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Comparison of analytical and numerical biodegradation models with application to aquifer remediation

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COMPARISON OF ANALYTICAL AND NUMERICAL BIODEGRADATION MODELS WITH APPLICATION TO AQUIFER REMEDIATION

by

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ABSTRACT

COMPARISON OF ANALYTICAL AND NUMERICAL BIODEGRADATION MODELS WITH APPLICATION TO AQUIFER REMEDIATION

SARAH E. ALDER-SCHALLER

Contaminant transport in ground water is predicted through the use of analytical and numerical models. The horizontal plane source analytical code (HPS) was compared to the USGS solute transport numerical code (MOC) for different problem configurations.

BIOPLUME II is a sophisticated numerical model which estimates aerobic biodegradation of benzene, toluene, and xylene in ground water. Predictions of biodegradation obtained using the BIOPLUME II model were matched with predictions from an analytical first order decay solution by varying the first order decay rate.

Numerical models are useful tools for evaluating different well patterns in the design of an aquifer remediation scheme. The effect of oxygen injection in aquifer remediation schemes was numerically simulated using BIOPLUME II. The effect of varying oxygen levels was evaluated for different well patterns and the results were used to simulate aquifer restoration at an aviation fuel spill site.
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But most of all, I would like to thank my husband, Ron Schaller, for his unwavering faith in me and belief in the impossible, now made reality with the completion of this manuscript.

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1.0 INTRODUCTION

Mathematical models are often used to determine the extent of ground water contamination from surface and subsurface waste sources. Models for predicting contaminant transport vary in complexity and solution procedure. Numerical or analytical solutions are employed, depending on the complexity of the problem.

Analytical procedures give exact solutions to the equations which describe the problem. Analytical solutions have the advantages that they contain no numerical error and require little computational time. However, the derivation of an analytical solution may require simplifying assumptions which preclude solving complex 'real world' problems. Thus, to perform a site investigation using an analytical model, one must determine the applicability of the model's simplifying assumptions to the waste site in question.

Numerical procedures, on the other hand, allow the solution of complex, heterogeneous systems without simplifying the problem. Numerical solutions are more difficult to code, require longer run times and/or greater computational power, and may contain numerical error. These models require the proper selection of numerical parameters to minimize computational effort and numerical error. Thus, a knowledge of the numerical procedures used in the model is requisite to the proper implementation of the code.

These distinctions are important because mathematical models are being implemented in the regulatory process for ground water contaminants, and the choice of solution procedures can have a significant effect on the prediction of the extent of contamination. For instance, the Environmental Protection Agency (EPA) is proposing to use their Composite Landfill Model (EPACML) (Woodward-Clyde consultants, 1988) to regulate land disposal of wastes. Some compounds such as benzene, toluene, and xylene (BTX) biodegrade
aerobically in the environment, and it has been shown that biodegradation is an important means of attenuating the contaminant plume. The EPACML model is a semi-analytical code which only allows for first order decay (FOD) as a means for simulating degradation. However, there are sophisticated numerical models which simulate the processes that govern the transport and biodegradation of these compounds with greater accuracy.

Despite their limitations, analytical codes are being used by researchers as well as regulators. Therefore, it is important to understand the way in which analytical and numerical models compare in their calculations of the transport and biodegradation of compounds in ground water. In this investigation, a comparison was made between an analytical model (HPS, Galya, 1988) and a numerical model (the USGS solute transport model (MOC), Konikow and Bredehoef, 1978) for ground water transport. This comparison determined how well HPS matched the MOC model results for different problem configurations.

BIOPLUME II (Rifai et al., 1987) is a sophisticated numerical model which estimates the biodegradation of BTX in ground water. An investigation was performed to match predictions of biodegradation obtained using BIOPLUME II with predictions from a FOD analytical solution. The total mass biodegraded in a BIOPLUME II numerical run was matched with an FOD analytical simulation by varying the value of the FOD coefficient. The FOD rates obtained can be used in analytical models to approximate biodegradation calculated by BIOPLUME II.

Much research has been done in the area of design of aquifer remediation schemes (Wilson, 1984, Javandel and Tsang, 1986, Satkin, 1987). This research, however, has considered only the hydraulic capability of the remediation designs and has not investigated the effect of biodegradation. In
In this research, BIOPLUME II was used to numerically simulate the removal of contaminants from a system where biodegradation is the only sink. Remediation-well configurations were taken from Satkin (1987), and evaluated for cases when oxygen is injected into the system. The results of this investigation will be useful in the design of bioremediation schemes.
2.0 PREVIOUS WORK

Ground water is one of the main sources of water for domestic, agricultural and industrial uses (Bedient and Huber, 1988). However, despite the importance of our ground water supply, many aquifers have become contaminated by organic compounds through accidental spills, improper disposal of wastes, and agricultural practices. Remediation of these contaminated aquifers can be attempted using a number of techniques which include: physical containment, withdrawal and treatment processes, and in situ treatment (Lee et al., 1988).

Physical containment processes separate contaminated soil and ground water from the surrounding environment. Techniques for isolating contamination include excavation and removal; and supplying barriers to ground water flow such as slurry walls, grout curtains or clay liners. Hydrodynamic control, which uses injection and production wells to create a ground water divide around a contaminated region, is also implemented as a containment measure. Finally, surface controls which divert uncontaminated water away from sites and minimize the amount of infiltration into the area also serve to isolate contaminants (Thomas et al., 1987).

Withdrawal and treatment processes use physical, chemical and biological processes to treat contaminated water and soil removed from an aquifer. The physical processes used can include activated carbon adsorption, density separation, filtration, incineration, and air stripping. Chemical processes such as neutralization, precipitation, oxidation-reduction, wet air oxidation, ozonation, addition of hydrogen peroxide, and coagulation can be used to treat contaminated water ( Ehrenfeld and Bass, 1984). However, chemical treatments may be ineffective in removing dissolved contaminants. Also, the use of
chemicals to treat heavily contaminated material can create a potentially hazardous sludge by-product. Therefore, chemical treatment is generally used in combination with other processes. Biological methods utilize conventional biological wastewater treatment processes such as activated sludge, lagoons, waste stabilization ponds, trickling filters, sequencing batch reactors etc., to treat contaminated water (Thomas, et al., 1987).

*In situ* treatment can be accomplished by using chemical agents to inactivate or immobilize contaminants or by stimulating subsurface microbial populations to enhance the biodegradation process. *In situ* treatment has the advantage that it can remediate contaminated materials in place, without transferring contaminants elsewhere in the environment. (Lee et al., 1988).

Petroleum-derived hydrocarbons are an important class of organic contaminants that are of concern for ground water. Some of the contaminants which are soluble in water, such as benzene, have been shown to be carcinogenic (Wilson and Ward, 1987). In an effort to try to deal with the problem of contaminated ground water, much research has been done in the area of aquifer remediation.

In a remediation effort, determining the extent of ground water contamination is a difficult problem. Initially, costly procedures, such as taking and analyzing core samples and installing monitoring wells, are often performed in an attempt to assess the location and level of contamination. Once the contaminant source and hydrogeology of the waste site are characterized, plume migration and remediation options are often analyzed using mathematical models.

The governing equations for ground water flow and contaminant transport are given in the literature (Bear, 1979; Freeze and Cherry, 1979; Bedient et al., 1985). These equations have been solved using both analytical and numerical
approaches. Analytical solutions to the advection dispersion equation for simplified boundary and initial conditions are available in the literature (Bear, 1979; Javandel et al., 1984). The most commonly used numerical solutions solve the transport equation in two dimensions. These numerical models are more flexible than their analytical counterparts because numerical solutions allow for complex geometries and combinations of recharge and production wells. (Bedient et al., 1985).

Analytical solutions to the advection dispersion equation require simplifying assumptions to the initial and boundary conditions which often preclude application to field sites. There are three numerical solution methods which are often used to solve the solute transport problem. These numerical techniques include finite difference approximations, finite element solutions, and the method of characteristics (MOC) combined with finite difference approximations.

Finite difference approximations are subject to numerical error which can invalidate the solution. Conversely, finite element solutions, in general, are subject to less numerical error than finite difference approximations. However, Huyakorn and Taylor (1977) have shown that for some systems where advection dominates the mass transport regime, large numerical dispersion may be produced by the standard Galerkin finite-element formulation.

The MOC solution procedure replaces the partial differential equation for advective dispersive transport with a set of ordinary differential equations. The ordinary differential equations are then approximated by finite differences (Wang and Anderson, 1982). The idea behind the MOC method is to decouple the advective and dispersive parts of the advection dispersion equation and solve these parts successively. There are two different ways of handling the dispersion term in the solute transport equation; one is the particles in cells method (PIC), and the other is the discrete parcel random walk method (DPRW)
(de Marsily, 1986).

In the PIC method, the governing equation for ground water flow is solved first, and the velocity in each grid cell is determined. Then, at each source location in the model, a large number of particles is introduced. Adveotive solute transport is represented by tracking the coordinates of these particles as they are moved by the ground water flow. Particles in the PIC method represent solute concentration. After the particles have been moved by the advective velocity, a new concentration for each grid cell is calculated by averaging the concentrations of all the particles in the cell. The dispersive part of the solute transport equation is solved using the concentrations calculated for each grid cell. The new concentration of each particle is the sum of its concentration at the end of the advective step plus the change in concentration calculated in the dispersive step (de Marsily, 1986).

In the DPRW method, each particle represents a solute mass. Concentrations for each grid cell are obtained by dividing the total mass in the cell by the volume of water in the cell. The dispersive part of the solute transport equation is represented by giving each particle an additional random displacement at the end of each advective step. This random displacement represents Brownian motion, responsible for molecular diffusion (de Marsily, 1986).

Khaleel and Reddell 1987, used the MOC solution to analyze four convective dispersive problems. The problems which were analyzed included longitudinal dispersion in one-dimensional flow, longitudinal dispersion in two-dimensional flow, longitudinal and lateral dispersion in one-dimensional flow, and longitudinal and lateral dispersion in two-dimensional flow. The numerical solutions were compared with available analytical solutions, and shown to be in excellent agreement.
One of the most widely used two-dimensional ground water transport models is the USGS method of characteristics (MOC) code (Konikow and Bredehoeft, 1978). Freeberg et al. (1987) used the MOC code to model trichloroethylene (TCE) contamination and recovery in a shallow sandy aquifer. In this effort, leakage of TCE from an underground storage tank was modeled using an injection well source definition. Although the actual rate of release of contaminants into the aquifer was unknown, the predicted values of TCE in the simulated plume matched observed concentrations reasonably well. A contaminant recovery effort consisting of a four-well withdrawal system was also modeled, in which model predictions of hydraulic head in the aquifer and TCE concentrations matched data at two points in time.

Satkin (1987) used the USGS MOC code to evaluate different well patterns for aquifer restoration under variable hydrogeologic conditions. He studied seven different well patterns to determine which was the most efficient for contaminant reduction. Among the well patterns investigated, was the double cell configuration (see Figure 7.1). The double cell well containment system was presented by Wilson, 1984. This well pattern utilizes four wells along a line bisecting the plume, with the two upgradient wells injecting, and the two downgradient wells pumping. This well configuration hydraulically isolates the plume while simultaneously withdrawing water for treatment. The inner cell, (inner injection/production pair), captures the plume and sets up a hydraulic gradient which is higher than the background, facilitating contaminant removal. The outer cell circulates a larger volume of water than the inner cell, and sets up a steep hydraulic gradient through the plume, further isolating the contaminant.

