BIOPLUME II

COMPUTER MODEL OF
TWO-DIMENSIONAL CONTAMINANT
TRANSPORT UNDER THE INFLUENCE OF
OXYGEN LIMITED BIODEGRADATION
IN GROUND WATER

USER'S MANUAL - VERSION 1.0

National Center for Ground Water Research

Rice University
P. O. Box 1892
Houston, Texas 77251

October 1987

Disclaimer

Readme

The following will be consistent throughout the documents distributed by the Center for Subsurface Modeling Support via Acrobat Reader:

- Red text signifies a link.
- Bookmarks have been developed and will vary from document to document and will usually include table of contents, figures, and/or tables.
- Most figures/graphics will be included at the end of the document.

BIOPLUME II

by

Hanadi S. Rifai[1]
Philip B. Bedient[1]
Robert C. Borden[2]
John F. Haasbeek[1]

[1]National Center for Ground Water Research
Rice University
P. O. Box 1892
Houston, Texas

(713) 527-4951

[2]North Carolina State University Department of Civil Engineering Box 7808
Raleigh, North Carolina 27695-7908

(919) 737-2331

Cooperative Agreement No. CR-812808

Project Officer
John T. Wilson
Processes and Systems Research Division
Robert S. Kerr Environmental Research Laboratory
Ada, Oklahoma 74820

ROBERT S. KERR ENVIRONMENTAL RESEARCH LABORATORY
OFFICE OF RESEARCH AND DEVELOPMENT
U.S. ENVIRONMENTAL PROTECTION AGENCY
ADA, OKLAHOMA 74820

BIOPLUME II Version 1.1

October 1989

Update Summary

The following are the main differences between version 1.0 and version 1.1:

1. The data input format for version 1.1 has been changed from fixed format to free format. Both the preprocessor and the executable runtime modules accept input as free format. Users should be cautious when attempting to modify or run a previously prepared file in fixed format.

2. Version 1.1 will allow the user to input the stoichiometric ratio, F, of oxygen to contaminant utilized The parameter, F, is entered on card 4 as the last parameter on that card. The data to be specified on card 4 (Appendix A, page A-3) in version 1.1 are then:

```
DK
RHOB
THALF
DEC1
DEC2
F
```

It is noted that the value for F is not echoed in the output data set and the user needs to keep in mind what value is being used for the runs in question

3. Some changes were implemented to the preprocessor to adjust some of the previous problems reported by other users. These changes only enhance the preprocessor and do not affect the way the preprocessor works

4. A status message screen has been included in the runtime module to inform the user of the number of moves required to complete a simulation run. The status message screen informs the user of the present move being computed. This addition should help users figure out whether there is a problem with the input data and will give the user an idea of how long it will take to complete the run in question

5 .The graphic output files generated during a computer run (see pages 3-10 to 3-12 in the manual) in version 1.1 are generated with real numbers instead of integer values for the heads, oxygen concentrations and contaminant concentrations. This allows the user to plot the model results more accuratately.

Acknowledgements

We would like to acknowledge the following people for their valuable assistance with this project:

The Robert S. Kerr Environmental Laboratory (RSKERL) of the U. S. Environmental Protection Agency for providing us with the opportunity to develop BIOPLUME II. In particular, we thank John T. Wilson, James F. McNabb, Marion R. Scalf, Bert E. Bledsoe, and Don H. Kampbell.

L. F. Konikow and J. D. Bredehoeft for developing the USGS 2-D solute transport model which provided the basis for our code.

Dr. John M. Armstrong of the Traverse Group, Inc. for providing valuable field data from the Traverse City field site in Michigan for testing BIOPLUME II, and U. S. Coast Guard Commander John H. Sammons for providing us with the opportunity to work at the Traverse City field site.

Pamela J. Ross for providing her technical skills, time and effort in developing this document. Jill A. Oglesby and Karen M. Miller for testing BIOPLUME II. Charles J. Newell for his valuable advice throughout this project.

Disclaimer

The information in this document has been funded wholly or in part by the United States Environmental Protection Agency under Cooperative Agreement No. CR-812808 to Rice University. It has been subjected to the Agency's peer and administrative review, and it has been approved for publication as an EPA document. Mention of trade names or commercial products does not constitute endorsement or recommendation for use.

Foreword

EPA is charged by Congress to protect the Nation's land, air and water systems. Under a mandate of national environmental laws focused on air and water quality, solid waste management and the control of toxic substances, pesticides, noise and radiation, the Agency strives to formulate and implement actions which lead to a compatible balance between human activities and the ability of natural systems to support and nurture life.

The Robert S. Kerr Environmental Research Laboratory is the Agency's center of expertise for investigation of the soil and subsurface environment. Personnel at the Laboratory are responsible for management of research programs to: (a) determine the fate, transport and transformation rates of pollutants in the soil, the unsaturated and the saturated zones of the subsurface environment; (b) define the processes to be used in characterizing the soil and subsurface environment as a receptor of pollutants; (c) develop techniques for predicting the effect of pollutants on ground water, soil, and indigenous organisms; and (d) define and demonstrate the applicability and limitations of using natural processes, indigenous to the soil and subsurface environment, for the protection of this resource.

This project was initiated to provide a computer model that could be used to screen hazardous waste sites and determine whether natural biological processes could be used to contain the spread of pollution, or remediate the source of contamination. The computer model is designed to run on a personal computer instead of a mainframe, which makes the model readily available to regional and state regulators.

Clinton W. Hall
Director
Robert S. Kerr Environmental
Research Laboratory

System Requirements

To run BIOPLUME ll, you need the following:

1. IBM PC/AT or compatible
2. DOS version 2.0 (or later)
3. 640K of machine resident memory (RAM)[1]
4. 80287 math co-processor chip
5. Hard disk[2]

Optional hardware includes:

6. Graphics adapter (CGA, EGA, or Hercules)[3]
7. SURFER suppported graphics printer or plotter
   (see Appendix D of SURFER manual)

System Setup

In order to run the programs, the following command must be included in the file CONFIG.SYS on your system disk:

DEVICE = ANSI.SYS

Note that the file ANSI.SYS, included with the DOS package, must reside in the same directory as CONFIG.SYS. Otherwise a pathname must be included in the file. Please refer to your DOS reference manual for details on this command.

---

[1]A minimum of 550K of RAM is necessary to load the model with the menu preprocessor. To check available RAM, type the command CHKDSK. If there is less memory available, the model (DRIVER.EXE) may still be loaded without the menu preprocessor. Please contact Rice University if you have any questions.

[2]It is possible to run the model using a high-density floppy drive if a hard disk is not available in your system.

[3] The VIEW program and the View option in TOPO and SURF both require a graphics card (adapter). However, if your system does not have a graphics card, SURFER may still be used to generate graphics on a graphics printer or plotter (Golden Software, Inc., 1987).

Table of Contents

List of Figures

List of Tables

Abstract

This manual presents a two-dimensional computer model, BIOPLUME ll, that simulates the transport of dissolved hydrocarbons under the influence of oxygen-limited biodegradation. BIOPLUME ll also simulates reaeration and anaerobic biodegradation as a first order decay in hydrocarbon concentrations.

The model is based on the USGS solute transport two-dimensional code (Konikow and Bredehoeft, 1978). The model computes the changes in concentration over time due to convection, dispersion, mixing, and biodegradation. The same numerical techniques that are used in the USGS code are maintained in BIOPLUME ll.

BIOPLUME ll solves the solute transport equation twice: once for hydrocarbon and once for oxygen. As a result, two plumes are computed at every time step. The model assumes an instantaneous reaction between oxygen and hydrocarbon to simulate biodegradation processes. The two plumes are combined using the principle of superposition.

The model is extremely versatile in that it can be used to simulate natural biodegradation processes, retarded plumes, and in-situ biorestoration schemes. BIOPLUME ll allows injection wells to be specified as oxygen sources into a contaminated aquifer. This means that alternate methods for aquifer reclamation can be investigated to design the most economically feasible scheme.

The model provides three additional sources of oxygen into an aquifer: initial dissolved oxygen in the uncontaminated aquifer, natural recharge of oxygen across the boundaries, and vertical exchange of oxygen from the unsaturated zone (reaeration). All three sources of oxygen can be used to simulate a contaminant plume that is being naturally biodegraded.

BIOPLUME ll runs on an IBM PC/AT or compatible system. A menu-driven preprocessor was developed to assist the user in applying the model. The preprocessor provides three options: data input or data edit, performing a simulation run, and developing graphical output. A graphics software program, SURFER, from Golden Software, Inc. (1987), was selected to provide the user with contour and surface plots of hydrocarbon and oxygen concentrations and water table elevations.

Introduction

This manual describes a computer model for simulating transport of hydrocarbons (HC) in ground water under the influence of oxygen (O_2) limited biodegradation. The model core is based on the USGS 2-D solute transport model (Konikow and Bredehoeft, 1978). Although this manual is self-contained and will allow the user to run BIOPLUME ll easily, it is recommended that the user be familiar with the USGS code beforehand. A user-friendly menu-driven preprocessor has been built in the code. The preprocessor provides the user with three options: 1)data input/editing; 2) simulation run performance; and 3) graphical representation of output. The model is designed to run on an IBM PC/AT or compatible system.

The purpose of the simulation model is to compute the concentration of a dissolved hydrocarbon that is undergoing biodegradation in an aquifer. Changes in chemical concentration occur primarily due to four distinct processes: 1) convective transport, in which dissolved chemicals are moving with the flowing ground water; 2) hydrodynamic dispersion, in which molecular and ionic diffusion and small scale variations in the velocity of flow through the porous media cause spreading of the contaminant front; 3) fluid sources or sinks, such as pumping or injecting wells, and; 4) reactions, in which the concentration of the contaminant may increase or decrease due to chemical and physical reactions within the ground water or between the water and the solid aquifer material.

The standard 2-D USGS code assumes that no reactions occur which affect the concentration of the species of interest. BIOPLUME ll, on the other hand, assumes an instantaneous reaction between HC and O_2. The instantaneous reaction decreases the concentration of HC by an amount that is proportional to the available O_2 in the aquifer (it is assumed that 3 units of O_2 are required to completely biodegrade 1 unit of HC).

