioning problem where cool water is brought to the surface, run through an air conditioning unit, and then injected back into the subsurface. In this problem the amount of circulation occurring between the extraction and injection well should be minimized to prevent thermal contamination of the pumped water (Dacosta and Bennett, 1960). By taking the difference between the streamfunction located at stagnation points (points where velocity in all directions equals zero) associated with each well (Bear, 1972) Dacosta and Bennett (1960) were able to analytically solve for the interflow between wells as a function of the flow rate in the wells, the distance between the wells, the regional Darcy velocity, the aquifer depth and the angle of the regional flow. This same problem was subsequently solved by several authors for the specific case where a pumping well is directly up-gradient of an injection well (Bear, 1979; Strack, 1989; Haitjema, 1995). Hunt (1985) took a slightly more general approach to determine that there are three possible flow patterns that occur when the injection well is upstream of the pumping well and four possible patterns when the injection well is downstream from the pumping well given unequal flow rates in the two wells.

Since these papers, much work has been done investigating the use of type curves to design pump-and-treat systems to capture contaminant plumes (Domenico and Schwartz, 1990; Fetter, 1994). Javandel and Tsang (1986) presented a relatively simple method for determining the capture zone width for a confined aquifer. Their methodology was applied to determine the capture zone width for one, two, three, and four pumping wells in a regional flow field. This methodology has since been expanded for the estimation of non steady-state and steady-state capture zones for pumping wells in confined, unconfined or confined/unconfined aquifers (Grubb, 1993).

Due to the increasing popularity of *in situ* remediation, modeling work has recently been focused on injection/extraction well systems. The method of images has been used to model horizontal line sources and sinks in saturated (Tarshish, 1992) and unsaturated conditions (Falta, 1995). The calculation of streamlines for vertical circulation wells can be done numerically (Herrling *et al.*, 1991a; Herrling *et al.*, 1991b; Herrling and Stamm, 1992) or analytically (Philip and Walter, 1992; MacDonald and Kitanidis, 1993). Important to the operation of vertical circulation wells are the effects that anisotropy has on a system. Zlotnik (1997), using dimensional analysis, shows that when the pumping rate is small compared to the scaled regional flow velocity or the well has a low degree of penetration, then anisotropy becomes an important parameter in the delineation of three-dimensional capture zones.

A key to determining the capture zone width and the interflow between injection and extraction wells is determining the location of the stagnation point. Bakker and Strack (1996) have recently presented an efficient numerical method for solving for the stagnation points in a uniform flow field. Once these stagnation points are found then the capture zone envelope and the interflow can be calculated. Christ and Goltz (1997) present a method for analytically determining the stagnation points, streamfunctions, interflows and capture zones for two, four, six and eight co-linear wells. They also present an algorithm for numerically determining these parameters for the general N-well case. In this thesis, the model discussed above (Christ and Goltz, 1997) will be used to analyze different well patterns.

2.3.4 System Optimization

The above discussion provides a lead in to a brief discussion of optimization methods. Although optimization is beyond the scope of this thesis, a short review will serve as a starting point for future research.

An objective function is a mathematical description of the goals that a certain project is trying to achieve. An example objective would be to minimize the pumping costs (Gorelick *et al.*, 1993). This objective function is also subject to constraints based on state variables such as maximum allowable drawdown and maximum pumping rate

(Gorelick *et al.*, 1993). These constraints restrict the feasible region of a design and aid in the identification of an optimal solution.

The objective function, minimize pumping rate, is one that is often used due to its simplicity and linearity. Many authors have provided optimization methods to solve for the locally optimal solution (Gorelick, 1983; Gorelick *et al.*, 1984; Colarullo *et al.*, 1984; Lefkoff and Gorelick, 1985, 1986; Gorelick and Wagner, 1986). Others have integrated risk-based engineering considerations and sensitivity and probability theory into the objective function making the solutions more complex (Massman and Freeze, 1987; Ahlfeld *et al.*, 1988a, 1988b; Gailey and Gorelick, 1993; Sawyer *et al.*, 1995). Many of these more complex problems require non-linear objective functions and constraints. To solve these nonlinear problems new heuristics for optimization based on hydraulic control have been developed (Greenwald and Gorelick, 1989; Aral, 1989; Ahlfeld and Sawyer, 1990; Rogers, 1991; Ratzlaff *et al.*, 1992). In addition, recent advances in computational efficiency have allowed for the use of much more complicated optimization solution techniques using genetic algorithms and neural networks (Rogers *et al.*, 1995; Huang and Mayer, 1997; Wang and Zheng, 1997). These solution techniques have the advantage of solving problems that have highly nonlinear objective functions and constraints and also of finding globally optimal solutions.

2.4 AEROBIC COMETABOLIC TRANSPORT MODELS

This final section provides a brief review of the models which combine biological and flow processes to describe *in situ* aerobic cometabolic bioremediation.

The studies discussed in section 2.2 describe how the primary substrate, the secondary substrate (target contaminant) and the electron acceptor (oxygen source) interact during aerobic cometabolism. One way of modeling these interactions is through the use of a double Monod kinetics term which incorporates competitive inhibition. The Monod terms will be explicitly defined in the following chapter. Suffice it here to say they mathematically describe the observed kinetics of chemical degradation (Criddle, 1993). Sturman *et al.* (1995) provide a review of transport models that have been used to describe bioremediation; however, only two are identified as accounting for cometabolism.

The earliest model documented in the above review is a one-dimensional, non-steady-state model which accounted for advection, dispersion, equilibrium sorption and cometabolism. Cometabolism was modeled using a single Monod term to describe contaminant degradation (Kindred and Celia, 1989).

A second model took a slightly more complicated approach. A double Monod kinetics model was developed (Semprini and McCarty, 1992) to describe contaminant degradation based on both electron donor and electron acceptor concentration. This model also allowed for competitive inhibition and microbial deactivation. The model relatively accurately simulated the Moffett field investigation (Semprini and McCarty, 1992). Lang (1995) and Goltz *et al.* (1995) applied the Semprini and McCarty (1992) model in two dimensions. They did this by using a semi-analytical code (RESSQ) which calculated streamtubes. The one-dimensional model developed by Semprini and McCarty (1992) was then applied along the streamtube. This model incorporated two-dimensional steady-state flow with one-dimensional advection, dispersion, and rate-limited sorption along with the microbial processes of bacterial growth, primary substrate and oxygen utilization, and cometabolic transformation of TCE (Goltz *et al.*, 1995).

The final model to be discussed was one that was used to describe the field demonstration at the Savannah river site (See section 2.2.3). This model is based on the TRAMPP code which allows for transport in the vadose and groundwater zones, unsteady air and water flow, toxicity, triple Monod cometabolic kinetics, kinetic sorption and predator grazing (modeled using Monod kinetics) (Travis and Rosenberg, 1997). TRAMPP does not account for competitive inhibition. Travis and Rosenberg (1997) apply their model to the SRS demonstration and show that neglecting the effects of microbial interaction (i.e. predation) can lead to overestimates of TCE degradation on the order of 25%.

3.0 METHODOLOGY

3.1 OVERVIEW

In this chapter, the model used in this thesis is derived. In the first section, a method for predicting steady-state degradation in the bioactive zone (BAZ) is developed. The second section provides the derivation of the analytical flow model which can be used to determine the interflow between multiple well pairs. The third section shows how these two components can be combined to obtain an overall system treatment efficiency. The final section develops the objective function and constraints to be used in model optimization.

3.2 BIOLOGICAL MODEL

Due to toxicity effects on microorganisms at higher concentrations, *in situ* aerobic cometabolic bioremediation does not lend itself to treatment near the source of a plume (McCarty and Semprini, 1992). However, in combination with hydrodynamic control (system of injection and extraction wells) it serves as an excellent treatment barrier to further contaminant migration. The derivation and description of the biodegradation occurring in the bioactive zones surrounding the injection wells follows.

The biological portion of the model is based upon simplifying assumptions which can be made to obtain an analytical expression for the percent degradation of a contaminant on a single pass through the BAZ. This "single-pass" treatment efficiency can then be combined with the steady-state flow model (to be derived in the second section) to obtain an analytical expression for the overall efficiency of a system of treatment wells placed down gradient of a migrating plume.

If we can assume steady-state, then we no longer need be concerned with transient conditions at the start-up of the technology. That is, the flow field, microbial growth, and degradation can be assumed constant with time. One method of depicting this constant flow field is through the use of streamtubes. A streamtube is a section of the flow-field (two-dimensional in this case) which carries a specified amount of flow through the aquifer (Bear, 1972, 1979). To model degradation we must start by determining the reactions that occur along the longitudinal direction in a streamtube. Monod kinetics is a common method to account for the first order microbial growth that occurs at low concentrations, followed by zero order growth at high concentrations, when the substrate is not limiting (Criddle, 1993). The following set of equations (1-4), as developed by Semprini and McCarty (1992), can be used under transient conditions to describe the cometabolic degradation of a contaminant (C) when competitive effects between the primary substrate (C_D) and the contaminant are occurring and equilibrium sorption is considered. Notice that the equations are only written in one dimension (x) for simplicity.

$$\frac{\rho_B}{\theta}\frac{\partial S}{\partial t}+\frac{\partial C}{\partial t}=D\frac{\partial^2 C}{\partial x^2}-v\frac{\partial C}{\partial x}-F_a X K_2\left(\frac{C}{K_{s2}+C+\frac{K_{s2}C_D}{K_{sD}}}\right)\left(\frac{C_A}{K_{sA}+C_A}\right) \qquad (1)$$

where $S = K_d C$ (equilibrium sorption)

$$\frac{\partial C_D}{\partial t}=D\frac{\partial^2 C_D}{\partial x^2}-v\frac{\partial C_D}{\partial x}-XK\left(\frac{C_D}{K_{sD}+C_D}\right)\left(\frac{C_A}{K_{sA}+C_A}\right) \qquad (2)$$

C = Contaminant Concentration [M/L^3]

C_D = Primary Substrate Concentration [M/L^3]

C_A = Electron Acceptor Concentration [M/L^3]

X = Biomass Concentration on pore volume basis [M/L^3]

D = Longitudinal Dispersion Coefficient [L^2/T]

v = Average Linear Groundwater Velocity [L/T]

S = Sorbed Contaminant Concentration [M/M]

ρ_B = Bulk Density of the Solid Matrix [M/L^3]

θ = Water Content [-]

K_d = Partition Coefficient [L^3/M]

K_{SA} = Electron Acceptor Half-saturation Constant [M/L^3]

K_{SD} = Primary Substrate Half-saturation Constant [M/L^3]

K_{S2} = Contaminant Half-saturation Constant [M/L^3]

K_2 = Maximum Utilization Rate of Cometabolism [M Contaminant/M Cell - T]

F_a = Fraction of total population which is active towards the cometabolic transformation

$$\frac{\partial C_A}{\partial t} = D\frac{\partial^2 C_A}{\partial x^2} - v\frac{\partial C_A}{\partial x} - XFK\left(\frac{C_D}{K_{sD}+C_D}\right)\left(\frac{C_A}{K_{sA}+C_A}\right) - d_c f_d bX\left(\frac{C_A}{K_{sA}+C_A}\right) \qquad (3)$$

b = Cell Decay Coefficient [1/T]

d_c = Cell decay Oxygen Demand [M Acceptor/M Cell]

f_d = Fraction of cells that are biodegradable

F = Stoichiometric ratio of electron acceptor to electron donor utilization for biomass synthesis [M Acceptor/ M Donor]

$$\frac{\partial X}{\partial t} = XKY\left(\frac{C_D}{C_D + K_{SD}}\right)\left(\frac{C_A}{K_{SA} + C_A}\right) - bX\left(\frac{C_A}{K_{sA} + C_A}\right) \tag{4}$$

Y = Yield Coefficient [M Cell/ M Donor]

K = Maximum Utilization Rate [M Donor/M Cells - T]

The first equation (1) describes the advection, dispersion, sorption and degradation of the target contaminant (Cometabolized substrate). The second and third equations describe advection, dispersion and degradation (assuming no sorption), for the primary substrate (2) and the electron acceptor (3). The final equation (4) describes the growth and decay of the microbial population. Notice that although several models have been developed which consider the transport of microorganisms in the subsurface, they are not considered in this analysis (Taylor and Jaffe, 1990a; Taylor *et al.*, 1990b; Taylor and Jaffe, 1990c).

The first simplifying assumption made is that steady-state conditions exist. This assumption is true after the system has been given time to equilibrate. When this is the case the partial derivatives with respect to time on the left hand side (LHS) of the partial differential equations (1-4) drop out. At steady-state the contaminant that is being added to the system is equal to the contaminant that is being removed from the system. If we also assume that enough oxygen is being added into the system so the bioactive zone around the well is always aerobic, then the electron acceptor equation is unnecessary and all of the electron acceptor Monod terms ($C_A/(K_{sa}+C_A)$) can be approximated by 1. This leaves the following set of equations

$$F_a X K_2 \left(\frac{C}{K_{s2} + C + \frac{K_{s2} C_D}{K_{sD}}}\right) + v \frac{dC}{dx} = D \frac{d^2 C}{dx^2} \tag{5}$$

$$X K \left(\frac{C_D}{K_{sD} + C_D}\right) + v \frac{dC_D}{dx} = D \frac{d^2 C_D}{dx^2} \tag{6}$$

$$bX = XKY\left(\frac{C_D}{C_D + K_{SD}}\right) \tag{7}$$

To further simplify the model several other assumptions can be made. By assuming plug flow, the dispersion terms drop out of the equations ($D = 0$). If we also assume that all of the microbial population is active towards cometabolism then $F_a = 1$. Finally, we can neglect the competitive effects($K_{s2}C_D/K_{sd} << K_{s2}$), and since this system is employed at the edge of a plume where low contaminant concentrations exist, we can assume that the contaminant concentrations are small compared to the contaminant half-saturation constant ($C << K_{s2}$). That is, the degradation of the contaminant is assumed to be first order. Employing these assumptions we can use the following equations to describe the degradation of the contaminant

$$v \frac{dC}{dx} = -XK_2\left(\frac{C}{K_{s2}}\right) = -XK'C \tag{8}$$

where $K' = K_2/K_{s2}$

$$XK\left(\frac{C_D}{K_{sD}+C_D}\right)=-v\frac{dC_D}{dx} \tag{9}$$

Since we know that velocity is the distance traveled over a given time period (dx/dt) we can rearrange the differential on the LHS of equation (8) to be a change in concentration with respect to travel time through the BAZ (dC/dt). This is essentially saying that under steady-state conditions, contaminant concentration is decreasing as the contaminant travels through the BAZ in accordance with the first order rate expression below

$$\frac{dC}{dt}=-XK'C \tag{10}$$

so

$$\frac{C_e}{C_i}=e^{-XK't} \tag{11}$$

where

C_i = The influent concentration up gradient of the BAZ [M/L^3]

C_e = The effluent concentration down gradient of the BAZ [M/L^3]

Time (t) is the time the contaminant is in the bioactive zone, and is equal to the volume of the BAZ (V) divided by the flow rate (Q). To determine the steady-state concentration of microorganisms in the BAZ (X) we can equate the mass of microorganisms being produced in the BAZ (QYC_D) with the mass of microorganisms dying (bVX) (Jenal-Wanner and McCarty, 1997):

$$YC_DQ = XVb \tag{12}$$

where Q = Flow Rate of the well $[L^3/T]$

X = Steady-state Microbial Concentration $[M/L^3]$

V = Volume of the Bioactive Zone $[L^3]$

Rearranging we can solve for the steady-state microbial concentration (Semprini and McCarty, 1991; Jenal-Wanner and McCarty, 1997)

$$X = \frac{YQC_D}{Vb} \tag{13}$$

Recalling that $t = V/Q$, we can substitute equation (13) into equation (11) to obtain the following equation (Jenal-Wanner and McCarty, 1997)

$$\frac{C_e}{C_i} = e^{-\frac{YK'C_D}{b}} \tag{14}$$

The above equation approximates the extent of contaminant degradation that occurs in a single pass through the BAZ. The assumptions inherent in this equation are listed in table 3.1.