In Satkin's investigation, eight hydrogeologic conditions were modeled using various combinations of drawdown, hydraulic gradient, and dispersivity. The remediation schemes were evaluated on the basis of clean-up time,
volume of water circulated, and volume of water requiring treatment. The best
well pattern for ground water remediation was found to be a site-specific
parameter. Also, the rate of clean up of the aquifer was found to be controlled
by the well locations, pumping rates, transmissivity, dispersivity, and hydraulic
gradient.

One of the most commonly used remediation techniques involves the use
of recovery well systems. However, much of the recent research has been
directed toward understanding microbial processes and their affect in
attenuating ground water contamination. Research has indicated that microbes
in the subsurface are metabolically active (Lee et al., 1988). Biodegradation in
the subsurface environment seems to be limited by an essential nutrient such
as nitrogen or phosphorus. The lack of an electron acceptor, such as oxygen,
may also limit biodegradation. The addition of the missing nutrient(s) and
electron acceptor can stimulate the microbial populations and increase the
biodegradation potential of the aquifer. Where possible, the use of \textit{in situ}
biodegradation processes has the advantage of reducing or eliminating
contamination without transferring contaminants to another phase in the

Raymond et al. were the first to demonstrate the applicability of
degradation to the restoration of gasoline-contaminated ground water (Lee and
Ward, 1985 a). Raymond (1974) has patented a process that biologically
removes hydrocarbons from contaminated ground water by stimulating existing
microbial populations with nutrients and oxygen. Raymond (1975) applied the
process to the site of a pipeline leak Ambler Pennsylvania.

Flatham and Caplan (1985) present two case histories which demonstrate
the use of biological techniques in remediation of areas contaminated by
organic compounds. In the first case history, phenolic compounds in the soil at
a hazardous waste site were destroyed through in situ biodegradation. Physical measures were employed to prevent further migration of the contaminants and 1700 cubic yards of contaminated soil were seeded with bacterial strains, and treated with nutrients. In the second case history, biological techniques were used to successfully remediate ground water contaminated by ethylene glycol. An injection/recovery system was used to maintain an environment favorable to biodegradation while, at the same time, flushing the ethylene glycol from the system. The average concentration of ethylene glycol was reduced by more than 85 and 92 percent respectively, at two downgradient recovery wells.

Barker et al. (1987) examined the migration of contaminants in a unconfined sandy aquifer, after the introduction water containing BTX. The BTX in the system experienced sorptive retardation, and migrated slightly slower than the ground water. Within 434 days of injection, all the BTX mass was lost due to biodegradation. The BTX biodegradation was controlled by the amount of dissolved oxygen available in the system, with BTX levels persisting in layers low in dissolved oxygen. The decrease in mass loss rates with time was attributed to small masses of BTX remaining in anoxic layers.

A natural gradient field experiment was performed at Canada Forces Base Borden to evaluate the injection of nitrates as a means of remediating gasoline contaminated ground water (Berry-Spark and Barker, 1987). In the investigation, two gasoline plumes were injected into the unconfined sand aquifer. Upgradient of one plume, ground water spiked with nitrate was then injected into the aquifer. The second plume acted as a control. Comparison of the contaminant masses remaining in plumes showed a small but significant difference in the mass removal rates; nitrate addition apparently accelerated the bioremediation process.
Major et al. (1988) investigated the biodegradation of BTX in anaerobic batch microcosms containing aquifer material. The laboratory results showed that microorganisms can degrade BTX under denitrifying and aerobic conditions. The researchers concluded that addition of nitrate to ground water contaminated by gasoline could serve as an addition to current bioremediation techniques. Because nitrate has a higher solubility in water than oxygen, the addition of nitrate may prove to be more economical and effective than the injection of oxygen.

Field and laboratory studies at an abandoned wood-creosoting site, showed evidence of biodegradation of the polynuclear aromatics in the contaminant plume (Borden et al., 1984). Borden and Bedient (1986) developed equations describing the growth, decay and transport of microorganisms, as well as the transport and depletion of oxygen and hydrocarbons. In a companion paper (Borden and Bedient, 1986) this model was applied to an abandoned creosoting site where oxygen limited biodegradation was known to occur. Two-dimensional horizontal simulations were performed using a modified USGS MOC code.

Rifai and Bedient (1987) adapted Borden's equations to the USGS MOC code. The model developed, BIOPLUME II (Rifai et al., 1987), generates two sets of independent tracer particles for tracking the change in oxygen and hydrocarbon concentrations. At each time step the solute transport equation is solved twice, once for oxygen and once for the contaminant. An instantaneous reaction between the two plumes is simulated using the principle of superposition and a ratio of three parts oxygen to one part hydrocarbon is assumed.

Rifai et al. (1988) applied the model to the site of an aviation fuel spill in Traverse City Michigan where biodegradation is known to occur. The model
was calibrated to field data collected from the site before an interception pumping system was installed. Field conditions at the site were then simulated for a two year period after the pumping system was in operation. Concentrations predicted by the model matched the observed concentrations reasonably well. Also, the loss mass calculated by the model showed a reasonable match to the losses observed in the field.

Chiang et al., (1989) investigated the aerobic biodegradation of benzene, toluene, and xylene in a sandy aquifer and calculated a natural attenuation rate for the site. They investigated biodegradation at the site using two models: the method of characteristics model with a first order decay term, and the BIOPLUME II model. Using the MOC model and varying the leakage/spill rates between two sources at their site, and the dispersivities in the aquifer, a good correlation between observed and predicted values of benzene was obtained. Because of this correlation, it was felt that the estimated natural aerobic biodegradation rate may be the typical average rate to be expected in situ at the site. The results from the BIOPLUME II simulation showed a good correlation for the BTX plume. However, the simulated and measured concentrations for dissolved oxygen did not agree. It was felt that this dissimilarity may be due to a number of factors such as difficulties in quantifying the dissolved oxygen influx rate from the source and the reaeration rate from the unsaturated zone, and the possibility that due to growth of soil bacteria on the hydrocarbon substrate, the mass ratio for dissolved oxygen versus BTX may be less than is assumed in BIOPLUME II.

Through ongoing research, biodegradation has been shown to be an important means of attenuating ground water contamination. However, not all researchers use complicated numerical codes, like the ones previously discussed, to estimate the extent of ground water contamination and possible
remedial actions. Numerical solutions may introduce error into the solution. El-Kadi (1988) examined the accuracy the the USGS MOC code in situations which commonly exist in remedial actions using recovery wells. His investigation looked at situations dominated by radially convergent and divergent flow around wells. For the well configurations studied, El-Kadi found that inaccuracies occurred especially for the case of the recharge/recovery doublet, for long simulation times. He found that these inaccuracies, in part, were due to the arrival of contamination at sink nodes. It was concluded that care was needed in the application of the USGS code to simulations where production or injection wells are close together.

Other models are available for simulating contaminant transport and bioremediation. Srinivasan and Mercer (1988) present a one-dimensional finite-difference model for the simulation of biodegradation and sorption in saturated porous media. This model allows for advective and dispersive transport of a substrate and oxygen; aerobic biodegradation; first-order degradation for both substances; sorption using linear, Freundlich, or Langmuir equilibrium isotherms for either substance; and Dirichlet, Neumann, or Cauchy boundary conditions which are constant in time or include first-order degradation. The problem is solved using a Newton-Raphson iterative procedure. This code has several limiting assumption; these include one-dimension transport, a uniform flow field, and uniform material properties of both substances throughout the medium.

Analytical models are also available for ground water modelling. Galya (1987) presents a horizontal plane source model (HPS) for ground water transport. This model simulates three-dimensional contaminant transport from a horizontal plane source through the use of Green's functions. This model can simulate retardation, decay (as a first order process), and varying source
emission rates. The HPS model can be used to simulate contaminant transport from landfills, waste lagoons, and land treatment facilities.

Mathematical models are used in regulatory programs governing ground water contamination, and the assumptions inherent in these models sometimes must be adapted to simulate real world conditions. The Environmental Protection Agency (EPA) is proposing to use a Composite Landfill Model (EPACML) (Woodward Clyde consultants, 1988) to regulate land disposal of wastes. This Composite Landfill model simulates transport of contaminants in the unsaturated and saturated zones. The EPACML model simulates transport in the unsaturated zone with a numerical module. Output from the unsaturated zone module is expressed as a contaminant flux (mass/source area/time). This flux is used as input into the saturated zone module. Transport in the saturated zone is modeled with a semi-analytical procedure which accounts for advection, dilution, dispersion, adsorption, and first order decay.

A review of EPACML (Bedient et. al, 1988) has shown that aerobic biodegradation, as represented in the model, is an important means of attenuating plumes containing organic constituents. Although there are sophisticated numerical models which simulate the transport and biodegradation processes in the saturated zone, EPACML is limited to a first order decay (FOD) model as a means of approximating degradation. While FOD rates for some organic compounds can be found in the literature (Swindoll et al, 1987; Ghiorse and Wilson, 1988) these rates do not take into account the oxygen limited nature of the biodegradation of these compounds.

It can be seen that the issue of ground water contamination is of concern to researchers. Ground water solute transport is modeled using analytical and numerical models which help to define the extent of ground water contamination and possible remediation schemes. Biodegradation has been
found to be an important means of attenuating ground water contaminant plumes and researchers are now trying to find ways to quantify this process. Among the possibilities are sophisticated numerical models such as BIOPLUME II which simulates instantaneous reaction and superposition of contaminant and oxygen plumes in the aquifer. Also available as a means of simulating biodegradation is the use of first order decay to estimate the attenuation process. Trying to quantify biodegradation as first order decay may be important because a semi-analytical model may be implemented into the regulatory process.
3.0 OBJECTIVES

The objectives of this research were threefold. First, a numerical solution procedure for determining contaminant transport was compared to an analytical solution procedure, using two computer models. The HPS analytical model was compared to the USGS solute transport numerical code. The comparison determined how well HPS results match the MOC model results for different problem configurations. Three source definitions of varying sizes were used in the matching procedure, and a comparison using first order decay was also performed.

This comparison was performed because analytical codes are being used by investigators and regulators in the area of ground water contamination. Analytical codes, however, require many simplifying assumptions such as homogeneity in the aquifer. Numerical codes, on the other hand, allow the solution of more complex problem configurations. Because analytical codes are being used, a knowledge of the way analytical and numerical solutions compare is of importance. The results of this research will be useful to researchers trying to model the extent of ground water contamination.

The second objective of this research was to match BIOPLUME II predictions of biodegradation with predictions from a FOD analytical solution. Estimates of aerobic biodegradation of BTX obtained using BIOPLUME II were matched with estimates from a first order decay model. The FOD model used in this investigation was simply a version of BIOPLUME II in which no oxygen is input into the model. In this form, BIOPLUME II basically reduces to the USGS two dimensional model (MOC), and simulates biodegradation as a first order decay process. A match between the BIOPLUME II and MOC FOD plumes would require that the same amount of mass be degraded by both models. Matching
the total mass degraded was accomplished by varying the FOD coefficient. An attempt to match overall plume configuration (size, shape and contaminant concentrations) was also made. This research will be useful to investigators using an analytical code who wish to know how well they can match biodegradation results obtained using the numerical procedure in BIOPLUME II.