BIOPLUME ll solves the solute transport equation twice, once for HC and once for O_2. This allows the simultaneous simulation of two plumes; an HC plume and an O_2 plume. The two plumes are combined using superposition at every particle move to simulate the reaction between HC and O_2.

BIOPLUME ll is extremely versatile: it allows the simulation of a retarded HC plume undergoing biodegradation and it provides the user with the capability to simulate *in-situ* biorestoration schemes such as the injection of oxygenated water. Moreover, the model simulates anaerobic biodegradation and reaeration as a first order decay in HC concentrations.

1. Theoretical Background

1.1 Literature Review

1.1.1 Biodegradation Processes

Recent studies have indicated that many subsurface microorganisms are metabolically active and are able to degrade a wide variety of contaminants. Ghiorse and Balkwill (1983, 1985) observed population densities of approximately 10^6 cells per gram aquifer material at sites in Louisiana and Oklahoma using epifluorescent microscopy.

The microorganisms present appear to be predominantly bacteria (Hirsh and Rades-Rohkohl, 1983), but a few higher life forms have been detected (Wilson *et al.,* 1983; Ghiorse and Balkwill, 1985; White et al., 1983). Some eucaryotic forms which may be fungal spores or yeast cells have been observed in the upper 10 m of a soil profile (Ghiorse and Balkwill, 1983; Federle *et al.,* 1986).

There are many environmental factors which limit the biodegradation of subsurface organic pollutants, even in the presence of adapted microorganisms (Thomas *et al.,* 1987). These factors include the lack of an essential nutrient, substrate concentration, substrate inaccessibility, and the presence of toxicants (Alexander, 1975). The transport of contaminants in the subsurface also affects biodegradation.

Biodegradation of many organic pollutants in the subsurface may be limited by insufficient oxygen. Lee and Ward (1985) found that the rate and extent of biotransformation of naphthalene, 2-methyl naphthalene, dibenzofuran, fluorene, and phenanthrene were greater in oxygenated water than in oxygen-depleted water.

Recent research has also indicated that biodegradation can occur under anaerobic conditions. Kuhn et al. (1985) reported mineralization of xylenes in samples of river alluvium under denitrifying conditions. In addition, benzene, toluene, xylenes, and other alkylbenzenes were metabolized in methanogenic river alluvium that had been contaminated with landfill leachate (Wilson and Rees, 1986).

In addition to oxygen, other nutrients may limit the biodegradation of organic pollutants in the subsurface. Inorganic nutrients, such as nitrogen and phosphorous, may be limiting when the ratios of carbon to nitrogen or phosphorous exceed that necessary for microbial processes (Thomas et al., 1987). Also, the presence of sulfate may inhibit methanogenic bacteria that have been reported to dehalogenate and mineralize many chlorinated aromatic compounds (Suflita and Gibson, 1985; Suflita and Miller, 1985).

1.1.2 In-Situ Biorestoration

Microbial processes may be used to degrade contaminants *in-situ* by stimulating the native microbial population (Thomas *et al.,* 1987). Addition of electron acceptors, such as oxygen, and inorganic nutrients, typically nitrogen, phosphorous, and trace metals may provide the microorganisms with essential nutrients that are limiting in the presence of high concentrations of pollutants (Thomas *et al.,* 1987).

Inoculation of a specialized microbial population and the addition of surfactants to increase the availability of contaminants to the microorganisms can also be used. In general, biological processes, when possible, may offer the advantage of partial or complete removal of the contaminants rather than simply transferring the pollutants to another phase in the environment (Thomas *et al.,* 1987).

The application of *in-situ* biorestoration technology to site remediation is relatively new. Raymond (1974) received a patent on a process designed to remove hydrocarbon contaminants from ground water by stimulating the indigenous microbial population with nutrients and oxygen. The process was applied at a

site in Ambler, Pennsylvania where a pipe line leak had introduced an estimated 380,000 liters of high octane gasoline into the underlying aquifer.

Approximately two-thirds of the gasoline was recovered using conventional pump/treat systems, however, the time estimated for complete restoration using these systems was more than 100 years. A nutrient amendment scheme was implemented at the site. The nutrients added were oxygen, ammonium sulfate, disodium phosphate, and monosodium phosphate. During the period of nutrient addition, the concentration of gasoline in the ground water did not decline, however, ten months later gasoline could not be detected in the ground water (Raymond *et al.,* 1975).

There are many methods of introducing oxygen into contaminated aquifers. Brown *et al.* (1985) used air sparging at a gasoline contamination site. Wilson and Ward (1987) have suggested other methods, such as soil venting or air flooding. The problem that one faces is that these methods can only provide dissolved oxygen concentrations of 8 to 12 mg/l depending on the temperature of the ground water. Hydrogen peroxide, pure oxygen and ozone have been proposed as more efficient methods of supplying oxygen into contaminated aquifers. Concentrations of 40 to 50 mg/l can be achieved with pure oxygen, but pure oxygen is somewhat expensive, may bubble out of solution before the microorganisms can use it, and is extremely flammable (Brown *et al.,* 1984).

Hydrogen peroxide is another possible source of oxygen, however, it is used as a sterilant at concentrations of 3 percent and levels as low as 200 ppm can be toxic to microorganisms (Thomas *et al.,* 1987). In a column study in which oxygen concentration was varied from 8 to 200 ppm using air, pure oxygen, or a hydrogen peroxide solution, microbial growth and gasoline degradation were greater in columns amended with hydrogen peroxide which provided the highest concentration of available oxygen (Brown *et al.,* 1984). A more thorough review of field studies using hydrogen peroxide can be found in Thomas *et al.* (1987). Ozone can also be used as a source of oxygen, but very little research has been done on it.

1.1.3 Biodegradation Modeling

Modeling biodegradation and biorestoration processes involves: 1) description of the kinetics of biotransformation in the subsurface, 2) description of transport processes of the contaminant and available nutrients, and 3) an appropriate procedure for predicting the effect of biorestoration. A few investigators have begun work on describing some of these processes.

Kosson *et al.* (1985) use a simple one-dimensional finite difference solution to simulate the movement of hazardous industrial wastewater through an acclimated soil column. The model adequatly matches experimental data from the later portion of the column where an acclimated microbial population has developed.

Angelakis and Rolston (1985) present a mathematical model for simulating the movement of insoluble and soluble organic carbon through the unsaturated soil profile. The results of the simulation compare favourably with experimental data from a series of column tests performed using primary wastewater effluent. Baehr and Corapcioglu (1985) present a one-dimensional model for simulating gasoline transport by air, water, and free hydrocarbon phases. No experimental data are presented to test the model.

Molz *et al.* (1986) present a numerical model for simulating substrate and oxygen transport and use by attached microorganisms. The microbial population is assumed to be immobile and present in microcolonies of an average radius and thickness. Transport into the microcolonies of oxygen and substrate is limited by diffusion through a stagnant layer adjacent to the microcolony. Laboratory testing of the model is planned.

Borden and Bedient (1986) present a numerical model of oxygen-limited biodegradation of hydrocarbons in the saturated zone. Their model is discussed in detail in the following section as it provides the basis for the development of BIOPLUME ll. Borden et al. (1986) have applied the model to simulate oxygen-limited biodegradation of creosote wastes at a Superfund site. The model gave an

adequate description of the observed hydrocarbon and oxygen distributions in the shallow aquifer and was used to study various remedial actions at the site.

1.2 Model Development

1.2.1 Equation Formulation

Borden and Bedient (1986) present the theoretical basis for the development of BIOPLUME ll. A summary of their discussion is presented in this section for completeness. Borden and Bedient (1986) simulate the growth of microorganisms and removal of hydrocarbon and oxygen using a modification of the Monod function where:

$$\frac{dH}{dt} = -M_t \bullet k \quad \frac{H}{(K_h + H)} \quad \frac{O}{(K_o + O)} \qquad (1)$$

$$\frac{dO}{dt} = -M_t \bullet k \bullet F \quad \frac{H}{(K_h + H)} \quad \frac{O}{(K_o + O)} \qquad (2)$$

$$\frac{dM_t}{dt} = M_t \bullet k \bullet Y \quad \frac{H}{(K_h + H)} \quad \frac{O}{(K_o + O)} + K_c \bullet Y \bullet OC - b \bullet M_t \qquad (3)$$

where

H = hydrocarbon concentration
O = oxygen concentration
M_t = total microbial concentration
k = maximum hydrocarbon utilization rate per unit mass microorganism
Y = microbial yield coefficient (g cells/g hydrocarbon)
K_h = hydrocarbon half saturation constant
K_o = oxygen half saturation constant
K_c = first order decay rate of natural organic carbon
OC = natural organic carbon concentration
b = microbial decay rate
F = ratio of oxygen to hydrocarbon consumed

Equations (1) and (2) for oxygen and hydrocarbon removal were combined with the advection-dispersion equation (Bear, 1979) for a solute undergoing linear instantaneous adsorption and the following equations were obtained:

$$\frac{\partial H}{\partial t} = \frac{\nabla(D\nabla H - vH)}{R_h} - \frac{M_t \bullet k}{R_h} \quad \frac{H}{(K_h + H)} \quad \frac{O}{(K_o + O)} \qquad (4)$$

$$\frac{\partial O}{\partial t} = \nabla(D\nabla O - vO) - M_t * k * F \frac{H}{(K_h + H)} \frac{O}{(K_o + O)} \qquad (5)$$

where

D = dispersion tensor

v = ground water velocity vector

R_h = retardation factor for hydrocarbon

The exchange of microorganisms between the solid surface and the free solution was assumed to be rapid and follow a linear relationship with total concentration. The movement of microorganisms was simulated using a simple retardation factor approach (Freeze and Cherry, 1979):

$$\frac{\partial M_s}{\partial t} = \frac{\nabla(D\nabla M_s - vM_s)}{R_m} + M_s \bullet k \bullet Y \frac{H}{(K_h + H)} \frac{O}{(K_o + O)} \qquad (6)$$

$$+ \frac{K_C \bullet Y \bullet OC}{R_m} - b \bullet M_s$$

where M_s = concentration of microbes in solution

M_a = concentration of microbes attached to solids

K_m = ratio of microbes attached to microbes in solution

R_m = microbial retardation factor

$M_a = K_m \bullet M_s$

$M_t = M_s + M_a$

$= (1 + K_m) \bullet M_s$

$= R_m \bullet M_s$

1.2.2 One-Dimensional Simulations

Studies with the one-dimensional solution indicated that there are three general regions where different processes control the rate and extent of degradation. Figure 1.1 shows the location of these regions and the variation in oxygen and hydrocarbon with distance. The rate of biodegradation will be very high in the region closest to the source where a large microbial biomass will develop and result in nearly complete removal of oxygen.