Table 3.1: Biological model assumptions

Assumptions for Single Pass Degradation Derivation (Equation 14)
No deactivation of biomass
No competitive inhibition effects
Plug flow in a streamtube
Contaminant concentration (C) much less than contaminant saturation coefficient K_{S2}
Primary substrate is completely consumed
Oxygen is not limiting
Steady-state conditions
All microbial growth is due to the primary substrate

When compared with a numerical model constructed to solve the transient model (eq. 1-4) this steady-state approximation (eq. 14) gave consistently accurate (order of magnitude) results.

3.3 FLOW MODEL

Overall contaminant reduction through a groundwater circulation well (GCW) or injection/extraction well system depends on two factors: (1) contaminant removal for each pass of water through the treatment zone, and (2) fraction of treated water which is recycled back through the treatment zone. Treatment can occur within the well (Herrling *et al.*, 1991; Gvirtzman and Gorelick, 1993) or in the aquifer adjacent to the injection well screen (Christopher *et al.*, 1997; McCarty *et al.*, 1997; Spuij *et al.*, 1997). Contaminant reduction for each pass of water through the treatment zone was derived above and depends on equation (14) while fraction recycle depends upon the system hydraulics. Thus, for a given single-pass contaminant removal efficiency, overall treatment efficiency can be determined by knowing the fraction of water recycled. A simple analytical two-dimensional solution is presented which permits calculation of fraction recycle in two-, four-, six-, and eight-well GCW and injection/extraction well systems, given (1) steady, uniform regional flow in a homogeneous isotropic confined aquifer with known groundwater velocity and aquifer thickness, (2) constant well pumping/extraction rates, and (3) co-linear well locations. A numerical method is also presented which may be used to calculate total recycle for a greater number of wells, located arbitrarily and pumping at different rates. These methods may be used to aid in design of GCW and injection/extraction well *in situ* treatment systems.

3.3.1 Methodology

Assuming a homogenous, isotropic confined aquifer under steady-state conditions with a uniform thickness (B) and a constant regional Darcy velocity (U), complex potential theory can be used to describe the pattern of flow in the vicinity of any number of sources and sinks. N total wells (injection plus pumping) will be used in this analysis. As shown in equation (15), the complex potentials (W) due to the uniform flow and well sources and sinks are superposable due to the linearity of Laplace's equation (Javandel, *et al.*, 1984).

$$W = \phi + i\psi = -U Z e^{-i\alpha} + \frac{1}{2\pi B}\sum_{j=1}^{N} Q_j (-1)^j \ln[Z - Z_j] + C \qquad (15)$$

W = the overall complex potential of the system [L^2/T]

U = Darcy velocity of uniform regional flow [L/T]

α = angle between the direction of regional flow and the positive x-axis (measured counter-clockwise from the x-axis) [-]

B = Aquifer thickness [L]

Q_j = Pumping/ Injection rate of j^{th} well (j odd for injection wells, even for pumping wells) [L^3/T]

N = Total number of pumping and injection wells

Z = Location in the complex plane at which W is being evaluated (x+iy)

Z_j = Location in the complex plane of the jth well (x_j+iy_j)

i = √-1

C = Constant

The complex potential can be separated into a real velocity potential (ϕ)

$$\phi = -U(x\cos\alpha + y\sin\alpha) + \frac{1}{4\pi B}\sum_{j=1}^{N}(-1)^j Q_j \ln[(x-x_j)^2 + (y-y_j)^2] + C_1 \qquad (16)$$

and an imaginary stream function (ψ) (Javandel *et al.*, 1986):

$$\psi = U(x\sin\alpha - y\cos\alpha) + \frac{1}{2\pi B}\sum_{j=1}^{N}(-1)^j Q_j \tan^{-1}\left[\frac{y-y_j}{x-x_j}\right] + C_2 \qquad (17)$$

where C_1 and C_2 are constants.

In order to calculate the interflow for the injection/extraction well system, it is necessary to determine the location of the system's stagnation points. With the stagnation points known, the interflow can be calculated by taking the difference in the value of the stream function at the stagnation points (DaCosta and Bennett, 1960). To find the stagnation points, set the derivative of the complex potential (W) with respect to Z equal to zero and solve for Z. The x,y coordinates for Z in the complex plane represent the coordinates of the stagnation points in the real plane (Haitjema, 1995; Javandel and Tsang, 1986). Taking the derivative with respect to Z of equation (15) and setting it equal to 0 results in:

$$\frac{dW}{dZ} = -Ue^{-i\alpha} + \frac{1}{2\pi B}\sum_{j=1}^{N}\frac{Q_j(-1)^j}{Z - Z_j} = 0 \qquad (18)$$

Equation (18) is, in general, not amenable to analytical solution. However, by making certain simplifying (yet, realistic) assumptions, an analytical solution to equation (18) may be obtained. In the general case, equation (18) can be solved numerically using a number of well-known techniques (e.g. Newton-Raphson numerical root-finding (Press *et al.*, 1996)). Bakker and Strack (1996) recently presented an efficient algorithm for numerically locating stagnation points.

Assume an even number (N) of total wells (injection plus pumping), with all wells pumping at equal rates (Q), so that there is no net gain or loss of groundwater. Wells are equally spaced along the x-axis at a distance 2d between each injection and extraction well. The well at the most negative x value is a pumping well. With these assumptions, equation (17) may be rewritten as:

$$\psi = U(x\sin\alpha - y\cos\alpha) + \frac{Q}{2\pi B}\sum_{j=1}^{N}(-1)^j \tan^{-1}\left[\frac{y}{x - d(1 + N - 2j)}\right] + C_2 \qquad (19a)$$

or

$$\psi = U(x\sin\alpha - y\cos\alpha) + \frac{Q}{2\pi B}\sum_{j=1}^{N}(-1)^j \theta_j + C_2 \qquad (19b)$$

and equation (18) as:

$$\frac{dW}{dZ} = -Ue^{-i\alpha} + \frac{Q}{2\pi B}\sum_{j=1}^{N}\frac{(-1)^j}{Z-d(1+N-2j)} = 0 \tag{20}$$

where the angle θ_j in equation (19b) is defined as the angle between the positive x-axis and a line connecting the jth well with any point in the x-y plane. $0 \leq \theta < \pi$ for x,y in the first and second quadrants, and $-\pi < \theta \leq 0$ for x,y in the third and fourth quadrants. Note that the angle θ is discontinuous by an amount 2π along the branch cut that is the negative x-axis (Strack, 1989).

Equation (20) can be analytically solved and stagnation points determined for N=2, 4, 6, and 8. The analytical solution for these cases follows.

3.3.2 Two Well Case (N = 2)

For the two well case (pumping well at (-d, 0) and injection well at (d, 0)) with both wells pumping at rate Q, equation (20) results in:

$$\frac{dW}{dZ} = -Ue^{-i\alpha} + \frac{Q}{2\pi B(Z+d)} - \frac{Q}{2\pi B(Z-d)} = 0 \tag{21}$$

which upon rearranging gives the quadratic equation:

$$Z^2 - d^2 + \frac{dQ}{\pi BU}e^{i\alpha} = 0 \tag{22}$$

Solving for Z we obtain the stagnation points in the complex plane

$$Z = x + iy = \pm\sqrt{d^2 - \frac{dQ}{\pi BU}e^{i\alpha}} \tag{23}$$

These two roots provide the x and y coordinates for the two stagnation points in the x-y plane.

3.3.3 Four Well Case (N = 4)

Expanding equation (20), substituting m = Z^2, and rearranging, we obtain the following polynomial for the four well case

$$m^2 + \left(\frac{2dQ}{\pi UB} e^{i\alpha} - 10d^2 \right) m + 9d^4 + \frac{6d^3 Q}{\pi UB} e^{i\alpha} = 0 \tag{24}$$

Solving equation (24) for m and substituting Z = ±√m we obtain the following four roots of the equation which correspond to the four stagnation points in the x-y plane:

$$Z = \pm \sqrt{5d^2 - \frac{dQ}{\pi UB} e^{i\alpha} + 2d \sqrt{\left(\frac{Qe^{i\alpha}}{2\pi UB} \right)^2 - \frac{4dQ}{\pi UB} e^{i\alpha} + 4d^2}} \tag{25a}$$

$$Z = \pm \sqrt{5d^2 - \frac{dQ}{\pi UB} e^{i\alpha} - 2d \sqrt{\left(\frac{Qe^{i\alpha}}{2\pi UB} \right)^2 - \frac{4dQ}{\pi UB} e^{i\alpha} + 4d^2}} \tag{25b}$$

3.3.4 Six Well Case (N = 6)

Equation (20) for the six well case can be simplified to a cubic equation by substituting m = Z^2. Doing this and expanding the sum we obtain the following polynomial

$$m^3 + \left(\frac{3dQ}{\pi UB} e^{i\alpha} - 35d^2 \right) m^2 + \left(259d^4 - \frac{6d^3 Q}{\pi UB} e^{i\alpha} \right) m + \left(\frac{195Qd^5}{\pi BU} e^{i\alpha} - 225d^6 \right) = 0 \tag{26}$$

Letting b equal the coefficient of the second order term, c equal the coefficient of the first order term and D equal the constant on the left hand side of equation (26), we can solve the cubic equation using the method presented by Abramowitz and Stegun (1965), obtaining the following six roots:

$$Z_1 = \pm\left[(s1+s2) - \frac{b}{3}\right]^{\frac{1}{2}} \tag{27a}$$

$$Z_2 = \pm\left[-\frac{1}{2}(s1+s2) - \frac{b}{3} + \frac{i\sqrt{3}}{2}(s1-s2)\right]^{\frac{1}{2}} \tag{27b}$$

$$Z_3 = \pm\left[-\frac{1}{2}(s1+s2) - \frac{b}{3} - \frac{i\sqrt{3}}{2}(s1-s2)\right]^{\frac{1}{2}} \tag{27c}$$

where

$$s1 = \left[r + (q^3 + r^2)^{\frac{1}{2}}\right]^{\frac{1}{3}} \qquad \textit{and} \qquad s2 = \left[r - (q^3 + r^2)^{\frac{1}{2}}\right]^{\frac{1}{3}}$$

$$q = \frac{1}{3}c - \frac{1}{9}b^2 \qquad \textit{and} \qquad r = \frac{1}{6}(cb - 3D) - \frac{1}{27}b^3$$

3.3.5 Eight Well Case (N = 8)

The stagnation points in the eight well case may be found by solving the following quartic equation, which was obtained by substituting $m=Z^2$ into equation (20).

$$m^4 + \left(\frac{4dQ}{\pi UB}e^{i\alpha} - 84d^2\right)m^3 + \left(1974d^4 - \frac{92d^3Q}{\pi UB}e^{i\alpha}\right)m^2 + \left(\frac{1324d^5Q}{\pi UB}e^{i\alpha} - 12916d^6\right)m$$
$$+\left(11025d^8 + \frac{7980d^7Q}{\pi UB}e^{i\alpha}\right) = 0 \tag{28}$$

Though somewhat tedious, the solution to a quartic is straightforward (Abramowitz and Stegun, 1965).

3.3.6 Interflow and Capture Zone Width Calculations

When considering the use of groundwater circulation wells or injection/extraction well pairs to implement an *in situ* treatment, the fraction of interflow between wells and the width of the capture zone are two important design parameters. The fraction of water recycled through the treatment system, and hence, the overall efficiency of the system in treating contaminant for a given single-pass removal efficiency, is determined by the interflow. The effectiveness of the well system as a barrier to contain and treat a contaminant plume is a function of the capture zone width.

Knowing the stagnation points, interflow may be calculated using the fact that the total flow through a streamtube can be determined by taking the difference in the value of the stream function of the two streamlines bounding the streamtube (e.g. Bear, 1972, 1979; Haitjema, 1995; Strack, 1989). Thus, equation (19) may be used to find the stream function at the stagnation points, and the interflow determined by taking the difference between the two stream functions. There is a caveat to this method, however, due to the existence of the branch cut along the x-axis (see Figure 3.1). Recall that the angle θ is discontinuous by an amount 2π along the branch cut that is the negative x-axis. Thus, when determining the interflow between points that have a branch cut between them, it is necessary to account for the branch cut by adding a constant 2π.

The following equation may be used to calculate the interflow between stagnation points in a system of N pumping and injection wells. If we designate the stagnation points 1 and 2 located at (x_1, y_1) and (x_2, y_2), respectively, we find:

$$I = \frac{(\psi_1 - \psi_2 + K_1)}{Q/B} \tag{29a}$$

$$I = \frac{UB}{Q}\left[(y_2 - y_1)Cos(\alpha) - (x_2 - x_1)Sin(\alpha)\right] + \frac{1}{2\pi}\left[\sum_{j=1}^{N}(-1)^j\theta_{j1} - \sum_{j=1}^{N}(-1)^j\theta_{j2} + K_2\right] \tag{29b}$$

where

I = Interflow (-)

ψ_1 = stream function calculated at stagnation point 1 [L^2/T]

ψ_2 = stream function calculated at stagnation point 2 [L^2/T]

θ_{j1} = angle between the positive x-axis and the line connecting well j and stagnation point 1 (injection wells at j odd, pumping wells at j even)

θ_{j2} = angle between the positive x-axis and the line connecting well j and stagnation point 2 (injection wells at j odd, pumping wells at j even)

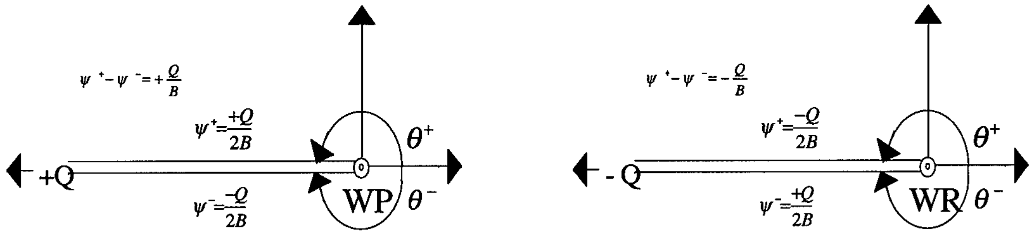
K_1 = Q/B when the path between the stagnation points crosses a branch cut [L^2/T]

= 0 when the path between the stagnation points does not cross a branch cut

K_2 = 2π when the path between the stagnation points crosses a branch cut [L^2/T]

= 0 when the path between the stagnation points does not cross a branch cut

The value of K_1 in equation (29a) stems from the branch cut (Strack, 1989; Haitjema, 1995). The stream function for a pumping well has the value +Q/2B just above the branch cut and -Q/2B just below it (see Figure 3.1a) while for an injection well the values just above and below the branch cut are -Q/2B and +Q/2B, respectively (see Figure 3.1b). This two valuedness appears to violate the single-valuedness feature of the stream function and is due to the fact that the center of the well represents a singularity in the flow field. Haitjema (1995) provides a physical interpretation that water being pumped out of the aquifer by the well flows along the branch cut that is the negative x-axis to infinity, where it is returned to the aquifer and flows toward the well again. Thus, the branch cut is a fictitious slit in the flow domain, with a fictitious flow of magnitude Q going through it (away from the well in the case of a pumping well, toward the well in the case of an injection well).