The third objective in this research was to numerically simulate the removal of a contaminant plume using different well configurations, for the case when biodegradation of the contaminant is occurring. In this investigation, BIOPLUME II was used to simulate contaminant transport and removal in the system. The aquifer and well configurations were taken from Satkin, 1987. This investigation expanded upon Satkin's work and showed, for the cases he studied, the effect that biodegradation and oxygen injection have on ground water remediation. The effect of varying levels of oxygen on aquifer remediation for the various well configurations were examined and the results were applied to a field site in Traverse City Michigan site, in an attempt to remediate the TCM contaminant plume.
4.0 MODEL DESCRIPTIONS

4.1 Horizontal Plane Source Model

HPS (Galya, 1987) is a three dimensional horizontal plane source model which simulates contaminant transport in a homogeneous ground water aquifer. This analytical model solves the advection dispersion equation in three dimensions using Green's functions. The governing equation describes transport as unidirectional advection (x direction) and three dimensional dispersion, and allows for retardation and first order decay of the contaminants. For a horizontal plane source, the Green's function solutions are formulated as equivalent line sources in the horizontal plane and a point source in the z direction. For a plane source, the x and y direction Green's functions are found by spatially integrating the point source solution. In the z direction, the Green's function for the conditions specified is obtained through the addition of an infinite number of image sources. The governing equation, boundary conditions, and solution presented by Galya are given below.

Governing equation:

$$\frac{\partial C}{\partial t} + \frac{u \partial C}{\partial x} = \frac{D_x \partial^2 C}{\partial x^2} + \frac{D_y \partial^2 C}{\partial y^2} + \frac{D_z \partial^2 C}{\partial z^2} - \lambda C + \frac{M_S}{\theta} \quad (4-1)$$

C = concentration of contaminant
u = pore velocity in x direction (= Darcy velocity/θ)
t = time
Dx = dispersion coefficient in x direction
Dy = dispersion coefficient in y direction
Dz = dispersion coefficient in z direction
λ = decay or degradation coefficient
R = retardation factor
kd = distribution coefficient
θ = porosity
MS = mass flux of contaminant source
Initial Condition:

\[ C = 0 \quad t = 0 \quad (4-2) \]

Boundary conditions:

\[ C = 0 \quad y = \pm \infty \quad (4-3) \]

\[ D_z \frac{\partial C}{\partial z} = 0 \quad z = 0 \quad (4-4) \]

\[ D_z \frac{\partial C}{\partial z} = 0 \quad z = H \quad (4-5) \]

\[ C = 0 \quad z = \infty \quad (4-6) \]

Galya developed the three-dimensional analytical solution using Green's functions. The source has a length L in the x direction, width B in the y direction, and an input source mass rate of \( M_S \). Green's functions have been used for the solution of the advection dispersion equation previously, including applications to heat flow (Carslaw and Jaeger, 1959) and ground water contaminant transport (Codell and Schreiber, 1977). Carslaw and Jaeger state that the solutions of a multidimensional partial differential equation can be obtained by multiplying the solutions for each of the dimensions. The solution presented by Galya is given below.

Solution:

\[ C = \frac{1}{\theta R} X_0(x,t) \quad Y_0(y,t) \quad Z_0(z,t) \quad T(t) \quad (4-7) \]

where

\[ T = \quad \text{degradation function due to degradation or decay of contaminants (includes the effects of biodegradation hydrolysis, chemical reaction, etc)} \]
\[ \exp(-\lambda t) \text{ for first-order degradation} \]

\( X_0, Y_0, Z_0 \) Green's functions for transport in \( x, y, \) and \( z \) directions respectively.

\[
X_0 = \frac{1}{2L} \left( \text{erf} \left( \frac{L}{2} + x - x_s - \frac{ut}{R} \right) \frac{1}{\sqrt{4D_xt/R}} + \text{erf} \left( \frac{L}{2} - x + x_s - \frac{ut}{R} \right) \frac{1}{\sqrt{4D_xt/R}} \right) \tag{4-8}
\]

\[
Y_0 = \frac{1}{2B} \left( \text{erf} \left( \frac{B}{2} + y - y_s - \frac{ut}{R} \right) \frac{1}{\sqrt{4D_yt/R}} + \text{erf} \left( \frac{B}{2} - y + y_s - \frac{ut}{R} \right) \frac{1}{\sqrt{4D_yt/R}} \right) \tag{4-9}
\]

\[
Z_0 = \frac{1}{H} \left( 1 + 2 \sum_{n=1}^{\infty} \exp \left( -\frac{n^2 \pi^2 D_z t}{H^2 R} \right) \cos(n\pi z/H) \cos(npz_s/H) \right) \tag{4-10}
\]

where \( x, y, \) and \( z \) = distance in \( x, y, \) and \( z \) directions, respectively, to calculation point.

Equations (4-8) - (4-10) are substituted into equation (4-7). Applying a convolution integral with respect to time gives the concentration due to a continuous or transient source with a rate \( M_s(t) \) as given below:

\[
C(x,y,z,t) = \frac{1}{\theta R} \int_0^t \left( M_s(\tau) \ X_0(x,t-\tau) \ Y_0(y,t-\tau) \ Z_0(z,t-\tau) \ T(t-\tau) d\tau \right) \tag{4-11}
\]

Where \( M_s(t) \) = mass release rate at time \( t; \) and \( t \) = time variable for integration.

Equation (4-11) is applied to predict concentrations due to time dependent source terms.
The HPS code was developed by Galya for the American Petroleum Institute to supplement regulatory tools currently being proposed by the EPA. The HPS model simulates contaminant transport from horizontal plane sources such as landfills or land treatment facilities. In this model, the source term covers the entire contaminant area and may be a more appropriate definition for this type of waste facility than a point source. Also, this semi-analytical model can simulate biodegradation of contaminants as a first order decay process, thereby allowing attenuation of the contaminant plume.

4.2 USGS Solute Transport Code (MOC)

The USGS method of characteristics code is a widely used solute transport model, which can simulate steady-state or transient flow in one and two dimensions. The model allows for a heterogeneous and/or anisotropic aquifer, and assumes that the solute is nonreactive. A finite difference approximation to the ground water flow equation is made and then solved using an iterative alternating direction implicit (ADI) solution procedure. The solute transport equation is solved using the method of characteristics. (Bedient et al., 1985).

The USGS MOC code uses particle-tracking to simulate convective transport, and solves the finite-difference equations which describe the effects of hydrodynamic dispersion, fluid sources and sinks, and divergence of velocity using a two-step explicit procedure. The USGS model is able to simulate production and injection wells operating over different pumping periods, streams and ponds (as constant head boundaries or regions), regions of diffuse recharge or discharge, and observation wells. The model output includes head distribution and draw down maps, x and y direction velocity distributions, concentration values at each grid location, and the chemical mass balance.
4.3 BIOPLUME II

BIOPLUME II is a numerical model which is based on the USGS two dimensional transport model. BIOPLUME II is a dual particle mover model which solves the solute transport equation twice: once for the contaminant and once for oxygen. This model assumes an instantaneous reaction between the contaminant and oxygen, in which three units of oxygen are required to completely biodegrade one unit of contaminant. The 3:1 oxygen contaminant ratio is the stoichiometric average for BTX and can be changed in the model if a different ratio is needed. The principle of superposition is used to combine the oxygen and contaminant plumes at every particle move. The degradation equations used in this model are of the form:

\[ \frac{\partial (Hb)}{\partial t} = \frac{1}{R_h} \left( \frac{\partial}{\partial x_i} \left( bD_{ij} \frac{\partial H}{\partial x_j} \right) - \frac{\partial}{\partial x_i} \left( bHV_i \right) \right) - \frac{H'W}{n} \]  \hspace{1cm} (4-12)

\[ \frac{\partial (Ob)}{\partial t} = \left( \frac{\partial}{\partial x_i} \left( bD_{ij} \frac{\partial O}{\partial x_j} \right) - \frac{\partial}{\partial x_i} \left( bOV_i \right) \right) - \frac{O'W}{n} \]  \hspace{1cm} (4-13)

where \( H \) and \( O \) = concentration of contaminant and oxygen respectively, \( H' \) and \( O' \) = concentration of hydrocarbon and oxygen in a source or sink fluid, \( n \) = effective porosity, \( b \) = saturated thickness, \( t \) = time, \( x_i \) and \( x_j \) = cartesian coordinates, \( W \) = volume flux per unit area, \( V_i \) = seepage velocity in the direction of \( x_i \), \( R_h \) = retardation factor for contaminant, and \( D_{ij} \) = coefficient of hydrodynamic dispersion.
The two plumes are combined using the principle of superposition to simulate the instantaneous reaction between oxygen and the contaminants. This approximation can be written as:

\[ H(t+1) = H(t) - \frac{O(t)}{F} ; O(t+1) = 0 \]
where \( H(t) > \frac{O(t)}{F} \) \hspace{1cm} (4-14)

\[ O(t+1) = O(t) - H(t) \cdot F ; H(t+1) = 0 \]
where \( O(t) > H(t) \cdot F \) \hspace{1cm} (4-15)

where \( H(t) \), \( H(t+1) \), \( O(t) \) and \( O(t+1) \) are the concentrations of contaminant and oxygen at time \( t \) and \( t+1 \), respectively.

4.4 First Order Decay Model

In a model which simulates biodegradation as a FOD process, degradation is approximated using an equation of the form:

\[ \frac{dC}{dt} = -k_1 C \]

\hspace{1cm} (4-16)

\[ C = C_0 e^{-k_1 t} \]

\hspace{1cm} (4-17)

Where \( k_1 \) is the FOD coefficient (day\(^{-1}\)).

Simulation of biodegradation using a first order decay model was performed with a modified BIOPLUME II run. In this instance, aerobic biodegradation was prevented from occurring by removing oxygen from the system. This procedure essentially reduces BIOPLUME II to the USGS MOC code upon which it is
based. An FOD coefficient was then added to the input data set to calculate first order decay.
5.0 NUMERICAL VS ANALYTICAL METHODS FOR CONTAMINANT TRANSPORT

In this investigation, a comparison was made between analytical and numerical solution procedures. The HPS analytical model (see Section 4.1) was compared to the USGS solute transport numerical code. The comparison determined how well HPS matched the MOC model results for different problem configurations. Three source definitions of varying sizes were used in the matching procedure, and a comparison using first order decay was performed.

5.1 Model Set-up

In order to compare the HPS model with the MOC model, a base run problem definition was created. Figure 5.1 shows the 15 x 25 cell grid system which was used for the MOC simulations. The hydraulic gradient used was 0.004 ft/ft, and the contaminant source was modeled as a recharge cell, with a recharge rate of 8 x 10^-8 feet per second. This recharge rate is equivalent to a point source injection rate (i.e., an injection source cell) of 0.002 cubic feet per second spread over the entire area of the source cell. The assumed contaminant concentration was 100 mg/l, and the background oxygen was set as 8 mg/l. Table 5.1 gives the aquifer parameters for the base run. All runs were done assuming steady state hydraulic conditions, and all output was analyzed after three years of simulation time.