The mass transfer between oxygen in the formation water and hydrocarbon in the plume will limit the rate of biodegradation in the "heart" of the plume. At the leading edge of the plume, a zone of reduced oxygen and hydrocarbon concentrations will develop. As the plume continues to move, the zone of reduced oxygen and hydrocarbon concentrations will increase in size and limit mass transfer. In the third region, downstream of the contaminant plume, oxygen is present in excess and hydrocarbon will be absent or present at trace concentrations.

Sensitivity analysis with the one-dimensional model indicated that the various microbial parameters (K_h, K_o, k, Y, F) had little or no effect on the hydrocarbon distribution in the body of the plume and on the time to hydrocarbon breakthrough. This suggested that the consumption of hydrocarbon and oxygen by microorganisms in the body of the plume (Region 2, Figure 1.1) can be approximated as an instantaneous reaction between oxygen and hydrocarbon. In explicit finite difference form, this approximation is written as:

$$H(t+1) = H(t)-O(t)/F \qquad (7)$$

$$O(t+1) = 0$$

where $H(t) > O(t)/F$

$$O(t+1) = O(t)-H(t) \bullet F \qquad (8)$$

$$H(t+1) = 0$$

where $O(t) > H(t) \bullet F$

where H(t), H(t+1), O(t), O(t+1) are the hydrocarbon and oxygen concentrations at time t and t+1.

Results obtained using the instantaneous reaction approximation were compared with the complete one-dimensional solution in Figure 1.1. The instantaneous reaction approximation closely matched the complete solution except in Region 1. The width of this region will depend on the mixing properties of the aquifer near the contaminant source, the ground water velocity and the nature of the contaminant. If ground water velocities are very high or the hydrocarbon is poorly degradable, the area in which the instantaneous reaction assumption is not applicable may be significant.

1.2.3 Two-Dimensional Simulations

1.2.3.1 Vertical 2-D Simulations

Borden and Bedient (1986) conclude that vertical exchange of oxygen with the unsaturated zone could potentially result in significant fluxes of oxygen into a hydrocarbon plume and that this exchange would be most important for contaminants such as gasoline which occur at or near the water table. Simulation results with the two-dimensional vertical model indicated that the effect of vertical exchange of oxygen with the unsaturated zone can be approximated as a first order decay in hydrocarbon concentrations. Sensitivity analysis with the two-dimensional model indicated that the vertical dispersion coefficient and the saturated thickness had the greatest impact on the first order decay rate.

1.2.3.2 Horizontal 2-D Simulations

Two-dimensional simulations generated plumes with similar characteristics to the one-dimensional simulations. The most notable characteristic was the lack of lateral spread, i.e, the plumes were long and narrow. The HC plume has a somewhat lower peak concentration and is much narrower in the cross-

section than the plume for a nonreactive tracer such as chloride when the source concentration for both are equal. For non-adsorbing hydrocarbons, the major source of oxygen into a plume seems to be transverse mixing. Longitudinal mixing has little impact on oxygen exchange with the plume possibly because the plumes are narrow in width.

Figure 1.1 Process Control Regions

2. Overview of the Model

2.1 Description of the Program

The purpose of this section is to describe the overall structure of the program and to present a detailed description of the model's capabilities. This section is not intended to discuss the numerical methods and techniques used to solve the flow and transport equations since these methods are discussed in detail in the USGS manual (Konikow and Bredehoeft, 1978). It should be noted, however, that most numerical limitations of the USGS code apply to BIOPLUME ll and the user needs to be aware of these limitations. The user also needs to be aware of the limitations of the method of characteristics for solving the transport equation.

The major steps in the calculation procedure are summarized in Figure 2.1, which presents a simplified flow chart of the overall structure of the computer program. The flow chart illustrates that two independent sets of particles, O_2 tracer particles and HC tracer particles, are generated. Since the tracer particles may have to be moved more than once to complete a given time step and the reaction between O_2 and HC is assumed instantaneous, the O_2 and HC tracer particles are moved independently and their subsequent concentrations are also computed independently. The resulting two plumes (HC and O_2) are combined after every particle move time step to simulate the reaction between O_2 and HC. In this version of the model, it is assumed that three units of oxygen are required to completely mineralize one unit of hydrocarbon (parameter F, equations 7 and 8, section 1.2.2). More work is necessary before this parameter can be defined on a compound by compound basis. This technique, although it probably requires more computational time, is extremely beneficial due mainly to the following reasons:

1) It provides the capability to simulate retarded HC plumes undergoing biodegradation.

2) It allows the simulation of in-situ biorestoration since one can model the injection of oxygenated water.

3) It maintains the modular structure of the program which makes future updates relatively simple.

For the case of retarded HC plumes undergoing biodegradation, the model automatically computes the maximum time increments allowable for the explicit calculations for the retarded HC plume and for the non-retarded O_2 plume. The model then uses the smaller of the two time steps for the explicit solution of the solute transport equation (i.e. the larger number of particle moves is used to complete the given time step).

The flow chart also illustrates that hydraulic gradients are computed once for the aquifer in question. The flowrates specified for pumping or injection wells are used in the computation. However, if one specifies an injection well, then that well can be used to simulate a contaminant source, an oxygen source, or both, by specifying the concentration of HC and/or O_2 in the injected water.

Mass balance computations are performed for both O_2 and HC independently at the end of every particle move. The mass balance computations are then adjusted to account for the mass loss due to biodegradation after the two plumes have been superimposed. The amount of mass loss due to biodegradation is printed as part of the chemical mass balance output. This is extremely useful since one can correlate the simulated mass loss with the observed mass loss from field data. The mass balance computations for O_2 are necessary to insure the accuracy of the numerical technique when one is simulating an O_2 injection scheme.

In addition to aerobic biodegradation, the model provides two other sources for biodegradation: anaerobic decay and reaeration. Both are simulated as a first order decay in HC concentrations, and the only input requirement is the coefficient of decay. The decay terms are applied at the nodes and not at the particles. This provides more numerical stability in case the coefficient of decay is much smaller than the

move time step. The chemical balance output also provides the user with the amount of mass loss due to reaeration and anaerobic decay.

It should be mentioned that the model can be used to simulate plumes without biodegradation terms. The user would have to set all the oxygen sources in the model to zero. The output for the oxygen plume is not suppressed. Instead, a null plume for oxygen is printed.

2.1.1 Incorporated Revisions of the USGS MOC Code

The USGS MOC Code has been modified several times since it was first introduced. The following changes (referred to by date) have been incorporated in this version of BIOPLUME ll:

May 16, 1979
March 26, 1980
August 26, 1981
October 12, 1983
June 10, 1985
July 26, 1985
July 31, 1985
August 2, 1985
August 8, 1985
August 12, 1985

Future revisions to the USGS MOC Code will be incorporated and released as upgraded versions of BIOPLUME ll.

2.1.2 Code Verification

The accuracy of a numerical solution is usually evaluated by comparing the results from the numerical solution to the results from an analytical solution for a particular problem. The USGS MOC code has been compared to several analytical solutions and the user is referred to the documentation on the code for more details (Konikow and Bredehoeft, 1978).

2.2 Program Capabilities

BIOPLUME ll is designed basically to handle two different types of simulations:

1) Simulation of a hydrocarbon plume that is being naturally biodegraded.

2) Simulation of in-situ biorestoration schemes by injecting oxygenated water into the contaminated aquifer.

The model also has the capability to simulate anaerobic biodegradation and reaeration as a first order decay in HC concentration.

2.2.1 Simulation of Naturally Occurring Biodegradation

The basic data requirements for this type of simulation would be the physical parameters for the aquifer and some information about the amount of oxygen available in the aquifer prior to contamination. BIOPLUME ll simulates four sources of O_2 in the aquifer:

1) Initial Oxygen Concentration: The initial O_2 concentration refers to the dissolved oxygen available in the aquifer prior to contamination.This value is obtained by performing adissolved oxygen measurement in the field from a pristine or uncontaminated zone. The background O_2 value is input in the array CONC1 (Data Set 10, Appendix A).

2) Natural Recharge of Oxygen: The natural recharge of O_2 refers to the dissolved oxygen that would be transported into the aquifer due to the flow of ground water. The user can assign an O_2 concentration to the constant head nodes. This value is input as the variable FCTR4 (Data Set 7, Appendix A).

3) Vertical Exchange of Oxygen with the Unsaturated Zone: Vertical exchange of O_2 or reaeration is simulated as a first order decay in HC concentration. A constant decay coefficient (DEC2) is required as input to the model (Card 4, Appendix A). The first order decay is applied at the nodes and not to the particles. (This technique prevents any numerical instabilities that could occur if the coefficient of decay was small relative to the particle movement time step.)

4) Injection of Oxygenated Water: The fourth source of O_2 into the aquifer is through injection of O_2 rich water. Injection wells specified in Data Set 2 (Appendix A) can be simulated as contaminant sources, O_2 sources, or both. The concentration of O_2 is input as the variable CNRECO (Data Set 2, Appendix A).

The first three sources of O_2 are used to simulate natural biodegradation of a contaminant plume. Test Problem #1 (Section 4.1) illustrates the simulation techniques for a contaminant plume undergoing natural biodegradation using the first two sources of oxygen (initial oxygen and natural recharge). Test Problem #2 (Section 4.2) illustrates the use of reaeration as an additional source of oxygen into an aquifer.

2.2.2 Simulation of In-Situ Biorestoration

In order to simulate in-situ biorestoration schemes, the user must specify the following:

1) The concentration distribution of HC in the aquifer: The HC plume to be cleaned up is input in the array CONC (Data Set 9, Appendix A). This plume could be obtained from field measurements or from a previous BIOPLUME ll simulation effort (with or without natural biodegradation depending on the particular field conditions).

2) The concentration distribution of O_2 in the aquifer: The O_2 distribution in the aquifer is input in the array CONC1 (Data Set 10, Appendix A). This plume can be obtained from a previous BIOPLUME ll simulation if the HC plume was being naturally biodegraded. For other cases, the O_2 distribution would be obtained from field measurements.