(a)

(b)

Figure 3.1: Branch cut discontinuities in flow field for (a) a pumping well (WP) and (b) an injection well (WR).

In the case of a pumping/injection well pair, the branch cut only extends from the pumping to the injection well. Based on the sign conventions presented in this thesis, the branch cuts for a system of co-linear wells, with pumping and injecting wells alternating, are shown in Figure 3.2. When calculating the interflow between stagnation points, where a branch cut is not crossed, $K_1 = K_2 = 0$. When a branch cut is crossed, $K_1 = Q/B$ or $K_2 = 2\pi$.

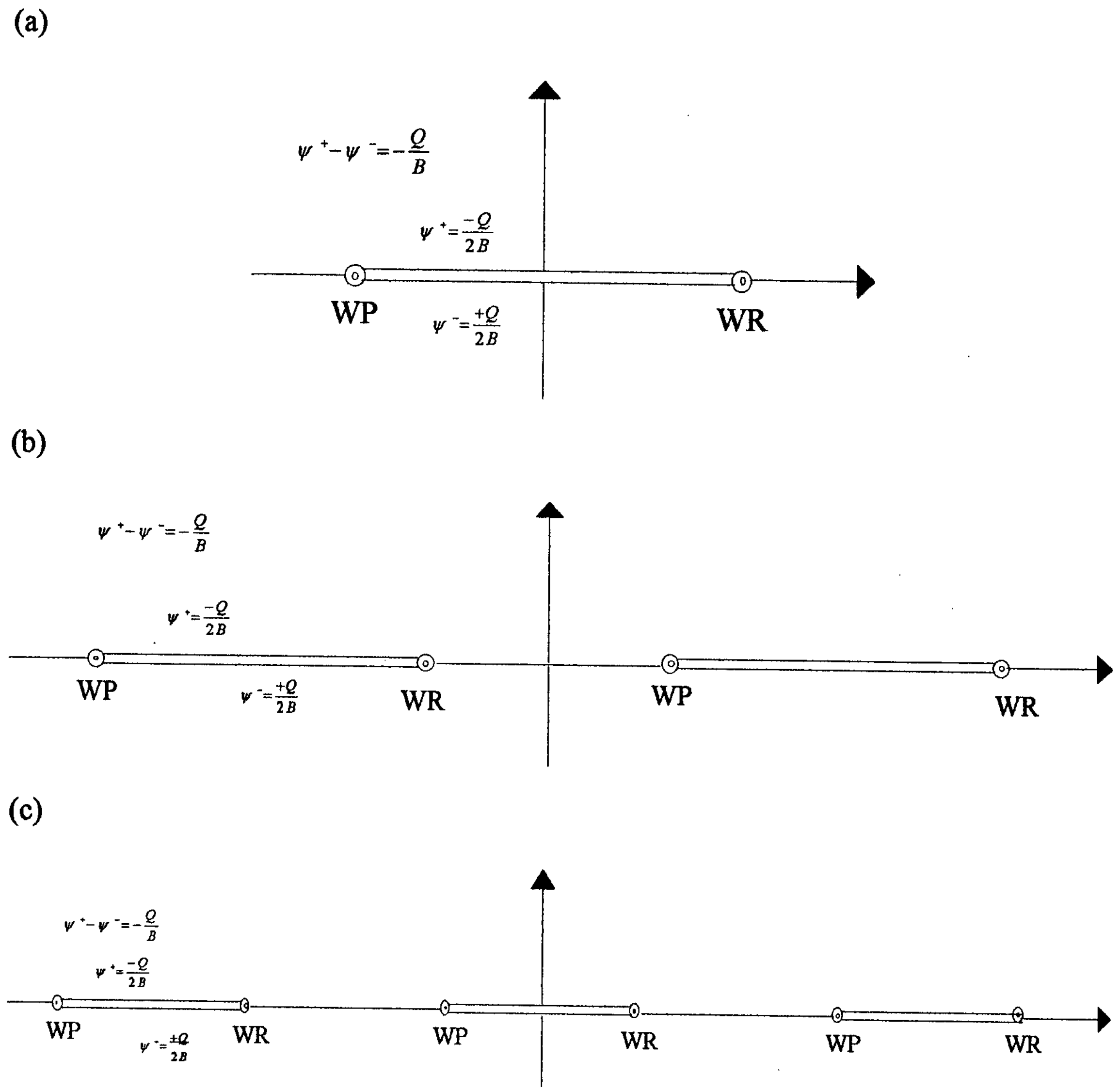
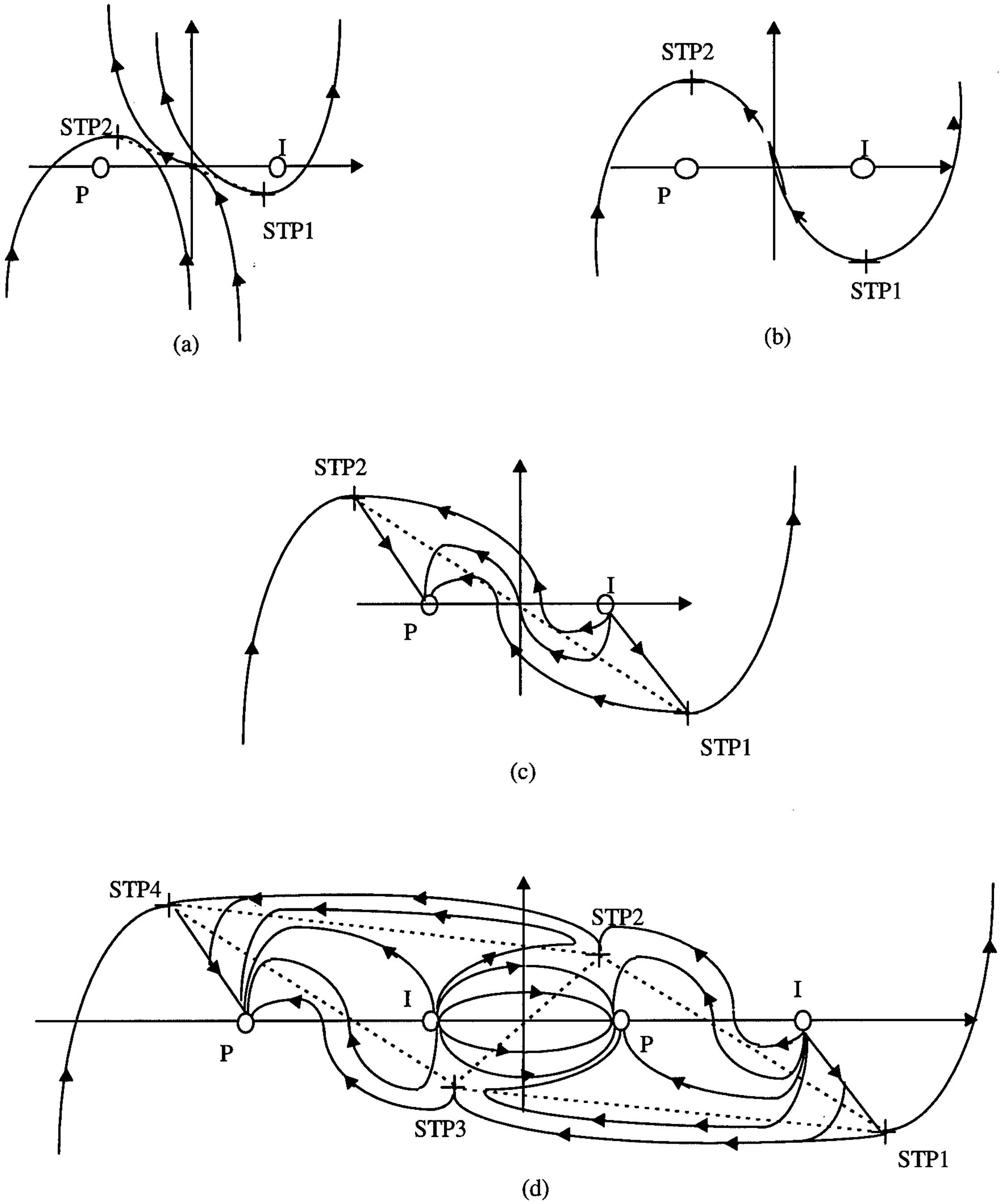


Figure 3.2: Branch cut discontinuities in flow field for several well cases (a) two-well system, (b) four-well system, and (c) six-well system

Conceptually, interflow (I) calculated in equation (29) is a measure of the flow crossing a line connecting two stagnation points (one point associated with a pumping well, the other with an injection well) in a flow field (normalized by the flow through the pumping well). Previous work using two-well systems with both wells pumping at the same rate, found interflow could take on any value less than one, including negative values (Dacosta and

Bennett, 1960). However, for the purposes of this work, the range of values for which interflow is valid includes values greater than one, to account for unbalanced flow conditions (wells not operating at equal flow rates) and multiple well (N>2) treatment systems. In these cases, the amount of flow crossing between two stagnation points can be greater than the flow through the pumping well.

Figure 3.3 shows several scenarios which depict, conceptually, how interflow values can vary. In Figure 3.3a we see a case in which the interflow value is less than zero. In this case there are no flow lines going from the injection to the extraction well as regional flow is passing in between the two wells and flow lines cannot cross. The absolute value of (I) corresponds to the amount of flow passing between the two wells (higher value indicative of greater flow). A value less than negative one means that the amount of flow "breaking through" between the two treatment wells, is larger than the amount of flow in a treatment well. Starting with the Figure 3.3a scenario, if the flow rates in the treatment wells increase, the stagnation points will shift and eventually the situation depicted in Figure 3.3b will be seen. In this case the interflow is equal to zero and although there are no regional flow lines passing in between the two wells, there is no interflow between them either. As the flow rates in the wells continue to increase the stagnation points continue to separate and there is interflow between the wells as shown in Figure 3.3c ($I > 0$).



P = Pumping Well
I = Injection Well
STP = Stagnation Point

·············· Line connecting STP's

Figure 3.3: Conceptual flow diagram for illustration of interflow when (a) I < 0, (b) I = 0, (c) I > 0, (d) I > 1. (α = 90 deg.)

The above cases are scenarios that can arise when analyzing a two-well balanced flow system (Dacosta and Bennett, 1960; Bear, 1972, 1979). In this work, which expands on prior work by allowing for multiple well pairs ($N > 2$), the value of interflow can be greater than one. This means that more water is crossing the line connecting the two stagnation points than is flowing in the pumping well. This scenario is depicted in Figure 3.3d, where it can be seen that due to the presence of multiple wells, the amount of flow crossing a line connecting two stagnation points of interest (for example, STP-2 and STP-4) is not limited by the flow in a single pumping well. Again referring to Figure 3.3d, we also see that the sum of the interflow between STP-1 and STP-2 and between STP-2 and STP-3, for example, can be greater than unity due to interflow between non-adjacent wells. A second cause for values of (I) exceeding unity, unbalanced flow, will be discussed in a later section.

Knowing the interflows between stagnation points allows us to determine the fraction of total flow in a pumping well that is coming from upgradient and the fraction that is coming from injection wells. Figure 3.4 illustrates how this calculation can be done, for a four-well system.

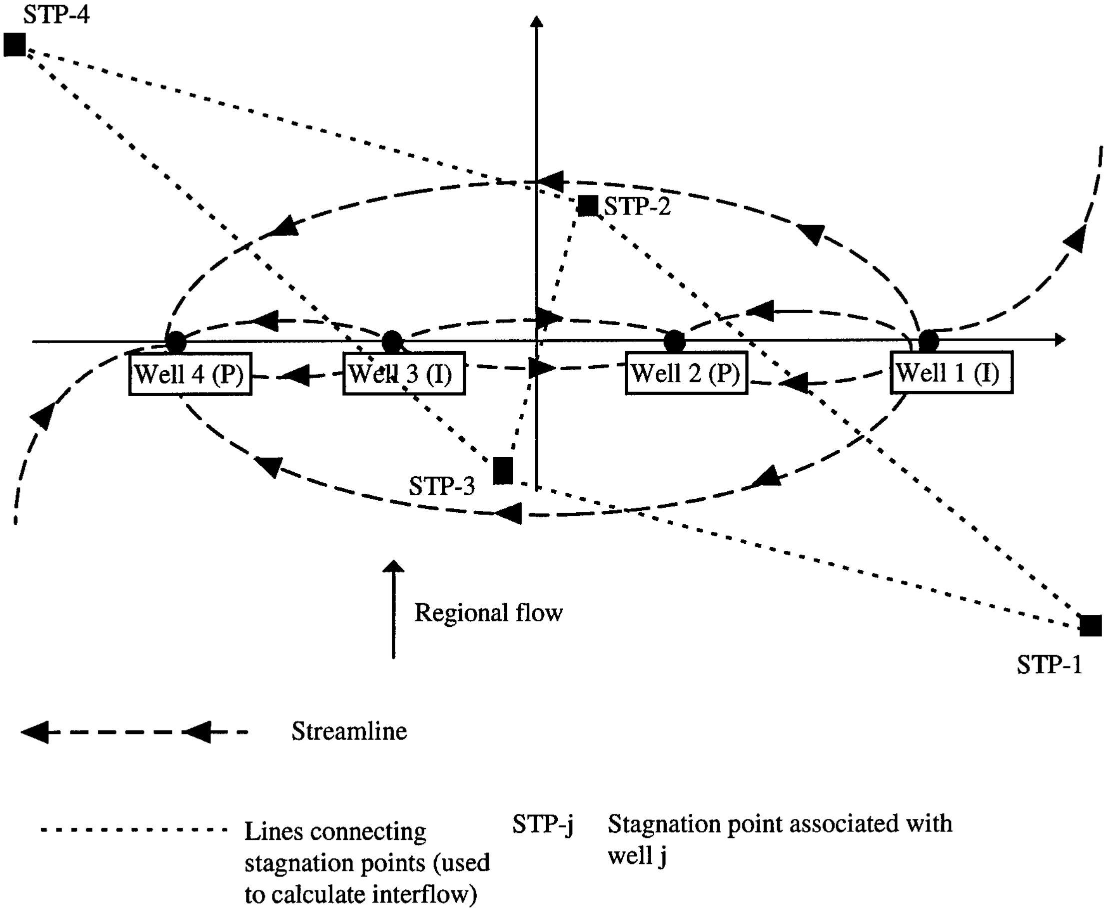


Figure 3.4: Flow field for a four well system with pumping (P) and injection (I) wells alternating.