The same parameters were input into the HPS model, except that all units were converted to the metric scale. Also, an allowance was made for the fact that HPS is a three dimensional solute transport model, whereas MOC is a two dimensional model. The MOC model assumes that output concentrations are an average of the concentrations generated at the surface and the bottom of the aquifer. Therefore, all concentrations from the HPS model were calculated as
FIGURE 5.1
Model Grid

Scale: 1" = 100'

LEGEND
- Constant Head Cells
- Injection Wall
<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Transmissivity (ft$^2$/s)</td>
<td>$3.28 \times 10^{-3}$</td>
</tr>
<tr>
<td>Thickness (ft)</td>
<td>10</td>
</tr>
<tr>
<td>Dispersivity (ft)</td>
<td></td>
</tr>
<tr>
<td>• Longitudinal</td>
<td>10</td>
</tr>
<tr>
<td>• Dt/DI</td>
<td>0.30</td>
</tr>
<tr>
<td>Porosity</td>
<td>0.30</td>
</tr>
<tr>
<td>Storativity (steady state conditions)</td>
<td>0.0</td>
</tr>
</tbody>
</table>
an average of the output concentrations at the top (depth = 0 m) and the bottom (depth = 3 m) of the aquifer.

5.2 Evaluation of Numerical Problems Near the Source

The first comparison between the numerical and analytical models was performed for the base run problem configuration. Figure 5.2 shows plots of concentration down the plume centerline for both the HPS and MOC runs. These plots show that the results from the two models match well. Figure 5.2 also shows an interesting anomaly in the results from both the HPS and MOC models. In both model simulations, the contaminant concentration 50 feet down gradient from the source is higher than the concentration at the source itself. Since this theoretically should not occur, it was suspected that there was some problem with the way the codes were handling the concentration calculations near the source. Because the MOC curve was not smooth, it was thought that there might be a numerical problem for the configuration being examined.

Table 5.2 shows the series of runs used to examine the anomaly in the concentration results from the MOC code. In this examination, a series of parameters were varied to determine which variables have an effect on the anomaly. The parameters varied in this investigation were: source definition, cell distance (celdis is a numerical parameter which specifies the maximum cell distance a particle can displace itself per particle move), and hydraulic conductivity.

MOC model runs were performed with the source defined as a recharge area and as an injection well. The contaminant loading for both source configurations was the same. Figures 5.3 and 5.4 show that for each source definition there is an increase in contaminant concentration down gradient of
Figure 5.2  MOC1 vs HPS1
Base run configuration

Concentration (mg/l)

MOC1
HPS1

XDEL (ft)
<table>
<thead>
<tr>
<th>RUN #</th>
<th>CELDIS</th>
<th>SOURCE DEF</th>
<th>HYDR COND. (cm/s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>.25</td>
<td>Recharge cell</td>
<td>$10^{-2}$</td>
</tr>
<tr>
<td>2</td>
<td>.50</td>
<td>Recharge cell</td>
<td>$10^{-2}$</td>
</tr>
<tr>
<td>3</td>
<td>.25</td>
<td>Injection well</td>
<td>$10^{-2}$</td>
</tr>
<tr>
<td>4</td>
<td>.50</td>
<td>Injection well</td>
<td>$10^{-2}$</td>
</tr>
<tr>
<td>5</td>
<td>.25</td>
<td>Recharge cell</td>
<td>$10^{-3}$</td>
</tr>
<tr>
<td>6</td>
<td>.25</td>
<td>Recharge cell</td>
<td>$2 \times 10^{-3}$</td>
</tr>
<tr>
<td>7</td>
<td>.25</td>
<td>Recharge cell</td>
<td>$5 \times 10^{-3}$</td>
</tr>
<tr>
<td>8</td>
<td>.25</td>
<td>Recharge cell</td>
<td>$7.5 \times 10^{-3}$</td>
</tr>
</tbody>
</table>
Figure 5.3  Concentration down plume centerline: MOC recharge source - Infil rate = 8 x E-08 ft/s

Figure 5.4  Concentration down plume centerline: MOC injection well source - Injec rate = 0.0002 cfs
the source for the original cell distance of 0.25, although there is less of an increase for the injection well source definition. Figures 5.3 and 5.4 also show that varying the cell distance does shift the peak contaminant concentration to the source cell. For this configuration, a cell distance of 0.5 smooths the output and corrects the problem.

As stated before, celdis is a numerical parameter. Lowering celdis often decreases mass balance errors in the program, but increases the run time. For the original base run a celdis of 0.25 was chosen because this value gives a mass balance error of approximately 6 percent, whereas a celdis of 0.5 results in a mass balance error of 13 percent. Figures 5.3 and 5.4, however, show that the higher celdis (and higher mass balance error) yields theoretically more reasonable results. The larger celdis, therefore, increases numerical stability. A further increase in celdis to 1.0 (Figure 5.5) shows that the anomaly does not reappear.

Initially, it is not apparent why an increase in celdis would produce greater numerical stability. However, an examination of the interrelationship of two user options (initial number of particle per cell (NPTPND), and celdis) explains this phenomenon. For the problem configurations described above, NPTPND was set to nine. The user is allowed to select a value of 4, 5, 8, or 9 for this parameter. An analysis by Konikow and Bredehoef, 1978, demonstrated that the accuracy and precision of the program results were directly proportional to the initial particle density, although the solution efficiency was inversely proportional to NPTPND. Analysis of the effect of celdis on the solution accuracy and precision (with NPTND equal to nine) showed that there is a relationship between celdis and the mass balance error in the solution. A celdis of 0.5 gave the best results, whereas a celdis of 0.25 showed strong oscillation in the error for the initial time steps (approximately 1.5 years).
Figure 5.5  Concentration down plume
centerline: MOC recharge source -
Infill rate = 8 X E-08 ft/s

celdis = 1.0
For a NPTPND of 9 and a celdis of 0.25, this oscillation occurred because the maximum amount a particle was allowed to move (25 percent of the grid dimension) was less than the space between the particles (33 percent of the grid dimension). Therefore, advective transport across cell boundaries could not be simulated adequately, for any time step, in grid areas where concentrations were changing significantly with time. (Konikow and Bredehoeft, 1978). Thus, increasing the celdis to 0.5 in this investigation allowed a more adequate representation of convective transport. Figures 5.3 and 5.4 demonstrate that, for a given source definition, the concentration in the source cell is not the same for a celdis of 0.5 and a celdis of 0.25. This difference in source concentration for varying celdis is also an effect of the numerical instability, caused by the improper choice of celdis.

Figures 5.3 and 5.4 also show that for a given celdis, the recharge source and injection well source configurations do not have the same concentrations in the source cell. The MOC code treats the recharge and injection well sources identically, when calculating the heads and velocity field in the aquifer. Therefore, these two source definitions should have identical concentrations at the source cell. However, an investigation of the USGS code showed that this model does not treat the injection well and recharge cell source definitions the same when calculating the particle concentrations in the source cell.

As discussed previously, in the particle in cells (PIC) method of treating dispersion in MOC, each particle represents a concentration of solute. The particles are moved with the advective velocity and a new concentration in each grid cell is calculated as the average of each particle concentration in the mesh. This concentration is placed at the center of the grid. Then, the dispersive part of the transport equation is solved and the grid concentrations calculated during the advective step are modified. In the USGS model, for the recharge source
configuration, the new concentrations for the particles in each cell are
calculated as the sum of the particle concentration at the end of the advective
step plus the change in concentration calculated for that grid cell during the
dispersive step. Thus, the concentration gradient existing in the cell (if any) at
the beginning of the time step is preserved.

For the injection well source definition, the change in concentration
computed at the source node (due to the dispersive step) is not applied to each
of the particles in the cell directly. Instead, the new concentration of each
particle at the end of a time step is set equal to the final node concentration.
This procedure prevents the concentrations of individual particles from
deviating from the average source concentration. In other words, no
concentration gradient is allowed in the source cell. Therefore, when
comparing the injection well source configuration to a source configuration
which contains concentration gradients in the source area (i.e., the recharge
source cell), a difference in the source concentrations may be expected.

It should also be noted that in the USGS code there are a set of constraints
applied to the injection well source configuration which prevent source cell
concentrations from exceeding the concentration in the source itself. However,
these constraints are not applied to the recharge source definition. For cases of
high contaminant loading, the recharge source definition may give contaminant
concentrations in the source cell higher than the concentrations in the source
itself.

Figure 5.3 shows that for the recharge source cell with celdis equal to 0.5, a
numerical perturbation occurs 250 feet down gradient of the source. This
distance is the point at which the velocity field levels out from the mounding
caused by the loading at the source cell. The contaminant influx in the source
area causes an increased gradient (and increased velocities) near the source.
Further away from the source, the velocity decreases until a constant Darcy velocity (velocity determined by the background hydraulic gradient) of the system is reached. The perturbation seen in Figure 5.3 may be caused by the code having numerical difficulty in the conversion from the recharge velocity to the Darcy velocity, when the celdis is equal to 0.5.

A set of runs was performed to test the theory that the perturbation is due to numerical difficulties in the velocity field. In these runs, the value of hydraulic conductivity (k) was lowered, thereby lowering the recharge velocity. This change in the recharge velocity decreased the difference between the recharge and Darcian velocities of the system. It was felt that at the lower velocity the perturbation in the results would disappear.

Figure 5.6 shows the results of the runs performed with a lower recharge velocity. The value of hydraulic conductivity was initially decreased by one order of magnitude to $10^{-3}$ cm/s. At this value of k, the perturbation does not appear in the results. The hydraulic conductivity was then gradually increased to determine the value at which the perturbation would begin to occur in the results. It is interesting to note that at a value of k equal to $2 \times 10^{-3}$ cm/s the contaminant concentration 50 feet down gradient of the source is once again higher than at the source (the celdis is 0.5 for all of these runs).

Figure 5.6 also demonstrates that for the different values of k (and thus different values in the velocity field), different values of concentration at the source are obtained. In the PIC method, the concentration in the source cell is calculated as the dilution of the flux of solute in the grid cell where the contaminant is input. In other words, the initial contaminant concentration is the mass of the solute input into the source cell divided by the volume of water in that grid cell. Therefore, the higher the background velocity in the system, the greater the amount of water entering the cell, and the greater the dilution of the
Figure 5.6 Concentration down plume centerline: Various values of hyd. cond.

- $k=10^{-3}$ cm/s
- $k=2\times10^{-3}$ cm/s
- $k=5\times10^{-3}$ cm/s
- $k=7.5\times10^{-3}$ cm/s

Figure 5.7 Concentration down plume centerline: MOC11 - $k=7.5\times10^{-3}$ cm/s
solute. Thus, for higher velocities, the initial contaminant concentrations in the source will be smaller, as seen in Figure 5.6.

At $k$ equal to $7.5 \times 10^{-3}$ cm/s the perturbation reappears in the results and the anomaly in contaminant concentrations near the source disappears. Figure 5.7 shows a plot of contaminant concentration down the centerline of the plume for $k$ equal to $7.5 \times 10^{-3}$ cm/s.

5.3 Effect of Varied Source Sizes

In the next series of runs, the HPS and MOC models were compared for varying source sizes. Table 5.3 shows the source sizes and loadings used in this comparison. It should be noted that in the first series of runs (runs 1-3) the contaminant loading per source cell area was held constant. Thus, as the source size was increased, the total contaminant loading on the system also increased. These runs simulated contaminant transport only, with no biodegradation occurring in the system. A value of 0.25 was used for the celdis in these simulations. This value results in higher contaminant concentrations down gradient of the source in the MOC runs but gives a better match to the results generated by the HPS model. Figure 5.8 shows plots of contaminant concentration down the plume centerline for source sizes of 50' x 50' (one cell), 100' x 100' (four cells), and 150' x 150' (nine cells), for both models. Figure 5.8 shows that the results from HPS and MOC compare well for the smallest source, but the results begin to deviate for larger source configurations.