3) Injection well data: The location, rate, and concentration of injected water are input in Data Set 2 (Appendix A). The concentration of O_2 in the injected water is input as the variable CNRECO (Data Set 2, Appendix A).

Test Problem #3 illustrates modeling of an in-situ biorestoration scheme. A doublet injection/production scheme is used to predict the clean-up time required to restore the contaminated aquifer modeled in Test Problem #1.

2.3 Sensitivity Analysis

In order to define which parameters have the most effect on biodegradation in BIOPLUME ll, the following detailed sensitivity analysis was performed. The parameters that were investigated included: hydraulic conductivity, dispersivity (longitudinal and transverse), porosity, reaeration, and retardation.

A hypothetical contaminant plume was generated using a single continuous hydrocarbon source. The above mentioned parameters were then varied individually to determine their effect on biodegradation. The results from the sensitivity analyses indicate that biodegradation in the model is most sensitive to hydraulic conductivity, the coefficient of reaeration, and the coefficient of anaerobic decay. The following input data was utilized in the base run:

Simulation time	10 years
Grid size	20 x 30
Cell size	50 ft x 50 ft
Porosity	0.3
Longitudinal Dispersivity	10 ft
Transverse Dispersivity	3 ft
Txx	.0025 ft^2/s
Tyy	.0025 ft^2/s
Aquifer thickness	25 ft
Hydraulic Gradient	4.29E-3 ft/ft
Injection well at cell	X=10,Y=10
Injection rate	0.0002 cfs
Conc. of contaminant in injected water	150 mg/l
Conc. of oxygen in injected water	0.0 mg/l
Initial Conc. of oxygen	8.0 mg/l
Conc. of natural recharge of oxygen	8.0 mg/l

A detailed discussion of the sensitivity analyses is included in the following sections.

2.3.1 Variation of Concentrations with Hydraulic Conductivity

The hydraulic conductivity (K) was varied from 10^{-4} ft/sec to 10^{-7} ft/sec. Figure 2.3 is a plot of the contaminant and oxygen concentrations along the centerline of the plume (cross section A - A, Figure 2.2) for three values of hydraulic conductivity. It can be seen that the hydraulic conductivity has a significant effect on biodegradation. The maximum contaminant concentration varied from 29.6 mg/l (K = 10^{-4} ft/sec) to 130 mg/l (K = 10^{-7} ft/sec). The change in biodegraded mass with hydraulic conductivity is illustrated in Figure 2.4.

2.3.2 Variation of Concentrations with Retardation

The effect of retardation on biodegradation was studied by using a retardation factor, R, greater than 1. Figure 2.5 presents the variation in contaminant and oxygen concentrations along the centerline of the plume (section A - A, Figure 2.2) for three values of R. It can be seen that the mass of hydrocarbon remaining at the end of the simulation period decreases with increasing values of R. The percent of mass biodegraded relative to the total dissolved mass, however, decreases for increasing values of R (Figure 2.4b).

Table 2.1 lists the percent of mass biodegraded relative to the total dissolved mass and the percent of mass biodegraded relative to the total stored mass. Table 2.1 also lists the percent of mass adsorbed relative to the total stored mass for the three values of R. Table 2.1 indicates that the percent of biodegraded mass decreases with increasing values of retardation (columns A and B).

Table 2.1 - Percent Biodegraded Mass as a Function of the Retardation Factor (R)

R	A	B	C
1	30.25	30.25	0.00
2	27.73	13.86	50.00
3	25.74	8.58	66.67

A = BM/TDM
B = BM/TSM
C = AM/TSM

BM = Biodegraded Mass
AM = Adsorbed Mass
TDM = Dissolved Mass + Biodegraded Mass
TSM = Dissolved Mass + Biodegraded Mass + Adsorbed Mass

2.3.3 Variation of Concentrations with Dispersivity

The variation of contaminant concentrations with dispersivity was examined by looking at the longitudinal and transverse dispersivities independently.

2.3.3.1 Longitudinal Dispersivity

The longitudinal dispersivity was varied from 10 ft to 1 ft. Figure 2.6 presents the variation in contaminant and oxygen concentrations along the centerline of the contaminant plume (section A - A, Figure 2.2) for three values of longitudinal dispersivity. It can be seen that the longitudinal dispersivity also has a slight effect on biodegradation. The maximum contaminant concentrations varied from 29.6 mg/l (10 ft) to 41.7 mg/l (1 ft). The change in biodegraded mass with longitudinal dispersivity is illustrated in Figure 2.7.

2.3.3.2 Transverse Dispersivity

The transverse dispersivity was varied from 1 ft to 5 ft. Figure 2.8 shows the variation of contaminant and oxygen concentrations with transverse dispersivity along a transverse cross section through the centerline of the plume (cross section B - B, Figure 2.2). The transverse dispersivity does not seem to have an appreciable effect on biodegradation. The areal extent of the plume is not very sensitive to the transverse dispersivity, however, the maximum concentrations exhibit a wide range of variation. The maximum contaminant concentrations varied from 26.5 mg/l (5 ft) to 35.5 mg/l (1 ft). The change in biodegraded mass with transverse dispersivity is illustrated in Figure 2.7.

2.3.4 Variation of Concentrations with Porosity

The porosity was varied from 0.25 to 0.7. Figure 2.9 shows the variation of contaminant and oxygen concentrations with porosity along the centerline of the plume (section A - A, Figure 2.2). It is evident that porosity does not have a significant effect on biodegradation. The maximum contaminant concentrations varied from 29.0 mg/l (n = 0.25) to 35.0 mg/l (n = 0.5). The change in biodegraded mass with porosity is illustrated in Figure 2.4b.

2.3.5 Variation of Concentrations with Reaeration Coefficient

The reaeration coefficient, k, was varied from 0.0 day^{-1} to 0.005 day^{-1}. Figure 2.10 presents the variation of contaminant and oxygen concentrations with k along the centerline of the plume (cross section A - A, Figure 2.2). It is evident that the coefficient of reaeration has a significant effect on biodegradation. The areal extent of the contaminant plume as well as the maximum concentrations exhibit a wide range of variation with k. The maximum concentrations varied from 29.6 mg/l (k = 0.0 day^{-1}) to 17.6 mg/l (k = 0.005 day^{-1}). The change in biodegraded mass with k is presented in Figure 2.4a.

2.4 Model Output

Typical output from BIOPLUME ll includes an oxygen and hydrocarbon distribution matrix at selected points in time (see Appendix B). These matrices can be plotted as contour plots (Figure 4.1) or surface plots using the SURFER graphics package (Golden Software, 1987). The graphics option in the BIOPLUME ll preprocessor will transform the oxygen and hydrocarbon matrices to the required format for direct use in SURFER.

It can be seen from Figure 4.1 that whenever hydrocarbon is present in relatively high concentrations, then oygen is absent. The oxygen plume forms an envelope for the hydrocarbon plume with oxygen concentrations gradually increasing to initial background levels as one moves away from the contaminant plume. The model output also includes a mass balance computation for oxygen and hydrocarbon at the selected points in time. The dissolved mass present in the system for each is computed, as well as the biodegraded mass. The hydrocarbon mass balance computation details the biodegraded mass due to the different processes available in the model (aerobic, anaerobic, reaeration and radioactive decay). It is noted at this point that a detailed analysis of mass balance errors computed in BIOPLUME ll is being performed for a variety of conditions and geometries. The results of the analysis will be included in future updates to the manual.

2.5 Summary

BIOPLUME ll simulates hydrocarbon transport under the influence of oxygen limited biodegradation. A dual particle mover concept is used to compute an oxygen plume and a hydrocarbon plume. An instantaneous reaction between the solute (hydrocarbon) and the substrate (oxygen) is assumed and the method of superposition is utilized to represent the reaction between the two. An independent mass balance is performed for oxygen and hydrocarbon and is adjusted to account for the mass loss due to biodegradation.

The model can be used to simulate naturally occuring biodegradation processes and to simulate in-situ restoration processes. Injection wells can be used as oxygen sources in the model. Three other sources of oxygen are included in BIOPLUME ll: (1) dissolved oxygen in the aquifer; (2) natural recharge, and; (3) oxygen exchange fron the unsaturated zone.

The biodegraded mass in the model is most sensitive to hydraulic conductivity, the coefficient of reaeration, and the coefficient of anaerobic decay. The model has been applied to two sites: a wood creosoting process waste site in Conroe, Texas (Borden et al., 1986) and a jet fuel spill site in Traverse City, Michigan. The model application to the Traverse City site is presently being submitted for publication. The model provided a good match to field conditions at both sites. BIOPLUME ll is presently being used to design an in-situ bioreclamation field experiment at the Traverse City field site. Results from the experiment will also be published in the literature.

3. Use of the Preprocessor

A user-friendly menu-driven preprocessor has been written for BIOPLUME II. This preprocessor allows a user to create and/or edit data files, run the BIOPLUME ll program, and prepare graphics files. The preprocessor can be executed by typing the command:

```
menu
```

This command will cause a title screen to be displayed on the terminal. When the enter or carriage return key is pressed, a second title screen will appear. Pressing the enter key again will cause the main menu to be displayed:

```
1    Edit/Create an Input Data File
2    Run BIOPLUME II
3    Prepare Graphics Files
4    QUIT
```

To choose an option, simply type the number of the option and press the enter or return key (indicated by <ENTER> or <CR>). Each of the options of the main menu are discussed in more detail in the following sections.

Throughout the remainder of this manual, messages which the computer displays on the screen will be indicated in boldface type, such as that used above in the main menu. Commands or responses entered by the user will be indicated in smaller type such as the command

```
menu
```

Responses to the program may be made in either upper or lower case. The program will recognize an

```
N
```

and an

```
n
```

as the same response. You may stop at any point in the program simply by pressing CTRL C (hold down the CTRL key and press C at the same time). The following message will appear on the screen:

Press the <ENTER> key to continue . . .

Pressing the <ENTER> key will return you to the main menu.

3.1 Option 1: Edit/Create an Input Data File

Option 1 of the main menu allows one to either edit an existing data file or create a new data file. The editing program is structured to allow editing of an entire data file or any portion of a data file. When option 1 is selected, a message will appear on the screen which indicates the version of the editing program. A continuation prompt appears at the bottom of the screen. If you do not wish to continue, type an

N

and <ENTER>. (Remember that responses may be in either upper or lower case.) Pressing <ENTER> again will return you to the main menu.