Looking first at pumping well 2, we can use equation (29), traveling clockwise from stagnation point 1, to calculate the interflows between stagnation points 1 and 3, 3 and 2, and 2 and 1, which surround pumping well 2. Note that the sum of the three interflows must equal unity (the total flow into well 2). Depending on relative parameter values, this can result in several scenarios. If all interflows are positive, the interflow between stagnation points 1 and 2 would indicate the interflow between injection well 1 and pumping well 2. Similarly, the interflow between stagnation points 2 and 3 would indicate the interflow between injection well 3 and pumping well 2. Finally, the interflow between stagnation points 1 and 3 would indicate the upgradient flow going into pumping well 2. A second scenario may occur if there's a negative interflow between stagnation points 1 and 2 and points 2 and 3. This means there is regional flow passing between wells 1 and 2 and wells 2 and 3, with the magnitude of the interflow indicative of the number of regional stream lines passing in between the well pairs (DaCosta and Bennett, 1960). Of course, in this case, the interflow between the two well pairs is zero. As the sum of interflows between stagnation points 1, 2, and 3 must equal unity, the interflow between stagnation points 1 and 3 must be positive. This would indicate the regional flow coming from upgradient with an amount Q being captured by pumping well 2. A third scenario is that both the interflows between stagnation points 1 and 2, and 2 and 3 are positive, while the interflow between stagnation points 1 and 3 is negative. This is the scenario depicted by the flow lines in Figure 3.4. In this scenario, there is flow from injection wells 1 and 3 into pumping well 2, with no regional flow coming into pumping well 2. In this case, the interflow between stagnation points 2 and 3 will tell us how much of the flow in pumping well 2 is coming from injection well 3. The flow going from injection well 1 into pumping well 2 is the sum of the interflows between stagnation points 1 and 2 (which is >0) and 1 and 3 (which is <0). The negative value of the interflow between stagnation points 1 and 3 indicates that some portion of the flow from injection well 1 that has crossed the line between stagnation points 1 and 2 also crosses the line between stagnation points 1 and 3, thereby leaving the influence of pumping well 2 and ultimately flowing to pumping well 4. As may be seen from Figure 3.4, there is a second portion of flow which also travels from well 1 to well 4. These stream lines pass downgradient of stagnation point 2 and are not accounted for in the interflow calculated between stagnation points 1 and 2. However, this portion of flow is accounted for when the interflow between stagnation points 2 and 4 is calculated, and in fact makes up the entire net flow passing between stagnation points 2 and 4 (just as the flow taking the "upgradient route" from well 1 to 4 makes up the entire net flow passing between stagnation points 1 and 3).

Note that if we define I_j as the interflow between the jth and (j+1)th stagnation points, and if all interflows between wells are positive, then the total interflow in the system (I_T) is simply

$$I_T = \sum_{j=1}^{N-1} I_j \tag{30}$$

where total interflow is defined as the ratio of the flow through all extraction wells that originated in injection wells and the flow through a single extraction well (Q). We may also define an average interflow, I_{AVG}, as the fraction of flow through all extraction wells that originated in injection wells. Note that I_{AVG} is equal to I_T divided by the number of extraction wells (N/2).

It may be of some use to chemical and sanitary engineers to relate the average interflow (I_{AVG}), to a concept they may be more familiar with, the recycle ratio (f). Often in treatment system design (for instance activated sludge systems) a portion of the treated water is recycled back to the influent (Metcalf and Eddy, 1991). The recycle ratio (f) is equal to the amount of recycled flow divided by the amount of untreated incoming flow. The recycle ratio concept can also be applied to the *in situ* aerobic cometabolic treatment technology. If it is assumed that the *in situ* treatment system acts like a bioreactor, the average interflow is equivalent to the recycled flow. The incoming flow to the remediation system is one minus I_{AVG}; $(1 - I_{AVG})$. Thus, the recycle ratio for this remediation application (f) can be expressed as $I_{AVG}/(1 - I_{AVG})$. As an example, an average interflow $I_{AVG} = 0.75$, is equivalent to a recycle ratio $f = 3$. Note that I_{AVG} can have negative values, when there is no interflow and regional flow is passing between treatment wells. In this case, of course, $f = 0$.

An alternate approach to that described in equation (30) may be used to determine total interflow through the circulating well system. By calculating the stream function difference of the two outer stagnation points (stagnation points 1 and 4 for the four-well system shown in Figure 3.4), the flow entering the well system from upgradient (or equivalently, leaving the system downgradient) may be determined. Subtracting this flow from the total flow going through the pumping wells gives the total interflow for the well system. This approach precludes the need to calculate interflows for each well pair.

$$I_T = \frac{N}{2} - \frac{\psi_1 - \psi_2}{Q/B} \tag{31}$$

ψ_1 = Stream function evaluated at stagnation point associated with left most pumping well (pumping well at location with the minimum x-value) $[L^2/T]$

ψ_2 = Stream function evaluated at stagnation point associated with right most injection well (pumping well at location with the maximum x-value) $[L^2/T]$

Being able to calculate the total system interflow allows us to determine the capture zone width (CZW) for the well system. We can equate flow into the system from upgradient

(CZW*U*B) with the portion of flow being pumped through the extraction wells that comes from upgradient (Q*N/2- Q*I_T) to calculate the capture zone width.

$$CZW = \frac{Q}{UB}\left[\frac{N}{2} - I_T\right] \tag{32}$$

3.4 OVERALL TREATMENT EFFICIENCY

Now that we have developed a model which calculates the single pass treatment efficiency and the amount of interflow passing between well pairs, were able to calculate an overall treatment efficiency (η) for a system of pumping/injection wells being used as a treatment barrier. If we define overall treatment efficiency as follows:

$$\eta = 1 - \frac{C_{out}}{C_{in}} \tag{33}$$

where

C_{out} = contaminant concentration downgradient of the well system [M/L^3]

C_{in} = contaminant concentration upgradient of the well system [M/L^3]

and define a single-pass treatment efficiency (η_{SP}) as the fraction of contaminant removed during a single-pass through a treatment zone or well, by mass balance we find

$$\eta = \frac{\eta_{SP}}{1 - I_{AVG}(1 - \eta_{SP})} \qquad \frac{C_{out}}{C_{in}} = \frac{(1-\eta_{SP})(1-I_{AVG})}{1 - I_{AVG}(1-\eta_{SP})} \tag{34}$$

Using equations (31), (32), and (34) we can find the total interflow, capture zone width, and overall treatment efficiency for an N well system of single screened injection and extraction wells operating in a single confined aquifer.

If, however, we wish to obtain the overall efficiency for a system of dual screened wells operating in two aquifers as used at the Edwards demonstration (See Chapter 2) we find the following equations for the upper and lower aquifer, respectively

$$C_{outU} = C_{in}\left[\frac{(1-I_L)(1-\eta_{spU})+I_L(1-I_U)(1-\eta_{spL})(1-\eta_{spU})}{1-I_U I_L(1-\eta_{spL})(1-\eta_{spU})}\right] \qquad (35a)$$

$$C_{outL} = C_{in}\left[\frac{(1-I_U)(1-\eta_{spL})+I_U(1-I_L)(1-\eta_{spL})(1-\eta_{spU})}{1-I_U I_L(1-\eta_{spL})(1-\eta_{spU})}\right] \qquad (35b)$$

η_{spU} = Average single-pass treatment efficiency in upper aquifer

η_{spL} = Average single-pass treatment efficiency in lower aquifer

I_U = Average interflow between upper well screens

I_L = Average interflow between lower well screens

C_{in} = Influent (upgradient) Concentration [M/L^3]

C_{outU} = Effluent (downgradient) Concentration in upper aquifer [M/L^3]

C_{outL} = Effluent (downgradient) Concentration in lower aquifer [M/L^3]

Notice that equation (35) does not allow for any short-circuiting interflow between the injection and extraction screens in a single well. Also note that equation (35) assumes upgradient concentrations are the same in the upper and lower aquifers. If we wish to determine the overall treatment efficiency for a case where conditions are isotropic (or no aquitard is present) and short-circuiting is allowed these equations must be modified to account for the short-circuiting which can occur between the well screens in a single well (in the z direction--see Figure 4.2). The following equations have been written to account for this

$$\frac{C_{outU}}{C_{in}} = \left[\frac{(1-\eta_{spU})(1-I_L - I_{ScU})}{(1-I_{scU} + I_{scU}\eta_{scU})} + \frac{I_L(1-I_U - I_{scL})(1-\eta_{spU})(1-\eta_{spL})}{(1-I_{scU} + I_{scL}\eta_{scU})(1-I_{scL} + I_{scL}\eta_{scL})} \right] x \left(\frac{1}{1 - \frac{I_U I_L (1-\eta_{spU})(1-\eta_{spL})}{(1-I_{scU} + I_{scL}\eta_{scU})(1-I_{scL} + I_{scL}\eta_{scL})}} \right) \quad (36a)$$

$$\frac{C_{outL}}{C_{in}} = \left[\frac{(1-\eta_{spL})(1-I_U - I_{ScL})}{(1-I_{scL} + I_{scL}\eta_{scL})} + \frac{I_U(1-I_L - I_{scU})(1-\eta_{spU})(1-\eta_{spL})}{(1-I_{scU} + I_{scL}\eta_{scU})(1-I_{scL} + I_{scL}\eta_{scL})} \right] x \left(\frac{1}{1 - \frac{I_U I_L (1-\eta_{spU})(1-\eta_{spL})}{(1-I_{scU} + I_{scU}\eta_{scL})(1-I_{scL} + I_{scL}\eta_{scL})}} \right) \quad (36b)$$

where

I_{scL} = Percentage of in-well flow (Q) short-circuiting from the lower injection screen to the upper pumping screen [-]

I_{scU} = Percentage of in-well flow (Q) short-circuiting from the upper injection screen to the lower pumping screen [-]

η_{scU} = Efficiency of the degradation occurring along the shortened flow path from the lower injection screen to the upper pumping screen.

η_{scL} = Efficiency of the degradation occurring along the shortened flow path from the upper injection screen to the lower pumping screen.

Notice that equation (36) will simplify to equation (35) when no short-circuiting occurs ($I_{scU} = I_{scL} = 0$) and equation (35) will simplify to equation (34) when only one aquifer is considered.

Although the above equations were developed assuming one line of co-linear wells, in some cases, it may be necessary to have multiple lines of wells. For instance, if contaminant concentrations are extremely high, two or more lines of wells in series may be needed to reduce concentrations enough to meet regulatory goals. Also, multiple lines of wells may be required to treat multiple contaminants. For example, a line of wells may treat PCE abiotically or anaerobically, followed by a second line of wells to treat TCE (and other less chlorinated ethenes) by aerobic cometabolism.

If several rows of wells are employed and there is enough distance between the rows to assume the interactions between multiple rows are negligible (the validity of this assumption is discussed in chapter 4) then the overall treatment efficiency for a system of multiple well rows is given by equation (37)

$$\eta = 1 - \prod_{j=1}^{M} \left(\frac{C_{out}}{C_{in}} \right)_j \tag{37}$$

where M = the number of treatment well rows and C_{out}/C_{in} is given by equation (34), (35) or (36) depending on the situation. The above equation is written for the more general case of varying treatment efficiencies due to differing treatment technologies (η_{sp}), interflows (I_T) and numbers of wells (N). However, if one is using the same technology in each treatment well row and the same number of wells pumping at the same rate then equation (37) simplifies to

$$\eta = 1 - \left(\frac{C_{out}}{C_{in}} \right)^{M} \tag{38}$$

Equations (37) and (38) can be used to aid in the design of a multiple well system.

3.5 OPTIMIZATION MODEL

The above three sections present the equations which define the interactions between engineered and environmental parameters. To design a system under specific environmental and site conditions, the engineered parameters should be adjusted, perhaps using a groundwater management model, to minimize cost, minimize time, or maximize destruction of TCE within cost and time constraints. Although application of a groundwater management model is beyond the scope of this thesis, the objective function and constraints for use in such a model will be formulated to lay the framework for a simplified optimization to be presented in the next chapter. Also, the formulation of an objective function may serve as a starting point for future work looking at application and optimization of this technology.

In this study, the goal will be to minimize total annualized cost (TC). TC represents all of the costs associated with the purchase, installation and operation of this technology. TC can be divided into capital costs and operating costs, each of which will be discussed below.

Capital costs: The capital costs include all of the costs associated with the initial purchase and start up of the system. The capital costs are a function of the well size, pump size, well depth, storage facilities, etc. This cost can be defined as:

$$TCC = Cost_C * N * f(y) \qquad (39)$$

where

TCC = Total annualized capital costs annualized over n time periods [$/yr]

$Cost_C$ = The Capital/installation/initial start-up costs per well [$]

N = Total number of wells

$f(y)$ = function used to annualize the capital costs based on an assumed interest rate and a planning horizon (Note: can be critical if capital costs are large or planning horizon is short).

Operating Costs

It is assumed operating costs will consist of pumping costs, and electron donor and acceptor costs (monitoring costs are neglected).