The deviation in results for larger source sizes may be due to a difference in the velocity fields for each of the models. Because MOC is a numerical model, the code is able to generate a well defined velocity field through its hydraulic calculations. This velocity field allows for a more accurate calculation of contaminant transport. The HPS model, on the other hand, allows only one
Table 5.3 MOC vs. HPS Runs

<table>
<thead>
<tr>
<th>RUN #</th>
<th>SOURCE SIZE</th>
<th>(per source cell)</th>
<th>MAX C (mg/l)</th>
</tr>
</thead>
<tbody>
<tr>
<td>MOC 1</td>
<td>1 CELL (50' X 50')</td>
<td>$8 \times 10^{-8}$</td>
<td>24.0</td>
</tr>
<tr>
<td>HPS 1</td>
<td></td>
<td></td>
<td>24.6</td>
</tr>
<tr>
<td>MOC 2</td>
<td>2 X 2 Source cells (100' X 100')</td>
<td>$8 \times 10^{-8}$</td>
<td>52.8</td>
</tr>
<tr>
<td>HPS 2</td>
<td></td>
<td></td>
<td>43.7</td>
</tr>
<tr>
<td>MOC 3</td>
<td>3 X 3 Source cells (150' X 150')</td>
<td>$8 \times 10^{-8}$</td>
<td>65.8</td>
</tr>
<tr>
<td>HPS 3</td>
<td></td>
<td></td>
<td>90.3</td>
</tr>
<tr>
<td>MOC 3A</td>
<td>3 X 3 Source cells (150' X 150')</td>
<td>$4 \times 10^{-8}$</td>
<td>37.5</td>
</tr>
<tr>
<td>HPS 3A</td>
<td></td>
<td></td>
<td>45.2</td>
</tr>
<tr>
<td>MOC 3B</td>
<td>3 X 3 Source cells (150' X 150')</td>
<td>$1 \times 10^{-8}$</td>
<td>11.3</td>
</tr>
<tr>
<td>HPS 3B</td>
<td></td>
<td></td>
<td>10.2</td>
</tr>
</tbody>
</table>
Figure 5.8 Concentration down plume centerline: Different source sizes

- MOC1
- HPS1
- MOC2
- HPS2
- MOC3
- HPS3

Concentration (mg/l) vs. XDEL (ft)
input value for the velocity. For areas of high contaminant loading, a mounding situation occurs and the velocity field is altered from the Darcy velocity created by the background gradient in the system. For the MOC runs, although there is a constant source loading for each source cell, the larger sources receive a larger loading over the entire source area because they have more source cells. The infiltration rates entered into the HPS model were raised to match the loading input to the MOC code.

The deviation in concentrations generated by the two models for larger source terms may be due to the effect of mounding from the elevated contaminant loading. Therefore, a set of runs was performed for the nine cell source configuration, with lowered values of contaminant loading (see Table 5.3). The results are shown in Figure 5.9. This figure demonstrates that for the larger source configuration, good matches between the two models are obtained for lower source loadings.

Figure 5.10 shows plots of the velocity distribution down the plume centerline for varied source sizes. Figure 5.10 demonstrates that for larger sources (which create larger contaminant loadings on the system) greater mounding in the velocity field occurs. Figure 5.11 shows plots of the velocity distribution down the plume centerline for the nine cell source configuration with decreasing values of contaminant loading. This figure demonstrates that for the larger source, as the contaminant loading is decreased, less mounding in the velocity field occurs.

5.4 First Order Decay Biodegradation

After comparing the models for simulations of contaminant transport only, runs were performed with biodegradation. The simulations were done with the base run configuration of one 50' x 50' source cell. This run was chosen for the
Figure 5.9  Concentration down plume centerline: 3X3 source configuration (varied loading rate)
Figure 5.10 Velocity Down Plume Centerline: Increasing Source Sizes and Contaminant Loading.

Figure 5.11 Velocity Down Plume Centerline: 3X3 Source Configuration Decreasing Values of Contaminant Loading
biodegradation simulation because the two models compared well for this problem definition without degradation.

Comparisons between the HPS and MOC models with first order decay were performed with a first order decay coefficient of 0.002 day⁻¹. The first runs using first order decay showed MOC values consistently lower than the HPS values. This shift in the curves indicated a difference in the way in which FOD was being handled in the source for each of the models: HPS was allowing the source to biodegrade while MOC was not.

In order to achieve a better match between the two models with biodegradation, MOC was run in a mode which allowed for decay of the source. To accomplish this, the decay coefficient was converted into a half-life of the solute and degradation was calculated as an exponential decay. A plot of the results in Figure 5.12 show a good match between the two models.
Figure 5.12 Concentration down plume centerline: Biodegradation represented as first order decay
6.0 EVALUATION OF EQUIVALENT FIRST ORDER AEROBIC DEGRADATION RATES

The objective of this investigation was to match BIOPLUME II predictions of biodegradation with predictions from a FOD analytical solution. Estimates of aerobic biodegradation of BTX obtained using BIOPLUME II were matched with estimates from a first order decay model. The FOD model used for this investigation was simply a version of BIOPLUME II in which no oxygen was input into the model. In this form, BIOPLUME II reduces to the USGS two dimensional model, upon which it is based, and simulates biodegradation as a first order decay process. A match between the BIOPLUME II and MOC FOD plumes would require that the same amount of mass be degraded by both models. Matching the total mass degraded was accomplished by varying the FOD coefficient. An attempt to match the overall plume configuration (size, shape and contaminant concentrations) was also made.

6.1 Model Set-up

In order to compare the MOC FOD and BIOPLUME II runs, a base run problem definition was created. The grid system presented in Figure 5.1 was also used for these simulations, the only change being that the source was modeled as an injection well instead of as a recharge cell. The contaminant source was modeled as an injection well occupying one source cell with an area of 2500 ft² (see Figure 5.1). Contaminant was injected at the source at a rate of 0.0002 cubic feet per second, which is equivalent to a recharge velocity over the source cell area of 7.7 m/yr. This recharge rate is not intended to model a rainfall infiltration rate, but instead simulates a situation created by a leaking contaminant pond. The assumed contaminant concentration was 100 mg/l. The hydraulic gradient used was 0.004 ft/ft, which gives a seepage
velocity in the system of 0.38 ft/day for the base run case. The background oxygen for the base run was set as 8 mg/l, which is an upper limit for oxygen levels occurring naturally in ground water. The national average for dissolved oxygen in ground water is approximately 3 mg/l.

Both models used are two dimensional codes and do not simulate transport or degradation in the vertical direction. The models therefore consider contaminant injection at the surface of the aquifer, and contaminant concentrations are assumed to be constant with depth. Table 5.1 gives the aquifer parameters for the base run.

All runs were done assuming steady state hydraulic conditions, and all output was analyzed after three years of simulation time. The three year simulations allowed runs to be made in a reasonable length of time. This time frame also prevented plumes in systems with higher seepage velocities from migrating to the no flow boundaries at the downgradient edge of the grid. However, in simulations with lower seepage velocities the system may not have reached chemical steady-state conditions after three years.

6.2 Plume Match Varying FOD Coefficient Only

In the first series of runs (Table 6.1), BIOPLUME II, MOC FOD and no degradation (Nodeg) simulations were performed. The Nodeg run was simply a base run simulation in which contaminants were injected into the aquifer, but were not allowed to degrade. The Nodeg run was compared to a BIOPLUME II run to confirm that the contaminant plumes generated by the two runs were significantly different. In other words, the Nodeg simulation was performed to confirm that model runs would predict significant levels of degradation occurring for the base run case, before trying to match BIOPLUME II and MOC FOD degradation.
Table 6.1 Seepage Velocity vs. FOD Coefficient & Ratio of Longitudinal to Transverse Dispersivity

<table>
<thead>
<tr>
<th>Run ID</th>
<th>Vs (ft/d)</th>
<th>k1 (1/day)</th>
<th>Dt/Dl</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bio1 k1</td>
<td>.08</td>
<td>.0005</td>
<td>.01-.07</td>
</tr>
<tr>
<td>Bio2 k2</td>
<td>.15</td>
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<tr>
<td>Baserun k7beta</td>
<td>.38</td>
<td>.0020</td>
<td>.01-.07</td>
</tr>
<tr>
<td>Bio4 k4</td>
<td>.72</td>
<td>.0040</td>
<td>.01-.07</td>
</tr>
<tr>
<td>Bio5 k5</td>
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<td>.01-.07</td>
</tr>
<tr>
<td>Bio3 k3</td>
<td>1.13</td>
<td>.01</td>
<td>.01-.04</td>
</tr>
</tbody>
</table>

*Di = 10 ft for all runs

**All results are given at time = 3 years
The FOD run was matched to the BIOPLUME II run by varying the FOD coefficient \( k_1 \) until the total mass degraded by the FOD simulation was within 5% of the total mass degraded by the BIOPLUME II simulation. For the base run case, a \( k_1 \) value of 0.002 day\(^{-1}\) generated mass degradation matching that in the BIOPLUME II run.

Plume configurations (Figures 6.1-6.3) show that the BIOPLUME II plume is much narrower than the FOD plume. This difference is due to the way that degradation is calculated in each of these runs. In BIOPLUME II, more biodegradation occurs on the plume edges because, in this area of lower concentrations, oxygen can fully degrade the contaminant. In the MOC FOD scenario, however, degradation is calculated using a first order decay rate throughout the contaminant plume. In this method, the contaminant concentration at each point across the plume area is calculated as the initial concentration multiplied by the exponential decay factor (see equation 6). Thus, the FOD method does not completely degrade the plume edges, as BIOPLUME II does.

6.3 Plume Match Varying FOD Coefficient and Dt/DI

A plot of contaminant concentration down the plume centerline (Figure 6.4) shows that the BIOPLUME II curve follows the Nodeg curve, but is shifted to lower concentrations. Figure 6.4 also shows that the MOC FOD curve has consistently lower concentrations than the BIOPLUME II curve on the interior of the plume. This difference is related to plume shape and the effect of differing degradation rates on the interior and edges of the plume, as described above. The MOC FOD plume, which is much broader than the BIOPLUME II plume, has the same amount of mass spread out over a larger area. It was therefore theorized that, if the FOD plume could be narrowed, a better match to the
Legend: Values represent upper limits for corresponding pattern.

Concentration

<table>
<thead>
<tr>
<th></th>
<th>0</th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
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</tr>
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<tr>
<td></td>
<td>28</td>
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</tr>
</tbody>
</table>

Figure 6.1 BIOPUME II RUN
Contaminant Plume

Legend: Values represent upper limits for corresponding pattern.

<table>
<thead>
<tr>
<th>Concentration</th>
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</thead>
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<tr>
<td>0</td>
</tr>
<tr>
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<tr>
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<td>22</td>
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<tr>
<td>28</td>
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</table>

Figure 6.2 No Degradation Run
Legend: Values represent upper limits for corresponding pattern.

Concentration

<table>
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</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>4</td>
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<tr>
<td></td>
<td>25</td>
</tr>
<tr>
<td></td>
<td>28</td>
</tr>
</tbody>
</table>

Figure 6.3 FOD RUN matched with k1 only
Figure 6.4  Concentration down plume centerline: Base run - FOD matched with k1 only

Concentration (mg/l) vs. Distance (ft)

- BIOPLUME II
- First Order Decay
- No Degradation
BIOPLUME II plume would be obtained.