If you do wish to continue with the Edit/Create option, enter the letter

Y

and press the <ENTER> key or simply press the <ENTER> key. The screen will clear and the following menu will appear.

```
Loader
Main Menu
1.      Edit file name
2.      Edit card 1 (Title)
3.      Edit card 2 (Grid/timing parameters)
4.      Edit card 3 (Grld/timing parameters)
5.      Edit card 4 (Reaction parameters)
6.      Edit data set 1 (Observation wells)
7.      Edit data set 2 (Pump/Inject wells)
8.      Edit data set 3 (Transmissivity map)
9.      Edit data set 4 (Thickness map)
10.     Edit data set 5 (Recharge map)
11.     Edit data set 6 (Nodeid map)
12.     Edit data set 7 (Nodeid code definitions)
13.     Edit data set 8 (Water table elevations)
14.     Edit data set 9 (Initial hydrocarbon conc.)
15.     Edit data set 10 (Initial oxygen conc.)
16.     Edit data set 11 (Pumplng periods)
17.     Write data to file
18      Quit

Enter the number of your cholce (1-18)
```

Selections 2 through 16 allow editing of groups of data. As each group of data is edited, variable names and values appear on the screen. If there is a limiting range of values which a variable can assume, that range will appear on the screen in the form (X..Y) where X is the lower bound and Y is the upper bound. In the event that there is only a lower bound the range will be in the form (X...).

A prompt will ask if you wish to change the value for that variable. Once all the variables on a Data Set or Card have been changed, the following prompt will appear:

```
    Hit the return key to continue with the next item or enter 'M'
to return to the main menu
```

Pressing the return key will cause the next item in the data file to appear on the screen. For instance, if you have just entered a new title card, the next item for editing would be the variables on Card 1. Entering an

```
M
```

and pressing the return key will return the editing menu to the screen.

3.1.1 Selection 1 - Editing an Existing Data File

Selection 1 will prompt for an input file name. This is the file from which existing data will be read. If the file does not exist, the prompt for the input file name will be repeated until a file name is entered which does exist. The program reads the data in the input file and assigns values to each variable. These values may then be edited using options 2 through 16 or by simply hitting the return key and continuing with the next item.

If an error should occur while the program is reading an input data file, the number of the Card or Data Set in which the error occurred will be displayed on the screen. If the data file was created with an editor other than the Preprocessor, use that editor to determine if the data is in the correct format (see Appendix A). In the event that the data file was created using the Preprocessor, make a note of the location of the error and report the problem by mailing in the software problem report sheet included in your package, or by calling the number listed in the front of the manual.

3.1.2 Creating an Input File

If an input file name is not entered (with option 1), default values are assigned to each variable. The default values have been set equal to the values used in Test Problem #1 (see Section 4.1). It is suggested that you try creating a data file with all default values, then run BIOPLUME ll using that file. Check the results and compare them to the output from Test Problem #1 (Appendix B). Any differences in the output data should be minor.

3.1.3 Selection 2 - Card 1

Card 1 is the title of the problem. Any title containing up to 80 alphanumeric characters can be entered.

3.1.4 Selection 3 - Card 2

Card 2 contains 18 variables pertaining to input and output control. Each of these variables are displayed on the screen, one at a time, in order. A definition of the variable and the range which it is limited to appear on the screen along with the prompt

```
Do you wish to change this value? (Y/N)
```

This prompt, or versions of it, appear throughout the Edit/Create program. It is referred to as the change prompt in the following discussions.

Once all 18 variables have been entered, you may continue to the next item by hitting the return key or enter an

```
M
```

and return to go back to the menu.

3.1.5 Selection 4 - Card 3

Card 3 contains 12 variables which describe the physical characteristics of the aquifer. Each of these variables are displayed on the screen, one at a time, in order. A definition of the variable and the range which it is limited to appear on the screen along with the change prompt. Once all the variables have been entered, continue to the next item or return to the menu.

3.1.6 Selection 5 - Card 4

Card 4 contains information necessary for retardation and/or decay. This card is skipped if NREACT=0. If NREACT=0, and selection 5 is chosen from the menu, a message will appear which reminds you that Card 4 is not needed when NREACT=0. Each of the variables for Card 4 are displayed on the screen, one at a time, in order. A definition of the variable and the range which it is limited to appear on the screen along with the prompt to change the value. Once all 5 variables have been entered, continue to the next item or return to the menu.

3.1.7 Selection 6 - Data Set 1

Data Set 1 contains the coordinates of the observation points. If there are no observation points (NUMOBS=0), then this data set is skipped. When observation points are specified (NUMOBS>0), then there will be one line for each point. The screen will display the number of observation wells specified, the well number, and the current X and Y coordinates of the well. The locations of the observation wells must be changed one at a time. To do this, enter a

```
Y
```

in response to the change prompt. Then enter the well number and the location (x,y) as integers. The integers may be separated by commas, spaces, or by a carriage return <CR>. For example, if NUMOBS=2, the screen will display the following:

```
There are  2 observation wells specified

 Well Number   X    Y
          1    0    0
          2    0    0
 Do you wish to change any of these? (Y/N)
```

To define an observation point at node 5,5 you would type:

Y

Then the program would prompt:

Enter Well Number, X, and Y as integers separated by commas.

Any of the following three responses would define the second observation point as being located at node 5,5.

```
2,5,5

2 5 5

2
5
5
```

After each well is changed, the screen will display the location of all the wells. Once all wells are properly defined by location, enter a negative response to the change prompt and continue to the next item or return to the menu.

3.1.8 Selection 7 - Data Set 2

Data Set 2 contains information about pumping/injection water wells. First, the program will display the number and location of these wells. (If NREC=0, this data set is skipped.) The locations should be defined in the same manner as the locations of the observation wells were defined.

In addition to the location, the pumping or injection rate and concentration must be defined. To indicate that a well is pumping, the rate (cfs) is entered as a positive value. Injection is indicated with a negative value. The variable CONC is the concentration of the contaminant which is being injected. The variable 02 CONC is the concentration of oxygenated water which is being injected. (See Appendix A for more detail on variable definition). Note that only injection wells will need to have a concentration defined.

Once all of the wells have been given a location, pumping/injection rate, and concentration, continue to the next item or return to the menu.

3.1.9 Selection 8 - Data Set 3

Data Set 3 contains transmissivity information. The program will display the current transmissivity map. To change the current map, enter a positive response to the change prompt. There are three ways to change the transmissivity map:

```
Enter a zero (0) for a constant Transmissivity,
       a one (1) if you wish to enter a map,
    or a two (2) if you w1sh to enter an individual value
```

Selection 0 is used to enter a constant transmissivity. When this selection is used, you will be asked for the value of transmissivity and a factor by which to multiply the transmissivity. This factor is used when the transmissivity is outside the bounds of the input format (see Appendix A). For instance, if you wish to input a constant transmissivity of 10,000 ft^2 /sec, you would have to enter a constant transmissivity of 100 ft^2 /sec with a multiplication factor of 100. The same is true of all multiplication factors throughout the program.

Selection 1 is used to enter a map of transmissivity. When this selection is used, you will be asked to enter transmissivity values by row. For instance, if the grid has 10 columns and the transmissivity along row one is all equal to 10, you would enter 10 ten times, each separated by a space, comma, or <ENTER>. This would be repeated for each row until the entire transmissivity map is defined. The program will then ask for the multiplication factor for these values.

Selection 2 allows an individual value to be entered into the map. When this option is selected you will be prompted to enter the location of the node (x,y) and the value of transmissivity at that node. Again, the program will ask for a multiplication factor.

An anisotropic aquifer can be modeled by entering a value for ANFCTR on Card 3 which is not equal to one. Then enter the values of T_{xx} into the transmissivity map. These values will be multiplied by ANFCTR to obtain the values for T_{yy}. Note that the multiplication factor which is entered with the transmissivity map is ***not*** the same as ANFCTR.

After the selection is completed, the transmissivity map will be displayed on the screen along with the change prompt. If the values are correct, enter a negative response and continue to the next item or return to the menu.

3.1.10 Selection 9 - Data Set 4

Data Set 4 contains aquifer thickness information. The program will display the map of the thickness and ask if you wish to make any changes. Changes are made in the exact same manner as for the transmissivity map (Data Set 3).

3.1.11 Selection 10 - Data Set 5

Recharge information is contained in Data Set 5. Changes to the recharge map are made in the same manner as for transmissivity and thickness (Data Set 3 and 4). Diffuse recharge should be entered as negative (-) values and discharge should be entered as positive (+) values.

3.1.12 Selection 11 - Data Set 6

Node identifications are contained in Data Set 6. Node identifications are used to define constant-head nodes or other boundary conditions. The number of node ids available is set by the variable NCODES on Card 2. The current node id map will be displayed on the screen along with the change prompt. The following methods are available to make changes:

```
Enter one of the following values:
0 - Constant node id for whole map.
1 - Node id = 1 along top and bottom edges.
2 - as for 1, with additional node ids specified.
3 - as is with additional node ids specified.
4 - enter whole map.
```

Selection 0 allows one to enter a constant node id for the whole map. Selection 1 sets the node identification to 1 along the top and bottom edges (rows 2 and NY-1). Selection 2 will set the same conditions as Selection 1 and allow you to enter additional node ids at specific points. When this option is used, you will be prompted to enter the number of additional points to be entered. Then each of those

points must be entered as a location (x,y) and node id value. Selection 3 will prompt for the number of points to be added to the map. These points are entered as a location (x,y) and value. The entire map can be entered by using Selection 4. This option operates in the same manner as Selection 1 of Data Sets 3 through 5, prompting for all values on each row.

After a selection has been executed, the map will reappear on the screen along with the change prompt. If the values are correct, enter a negative response and continue to the next item or return to the menu.