Pumping Costs: The pumping costs are a function of the flow rate in the well and the distance the water must be lifted. For the analysis presented in this thesis all of the well flow rates are equal. However, in the most general case the pumping rates of individual wells will vary. Equation (40) is written for the simplified case. The pumping costs are also a function of the periodic well redevelopment which was found at the Edwards demonstration (McCarty *et al.*, 1997) to be required to deal with the clogging at the well screens. The total pumping costs can be expressed as:

$$TPC = (P*N*Cost_P)/\eta + N*Cost_R \qquad (40)$$

$$P = \gamma*H*Q$$

where

TPC = Total annual pumping costs [\$/yr]

P = Power used to lift water $[(M\text{-}L^2)/T^3]$

Q = Annual Flow rate in each well $[L^3/yr]$

γ = Specific Gravity of water $[M/L^2\text{-}T^2]$

H = Distance to water table or distance the water is lifted [L]

N = Number of wells

$Cost_p$ = Pumping Costs $[\$\ M^{-1}L^{-2}T^2]$

$Cost_R$ = Well Redevelopment costs [\$/well-yr]

η = Pump efficiency (since all electricity isn't converted into pumping power, some electric power is lost)

Primary Substrate Costs: The primary substrate costs are a function of the primary substrate concentration and as shown earlier (see section 3.1) this concentration is a function of the desired single pass treatment efficiency. Primary substrate costs can be given as

$$TPSC = (N/2)*Q*C_D*Cost_{ps} \qquad (41)$$

where

TPSC = Total annual primary substrate costs

Q = Annual flow rate in each well [L^3/yr]

C_D = Primary Substrate Concentration [M/L^3]

$Cost_{ps}$ = Cost of Primary substrate [\$/M]

<u>Electron Acceptor Costs</u>: As with the primary substrate, this cost is primarily dependent on the electron acceptor concentration, which is related to the primary substrate concentration and the desired "single pass" treatment efficiency. Although the model used in this thesis assumes electron acceptor is not limiting, in general, the amount of electron acceptor that can be degraded will control the amount of electron donor that can be degraded. In the Edwards field demonstration, the cost of the hydrogen peroxide that was used to supply oxygen was a significant project cost (McCarty *et al.*, 1997). The electron acceptor cost is given as

$$TEAC = (N/2)*Q*C_A*Cost_{EA} \qquad (42)$$

where

TEAC = Total annual electron acceptor costs

Q = Annual flow rate in each well [L^3/yr]

C_A = Electron Acceptor Concentration [M/L^3]

$Cost_{EA}$ = Cost of Electron Acceptor [\$/M]

These costs can now be combined to obtain the overall objective function to be minimized

$$TC = TCC + TPC + TPSC + TEAC \tag{43}$$

Now that the objective function has been formulated we must determine constraints on the objective function. A constraint restricts the value of a decision variable (e.g. pumping rate or donor concentration) or limits a state variable such as hydraulic head (Gorelick, 1993). The decision variables are parameters that we exert direct control over. In this model the flow rate (Q), number of wells (N), distance between wells (2d), angle of regional flow (α), and primary substrate and electron donor concentration are all decision variables or parameters which we engineer.

Constraint 1: The most important constraint is that the down gradient contaminant concentration (C_{out}) must be below the concentration established by the appropriate regulation (C_R)

$$C_{out} \leq C_R \tag{44}$$

Constraint 2: This constraint restricts the value of the decision variable Q. Q must be less than some predetermined value, Q_{max}, which is based on a maximum allowable drawdown at the pumping well

$$Q \leq Q_{max} \tag{45}$$

Constraint 3: Either the entire plume or a large enough fraction of the contaminant plume must be captured to prevent significant amounts of untreated contaminated water to bypass the treatment system. This constraint restricts the minimum value of the capture zone width (CZW) to some specified width, P_W

$$CZW \geq P_w \qquad (46)$$

Although none of the decision variables are directly specified in this constraint, the flow rate, number of wells, distance between wells and angle of regional flow will all affect the capture zone width ($CZW = f(Q, N, d, \alpha)$).

Constraint 4: This constraint limits the concentration of the electron acceptor and primary substrate. The electron acceptor and primary substrate both contribute to the "single pass" treatment efficiency. The concentration of electron donor that can be degraded depends on the concentration of electron acceptor that can dissolve into solution and the stoichiometry of the degradation. The dissolved electron acceptor concentration will depend on the source of the electron acceptor (e.g. air, oxygen, hydrogen peroxide). Of course, electron acceptor cost also is a function of the source. This constraint limits the electron acceptor (and therefore donor) concentration based on the source of the acceptor.

Constraint 5: This constraint is concerned with the cost of start-up and operation of the system. It limits the capital costs of the system to be equal to or lower than the start-up budget and limits the operating and maintenance costs to be at or below some operating budget. In reality, the model must be restricted by some start-up and operating budget of the site owner. This constraint, from a start-up point of view, can restrict the number of wells drilled initially and from an operations point of view restrict the flow rate. In fact, this constraint might be one that creates infeasible solutions to the model based on cost considerations.

While optimizing the objective function under this set of constraints is beyond the scope of this work, the above discussion establishes the link between the management model and the fate and transport model. This shall serve as a starting point when considering technology application and future research into system optimization.

3.6 CONCLUSION

The method for calculating single pass treatment efficiency, interflow, and overall treatment efficiency introduced in this chapter is intended to provide a simple tool to determine the efficacy of multiple circulation wells at a site, given a limited number of engineering and environmental parameters. The final section in which the optimization model is developed provides a framework for the simplified analysis in the next chapter. With the growing employment of groundwater circulation wells and injection/extraction well systems as treatment barriers, the analytical and numerical methods discussed in this chapter should prove very useful in facilitating system conceptual design and application.

4.0 ANALYSIS

4.1 INTRODUCTION

This chapter includes an analysis of the model developed in this thesis and a methodology showing how the model can be employed to implement the technology in the field. The first section in this chapter compares model results with data from the Edwards AFB *in situ* bioremediation demonstration. In the second section, a sensitivity analysis is conducted in which environmental and engineered parameters such as hydraulic conductivity (K_h), regional gradient (i), well flowrate (Q), distance between wells (2d), and number of wells (N) are varied to determine their effect on the overall treatment efficiency (η) and capture zone width (CZW). Also in the second section, the effect of three-dimensional flow on overall treatment efficiency and capture zone width is examined. In the third section, the model is used to show the utility of implementing the technology with multiple rows of wells. This approach may be useful in remediating plumes with high concentrations, multiple contaminants or extended lengths. The final section of this chapter describes software, based on the model, which was developed for use by remedial project managers as a screening tool to determine whether *in situ* aerobic cometabolic bioremediation may be useful at remediating a particular contaminated hazardous waste site. The final section also provides a step-by-step methodology for using the model to help design and implement *in situ* aerobic cometabolic bioremediation at hazardous waste sites.

4.2 COMPARISON OF MODEL WITH DATA FROM THE EDWARDS AFB BIOREMEDIATION DEMONSTRATION

A recent demonstration of *in situ* aerobic cometabolic bioremediation at Edwards AFB motivated this thesis. The demonstration also provides field data that can be used for model verification. At the Edwards demonstration, groundwater contaminated with 500 to 1200 μg/L trichloroethylene (TCE) was successfully treated using the *in situ* aerobic cometabolic bioremediation technology (McCarty *et al.*, 1997). The demonstration lasted 410 days and consisted of two wells screened at two depths separated by an aquitard. As described in chapter 2, one well extracted contaminated water from an upper unconfined aquifer, amended the water with nutrients (toluene, the primary substrate and oxygen and hydrogen peroxide, the electron acceptors), and then reinjected the mixture into a lower confined aquifer (McCarty *et al.*, 1997). The second well operated in the upflow mode, withdrawing contaminated water from the lower confined aquifer, adding toluene and oxygen, and reinjecting it into the upper unconfined aquifer. The two wells were separated by 10 m, allowing recirculation (interflow) between the pumping and injection wells in each aquifer. Bioactive zones were established around the injection well screens in the upper and lower aquifer, where primary substrate was metabolized and TCE cometabolized. Due to recirculation, water passed through the bioactive zones more than once, so that the overall treatment efficiency of the system was 97 to 98 percent, even though the treatment efficiency of a single pass through the bioactive zone was only 83 to 87 percent (McCarty *et al.*, 1997). The successful field-scale demonstration of aerobic cometabolic *in situ* bioremediation showed that this is a promising remediation technology with potential to remediate TCE contaminated sites.

Three distinct steady-state periods were observed during the demonstration. In the first two steady-state periods, short-circuiting between the upper and lower screens in the down flow well created unbalanced flow conditions. Once the problem was realized, the flow rate in the upflow well was reduced, creating balanced flow conditions for the third steady-state period (McCarty *et al.*, 1997). The data collected during these three steady-state periods can be compared with model simulations, thereby helping to verify model performance.

In this section we will begin by comparing the analytical model developed in this thesis with a popular semi-analytical model, RESSQ, that was used by the investigators at the Edwards AFB demonstration to help design the system. We will then compare analytical model results with the actual field data taken over the 410 day demonstration. Finally, we will conduct a sensitivity analysis of the model to see how model results vary with input parameters.

4.2.1 Comparison with Semi-Analytical Model

RESSQ, a two-dimensional semi-analytical groundwater flow model, was used by McCarty *et al.* (1997) to evaluate the capture zone and interflow at the Edwards AFB demonstration site. RESSQ is a popular model which is often employed for site evaluations (Bair and Roadcap, 1992; Springer and Bair, 1992; Lang *et al.*, 1997). Using the RESSQ program, the investigators at Edwards AFB were able to determine the amount of interflow (recycle) that occurred between the pumping and injection wells in a single aquifer. Preliminary studies at the demonstration site found the hydraulic conductivity on the order of 3.4 x 10^{-3} cm/sec, the regional gradient was 0.007, and the upper and lower aquifer thickness' were 8 and 5 m, respectively (McCarty *et al.*, 1997). For the third steady-state period, effective flow rate in each of the treatment wells was 36.0 m^3/d (25.0 L/min) (McCarty *et al.*, 1997). If the two wells, which were 10 m apart, were assumed to lie on the x-axis, and were placed symmetric about the y-axis, the general direction of groundwater flow in the upper aquifer would make a 67.5° angle (α) measured counterclockwise from the positive x-axis (see Figure 4.1a). In the lower aquifer, because the relative position of the pumping and injection wells are transposed, the angle (α) would be the supplement of the upper aquifer angle (Figure 4.1b).

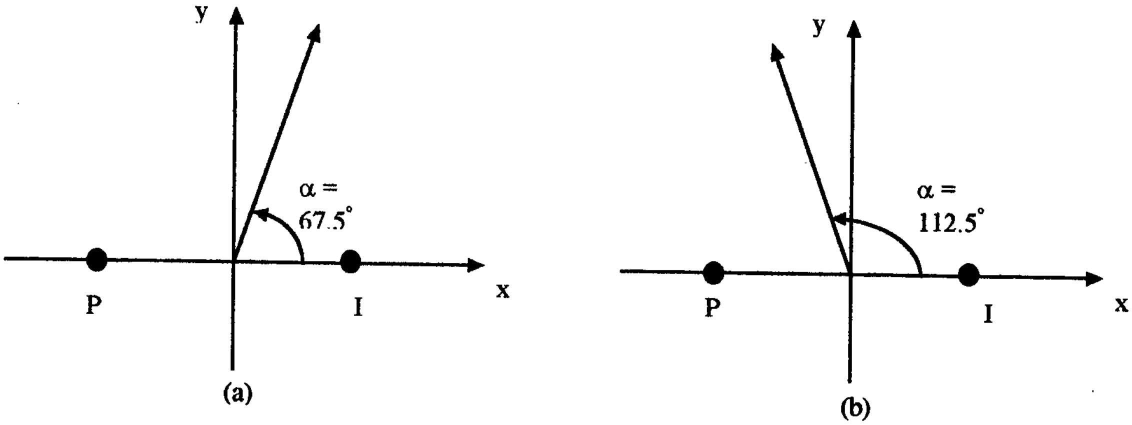


Figure 4.1 Angle of regional flow at the Edwards AFB bioremediation demonstration in the (a) upper aquifer and (b) lower aquifer.

Using these parameters, in conjunction with the RESSQ model, the researchers found that interflow in the upper aquifer accounted for 71 percent of the extraction well flow while interflow in the lower aquifer accounted for 85 percent of the extraction well flow (McCarty *et al.*, 1997). This means that 71 percent of the water being extracted from the upper aquifer by the downflow well originated in the upflow well while 85 percent of the water being extracted from the lower aquifer by the upflow well originated in the downflow well. The corresponding capture zone widths for each well were 62 m and 53 m in the upper and lower aquifers, respectively. Using the analytical model developed in this thesis, the same results are obtained. This agreement is not unexpected, since the equations which form the foundation for the model are the same as the equations RESSQ is based on. The thesis model simply provides an analytical method of solving these equations which forgoes the need to plot and count streamlines as was done using RESSQ. The real test of the model is to compare it to field data. Nevertheless, testing the model against an established model is an important first step in model verification.

4.2.2 Model vs. Field Data

To evaluate a model, "history matching" model output with real data collected in the field is an effective method (Bredehoeft and Konikow, 1993). This section accomplishes this comparison, using data from the Edwards AFB demonstration.

The three steady-state evaluation periods were approximately 70 days each. The first and second steady-state periods were slightly different than the third steady-state period. Due to installation problems, some of the water injected into the lower aquifer from the downflow treatment well short-circuited back to the upper screen in the same well (McCarty *et al.*, 1997). As verified by McCarty *et al.* (1997) in various aquifer and tracer tests, this short-circuiting reduced the effective flow in the downflow well from the desired 38 L/min to 25 L/min. This led to an unbalanced flow condition, since the upflow treatment well was pumping the full 38 L/min.

Using the analytical model developed in this thesis, interflow between the two wells can be calculated. The results of the calculations can then be compared to the interflows determined in the field based on mass balance. To find the field values for interflow based on mass balance, the TCE concentration was monitored at the injection screen of each of the treatment wells, and at a monitoring point adjacent to each extraction screen. The monitoring point was chosen along the line connecting the two treatment wells, so it could be assumed that water passing the monitoring point was interflow. By also assuming an up gradient concentration of 1000 μg/L and that the TCE concentration measured at the treatment well injection screen represented the concentration of up gradient water mixed with recirculated water, the interflow could be calculated using the following mass balance expression:

$$C_{well}Q = (1-I)Q1000 + IQC_{mp} \qquad (47)$$

where

C_{well} = TCE concentration measured in the treatment well [μg/L]

C_{mp} = TCE concentration measured at a monitoring point approximately 2 m from the extraction screen (assumed to represent concentration of TCE in the recirculated water) [μg/L]

Q = Well flow rate [L^3/T]

I = Interflow [-]

Table 4.1 compares the value of interflow calculated using the analytical model with field results calculated by equation (47).

Table 4.1: Interflow calculated from field (eq. (47)) and thesis model

Steady-State Period	Upper Aquifer Field Results	Upper Aquifer Model	Lower Aquifer Field Results	Lower Aquifer Model
days 145-204	96 %	91 %	71 %	66 %
days 212-271	97 %	91 %	77%	66 %
days 365-444	92 %	71 %	85%	85 %

As can be seen from the table, the interflows which were found from field data using mass balance matched quite well with the model in both aquifers and all time periods except for one. During the third steady-state period, in the upper aquifer, we see a poor match between the model and field values. This disagreement can stem from a number of factors: (1) the upper aquifer is unconfined, yet the equations are written for confined conditions, (2) the equations assume an isotropic homogeneous media, yet this is rarely observed in the field, (3) the mass balance calculations assumed a constant up gradient TCE concentration for both aquifers of 1000 μg/L, when it actually varied in time and space (McCarty *et al.*, 1997), and (4) the concentration from one selected monitoring well was used to represent the concentration of the entire recirculated flow entering the extraction well in each aquifer. Given the above factors, it is quite remarkable (and surely somewhat fortuitous) that model results and field measurements agree as closely as they did in Table 4.1.