A narrowing of the FOD plume was accomplished by varying the ratio of transverse to longitudinal dispersivity (Dt/Dl) in the FOD run. Decreasing this ratio while holding Dl constant in effect lowers the transverse dispersivity. A lower value of Dt decreases the lateral spreading of the contaminant, and produces a longer, narrower plume. The decrease in Dt/Dl is a curve fitting procedure which is performed to match BIOPLUME II model results with the results from a FOD model. This process does not reflect an actual decrease of this ratio in the field.

A ratio of 0.05 was determined to give a good fit. A plot of the concentration down the plume centerline and a transect of the plume at 150 feet down gradient of the source for the lower dispersivity ratio are shown in Figures 6.5 and 6.6, respectively. The plume configuration for this run is given in Figure 6.7.

Figure 6.5 also shows a small hump in the BIOPLUME II and FOD curves. This hump is related to the three year time period at which the results are being examined. For this problem configuration, the seepage velocity in the system is 0.38 ft/day. After three years the contaminant would have migrated approximately 420 ft downgradient. Referring to Figure 6.5, it can be seen that the hump begins at approximately this location. The hump therefore indicates a region downgradient which has not reached steady state.

Another run was performed using an expanded grid. In this run, output was analyzed after 8 years. This time frame allowed the contaminant to migrate approximately 1000 ft downgradient. In the 8 year run, the hump at 400 feet disappears. However, with the k1 value of 0.002 day\(^{-1}\) determined in the three year run applied to the 8 year simulation, the mass degraded in the BIOPLUME II run was only 70% of the mass degraded in the FOD run. Therefore, before reaching steady state contaminant condition, the k1 value is time dependent.
Figure 6.5 Concentration down plume centerline: Base run - FOD matched with $k_1$ & $D_t/D_l$
Figure 6.6 Transect of contaminant plume
150 ft downgradient of source
Legend: Values represent upper limits for corresponding pattern.

Concentration

<table>
<thead>
<tr>
<th></th>
<th>0</th>
<th>4</th>
<th>7</th>
<th>10</th>
<th>13</th>
<th>16</th>
<th>19</th>
<th>22</th>
<th>25</th>
<th>28</th>
</tr>
</thead>
</table>

Figure 6.7 FOD RUN matched with k1 and D/Dl
6.4 Relationship Between Seepage Velocity and FOD Coefficient

Having determined that BIOPLUME II results can be matched with a FOD simulation, an analysis was performed to determine if a relationship exists between the seepage velocity and the FOD coefficient required to match biodegradation simulated using BIOPLUME II. Velocity was chosen as a key variable because biodegradation is very sensitive to this parameter. Table 6.1 shows the different values of velocity and the corresponding $k_1$ values required to match the BIOPLUME II results within 5%. Also given in Table 6.1 is a range of values for $Dt/Dl$. The model runs revealed that lowering the ratio of $Dt/Dl$ to a certain value changed the plume configuration, and that lowering the ratio beyond this point did not result in any significant changes in the plume.

Figure 6.8 shows a plot of the relationship between seepage velocity and the value of the FOD coefficient. This figure shows that the relationship between these two parameters may be described by a simple curve. The relationship between the FOD coefficient and the seepage velocity is dependent on the initial amount of oxygen in the system. Figure 6.9 shows an approximately linear relationship between the FOD constant and the oxygen level in the system for the case of seepage velocity equal to 0.38 ft/day. Figure 6.9 indicates that the rate constant can be viewed as a function of the oxygen concentration. At the edge of the plume, the oxygen concentration is higher, and thus the rate constant will be larger, resulting in more biodegradation.
Figure 6.8 Relationship Between:
Seepage velocity & FOD coefficient

Oxygen Conc = 8 mg/l
Dv/Dk = .04
Figure 6.9  Relationship Between:
FOD coefficient & Oxygen level

$k_1$ (day$^{-1}$)

$O_2$ (mg/l)
7.0 NUMERICAL MODELING FOR AQUIFER BIOREMEDIATION

This section examines the effect of injecting oxygen in the standard pump and treat aquifer restoration scheme. Although the previous sections of this work examined the difference between analytical and numerical solution procedures, this investigation uses only numerical techniques. The use of a numerical model was required because no analytical solutions exist for the case of oxygen being injected in remedial pumping schemes.

Satkin, 1987, used the USGS solute transport code to evaluated different well configurations for standard pump and treat aquifer remediation under variable hydrogeologic conditions. He evaluated seven different well patterns on the basis of clean-up time, volume of water circulated and volume of water requiring treatment. This research used the BIOPLUME II code to examine three of Satkin's well configurations in two different hydrogeologic conditions for the case when biodegradation is assumed to occur. The effect of varying levels of oxygen on aquifer remediation for the various well configurations was examined and the results were applied to the Traverse City Michigan (TCM) site in an attempt to remediate the TCM contaminant plume.

7.1 Well Patterns

Five different well patterns were evaluated in this study. Three of the patterns were taken directly from Satkin's work (the 3-spot, double cell, and 5-spot patterns). The remaining two patterns used were variations on the 3-spot and 5-spot configurations. The variation patterns simply interchanged the injection and production wells in the original 3-spot and 5-spot well patterns. In other words, injection wells in the original scheme became production wells in the variation scheme. Similarly, the production well in the original scheme
became an injection well in the variation scheme. The 5-spot and 3-spot variation schemes were investigated because it was thought that injecting oxygen into the area of highest contaminant concentration, and pumping on the up and downgradient sides of this area might be a more efficient way to transport oxygenated water through the plume than provided by the original schemes. Figure 7.1 illustrates all five patterns.

7.2 Existing Contaminant Plume

Initially, a set of runs was performed to remediate an existing contaminant plume. Table 7.1 summarizes the aquifer characteristics and general problem configuration used in this set of runs. The transmissivity of the aquifer was 0.001 ft²/s (.93 cm²/s). The contaminant plume which was used is shown in Figure 7.2. The plume's maximum dimensions were 650 x 350 feet, and the initial dissolved contaminant mass in the system was equal to 1,100 kg.

Runs were performed for each of the well patterns previously described. For each well pattern, simulations were done with three different levels of oxygen in the system: no oxygen, oxygen injected at 3 mg/l, and oxygen injected at 20 mg/l. These three oxygen levels were chosen because they correspond to hydraulic cleanup only, the average level of oxygen occurring naturally in ground water, and a mid range level of oxygen achieved using pure oxygen, respectively. Table 7.2 shows the parameters used for these runs. The results for the double cell, 3-spot (2 wells injecting), and 5-spot (4 wells injecting) well patterns are shown in Figures 7.3-7.5, respectively. These figures show plots of percent of initial dissolved contaminant remaining in the system (present mass dissolved/initial mass dissolved) versus time. The figures for all three of the well patterns show only a small difference between the no oxygen curve and the curves with oxygen injected at 3 and 20 mg/l. The
Figure 7.1 Well Patterns
(from Satkin, 1987)
<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Transmissivity</td>
<td>0.001 ft²/s</td>
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<tr>
<td>Thickness</td>
<td>10 ft</td>
</tr>
<tr>
<td>Hydraulic gradient</td>
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<tr>
<td>Longitudinal dispersivity</td>
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</tr>
<tr>
<td>Transverse dispersivity</td>
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<tr>
<td>Effective porosity</td>
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<tr>
<td>Cell size</td>
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</table>
Figure 7.2 Initial Contaminant Plume
(from Satkin, 1987)
### Table 7.2 Aquifer Remediation Runs:
Different well patterns & Varying oxygen levels

<table>
<thead>
<tr>
<th>Run ID</th>
<th>Source</th>
<th>$O_2$ inj level (mg/l)</th>
<th>Transmissivity ($ft^2/s$)</th>
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<tbody>
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<tr>
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<td>0.001</td>
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<td>rs2b1</td>
<td>init plume</td>
<td>3</td>
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</tr>
<tr>
<td>rs2b2</td>
<td>init plume</td>
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</tr>
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Figure 7.3 Double cell well pattern

% Contaminant remaining (x 100)

- Rich2a -- no O2
- rs2b1 -- O2 inj @ 3 mg/l
- rs2b2 -- O2 inj @ 20 mg/l

Time (yr)
Figure 7.4 3 spot well pattern with 2 wells injecting

% Contaminant remaining (X 100)

Rich1a -- no 02
rs1b1 -- 02 inj @ 3 mg/l
rs1b2 -- 02 inj @ 20 mg/l

Time (yr)

0 1 2

Figure 7.5 5 spot well pattern with 4 wells injecting

% Contaminant remaining (X 100)

Rich3a -- no 02
rs3b1 -- 02 inj @ 3 mg/l
rs3b2 -- 02 inj @ 20 mg/l

Time (yr)

0 1 2
fact that there is only a small difference between the runs suggests that the
majority of the clean-up is occurring due to the hydraulics of the system. In
other words, most of the plume's contaminant mass is being pumped out of the
system before the contaminant has a chance to biodegrade. It is also
interesting to note that most of the hydraulic removal occurs in the first three to
six months after the beginning of the simulation, as evidenced by the sharp
decline in the percent contaminant remaining for the no oxygen runs for all
three well configurations during this time period.

In an attempt to see a greater variation between the no oxygen and oxygen
runs, more mass was added to the system. Two runs were performed for the 3-
spot (2 wells injecting) well configuration in which the initial plume
concentrations were increased first by a factor of three and then by a factor of
five. Again, in each of the two cases the no oxygen and oxygen curves differed
by less than 5%. Thus, for the hydrogeologic conditions and contaminant
concentrations studied, no appreciable benefit was found in the addition of
oxygen to the system, since the majority of the clean-up occurred hydraulically.

The variations on the 5-spot and 3-spot patterns (with only 1 well injecting
in each case) proved to be inefficient remediation configurations. Both of these
new patterns were unable to reduce the contaminant level as low as the
original scheme did, and took longer amounts of time in reducing the
contaminant levels overall. Figure 7.6 shows the percent contaminant
remaining versus time plot for the 3-spot, 1 well injecting simulation for no
oxygen, and oxygen injected at 3 mg/l. This figure shows some numerical
instability in the early time steps of the simulation. Figure 7.6 also shows that
with oxygen injected in the system, the contaminant plume is eliminated from
the aquifer after 1.5 years. For the original 3-spot (2 wells injecting) run,
contamination was eliminated from the system after only 0.75 years. Thus,
Figure 7.6 3 spot well pattern with 1 well injecting

- Rich1d -- no 02
- rs1b3 -- 02 inj @ 3 mg/l

% Contaminant remaining (x 100)

Time (yr)
although it originally seemed that the variation schemes would provide a more efficient way of flushing the contaminated zone with oxygen, thereby stimulating bioremediation, the new configurations actually demonstrated less remediation effects than the original schemes.

The inefficiency in the variation schemes is due to an inefficiency in the hydraulics. The original schemes which inject up and down gradient and pump in the center of the plume, in effect isolate the contaminant plume and flush oxygenated water toward the center. Since the plume cannot migrate, the contaminant throughout the area comes in contact with oxygen, and biodegrades or is pumped from the system. The variation scheme, on the other hand, does not have up and down gradient injection wells to contain the plume and some of the contaminant is able to escape the influence of the production wells and the injected oxygen.