3.1.13 Selection 12 - Data Set 7

Node identification codes are specified in Data Set 7. These are used to define the node identifications specified in Data Set 6. The program will display the node id codes which may be specified and the factors which can be set.

```
       There are   2 node identification codes specified
 Code  Leakance Contamlnant Conc  Oxygen Conc  Change recharge?  Recharge

   1   1.0000         .000             .000          No
   2    .0000         .000             .000          No
```

When the variable NODEID is equal to a node id code (ICODE), then the corresponding variables are set equal to the factors entered in this data set. To change node id codes, you must first enter a

Y

in response to the change prompt. Then you must enter the number of the id which you wish to change. The following options will appear on the screen:

```
Enter one of the following. . .

1 - Constant head
2 - Source cell
3 - Other
```

Selection 1 will set the leakance factor to 1 and all other factors will remain 0. Selection 2 will prompt for more information:

```
Enter 1 for a contaminant source,
      2 for an oxygen source
   or 3 for a combined source
```

If you enter a 1, you will be prompted for the contaminant concentration. If you enter a 2, the same prompts will be repeated except that the oxygen concentration will be asked for instead of the contaminant concentration. A 3 will cause both the contaminant and oxygen concentrations to be prompted for. For any of these three sources, leakance is assumed to be equal to 1. A source cell is assumed to have no recharge. Therefore, the recharge cannot be changed for this node id.

Selection 3 allows you to enter a code for nodes which do not fit into either of the other two options. Each of the variables will be prompted for individually. After the leakance and the contaminant and oxygen concentrations have been entered, the program will ask if you wish to change the recharge rate. If so, the program will then ask for the new rate. If not, the recharge will remain the same as specified in the recharge map (Data Set 5).

3.1.14 Selection 13 - Data Set 8

Data Set 8 contains the initial water table information. Though it is referred to as the water table map, the data entered here could also be the potentiometric elevation or constant head in a stream bed. The options to change the map are:

```
Enter a zero (0) for a constant water table,
       a one (1) if you wish to enter a map,
       a two (2) if you wish to enter values at a specified nod id
  or a three (3) if you wish to enter an individual value
```

Selections 0, 1, and 3 operate in the same manner as for the previous maps (see Data Set 3). Selection 2 allows one to enter the water table for those points which have been defined by a node id. When this option is executed, you will be asked for which node id you wish to specify the water table. The program will then prompt you for the water table at each of the nodes which are identified by that node id. For example, if the node ids have been set to 1 along the top and bottom edges of the node id map (option 1, Data Set 6) and you wish to def ine a water table along those same edges, you could do so by selecting option 2. Then enter a 1 when asked for the node id. The program would then ask for the water table elevation at column 2 row 2. After you enter a value, the program would ask for the water table elevation at column 3 row 2. This would continue until all the nodes defined by node id 1 had been assigned a value for the water table.

Once a selection has been executed, the water table map will reappear on the screen along with the change prompt. If the values are correct, continue to the next item or return to the menu.

3.1.15 Selection 14 - Data Set 9

Initial contaminant concentrations are contained in Data Set 9. The options to change the concentration map are:

```
Enter a zero (0) for a constant initial concentration,
       a one (1) if you wish to enter a map,
    or a two (2) if you wish to enter an individual value
```

These selections are executed in the same manner as previously described (see Data Set 3).

3.1.16 Selection 15 - Data Set 10

Data Set 10 contains the initial oxygen concentration. The options for changing the oxygen map are the same as for changing the contaminant concentration map (see Data Set 9).

3.1.17 Selection 16 - Data Set 11

Data Set 11 is used to revise several timing, printing, and pumping variables for each pumping period (see Appendix A). This data set is only used when the value of NPMP>1 (see Card 2). If NPMP>1, the program will display the current values of the variables and ask if you wish to change them for the next pumping period. A positive response will cause the program to prompt for each variable in turn. You must enter a value for all of the variables as they are prompted for. Once the variables have been entered for a pumping period, the procedure is repeated until the last pumping period has been reached.

3.1.18 Selection 17 - Write Data File

This option is used to write the edited data to a file. If a file name is entered which already exists, a prompt will ask if you want to overwrite the existing file. If so, the file will be overwritten. If not, you will be prompted for a new file name.

3.1.19 Selection 18 - Quit

Selection 18 returns the main menu to the screen. If data has been edited but not written to a file, the following prompt will appear:

```
     Any changes made have NOT been written to a file Do you wish
to write them before quitting? (Yes/No)
```

This ensures that you cannot accidentally quit the Edit/Create option of the main menu and cause any editing to be lost.

3.2 Option 2: Run BIOPLUME II

Option 2 allows a user to run the BIOPLUME II model from the main menu. When this option is selected, the program will prompt:

```
Enter name of input file . . .
```

Type in the name of an input file. This can be a file which was created using the Edit/Create option or by some other means. If the file does not exist, the program will display a message telling you that the file does not exist and repeat the prompt for the input file name. (Remember that CTRL C will return you to the main menu.) If the file does exist, the program will prompt:

```
Enter name of output file. . .
```

If this file name already exists, the program will ask if you wish to replace the existing file. If a negative response is received, the prompt for the output file name is repeated.

Once the proper input and output file names have been entered, BIOPLUME II is run using the data from the input file. Output is written to the output file. The program does take a few minutes to run, so please be patient.

If an error occurs, you can discover where it occurred by looking at the output data file. The DOS editor EDLIN or any other text editor may be used to examine the output file. (See your DOS manual for more information on EDLIN). Find the point at which the program stopped, or any input variable which was not read properly. Check the input data file to make sure that it contains the proper data. If you cannot locate the source of the error, call the phone number listed in the front of this manual or send in the software problem report sheet included in your package with the problem described in as much detail as possible.

3.3 Option 3: Prepare Graphics Files

Option 3 is used to convert the output from BIOPLUME ll into files which can be plotted using SURFER (Golden Software, 1987). The format for SURFER consists of three columns of data. This data is the form X, Y, Z and could be used with any other plotting package which uses that format.

BIOPLUME ll automatically writes output data to three files named HEADS.BIO, HPLUME.BIO and OPLUME.BIO. The file HEADS.BIO contains the array of computed head values at the end of each time step. HPLUME.BIO and OPLUME.BIO contain the HC and O_2 plumes, respectively.

The first line of the file HPLUME.DAT contains the variables NTIM, NPMP, NX, NY, NPNT, and NPNTMV. This line is read before converting any of the data from the files HEADS.BIO, HPLUME.BIO, and OPLUME.BIO into the graphical data format. It informs the program how often the chemical and hydraulic output was requested by the user. In other words, it tells the program just how many plumes can be converted for use with SURFER.

The files with the HC and O_2 plumes also contain a line of data before each plume. This line contains the pumping period number, time step number, and number of moves completed. This allows the program to determine which plume is being requested for conversion. It also allows you to convert and plot several plumes from the same output data.

When Option 3 is selected, the following menu will appear on the screen:

```
                Graphics Menu
1 -  Head map data
2 -  Hydrocarbon plume data
3 -  Oxygen plume data
4 -  Quit
Enter the number of your choice (1..4)...
```

When selections 1, 2, or 3 are chosen, the following prompt will appear on the screen:

```
    Enter a name for the output file You may specify a full path
and directory, up to 60 characters
```

Enter the file name you wish to have the data written to and press the <ENTER> key. It is suggested that you specify a file name with a DAT extension.

To convert HC and O_2 plume data, you must specify which plume you wish to use. After entering the name of the output file, a prompt will appear:

```
    You may graph plumes in any time step after multiples of 10
moves, or you may graph plumes at the end of the following time
steps
```

If NPNTMV > 0, another prompt will appear:

```
Enter a 1 to graph data after a number of moves,
   or a 2 to graph data at the end of a time step
```

The number of time steps for which plumes were computed will appear after the first prompt. The second prompt will not appear if NPNTMV = 0 since the only data requested for output was the data at the end of the time steps. If NPNTMV> 0, enter the option which you wish to use.

If there is more than one pumping period, the program will ask you to enter the pumping period you wish to use. Then you will be prompted to enter the time period desired. If you have chosen selection 2, the program automatically converts the data for the last move. If you have chosen selection 1, the move numbers which are available will be displayed. Enter the move number which you wish to use. For either option, the data for the plume will be converted and written to the output file specified and the Graphics Menu will reappear on the screen. If you wish to convert more data, repeat the above procedure. Selecting option 4 (Quit) will return the Main Menu to the screen.

The converted files are stored in the file name specified. To graph the data, it is suggested that you use a plotting package such as SURFER from Golden Software (1987). A SURFER manual is enclosed for those who have purchased the program along with BIOPLUME ll.

3.4 Option 4: QUIT

Selecting Option 4 will stop the program and return you to DOS.

4. Test Problems

4.1 Test Problem # 1 - Natural Biodegradation

4.1.1 Description:

Test problem #1 is an illustration of how to simulate a contaminant plume that is undergoing naturally occuring biodegradation. The problem simulates a single hydrocarbon source which could be a leaking underground storage tank or some other source of contamination. A hypothetical site with "typical" values for physical parameters is modeled for this problem.

Two sources of naturally occuring oxygen are used: initial dissolved oxygen in the aquifer prior to contamination, and recharge of oxygen across the boundaries of the hypothetical site. Steady state conditions are assumed and the source of contamination is modeled using an injection well.

4.1.2 Input Data:

The following data was assumed:

Simulation time	6 years
Grid size	11x20
Cell size	50ftx50ft
Injection well at cell	X=6,Y=6
Injection rate	0.0002 cfs
Conc. of Contaminant in injected water	100.0 mg/l
Conc. of Oxygen in injected water	0.0 mg/l
Initial conc. of oxygen	8.0 mg/l
Conc. of natural recharge of oxygen	8.0 mg/l

Note that even though the concentrations in the model have no units, it is important for the contaminant and oxygen concentrations to be expressed in the same scale, (i.e., if the contaminant concentration is input in mg/l, then the oxygen concentration needs to be in mg/l).

Data sets 2, 6, 7, and 10 will be discussed in detail to indicate where the oxygen data is input. The complete input data for this test problem are listed on the following pages.

```
Data set #2:      IX.IY,REC,CNRECH,CNRECO
                  IX = 6
                  IY = 6
                  REC = 0.0002 cfs
                  CNRECH = 100.0
                  CNRECO = 0.0
```

Note that the concentration of oxygen in the injected water (0 mg/l) is input as CNRECO.