4.3 Sensitivity Analysis

4.3.1 Hydraulic Conductivity and Regional Gradient

McCarty *et al.* (1997) present ranges for hydraulic conductivity and regional gradient values. To investigate the effect of varying these parameters, the final balanced flow steady-state period will be analyzed. In McCarty *et al.* (1997) the hydraulic conductivity (K_h) is reported to range between 1.5 x 10^{-3} and 5.5 x 10^{-3} cm/s. The regional gradient (i) is reported to be 0.004 in the upper aquifer and 0.010 in the lower aquifer (McCarty *et al.*, 1997). Using these values, a sensitivity analysis can be conducted to determine the effects of changes on the model parameters on interflow (see Table 4.2). Baseline parameters are those used in Table 4.1 for the third steady-state period.

Table 4.2: Sensitivity analysis on system interflow (I)

	Interflow (field data)	Interflow (Baseline)	Interflow (Low K_h^a)	Interflow (High K_h^b)	Interflow (Baseline K_h and varying i^c)	Interflow (Low K_h^a and varying i^c)	Interflow (High K_h^b and varying i^c)
Upper Aquifer	92 %	71 %	81 %	64 %	79 %	86 %	73 %
Lower Aquifer	85 %	85 %	90 %	81 %	82 %	88 %	77 %

a. $K_h = 1.5 \times 10^{-3}$ cm/s
b. $K_h = 5.5 \times 10^{-3}$ cm/s
c. i= 0.004 upper aquifer
   i= 0.010 lower aquifer

The above table shows the degree to which calculated interflow varies with relatively slight variations in aquifer parameters. The differences in the two aquifers stem from three factors, (1) the difference in the thickness of the aquifers, (2) the difference in the magnitude of the regional gradient in each aquifer, and (3) the position of the wells with respect to regional flow. In the upper aquifer the pumping well is located at (-d,0) and the injection well is located at (d,0). In the lower aquifer these positions are reversed (see Figure 4.1).

4.3.2 Hydraulic Conductivity and Anisotropy

Due to the presence of an aquitard separating the two aquifers at the Edwards demonstration site, all of the calculations performed above were completed assuming no vertical flow (i.e. two-dimensional flow). However, as was alluded to previously, vertical flow often occurs in the field and needs to be considered. This is especially true if the dual-screen well design is to be implemented at sites where there is no aquitard separating the two screened sections of the treatment wells (see Figure 4.2).

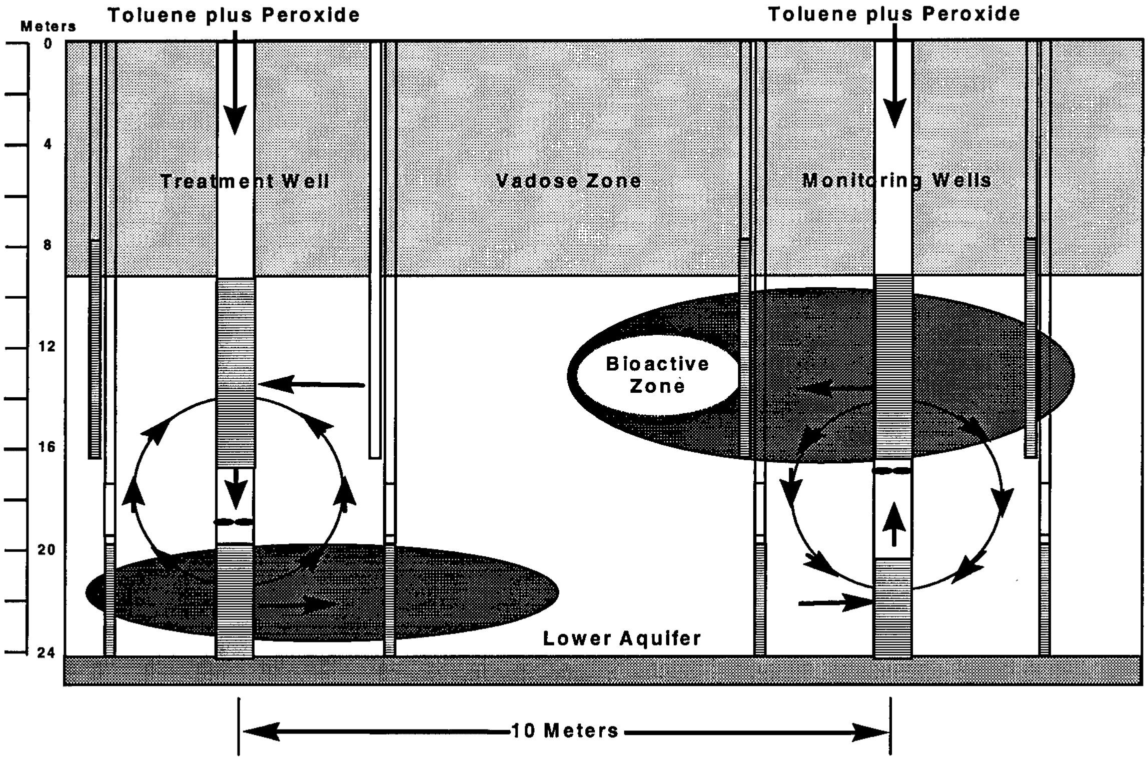


Figure 4.2: Bioremediation treatment system with short-circuiting between treatment well screens

To investigate the implications of flow in the vertical direction on treatment efficiency a numerical model (MODFLOW) was used. The numerical model allows for anisotropic conditions and multiple screened wells in a single aquifer. In an attempt to gain a better understanding of how the vertical flow (short-circuiting between well screens) affects the contaminant degradation, the Edwards AFB demonstration was modeled. All of the parameters used in the baseline case above were kept the same with the exception of flow rate and hydraulic conductivity. The flow rate in both wells was set at 38 L/min (54.7 m^3/d) and the vertical hydraulic conductivity (K_v) was allowed to vary from 0 cm/s (aquitard present - two-dimensional flow assumed) to 3.4 x 10^{-3} cm/s (isotropic conditions). By doing this, the anisotropy ratio (K_v/K_h) was varied to determine how vertical flow affected the degree of treatment. Figure 4.3 shows the mass of TCE degraded per day as a function of the anisotropy.

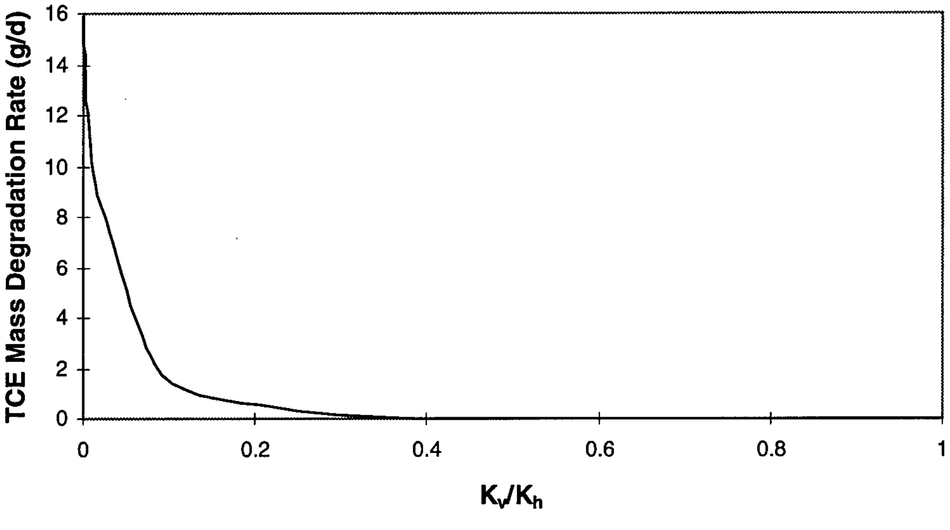


Figure 4.3: TCE degradation versus anisotropic ratio

There are several things that should be pointed out with respect to Figure 4.3. First, one should notice that $K_v/K_h = 0$ is equivalent to an aquitard being present. Therefore, the system can be modeled using the two-dimensional analytical model presented in this thesis, and in fact, results of the numerical model with $K_v/K_h = 0$ were verified using the analytical model. The second thing to notice from Figure 4.3 is that the amount of TCE which is degraded decreases as the system becomes more isotropic. At approximately $K_v/K_h = 0.3$ the treatment system is essentially rendered ineffective and no TCE is being degraded. The reason behind this is the short-circuiting effect and the assumption that short-circuited flow undergoes no treatment. When $K_v = 0$ there is no vertical flow and thus no short-circuiting. However, as K_v is increased it becomes easier for flow to move in the vertical direction. As vertical flow becomes easier, there is more short-circuiting between screens in a single well, and less treatment. In fact, when $K_v/K_h = 0.3$ all of the water being extracted by the pumping well is either originating in the injection screen of the same well or in the injection screen of the second treatment well. This means the system has become closed and the capture zone width has become zero. All of the water in the system is being treated to 0 µg/L, but no new water is being brought into the system. Thus, for the Edwards parameters, the horizontal hydraulic conductivity must be at least about 5 times greater than the vertical hydraulic conductivity for the system to work effectively. Note that an anisotropy ratio of less than 0.2 is not uncommon. On sites with higher ratios the treatment system can use single-screened wells, with water brought to the surface for amendment with primary substrate and oxygen. Alternatively, increasing the distance between screens in the treatment wells or decreasing the distance between wells can help improve the degree of treatment in relatively isotropic aquifers.

4.3.3 Engineered Parameters

The remainder of the analysis will focus on implementation of this technology for remediating a single isotropic aquifer with conventional injection/extraction treatment wells screened throughout the thickness of the aquifer.

An examination of the model developed in chapter 3 reveals the following engineered parameters which can be controlled by the user: (1) primary substrate concentration (C_D), (2) flow rate in the well (Q), (3) distance between wells (2d), (4) number of wells (N), and (5) angle the wells make with the general direction of groundwater flow (α). First the effect of varying these parameters will be qualitatively discussed. Following the qualitative discussion, the model will be applied to quantify how adjusting these parameters impacts interflow, capture zone width and treatment efficiency.

4.3.3.1 Qualitative Discussion

Primary Substrate Concentration: The primary substrate concentration is the amount of "food" provided to the microorganisms. This energy source allows the microorganisms to cometabolize the target contaminant. Primary substrates which have been demonstrated in the field to induce cometabolic degradation of TCE include methane (Semprini *et al.*, 1990), phenol (Hopkins *et al.*, 1993a), and toluene (McCarty *et al.*, 1997). There is a minimum concentration of primary substrate required to stimulate growth (Anderson and

McCarty, 1997a). Beyond this minimum concentration an increase in primary substrate increases the "single pass" treatment efficiency up to a point. However, due to competition between the primary substrate and the target contaminant for the active site on the enzyme, too much primary substrate can decrease the efficiency of the system (Semprini *et al.*, 1992). One should note that the simplified biological model presented in this thesis does not account for this deleterious effect.

Flow Rate: For the analysis in this chapter, all of the treatment wells are assumed to be pumping at equal rates. If this is the case, several statements can be made concerning the effects of the pumping flow rate on the flow field. First, an increase in the flow rate will result in an increased interflow. However, the flow rate is limited to some maximum value determined by the maximum allowable drawdown. Second, although an increase in flow rate causes an increase in interflow, the capture zone width also increases. This is due to the relative rates at which the flow rate, capture zone width and interflow increase. As the flow rate is incrementally increased, a portion of the increase is sustained through increased interflow, while the remainder is sustained through captured flow from up gradient. Third, increasing the flow rate with multiple wells can create interflow between non-adjacent pumping and injection wells. These non-adjacent interflows render the wells in between the non-adjacent wells inconsequential in determining the capture zone width, since they do not treat upgradient water (as flowlines cannot cross each other). These inner wells serve to increase total interflow, however, thereby increasing the overall efficiency of the treatment system.

Distance between treatment wells: The distance between the treatment wells (2d) is another parameter that can be used to control the capture zone width and interflow. If the wells are placed close together (2d is small) then the interflow will be high. As the wells move apart the interflow decreases while the capture zone width increases. Eventually, the wells will reach a point where the interflow between wells is zero. An interesting point when considering well systems where N>2 is the fact that the interflow between the center well pair will be the last to reach zero with increasing 2d. Even though all of the wells are the same distance apart as 2d increases, the interflows in the outer well pairs will reach zero first, followed by the interflow for the next inner well pair and so on, thus suggesting that adding wells outside of a well pair can increase the interflow between that well pair.

Number of wells: Throughout this analysis the number of wells has always been even. This does not have to be the case. One also could use the model to analyze an odd numbers of wells. To avoid having to treat and dispose of water, however, the quantity of extracted water should equal the quantity of injected water.

Angle of Regional flow: The angle the regional flow makes with the co-linear treatment well system is probably the least studied of the design parameters. Most studies up to this point have assumed the angle of regional flow to either be 0 ° (pumping well up gradient of extraction well) or 180 ° (injection well up gradient of the pumping well). The impact of varying flow angle, however, can easily be quantified using the model in this thesis. The angle of flow can have a major impact on the capture zone width and interflow.

When the angle of flow equals 0 °, the capture zone width is at its maximum and interflow at its minimum. As the angle of flow increases the interflow increases at the expense of the capture zone width. When the angle of flow equals 180 ° then the interflow is at a maximum (100 %) and the capture zone width is zero.

Related to the angle of flow is the location of the injection and pumping wells in relation to each other. For a two well system this is determined by α, however, for more wells ($N > 2$) the placement of the injection wells in relation to the pumping wells can significantly impact the interflow and capture zone width. For a non-colinear system of wells, when the injection wells are positioned slightly up gradient of the pumping wells then the interflow will increase and the capture zone width will decrease. On the other hand, when the injection wells are placed down gradient of the pumping wells the interflow will decrease and the capture zone width will increase. In this thesis, we will deal with colinear systems, but in general the position of the wells relative to each other must be considered when implementing and optimizing the technology.

4.3.3.2 Quantitative Discussion

The above discussion concentrated on qualitative aspects which should be considered when designing a treatment system. The section provided a brief description of the engineered parameters a designer could vary to adapt the technology to a particular site. This section builds on these ideas by quantitatively analyzing model results.

Using equations (31), (32), and (34) we can find the total interflow, capture zone width, and overall treatment efficiency for an N well system.

Table 4.3: Parameter evaluation for several well cases.

	2 Wells	4 Wells	6 Wells	8 Wells	10 Wells
Capture Zone Width (m)	76.5	110.	137.	160.	182.
Capture Zone Width/Pump Well (m)	76.5	55.0	45.6	40.1	36.4
Average interflow ($2I_T/N$) (%)	76.9	83.4	86.3	87.9	89.0
Overall System Treatment Efficiency (%)	96.7	97.6	98.0	98.2	98.4
Effluent[a] Conc. µg/L	33.4	24.2	20.1	17.7	16.2

a. Assuming influent contaminant concentration (C_{in}) is 1000 µg/L.