7.3 Constant Source Contaminant Plume

Contaminant sources at field sites often occur not as one discreet loading, as investigated in the previous section, but instead leach continuously into the aquifer. For the constant source problem, it is often not possible to remediate the system over a short period of time, using only hydraulic means (production and injection wells with surface treatment), and bioremediation can be a technique for dealing with the problem.

The next set of runs examined the effectiveness of the double cell, 3-spot (2 wells injecting), and 5-spot (4 wells injecting) well patterns in remediating an aquifer with a continuously leaking source (see Table 7.2). The aquifer conditions and initial plume concentrations from the initial set of runs were used in the constant source simulations. The continuous source was modeled as an injection well, injecting at a rate of $0.25 \times 10^{-4}$ cfs. This injection rate is
one order of magnitude greater than the rate used to generate the initial contaminant plume. The source concentration was set to 1500 units. The contaminant concentration must be of the same order of magnitude as the initial contaminant concentration in the injection cell, or high mass balance errors will result.

Figures 7.7 - 7.9 show plots of percent contaminant remaining versus time for the double cell, 3-spot, and 5-spot well patterns. Runs were done for no oxygen, and oxygen injected at 100 mg/l. Figures 7.7 - 7.9 show that, after one year, all three well configurations are able to reduce the contaminant level to less than 5% of the original. For each of the configurations, the runs with injected oxygen eliminated contamination in 0.75 years or less. Thus, after one year, the benefit of injecting oxygen is the reduction of the contaminant remaining in the system by only a few percent more than the reduction achieved by the no oxygen simulation.

7.3.1 Increase in source loading

Next, the continuous source injection rate was increased to 0.25 x 10^-3 cfs and simulations were performed for the double cell and 3-spot well patterns (see Table 7.2). The double cell runs were performed with no oxygen, and oxygen injected at 3 and 20 mg/l. Figure 7.10 shows the results for the double cell simulations. With no oxygen injected into the system, after 0.5 years the remediation levels off with approximately 20% of the initial contaminant mass remaining. With oxygen injected at 3 mg/l, approximately 0.1% of the original contaminant level remains after 0.5 years. For the simulation with oxygen injected at 20 mg/l contamination is eliminated at 0.5 years. Thus, there is approximately a 20 % difference in remediation levels between the oxygen and no oxygen schemes. After 0.5 years, there is no significant difference
Figure 7.7 Double cell well pattern:
Constant source @ 0.25 $\times 10^{-4}$ cfs

% Contaminant remaining ($\times 100$)

- rs2b3 -- no 02
- rs2b4 -- 02 @ 100 mg/l

Time (yr)
Figure 7.8  3 spot well pattern with 2 wells injecting: Constant source @ 0.25 E-04 cfs

% Contaminant remaining (X 100)

- rs1b5 -- no O2
- rs1b6 -- O2 @ 100 mg/l

Time (yr)

Figure 7.9  5 spot well pattern with 4 wells injecting: Constant source @ 0.25 E-04 cfs

% Contaminant remaining (X 100)

- rs3b5 -- no O2
- rs3b6 -- O2 @ 100 mg/l

Time (yr)
Figure 7.10 Double cell well pattern: Constant source @ 0.25 E-03
between simulations performed at oxygen levels of 3 and 20 mg/l. Figures 7.10 a), b), and c) show plume configurations for the Double cell well pattern with oxygen injection concentrations of 0, 3, and 20 mg/l respectively.

Runs for the 3-spot well pattern were performed for no oxygen and oxygen injected at 3, 20, and 100 mg/l. Figure 7.11 shows the results from the 3-spot runs. At 0.75 years, the percent contaminant remaining levels off at approximately 20% for the no oxygen run, and 10% for the run with oxygen injected at 3 mg/l. Contamination levels were eliminated at 0.75 years for the runs with oxygen injected at 20 and 100 mg/l. Therefore, the injection of oxygen into the system at levels greater than 20 mg/l reduces the level of contaminant remaining by approximately 20% more than the no oxygen simulation. However, increasing the oxygen level from 20 to 100 mg/l gave no significant improvement in remediation. Also, overall, the double cell configuration was able to eliminate contamination slightly faster than the 3-spot well pattern.

7.3.2 Decrease in aquifer transmissivity

In the next set of runs, the transmissivity in the aquifer was decreased by one order of magnitude to 0.0001 ft²/s. Runs were performed for the double cell, 3-spot and 5-spot well patterns with no oxygen and oxygen injected at 100 mg/l. The constant source for these runs was set to 0.25 x 10⁻⁴ cfs (see Table 7.2). Figures 7.12 - 7.14 show the results for the lower transmissivity runs.

The double cell well pattern showed the greatest difference between the oxygen and no oxygen simulations. Figures 7.12 a) and b) show Double cell plume configurations for oxygen injection levels of 0 and 100 mg/l, respectively. With no oxygen injected in the system, the percent contaminant remaining after 2.5 was approximately 32% of the original. However, with
Figure 7.10 a) CONCENTRATION OF CONTAMINANT (X 0.10 mg/l) after 0.50 years
rs2b5 -- no Oxygen

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Figure 7.10 b) CONCENTRATION OF CONTAMINANT (X 0.10 mg/l) after 0.50 years
rs2b6 -- Oxygen injected @ 3 mg/l

Figure 7.10 c) CONCENTRATION OF CONTAMINANT (X 0.10 mg/l) after 0.50 years
rs2b7 -- Oxygen injected @ 20 mg/l
Figure 7.11 3 spot well pattern with 2 wells injecting: Constant source @ 0.25 E-03 cfs
Figure 7.12  Double cell well pattern:
T=.0001 sq ft/s
Constant source @ 0.25 E-04 cfs

% Contaminant remaining (X 100)

- rs2a9 -- no O2
- rs2b9 -- O2 @ 100 mg/l

Time (yr)
Figure 7.12 a) CONCENTRATION OF CONTAMINANT (X 0.10 mg/l)
after 2.0 years

rs2a9 -- no Oxygen

Figure 7.12 b) CONCENTRATION OF CONTAMINANT (X 0.10 mg/l)
after 2.0 years

rs2b9 -- Oxygen injected @ 100 mg/l
Figure 7.13 3 spot well pattern:
\[ T = 0.0001 \text{ sq ft/s} \]
Constant source @ 0.25 E-04 cfs

[Graph showing contaminant remaining over time for rs1a15 and rs1b15 cases with and without oxygen injection]

Figure 7.14 5 spot well pattern
\[ T = 0.0001 \text{ sq ft/s} \]
Constant source @ 0.25 E-04 cfs

[Graph showing contaminant remaining over time for rs3a7 and rs3b7 cases with and without oxygen injection]
oxygen injected at 100 mg/l, contamination was almost completely eliminated from the aquifer, with only 3% of the original contaminant mass remaining after 2.5 years.

The 3-spot and 5-spot well patterns showed much less variation between the oxygen and no oxygen runs. For these two well patterns, over 40% of the original contaminant remained in the system after two and one-half years for the no oxygen simulations. With oxygen injected at 100 mg/l, the percent contaminant remaining after two and one-half years of simulation was still more than 30% for both well patterns. Therefore, for tighter systems, the double cell well configuration appeared to do a much better job in remediating the contaminant plume.

7.4 Application to TCM Field Site

7.4.1 Site History and Hydrogeology

The Traverse City field site is located on the U. S. Coast Guard Air Station base in the northwest portion of the lower peninsula of Michigan. In 1980, residents of the East Bay Township complained that water from private wells was discolored, foamed, and smelled. Investigations showed that the water from several domestic wells was contaminated by organic substances. Later in 1980, the Michigan Department of Natural Resources determined that the contaminant source was located on the Coast Guard Air Station. In 1985, the Coast Guard installed a line of withdrawal wells to stop contaminants from migrating across the site boundary.

The aquifer at the site is contaminated with organic chemicals originating from a spill of approximately 10,000 gallons of aviation fuel; the major contaminants at the site include BTX. The fuel has migrated through the
unsaturated zone, and acts as a continuous contaminant source. Some of the contaminants have become trapped in the pores of the aquifer material, and these compounds leach into the ground water as the water table rises due to seasonal changes, and as contaminants are solubilized by infiltrating rain water (Miller, 1989).

The coast guard base is underlain by glacial deposits which comprise two main layers: an upper sand and gravel layer and a lower clay layer. The sand and gravel zone is comprised of fine to medium grained sands with coarse sands and gravel found at lower depths. The sand and gravel unit is 10 to 40 m thick and the underlying clay measures about 30 m in depth. The hydraulic conductivity in the aquifer ranges from 28 to 50 m per day, with ground water velocities between 1 and 2 m per day. Ground water at the site flows toward the East Arm of the Grand Traverse Bay, in a northeasterly direction. (Twenter, 1985, Rifai et al., 1988, Miller, 1989).

7.4.2 Previous Research

Miller's (1989) thesis work examined the TCM field site in great detail. Miller applied BIOPLUME II to the waste site and calibrated site conditions with the model. She performed mass loss calculations, and found that the plume source was shrinking with time. The source change was incorporated into the calibration and model runs were performed to simulate field conditions two years after the start of plume remediation with an interdiction field (1986). Miller then compared various cleanup strategies to the existing interdiction field. In her remediation work, Miller used oxygen injection concentrations equal to 8 mg/l (level naturally occurring at TCM), and did not investigate the effect of increasing injected oxygen concentrations to the levels which can be obtained using pure oxygen or hydrogen peroxide. Miller concluded that for
the site conditions and remediation schemes studied, with the source remaining constant, the aquifer could never be completely remediated.

The purpose of this investigation was to expand upon Miller's work and incorporate the double cell well configuration, with varying levels of oxygen, into the simulations. The objective was to determine the effect of injecting oxygenated water (water with oxygen levels higher than those naturally occurring in the aquifer) on remediation of a constant contaminant source. One other well configuration, which takes advantage of the existing interdiction field, was also tested. A set of runs was then performed to determine the effect of varying well rates on the bioremediation process.

7.4.3 Model Set-up

The remediation schemes were performed for the 1986 model calibration from Miller's thesis. Figure 7.15 shows the grid used for these runs. Figure 7.15 also shows the cells which represent remediation wells, the interdiction field, the source, and areas of constant head.

7.4.4 Effect of Varying Oxygen levels

Runs were performed for two well configurations. Table 7.3 shows the parameters which were varied in the TCM modeling runs. In all remediation simulations, the interdiction field wells pictured in Figure 7.15 were assumed to remain in operation. The remediation scheme wells were added to the system in addition to the existing interdiction field and remediation wells under the assumption that, from a regulatory standpoint, the interdiction field and remediation wells would be required to remain operating.

The first well pattern used was the Double cell configuration discussed previously. The second configuration was an I pattern, which is pictured in
Figure 7.15 Model Grid for TCM Simulations
Table 7.3 Traverse City Michigan Field Site: Aquifer remediation runs

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<td>km5b1</td>
<td>20</td>
<td>entire simulation</td>
<td>0.04</td>
</tr>
<tr>
<td>km5b2</td>
<td>100</td>
<td>entire simulation</td>
<td>0.04</td>
</tr>
</tbody>
</table>
Figure 7.16. The I configuration utilized the existing down gradient interdiction field, and added an upgradient line of injection wells. One injection and one production well were placed along the centerline of the contaminant plume.