Data set #6: INPUT,FCTR
NODEID

INPUT = 1
FCTR = 1

NODEID :
00000000000
01111111110
00000000000
00000000000
00000000000
00000000000
00000000000
00000000000
00000000000
00000000000
00000000000
00000000000
00000000000
00000000000
00000000000
00000000000
00000000000
01111111110
00000000000

Data set #7: ICODE,FCTR1,FCTR2,FCTR4,FCTR3,OVERRD

ICODE = 1
FCTR1 = 1.0 ft/s (= leakance)
FCTR2 = 0.0 (= CNRECH)
FCTR4 = 8.0 (= CNRECO)
FCTR3 = 0 (= RECH)
OVERRD = 0

Note that the recharge concentration of oxygen across the constant head boundaries (8 mg/l) is input as FCTR4.

Data set #10: INPUT,FCTR
CONC1

INPUT = 0
FCTR = 8.0

Note that since the concentration of oxygen in the aquifer prior to contamination is constant (8 mg/l), the value was input as FCTR (i.e., there is no need to input the value in matrix form).

4.1.3 Output Data:

The complete output data for this problem are included in Appendix B. Figure 4.1 presents a contour plot of the contaminant and oxygen plumes for Test Problem #1 after 6 years. It can be seen that oxygen is absent wherever there is contamination. and contamination is absent wherever the concentration of oxygen is at pre-contamination levels (8 mg/l). It can also be seen that around the edges of the plume, there is a zone of reduced oxygen and hydrocarbon concentrations.

In order to illustrate the effects of natural biodegradation on contaminant plumes, the same problem was simulated without oxygen sources, i.e., without biodegradation. The resulting contaminant plume is plotted in Figure 4.2 and the concentration matrix is listed following the output data for this test problem (Appendix B). If the contaminant plumes of Figures 4.1 and 4.2 are compared, the following can be concluded:

1. The biodegraded plume is narrower than the non-biodegraded plume.

2. The maximum concentration in the biodegraded plume is less than that in the non-biodegraded plume.

3. The total contaminant mass in the biodegraded plume is less than that in the non-biodegraded plume.

Note: The mass loss due to biodegradation is printed as part of the chemical balance output and can be correlated with field data if available. This helps in the calibration effort by checking the projected mass loss against that from the measured concentration data in the field.

Input Data f or Test Problem #1

```
TEST PROBLEM #1 - NATURAL BIODEGRADATION                                          --- Card 1
  1     1    11         202000   1    7   1     100    1     9     1    0       0
0   0       0     1                                                               --- Card2
          6.0   0.001    0.3   10.    0   0   0     50.   50.   0.1   0.5   1.0   --- Card 3
0   0       0     0     0                                                         --- Card 4
 510                                                                              --- Data Set 1
6   6      -.0002          100.        0.                                         --- Data Set 2
0          .0025                                                                  --- Data Set 3
0            25.0                                                                 --- Data Set 4
0              0.0                                                                --- Data Set 5
1              1.0                                                                --- Start of Data Set 6
00000000000
01111111110
00000000000
00000000000
00000000000
00000000000
00000000000
00000000000
00000000000
00000000000
00000000000
00000000000
00000000000
00000000000
00000000000
00000000000
00000000000
00000000000
01111111110
00000000000                                                                       --- End of Data Set 6
1            1.0           0.0          8.0          0.0 0                        --- Data Set 7
1          1.0                                                                    --- Start of Data Set 8
        0.       0.       0.      0.       0.       0.      0.      0.      0.      0.       0.
        0.    100.     100.    100.    100.     100.    100.    100.    100.    100.       0.
        0.
        0.
        0.
        0.
        0.
        0.
        0.
        0.
        0.
        0.
        0.
        0.
        0.
        0.
        0.
        0.
        0.    97.       97.     97.     97.      97.     97.     97.     97.     97.        0.
0.       0.   0.         0.      0.      0.      0.       0.      0.      0.      0.          --- End of Data Set 8
```

```
0       0.0                                                    --- Data Set 9
0       8.0                                                    --- Data Set 10
```

4.2 Test Problem #2 - Natural Biodegradation with Reaeration

4.2.1 Description:

Test Problem #2 is similar to Test Problem #1 except that a third source of oxygen into the plume is simulated. The source is vertical exchange of oxygen from the unsaturated zone. The effect of reaeration is a first order decay in hydrocarbon concentrations (Chapter 2).

4.2.2 Input Data:

The coeffiecient of reaeration used in this problem is 0.0005 days . The value of the coefficient of reaeration is input in card #4 in the fifth field. (Note that NREACT, card #2, field 18, has already been set to 1 in Test Problem #1).

The input data for problem 2 are listed on the following pages.

4.2.3 Output Data:

The output data are included in Appendix C. If one compares the concentration matrix for problem #1 with that for problem #2, then it is evident that reaeration accounts for a significant reduction in contaminant concentrations. The mass loss due to reaeration is printed as part of the chemical balance output.

It is noted that reaeration can be used as a calibration parameter. For cases where the observed loss of mass is in excess of that projected by the model due to the two sources of oxygen utilized in problem #1, reaeration can be used to increase the projected mass loss due to biodegradation processes.

It should be also mentioned that anaerobic decay can be simulated in the same manner as reaeration, i.e., a coefficient of anaerobic decay needs to be specified in the fourth field of the fourth card. However, one must have an indication of anaerobic biodegradation processes from field data before the anaerobic decay option can be utilized for simulation runs.

Input Data for Test Problem #2.

```
TEST PROBLEM #2 - NATURAL BIODEGRADATION WITH REAERATION
 1      1      11      202000           1     7     1      100    1    9      1    0      0       0       0      0       1
6.00       .001    0.3     10.     0       0      0       50.    50.      0.1      0.5    1.0
0  0     0     0     0.0005    --- Reaeration Coefficient
 510
6 6       -.0002            100.          0.
0           .0025
0             25.0
0               0.0
1               1.0
00000000000
01111111110
00000000000
00000000000
00000000000
00000000000
00000000000
00000000000
00000000000
00000000000
00000000000
00000000000
00000000000
00000000000
00000000000
00000000000
00000000000
00000000000
01111111110
00000000000
 1       1.0                        0.0             8.0                   0.0 0
1        1 .0
       0.       0.       0.       0.       0.       0.       0.        0.        0.        0.        0.
      0.       100.     100.     100.     100.     100.     100.    100.     100     100.       0
       0.
       0.
       0
       0.
       0.
       0.
       0.
       0.
       0.
       0.
       0.
       0.
       0.
       0.
       0.
       0.
       0. 97. 97. 97. 97. 97. 97. 97. 97. 97. 0.
       0.  0.  0.   0.   0.   0.   0.   0.   0.   0.   0.
0        0.0
0        8.0
```

4.3 Test Problem #3 - In-Situ Biorestoration

4.3.1 Description:

Test Problem #3 is an illustration of how to simulate in-situ biorestoration. A doublet restoration scheme is simulated with one injection well and one production well. The injection well is used as an oxygen source and the production well basically pumps out contaminated water. The concentration of oxygen in the injected water is assumed to be 8 mg/l.

4.3.2 Input Data:

The problem is set up such that the contaminant and oxygen plumes from problem 1 are used as the initial condition in the aquifer. Data set #2 is discussed in detail to indicate how to simulate a well which is injecting oxygen for biorestoration. The complete input data for Test Problem #3 are listed in the following pages.

```
Data set #2:   IX.IY.REC,CNRECH,CNREC0

Injection Well:
      IX = 6
      IY = 5
      REC = - 0.0016
      CNRECH = 0.0
      CNREC0 = 8 mg/l

Production Well:
      IX = 6
      IY = 1 1
      REC = 0.0016
      CNRECH = 0.0
      CNREC0 = 0.0
```

4.3.3 Output Data:

The output data for problem #3 are listed in Appendix D. Figure 4.3 presents a contour plot of the contaminant plume after 6 years. For comparison the same well configuration was used to compute the contaminant plume without biodegradation after 6 years. Figure 4.3 also presents a plot of the non-biodegraded plume. It can be seen that the extent of cleanup is more with oxygen injection and the biodegraded plume is much smaller than the non-biodegraded plume. It is also noted that if the oxygen concentration in the injected water can be increased, then the cleanup time can be reduced considerably.

Input Data for Test Problem #3.

```
TEST PROBLEM NO 3 - IN-SITU BIORESTORATION
 1        1      11   202000         1   7   1   100      2   9   1    0    0    0    0    0   1
6.00.001    0.3     10.      0       0   0   50.  50.  0.1        0.5     1.0
0     0     0     0     0
    510
6 5       -.0016           0.0       8.0
611        .0016
0          .0025
0           25.0
0            0.0
1            1.0
00000000000
01111111110
00000000000
00000000000
00000000000
00000000000
00000000000
00000000000
00000000000
00000000000
00000000000
00000000000
00000000000
00000000000
00000000000
00000000000
00000000000
01111111110
00000000000
1          1.0               0.0             8.0          0.0 0
1       1.0
     0.    0.    0.    0.    0.    0.    0.    0.    0.   0.     0.
     0.    100.  100.  100.   100.   100.   100.   100.   100.  100.    0.
     0.
     0.
     0.
     0
     0.
     0.
     0.
     0.
     0.
     0.
     0.
     0.
     0.
     0.
     0.
     0.
     0.    97.   97.     97.     97.     97.     97.     97.     97.     97.     0.
```

```
 0.   0.  0.   0.   0.   0.   0.   0.   0.   0.   0.
1          1.0
        0    0    0    0    0    0    0    0    0    0    0
        0    0    0    0    0    0    0    0    0    0    0
        0    0    0    0    0    0    0    0    0    0    0
        0    0    0    0    0    0    0    0    0    0    0
        0    0    0    0    0    1    0    0    0    0    0
        0    0    0    0    0   30    0    0    0    0    0
        0    0    0    0    0   35    0    0    0    0    0
        0    0    0    0    6   30    6    0    0    0    0
        0    0    0    0    5   26    5    0    0    0    0
        0    0    0    0    0   18    0    0    0    0    0
        0    0    0    0    0    9    0    0    0    0    0
        0    0    0    0    0    1    0    0    0    0    0
        0    0    0    0    0    0    0    0    0    0    0
        0    0    0    0    0    0    0    0    0    0    0
        0    0    0    0    0    0    0    0    0    0    0
        0    0    0    0    0    0    0    0    0    0    0
        0    0    0    0    0    0    0    0    0    0    0
        0    0    0    0    0    0    0    0    0    0    0
        0    0    0    0    0    0    0    0    0    0    0
        0    0    0    0    0    0    0    0    0    0    0
1    1.0
        0    0    0    0    0    0    0    0    0    0    0
        0    8    8    8    8    8    8    8    8    8    0
        0    8    8    8    8    8    8    8    8    8    0
        0    8    8    8    8    7    8    8    8    8    0
        0    8    8    8    8    0    8    8    8    8    0
        0    8    8    8    7    0    7    8    8    8    0
        0    8    8    8    2    0    2    8    8    8    0
        0    8    8    8    0    0    0    8    8    8    0
        0    8    8    8    0    0    0    8    8    8    0
        0    8    8    8    1    0    1    8    8    8    0
        0    8    8    8    5    0    5    8    8    8    0
        0    8    8    8    7    0    7    8    8    8    0
        0    8    8    8    8    6    8    8    8    8    0
        0    8    8    8    8    8    8    8    8    8    0
        0    8    8    8    8    8    8    8    8    8    0
        0    8    8    8    8    8    8    8    8    8    0
        0    8    8    8    8    8    8    8    8    8    0
        0    8    8    8    8    8    8    8    8    8    0
        0    8    8    8    8    8    8    8    8    8    0
        0    0    0    0    0    0    0    0    0    0    0
```

5. References

Alexander, M., 1975, "Environmental and Microbiological Problems Arising from Recalcitrant Molecules", **Microb. Ecol**., 2, 17.