In Table 4.3, these values are calculated for two-, four-, six-, eight-, and ten-well systems. Table 4.3 calculations were made using the following representative parameter values: the pumping rate through each well in the N-well system $Q = 0.038\ m^3/min$, the regional Darcy velocity $U = 2.06\ cm/d$, the half-distance between the wells $d = 5\ m$, the aquifer thickness $B = 8m$, the angle of regional flow $\alpha = 67.5°$, and the single-pass treatment efficiency $\eta_{SP} = 87\%$. Stagnation points used to obtain the values in Table 4.3 were determined analytically for the two-, four-, six-, and eight-well cases (Equations (23), (25), (27), and (28), respectively). For the ten-well case, stagnation points were obtained by numerically finding the roots of equation (20). Looking at Table 4.3 we find that for the parameters chosen, an increased number of wells does not significantly increase the efficiency of the system, and that although capture zone width increases with an increasing number of wells, the capture zone width per well decreases.

In Table 4.4, we use equations (25) and (29) to calculate the individual interflows between wells in a four-well system. Parameter values were the same as used for Table 4.3, with three values of well pumping rate (Q).

Table 4.4: Effects of pumping rate on interflow for a four well system

Injection Wells				Pumping Wells			
Well 1				Well 2			
	Q=.038*	Q=.0038	Q=.001		Q=.038	Q=.0038	Q=.001
Flow to Well 2	0.651**	0.209	-0.654	Flow from Well 1	0.651	0.209	-0.654
Flow to Well 4	0.0171	0.00	0.00	Flow from Well 3	0.349	0.252	-0.459
Flow to down gradient	0.332	0.791	1.654	Flow from up gradient	0.00	0.538	2.11
Well 3				Well 4			
	Q=.038	Q=.0038	Q=.001		Q=.038	Q=.0038	Q=.001
Flow to Well 2	0.349	0.252	-0.459	Flow from Well 1	0.0171	0.00	0.00
Flow to Well 4	0.651	0.209	-0.654	Flow from Well 3	0.651	0.209	-0.654
Flow to down gradient	0.00	0.538	2.11	Flow from up gradient	0.332	0.791	1.65

* Units of Q are m^3/min

** Units of (m^3interflow/min)/(m^3 total flow/min)

From Table 4.4, we see the following. First, the system is symmetric. That is, the interflow between injection well 1 and pumping well 2 is equal to the interflow between injection well 3 and pumping well 4. At the highest value of Q ($Q=0.038\ m^3/min$) we see that there is no up gradient flow going to pumping well 2 and no flow from injection well 3 going down gradient. There is also a small flow that goes all the way from injection well 1 to pumping well 4. When the pumping rates through the wells are decreased by an order of magnitude, we see that there is no longer flow from well 1 to well 4, and water enters well 2 from up gradient, with an equal amount of water moving down gradient from well 3. When the well pumping rates are further decreased, there is no interflow between the wells. The negative interflows and interflows greater than unity at these very low pumping rates indicate the magnitude of the regional flow that breaks through in between the well pairs.

Just as interflows calculated using equation (29) can be less than zero (indicating regional flow breaking through between well pairs) inerflows greater than one can also be obtained. To illustrate this, a simple two-well system is shown in Figure 4.4. The wells are unbalanced so the pumping well is extracting more water than the injection well is injecting. Using the stagnation points to calculate interflow, a value of $I > 1$ is obtained. Looking at Figure 4.4, it is clear that the actual interflow is $I = 1$, as all the water injected by the injection well flows to the pumping well. The difference between the calculated I and $I = 1$ is due to the streamlines which enter the pumping well from upgradient, and are “counted” when calculating the interflow between the two stagnation points.

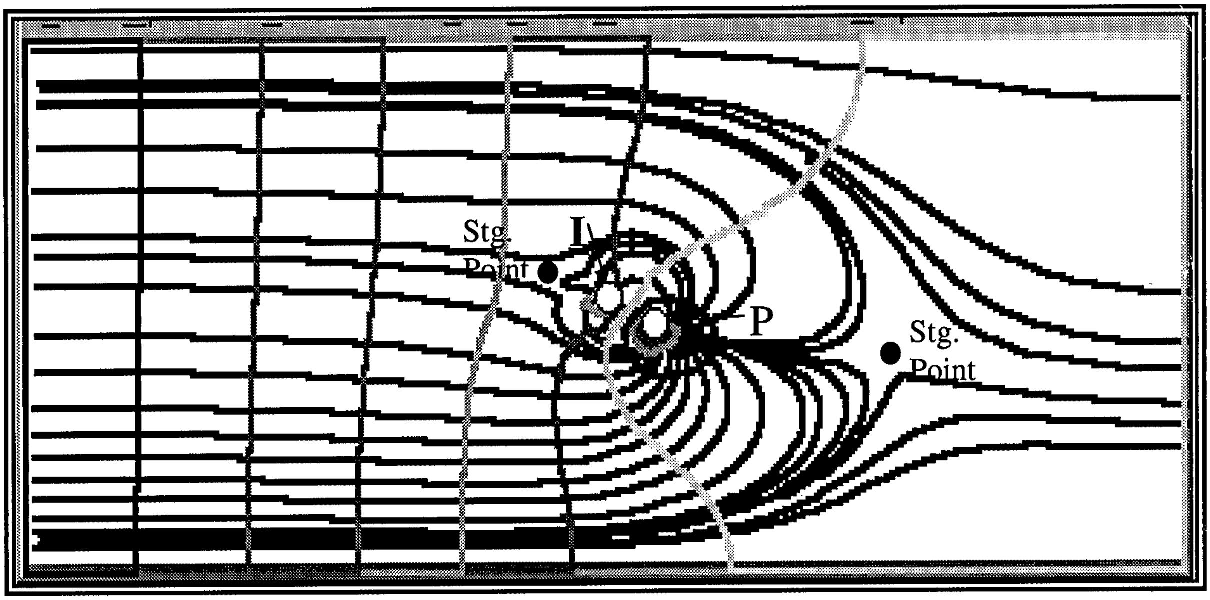


Figure 4.4: Stream line delineation for unbalanced flow conditions.

Figure 4.5 shows how the distance between wells (2d) affects interflow, overall treatment efficiency, and capture zone width (CZW) for the four-well system described above with Q=0.038 m^3/min. As expected, the capture zone width increases as the distance between the wells increases, at the expense of the total interflow. Note that at a distance 2d = 161m the interflow between wells 1 and 2 and wells 3 and 4 goes to 0. However, there is still some interflow between the two inner wells (wells 2 and 3). The interflow between the two inner wells eventually goes to 0.0 at 2d = 207m. Beyond this distance the extraction wells can be considered individual sinks in a uniform flow field each with a capture zone width of Q/UB.

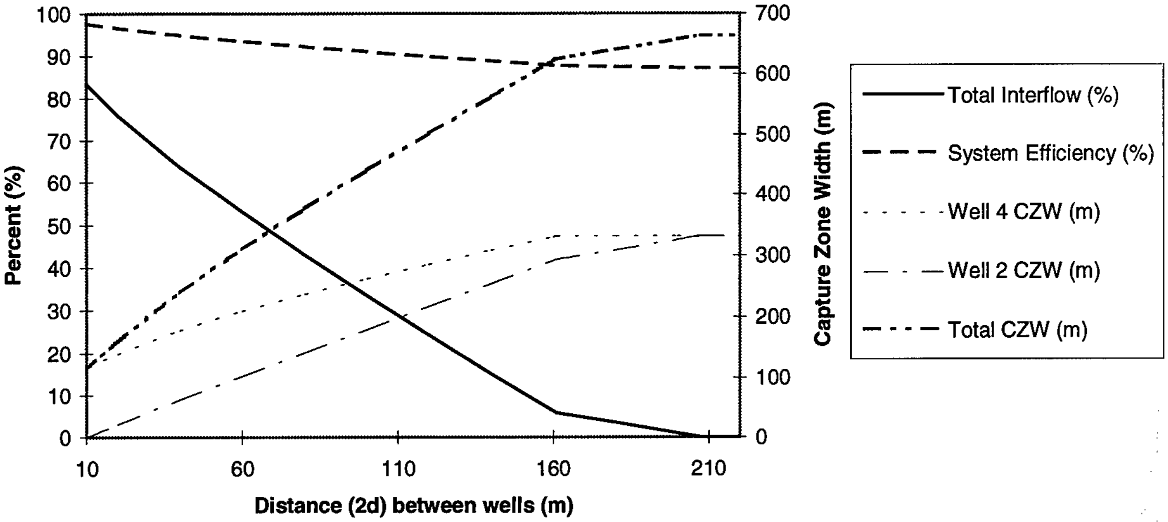


Figure 4.5: Four well analysis as a function of distance between wells.

Analyses similar to that in Figure 4.5 may be used when designing a treatment well system. For given parameter values based on the aquifer hydrogeology (U, B), and treatment system single-pass efficiency (η_{SP}), it is possible to determine a distance between wells in an N-well system that will meet treatment objectives (η and CZW) for a given Q. If no such distance can be determined, the number of wells (N) or the pumping rate (Q) must be increased. The maximum value of Q will be determined by the maximum allowable drawdown.

4.4 MULTIPLE ROW APPLICATION

Chapter 3 introduced the concept of using several rows of wells to remediate high concentration or multiple contaminant plumes.

In modeling a multiple row system of wells, we will make the assumption that the well rows are far enough away from each other that there is no interaction between rows. We can check this assumption by using equation (18) to numerically determine the stagnation points for a multiple row system and from the stagnation points we can calculate interflow. We are also able to calculate the interflow for each row of wells independently and thus can determine the validity of the assumption that there is no interaction between rows of wells.

We find that at relatively short distances a non-negligible interaction occurs with interflow between well rows. We also find that only at very long distances can each of the rows be treated independently. However, at moderate distances the multiple well rows can be assumed to act independently without introducing significant error (less than 3 %). Figure 4.6 plots non-dimensional distance between rows (R/d) versus τ, where R is the distance between well rows and τ is a ratio of the effect of the well system (Q/d) on the flow field (UB) ($\tau = Q/UBd$). Figure 4.6 shows the region where interaction between well rows can be considered negligible and each row can be treated independently. If the system is designed so that parameter values result in the system being in the negligible interaction region of Figure 4.6, then simple relationships can be used to calculate the overall treatment efficiency of a multiple line treatment system (i.e. equations (37) or (38)).

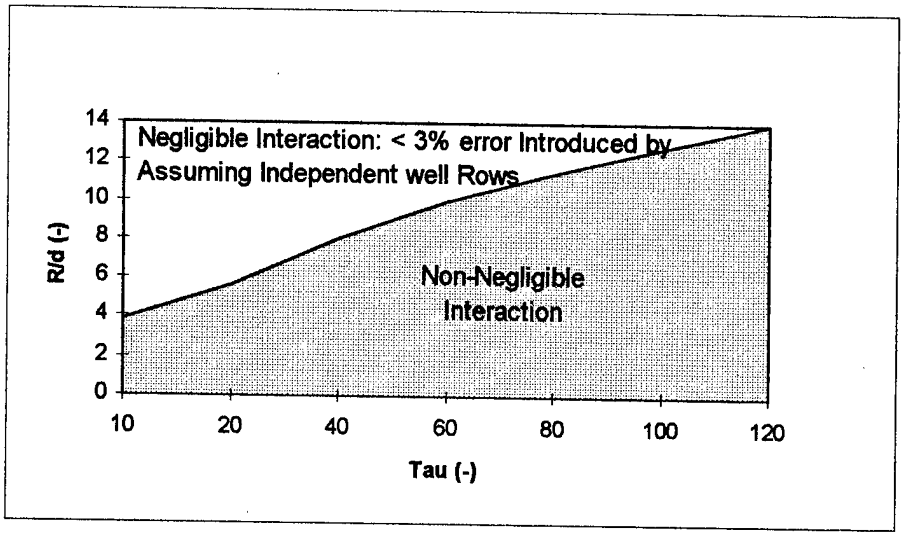


Figure 4.6: Plot showing region where multiple well rows can be modeled assuming no interaction between rows.

Analysis shows that adding two wells to an already existing two well design (resulting in a four-well row) will decrease the overall effluent concentration (C_{out}) by approximately 28%. However, adding two wells as a second row of wells behind an existing two-well row will decrease the overall effluent concentration by greater than 96%. Thus, the most efficient design is to use the least number of wells in a row which will still obtain the desired capture zone width. Then, if the system needs to be made more efficient, more wells should be added as additional rows placed down gradient of the initial row.

4.5 SCREENING SOFTWARE & SYSTEM DESIGN

4.5.1 Screening Software

As part of the thesis a computer program was developed to calculate a simple treatment system design and determine cost of implementation. The program is founded on basic engineering principles and makes many simplifying assumptions. Although not appropriate for an actual design, the program is an excellent screening tool that may be used to determine whether the technology is useable under given site conditions. The following discussion describes the program.

The first step is to calculate the maximum well flow rate based on allowable drawdown. To do this, one can use the simple aquifer hydraulic relationships found in many groundwater texts (e.g. Bear, 1979). Notice that equation (48) can be used for multiple wells even though it was formulated for a single well since our system is assumed to pump no water out of the aquifer. Thus, equation (48) will provide a conservative result.

$$Q_{\max} = \frac{2\pi T S_w}{\ln\left(R/r_w\right)} \tag{48}$$

where

T = Transmissivity $[L^2/T]$

r_W = radius of well (assumed to be 0.2 m)

R = Radius of influence $=3000*S_W*(K_h)^{0.5}$

S_W = Maximum Allowable drawdown in meters (assumed to be 30 % of aquifer thickness (B))

K_h = Horizontal hydraulic conductivity in m/s (note: these units must be used since R is determined empirically (Bear, 1979)).

Once the maximum flow rate (Q_{max}) is calculated then the required overall system efficiency (η_{Req}) must be determined based on existing upgradient concentration and required down gradient concentration ($\eta_{Req} = 1 - C_{out}/C_{in}$).

To calculate the "single-pass" treatment efficiency a simplified process is used. Rather than letting the primary substrate and electron acceptor concentrations vary, three dissolved oxygen concentrations are specified depending on whether air, oxygen gas or hydrogen peroxide is used as the oxygen source. Based on the results of the Edwards demonstration (McCarty *et al.*, 1997), it was shown that dissolved oxygen levels (D.O.) of 18 mg/L could be obtained if oxygen was used as the source of oxygen, and that D.O. levels of 30 mg/L were obtainable using hydrogen peroxide. Since air has about 20% the oxygen content of pure oxygen gas, it was assumed that the D.O. obtainable using air as the oxygen source is 3.6 mg/L. From these dissolved oxygen concentrations, the primary substrate concentration (C_D) can be calculated.

$$C_D = C_A/F \tag{49}$$

where

F = mass of dissolved oxygen required per mg primary substrate oxidized and incorporated into cell mass.

Since 2.1 mg D.O. is required per mg toluene oxidized and incorporated into cell mass (McCarty *et al.*, 1997) the primary substrate (toluene) concentrations can be calculated to be (1) air - 1.7 mg/L, (2) O_2 - 8.6 mg/L and (3) H_2O_2 - 14.3 mg/L. Now that the primary substrate concentrations are known, the "single-pass" treatment efficiencies can be determined using equation (14) with an organism decay rate b = 0.15 1/d, a yield coefficient Y = 0.77 mg/mg (Jenal-Wanner and McCarty, 1997) and the contaminant utilization constant K' (L/mg cell-d) as given in table 4.5 for several contaminants.