Figure 7.17 and 7.18 show the results of the TCM BIOPUMLE II runs for both well patterns. Also pictured, is a plot of contaminant removal provided by the existing interdiction field. Runs were performed at oxygen levels of 0, 20 and 100 mg/l. The plots for the TCM simulations show that for both well patterns, oxygen levels of 100 mg/l remediate the aquifer for BTX after one year. Simulations for both well configurations also show that with oxygen injected at 20 mg/l approximately ten percent of dissolved contaminant remains in the aquifer after two years.

7.4.5 Effect of Multiple Pumping Periods

Figures 7.17 and 7.18 also show that most of the hydraulic removal occurs in the first six months to one year after the beginning of the simulation, as shown by the sharp decline in the percent contaminant remaining for the no oxygen runs during this time period. The fact that hydraulic cleanup occurs over a short period of time at the beginning of the simulation could be of economic significance. Oxygen injection concentrations of 20 mg/l and 100 mg/l require the use of pure oxygen and hydrogen peroxide, respectively. Injection of pure oxygen and hydrogen peroxide, however, is an expensive procedure. Therefore, if a remediation scheme which cleans hydraulically only for a short period of time before initiating the injection of oxygenated water were as effective as a scheme which injected oxygenated water during the entire length of the project, a significant cost savings could be obtained.

A series of runs were performed with the Double cell well configuration which used two separate pumping periods. In the first pumping period, no
Figure 7.16. I Well Configuration for TCM Simulations

- Production Well
- Injection Well
Figure 7.17 TCM 1986 contaminant plume: Double cell well pattern

Figure 7.18 TCM 1986 contaminant plume: I well pattern
oxygen was injected with the water at the injection wells. During the second pumping period, oxygen was injected at a level of 100 mg/l. The results from these runs are shown in Figure 7.19. The wells in the Double cell configuration operated at 0.04 cfs for this series of runs.

Figure 7.19 shows four runs: no oxygen injected for three months, no oxygen injected for six months, no oxygen injected for one year, and oxygen injected for the entire simulation. The run with oxygen injected after 0.25 years shows the closest match to the simulation with oxygen injected for the entire time period. Also, the runs with no oxygen injected for 0.25 years and oxygen injected for the entire simulation reached zero percent contaminant remaining at the same time step (after 1 year). The runs with no oxygen for 0.5 years and 1.0 years showed a greater deviation from the run with oxygen injected for the entire simulation (see Figure 7.19).

Next, a set of runs was performed for the Double cell well configuration, with wells operating at 0.02 cfs (half the rate shown in Figure 7.19). Runs were done with oxygen injected for the entire simulation, and with oxygen injected after 0.25 and 0.50 years. Figures 7.20 and 7.21 show the results of these runs for oxygen injection concentrations of 20 mg/l and 100 mg/l, respectively. Figure 7.20 shows very little difference between the runs with oxygen injected after 0.25 years and 0.50 years and the run with oxygen injected for the entire simulation, for an oxygen injection concentration of 20 mg/l.

Figure 7.21 shows a greater variation between the runs with oxygen injected after 3 and 6 months and the run with oxygen injected for the entire simulation, for the case of oxygen injected at 100 mg/l. Figure 7.22 shows plots of plume concentrations down the ninth column of the grid, after 0.75 years of simulation time. Figure 7.22 demonstrates that, at intermediate time steps in the simulation, the runs with oxygen injected after 0.25 and 0.5 years
Figure 7.19  TCM 1986 Contaminant plume:
Oxygen injected for different time lengths
$Q = 0.04$ cfs  Inj concentration = 100 mg/l

% Contaminant remaining (X 100)

km2pp7 no 02 inj for 0.25 years
km2pp1 no 02 inj for 0.50 years
km2pp2 no 02 inj for 1.0 years
km4b2  02 inj for entire simulation

Time (yr)
Figure 7.20  TCM 1986 Contaminant plume:
Oxygen injected for different time lengths
Q = 0.02 cfs  Inj concentration = 20 mg/l

% Contaminant remaining (X 100)

Time (yr)

- km2pp3 02 inj after 0.25 years
- km2pp4 02 inj after 0.5 years
- km4b3 02 entire simulation

Figure 7.21  TCM 1986 Contaminant plume:
Oxygen injected for different time lengths
Q = 0.02 cfs  Inj concentration = 100 mg/l

% Contaminant remaining (X 100)

Time (yr)

- km2pp5 no 02 inj for 0.25 years
- km2pp6 no 02 inj for 0.50 years
- km4b4 02 inj for entire simulation
Figure 7.22 Plume Conc. (@ 0.75 yr) for different oxygen injection lengths -
Q = 0.02 cfs  02 inj @ 100 mg/l

- km4b4  02 inj during entire si
- km2pp5  02 inj after 0.25 yrs
- km2pp6  02 inj after 0.50 yrs

Distance (ft) from first source cell
(column 9)
had higher concentrations of contaminant than the run with oxygen injected during the entire simulation. Figure 7.21, however, shows that remediation of the contaminant plume occurs at approximately the same time for all three scenarios.

Figures 7.23 - 7.25 show the plume configurations for the runs with oxygen injected for the entire simulation, no oxygen injected for 0.25 years and no oxygen injected for 0.50 years. Figures 7.23 - 7.25 also show that there is a difference in the plume concentrations for the runs with oxygen injected for varying time lengths.
Figure 7.23 CONCENTRATION OF CONTAMINANT after 0.75 years

km4b4 02 injected for entire simulation
8.0 CONCLUSIONS

This research used three models to compare analytical and numerical biodegradation solution procedures: the Horizontal Plane Source Model (HPS), the USGS method of characteristics (MOC) solute transport code (with and without first order decay (FOD), and BIOPLUME II.

8.1 Numerical vs Analytical Methods for Contaminant Transport

The HPS analytical code was compared to the USGS solute transport numerical code to determine how well the two models compare for different problem configurations. For the series of runs performed, the HPS model results compared well to the MOC model results in cases where the velocity distribution remained close to the Darcian velocity created by the background gradient in the system. However, in cases where the velocity field experienced significant mounding (such as instances of large contaminant loading), results from the HPS and MOC models differed significantly.

The two models were also compared for estimation of contaminant biodegradation using first order decay. For the case of first order degradation, the HPS model biodegrades the source area as well as the generated contaminant plume, whereas MOC degrades only the plume. After performing the MOC simulation in a mode which degraded both the contaminate source and plume, the HPS and MOC model results matched well for the case of first order decay.

8.2 Evaluation of Equivalent First Order Aerobic Degradation Rates

Predictions of biodegradation obtained using BIOPLUME II were matched with predictions from a FOD analytical solution. The total mass biodegraded in a BIOPLUME II numerical run was matched with an MOC FOD analytical
simulation by varying the value of the FOD coefficient. For a given problem
definition, the BIOPLUME II generated contaminant plume was narrower and
showed higher concentrations down the centerline than the corresponding FOD
generated contaminant plume with equal mass degraded. The FOD
contaminant plume configuration was matched to the BIOPLUME II contaminant
plume configuration by altering the ratio of transverse to longitudinal dispersivity
(Dt/Dl) in the FOD simulation. Lowering this ratio narrowed and concentrated
the FOD contaminant plume.

The selected value for the FOD coefficient (k₁) which gave the best match
between the BIOPLUME II simulation and the FOD simulation seems to be
related to the seepage velocity modeled in the problem configuration. This
relationship allows the mass biodegraded in a BIOPLUME II numerical
simulation to be matched by an FOD analytical solution, and appears to be fitted
by a simple curve. The curve which relates the FOD coefficient to the seepage
velocity is also dependent on the initial amount of oxygen in the system. There
appears to be an approximately linear relationship between the selected FOD
constant and the oxygen level in the system for the case of seepage velocity
equal to 0.38 ft/day.

A decrease in the ratio of transverse to longitudinal dispersivity, in general,
narrows and concentrates the contaminant plume generated in an FOD
simulation, thus causing the FOD contaminant plume configuration to
approximate more closely that of the BIOPLUME II contaminant plume.
Decreasing Dt/Dl to a certain value causes changes in the FOD plume, and
then further variation in this parameter does not significantly alter the results.

These results imply that for the case studied, aerobic biodegradation as
simulated by the BIOPLUME II numerical procedure could be approximated by
an analytical model. With further investigation, the relationships of FOD
coefficient and $\frac{D_t}{D_l}$ vs. seepage velocity could be incorporated into an analytical model. The ability to incorporate these relationships into an analytical code could become important if a code such as EPACML is used in the regulatory process.

8.3 Numerical Modeling for Aquifer Bioremediation

Satkin, 1987, evaluated the effect of different well patterns for aquifer restoration under variable hydrogeologic conditions. This research took five well patterns from Satkin's work and expanded upon his research by incorporating the effects of biodegradation. In this investigation, oxygen was injected into the system at varying levels, and the effect on aquifer remediation was evaluated.

Although previous sections of this work evaluated the difference between numerical and analytical solution procedures, no analytical solution exists for the case of oxygen injection in remedial pumping designs. Therefore, the BIOPLUCE II numerical model alone was used for this study.

For an existing contaminant plume, only a small difference was seen between runs performed with no oxygen and oxygen injected at 3 and 20 mg/l. The lack of difference in results between oxygen and no oxygen simulations suggested that a majority of the remediation was occurring due to the hydraulics of the system. This means that most of the plume's contaminant mass was pumped out of the system before the contaminant had a chance to biodegrade. The Double cell and 3-spot well patterns proved to be the most effective in bioremediation.

Runs were then performed for a constant source contaminant plume. The aquifer transmissivity in these simulations was 0.001 ft$^2$/s. The constant source was modeled as an injection well, and a source injection rate of 0.25 x $10^{-3}$ cfs
showed an approximately 20% difference in remediation levels between the oxygen (100 mg/l) and no oxygen schemes for both the Double cell and 3-spot well patterns after one year of simulation. For the case of aquifer transmissivity decreased by one order of magnitude (to 0.0001 ft$^2$/s), the Double cell well pattern showed the greatest difference between the oxygen and no oxygen simulations, with over a 30% difference in percent contaminant remediated between the two runs. Thus, for the case of a constant source, biodegradation was seen to have a significant impact on remediation.

The effect of varying oxygen levels on remediation was also simulated for the Traverse City Michigan field site. Runs were performed for the 1986 plume calibration from Miller's thesis (1989), for oxygen levels of 0, 20 and 100 mg/l. For these runs, with an oxygen injection concentration of 100 mg/l, the TCM plume was remediated after one year. However, with no oxygen injected into the system, over 20% of the original contaminant mass remained after two years.

In the initial TCM simulations, a sharp decline in the percent contaminant remaining for the no oxygen runs during the first six months to one year of the simulations was seen. This decline suggested that contaminant remediation was occurring hydraulically during the initial time steps. Runs were performed with multiple pumping periods to determine the effectiveness of remediating the system hydraulically for a period of time before beginning bioremediation. Results showed that remediation in two phases (hydraulic clean-up first, followed by bioremediation) could remediate the contaminant plume in the same time frame as a remediation approach which incorporated biostimulation during the entire simulation. At intermediate points in time, the two phase scheme showed higher contaminant concentrations throughout the plume than the remediation approach which injected oxygen during the entire simulation.
9.0 REFERENCES


Rifai H. S., P. B. Bedient, R. C. Borden, J. F. Haasbeek. BIOPLUME II - Computer model of two-dimensional transport under the influence of oxygen limited biodegradation in ground water. Rice University, Houston, TX.