Table 4.5 Contaminant Utilization rates

Contaminant	Contaminant Utilization Rate K' (L/mg cell-d)
trichloroethylene (TCE)	0.07[a]
trans-dichloroethylene (trans-DCE)	0.25[b]
cis-dichloroethylene (cis-DCE)	0.035[b]
vinyl chloride (VC)	0.25[b]

a. Jenal-Warner and McCarty, 1997
b. Semprini and McCarty, 1992

We may now calculate the ratio of effluent to influent concentration and single pass treatment efficiency using equation (50):

$$\eta_{SP} = 1 - e^{-\frac{C_D Y K'}{b}} \tag{50}$$

Now that both the required overall treatment efficiency (η_{Req}) and the "single-pass" treatment efficiency (η_{SP}) are known, equation (34) can be rearranged to determine the required average interflow

$$I_{AVG} = \frac{\eta_{\mathrm{Re}q} - \eta_{SP}}{\eta_{\mathrm{Re}q}(1 - \eta_{SP})} \tag{51}$$

Knowing I_{AVG}, and recalling that $I_{AVG} = 2I_T/N$ the number of wells (N) can be calculated by setting the plume width (P_W) equal to the capture zone width (CZW) and rearranging equation (32)

$$N = \frac{2UBP_W}{Q_{Max}(1 - I_{AVG})} \tag{52}$$

Equations (48) through (52) can be used to obtain a design for the three sources of dissolved oxygen: air, oxygen and hydrogen peroxide. Once the design has been determined then the decision for the best alternative is made based on cost. Following Section 3.4, the costs in Table 4.6 may be used to determine total annualized cost.

Table 4.6: Simplified Management Model

CAPITAL COSTS	
Well Installation ($/well)	10,000[a]
OPERATING COSTS	
Well Redevelopment ($/well-yr)	1,000[b]
Electricity ($/Kw-hr)	0.1234[b]
Primary Substrate ($/kg)	0.2[c]
Electron Acceptor Air/O_2/H_2O_2 ($/Kg)	2.77[d]/1.74[d]/4.0[b]

a. Personal Communication with Dr. Mark Goltz (7 August 1997)
b. Hopkins letter to Edwards AFB Project Manager (6 August 1996)
c. McCarty *et al.*, 1997
d. Based on Ohio distributor cost

Running the program for various "typical" scenarios showed that oxygen gas is most often the best (cheapest) source of dissolved oxygen, with the number of wells usually ranging between 2 and 8. Air is rarely selected as the oxygen source since it supplies such low concentrations of electron acceptor. Hydrogen peroxide, due to its cost, is normally only selected when the effluent concentration is specified at a very low level so that high "single-pass" efficiencies are required.

The methodology presented in this program is very simplified and based on many assumptions. However, the program may be used as a technology screening tool, as well as a method for qualitative study. Once the screening program indicates a site may be amenable to treatment using *in situ* aerobic cometabolic bioremediation, a more detailed design analysis can be conducted. For details on program use, see Mandalas (1997).

4.5.2 System Design

The program discussed above is for a simplified case and is not intended to provide an optimal design. If one wishes to find an optimal solution then a different algorithm must be followed. Figure 4.7 is a flow diagram showing how the model can be used in an optimization algorithm to design a treatment system.

The first step in any modeling effort is to collect data. This model requires that hydrogeological data such as horizontal hydraulic conductivity (K_h), regional gradient (i), and aquifer thickness (B) be known. This model also requires a limited knowledge of the contaminant and microbiological parameters. Through laboratory experiments and literature review, parameters such as the yield coefficient (Y), the contaminant degradation coefficient (K'), the stoichiometric coefficient (F), and the organism decay rate (b) can be found (Jenal-Wanner and McCarty, 1997).

Once the initial data have been collected, reasonable values for engineering parameters (decision variables) can be selected and the variables which depend on these parameters can be calculated. These calculated variables can then be used to determine whether the current design meets the design constraints. If the constraints are violated then new engineering parameters must be selected and the process must run through again. The parameters should continue to be changed until a parameter set is selected which meets the design constraints. Once a parameter set which meets the constraints is found this represents a solution to the problem. However, to determine the optimum solution we must have some way to compare solutions. To do this we record the total cost of the selected solution. This allows several solutions to be compared to determine which one meets the objective of having the lowest cost. Once the solutions are compared based on cost then the locally optimal solution can be selected. To try and find the globally optimal solution the process can be rerun with new starting values (Gorelick, 1983). If the same solution as before is selected then there is a good chance that the solution is globally optimal. If the same solution is not selected then the new solution can be compared to the previous one to determine which one has the lowest cost. In this manner, the model can be used to select a viable and cost-effective solution.

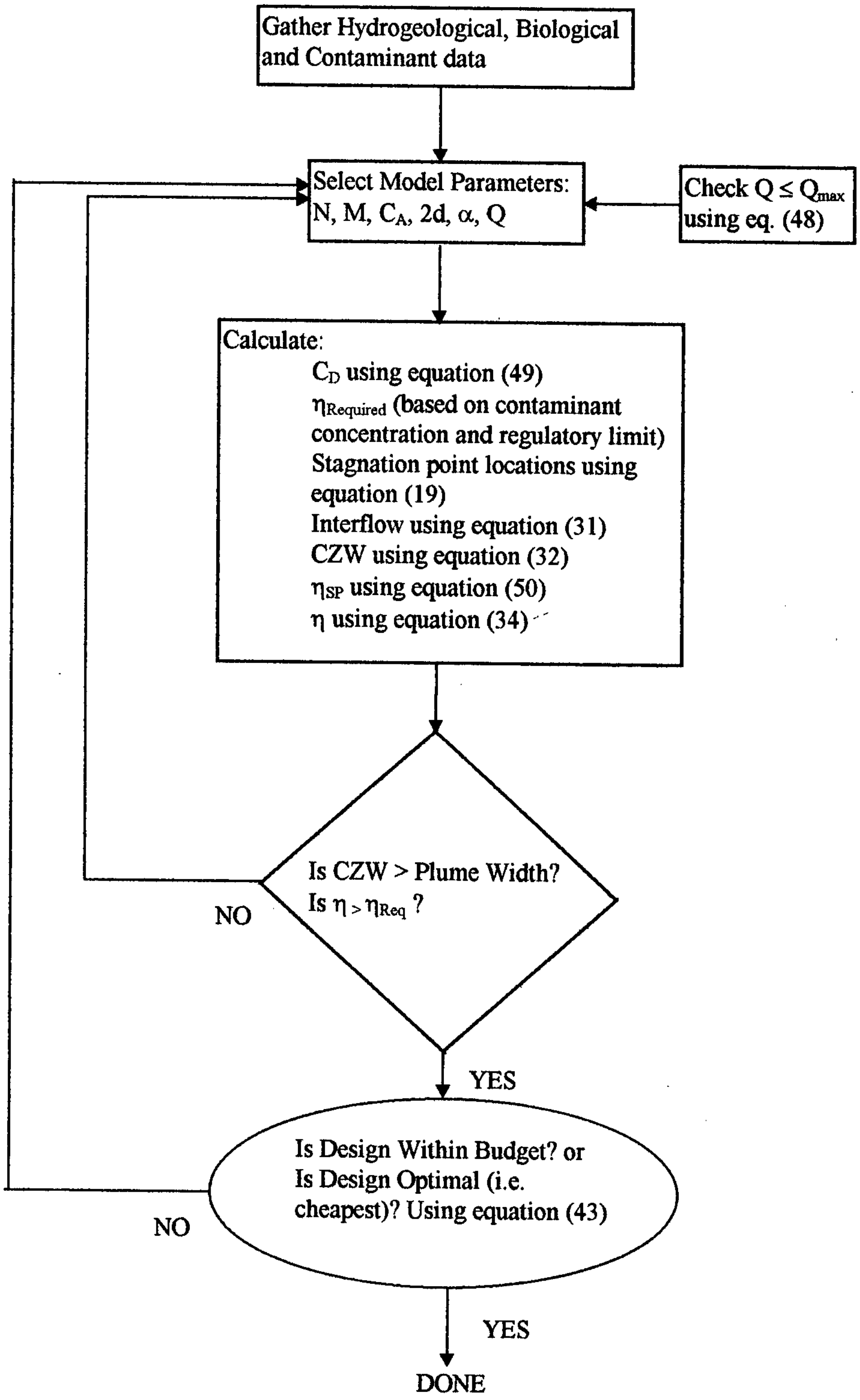


Figure 4.7 Flow diagram for system design

4.6 CONCLUSIONS

This chapter has used the thesis model to aid in implementing *in situ* aerobic cometabolic bioremediation in the field. It should be stressed, however, that many assumptions are built into the model presented here and therefore, it should not be used as the sole design tool. However, the model is an effective screening tool and a starting point for more detailed analysis.

5.0 CONCLUSIONS

5.1 SUMMARY

In this thesis a screening model which can be used to determine the efficacy of *in situ* aerobic cometabolic bioremediation under varying site conditions was developed. The model combines a simplified equation which describes cometabolic degradation of a contaminant with a novel analytical solution describing interflow in a system of injection/extraction wells in a regional flow field The model has been tested against field data obtained from the full-scale demonstration of *in situ* aerobic cometabolic bioremediation at Edwards AFB. Parameters from Edwards AFB were also used in conjunction with a three-dimensional numerical model to investigate the effects on treatment efficiency of hydraulic conductivity anisotropy. A sensitivity analysis of various engineering parameters, i.e. treatment well flow rate, distance between treatment wells, number of wells, number of well rows, angle of regional flow, primary substrate and electron acceptor concentration, has demonstrated their effect on the overall treatment system performance. A computer program was developed in conjunction with the model to help a technology user determine how the technology may best be applied to remediate groundwater contaminated with chlorinated aliphatic hydrocarbons.

5.2 CONCLUSIONS

- **Treatment system design using the dual-screen well is feasible in a single aquifer with typical hydraulic conductivity anisotropy.** The dual-screen treatment well used during the Edwards demonstration to remediate two contaminated aquifers eliminates the need to pump water to the surface for primary substrate and electron acceptor amendment. This reduces risk to workers, decreases the pumping costs and eliminates the need to obtain permits to reinject the treated water. This modeling study found that this same well design could be used to remediate sites with a single aquifer, if that aquifer had typical values of hydraulic conductivity anisotropy (i.e. vertical hydraulic conductivity less than 20% horizontal hydraulic conductivity).

- **Non-adjacent interflow can occur when multiple well pair (N > 2) treatment systems are designed.** At high treatment well flow rates (compared to regional flow), short distances between treatment wells, and N greater than two, interflow between non-adjacent wells may occur. This interflow, which occurs between two wells separated by at least one well pair, renders the inner well pairs ineffective at capturing up gradient flow since streamlines cannot cross each other. However, these inner wells increase the total interflow and therefore the overall treatment efficiency of the system.

- **Additional wells placed outside of an existing well pair will increase the interflow between the inner well pair.** As the distance between wells is increased the total interflow between wells decreases. In a multiple (N>2) well system, the non-adjacent interflow first becomes zero as distance between wells increases. This is followed by the interflow between the most external well pairs becoming zero. As distance between wells continues to increase, the interflows continue to go to zero for well pairs closer and closer to the center of the treatment system. The final well pair to reach an interflow of zero is the central well pair. This suggests, as found in the previous conclusion, that the addition of external wells increases the interflow between the central well pair.

- **Multiple well rows increase the overall treatment efficiency more than adding the same number of wells to a single well row.** Adding wells to an existing well row increases the total interflow and thus, the overall treatment efficiency. However, adding the same number of wells as a second well row placed down gradient of the existing well row causes a greater increase in the overall treatment efficiency. This analysis suggests that desired increases in overall treatment efficiency should be accomplished by adding wells as extra rows placed in series with existing well rows.

- **Molecular oxygen is usually the electron acceptor of choice when designing a treatment system using toluene as the primary substrate.** The screening program that was developed in conjunction with this thesis allowed for many different parameter combinations to be investigated. For the majority of these combinations, molecular oxygen was the selected electron acceptor. This is due to its relatively low cost and its ability to relatively efficiently introduce dissolved oxygen into the subsurface. Of the other oxygen sources available, air was rarely selected due to the relatively low concentration of dissolved oxygen it could introduce into the subsurface and hydrogen peroxide, due to its excessive cost, was selected only when high remediation efficiencies were required.

5.3 RECOMMENDATIONS

- **Compare the model with data from full-scale implementations of the technology.** As this technology is implemented more often as a full-scale remediation alternative, the model can be checked against these larger scale treatment systems to determine how well it agrees with the observed data.

- **Conduct an analysis with a 3-D model.** But for one analysis, all of the analyses conducted in this thesis were in two dimensions, as the model was motivated by the Edwards demonstration, for which a 2-D model was appropriate. In general, however, there is a need to be able to account for and model vertical flow. As shown by the 3-D modeling done in this thesis, the impact of vertical flow and short-circuiting in a single aquifer system is significant. Therefore, analysis of three-dimensional modeling studies will be required to extend the use of the technology to other sites.

- **Develop a solution which accounts for non-steady-state biodegradation.** Throughout this thesis, for simplicity, the assumption of steady-state biodegradation was made. However, to obtain a more accurate picture of treatment efficiency in the field, especially when primary substrate pulsing is used, a model which can account for transient conditions is required. Also, the model analyses in this work made many simplifying assumptions (no dispersion, equilibrium sorption, no competitive inhibition, etc.) some of which may be inappropriate. Further model/experimental analyses should be conducted to determine which processes are limiting and therefore, which require incorporation into the model.

- **Systematically select the engineered parameters using an optimization algorithm to obtain the most effective and cost-efficient design for technology implementation.** The screening software developed in conjunction with this thesis is a simplified routine that has utility in screening a site to approximate cost and performance of the technology under various site conditions. To actually design a treatment system, however, one will need to employ a formal optimization routine capable of varying all of the engineered parameters defined in this work, along with the well locations. This formal optimization will provide a methodology to design a treatment system which will prove both effective and cost efficient.

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The limitations of conventional groundwater remediation technologies have led to the development of innovative technologies which may achieve national hazardous waste site remediation goals. Before an innovative technology can be implemented in the field, remedial project managers, regulators and other stakeholders require adequate modeling tools to help assess the applicability of the technology at a particular site.

This modeling study investigates how an innovative technology, in situ cometabolic bioremediation, might be implemented to remediate a TCE-contaminated site, under different site conditions. A steady-state model is developed which couples an analytical expression to simulate the effect of flow between multiple pumping and injection wells, with an expression to calculate TCE removal as groundwater circulates through in situ bioreactors established around the injection wells. Varying site conditions and well configurations are investigated to determine their effect on the overall treatment efficiency of a system. A dual screen well design is found to be an effective method for contaminant capture and treatment given typical values of anisotropy. Investigation of a multiple row implementation concept proves it to be an effective configuration for site cleanup. The model is integrated into interactive software which serves as a technology screening tool.

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