Angelakis, A. N. and Rolston, D. E., 1985, "Transient Movement and Transformation of Carbon Species in Soil During Wastewater Application", **Water Resour. Res.**, 21, 1 141.

Baehr, A. and Corapcioglu, M. Y., 1985, "A Predictive Model for Pollution from Gasoline in Soils and Ground Water", in P**roc. Petroleum Hydrocarbons and Organic Chemicals in Ground Water - Prevention, Detection, and Restoration,** Nov. 1984, Houston, Texas, National Water Well Association, Worthington, Ohio, 144.

Bear, J., 1979, **Hydraulics of Ground Water,** McGraw Hill, New York.

Borden, R. C. and Bedient, P. B., 1986, "Transport of Dissolved Hydrocarbons Influenced by Oxygen-Limited Biodegradation: 1. Theoretical Development", **Water Resources Res.,** 22, 1973.

Borden, R. C., Bedient, P. B., Lee, M. D., Ward, C. H. and Wilson, J. T., 1986, "Transport of Dissolved Hydrocarbons Influenced by Oxygen-Limited Biodegradation: 2. Field Application", **Water Resources Res.,** 22, 1983.

Brown, R. A., Norris, R. D. and Brubaker, G. R., 1985, "Aquifer Restoration with Enhanced Bioreclamation", **Pollution Engineering,** 25.

Brown, R. A., Norris, R. D. and Raymond, R. L., 1984, "Oxygen Transport in Contaminated Aquifers", in **Proc. Petroleum Hydrocarbons and Organic Chemicals in Ground Water - Prevention, Detection, and Restoration,** Nov. 1984, Houston, Texas, National Water Well Association, Worthington, Ohio, 421.

Federle, T. W., Dobbins, D. C., Thornton-Manning, J. R. and Jones, D. D., 1986, "Microbial Biomass, Activity, and Community Structure in Subsurface Soils", **Ground Water,** 24, 365.

Freeze, R. A. and Cherry, R. B., 1979, **Ground Water,** Prentice Hall, Inc., Englewood Cliffs, New Jersey.

Ghiorse, W. C. and Balkwill, B. L., 1983, "Enumeration and Morphological Characterization of Bacteria Indigenous to Subsurface Environments", **Dev. Ind. Microbiol.**, 24, 213.

Ghiorse, W. C. and Balkwill, B. L., 1985, "Microbial Characterization of Subsurface Environments," in **Ground Water Quality**, Ward, C. H., Gieger, W. and McCarty, P. L., editors, John Wiley and Sons, Inc., New York, NY, 387.

Golden Software, Inc., 1987, **SURFER**, Version 3.00, Golden, CO.

Hirsch, P. and Rades-Rohkohl, E., 1983, "Microbial Diversity in a Ground Water Aquifer in Northern Germany", **Dev. Ind. Microbiol.**, 24, 183.

Konikow, L. F. and Bredehoeft, J. D., 1978, **Computer Model of Two-Dimensional Solute Transport and Dispersion in Ground Water**, Automated Data Processing and Computations Techniques of Water Resources Investigations of the U. S. Geological Society, Washington, D.C.

Kosson, D. S., Agnihotri, G. C. and Ahlert, R. C., 1985, "Modeling of Microbially Active Soil Columns", in **Computer Applications in Water Resour.** ASCE Torno, H. C., Ed., American Society of Civil Engineers, New York.

Kuhn, E. P., Colberg, P. J., Schnoor, J. L., Warner, O., Zehnder, A. J. B. and Schwarzenbach, R. P., 1985, "Microbial Transformation of Substituted Benzenes During Infiltration of River Water to Ground Water: Laboratory Column Studies", **Environ. Sci. & Technol.**, 19, 961.

Lee, M. D. and Ward, C. H., 1985, "Micr~bial Ecology of a Hazardous Waste Disposal Site: Enhancement of Biodegradation", in **Proc., 2nd Int'l Conference on Ground Water Quality Research**, Durham, N. N. and Redelfs, A. E., editors, Tulsa, Oklahoma, March 1984, OSU Printing Services, Stillwater, OK, 25.

Molz, F. J., Widdowson, M. A. and Benefield, L. D., 1986, "Simulation of Micrcobial Growth Dynamics Coupled to Nutrient and Oxygen Transport in Porous Media", **Water Resour. Res**., 22, 1207.

Raymond, R. L., 1974, **Reclamation of Hydrocarbon Contaminated Ground Water,** U. S. Patent 3, 846, 290, Nov. 5.

Raymond, R. L., Jamison, V. W. and Hudson, J. O., 1975, "Final Report on Beneficial Stimulation of Bacterial Activity in Ground Water Containing Petroleum Products", **Committee on Environmental Affairs,** American Petroleum Institute, Washington, D.C.

Rifai, H. S. and P. B. Bedient, 1987, "BIOPLUME ll - Two-Dimensional Modeling for Hydrocarbon Biodegradation and In Situ Restoration," **Proceedings**, NWWA/API Conference on Petroleum Hydrocarbons and Organic Chemicals in Ground Water - Prevention, Detection, and Restoration, Houston, Texas, National Water Well Association, Dublin, Ohio, (submitted).

Suflita, J. M. and Gibson. S. A., 1985, "Biodegradation of Haloaromatic Substrates in a Shallow Anoxic Ground Water Quality Research," in **Proc. 2nd Int'l Conference on Ground Water Quality Research**, Durham, N. N. and Redelfs, A. E., Eds., Tulsa, Oklahoma, March 1984, OSU University Printing Services, Stillwater, Oklahoma, 30.

Suflita, J. M. and Miller, G. D., 1985, "Microbial Metabolism of Chlorophenolic Compounds in Ground Water Aquifers", **Environ. Toxicol. Chem.**, 4, 751.

Thomas, J. M., Lee, M. D., Bedient, P. B., Borden, R. C., Canter, L. W. and Ward, C. H., 1987, **Leaking Underground Storage Tanks: Remediation with Emphasis on In-Situ Biorestoration,** Final Report, Cooperative Agreement No. CR-812808, U. S. Environmental Protection Agency, R. S. Kerr Environmental Laboratory, Ada, OK, p. 143.

White, D. C., Smith, G. A., Gehron, M. J., Parker, J. H., Findlay, R. H., Martz, R. F. and Fredrickson, H. L., 1983, "The Ground Water Aquifer Microbiota: Biomass, Community Structure, and Nutritional Status", **Dev. Ind. Microbiol.,** 24, 204

Wilson, J. T., McNabb, J. F., Balkwill, D. L. and Ghiorse, W. C., 1983, "Enumeration and Characterization of Bacteria Indigenous to a Shallow Water-Table Aquifer", **Ground Water**, 21, 134.

Wilson, B. H. and Rees, J. F., 1986, "Biotransformation of Gasoline Hydrocarbons in Methanogenic Aquifer Material", in **Proc. NWWA/API Conference on Petroleum Hydrocarbons and Organic Chemicals in Ground Water - Prevention, Detection, and Restoration**, Nov. 1984, Houston, Texas, National Water Well Association, Worthington, Ohio, 128.

Wilson, J. T. and Ward, C. H., 1987, "Opportunities for Bioreclamation of Aquifers Contaminated with Petroleum Hydrocarbons," **Dev. Ind. Microbiol.,** 27, 109.

Appendix A: Data Input Formats

Card	Column	Format	Variable	Definition
1	1-80	10A8	TITLE	Description of problem
2	1-4	I4	NTIM	Maximum number of time steps in a pumping period (1..100)*.
	5-8	I4	NPMP	Number of pumping periods. If NPMP > 1, then data set 11 must be completed.
	9-12	I4	NX	Number of nodes in the x direction (3..20).
	13-16	I4	NY	Number of nodes in the y direction (3..30).
	17-20	I4	NPMAX	Maximum number of particles (1..8100).
	21-24	I4	NPNT	Time step interval for printing hydraulic and chemical output data (1...).
	25-28	I4	NITP	Number of iteration parameters (usually 4..7).
	29-32	I4	NUMOBS	Number of observation points to be specified in a following data set (0..5).
	33-36	I4	ITMAX	Maximum allowable number of iterations in ADIP (usually 100..200).
	37-40	I4	NREC	Number of pumping or injection wells to be specified in a following data set (0..50).

*The possible ranges which a value may take are indicated in parentheses. The form (X..Y) indicates that X is a lower bound and Y is an upper bound. The form (X...) indicates that X is a lower bound and there is no upper bound.

Card	Column	Format	Variable	Definition
2	41-44	I4	NPTPND	Initial number of particles per node (4,5,8,9).
	45-48	I4	NCODES	Number of node identification codes to be specified in afollowing data set (1..9).
	49-52	I4	NPNTMV	Particle movement interval (IMOV) for printing chemical output data (0 to print only at end of time steps).
	53-56	I4	NPNTVL	Option for printing computedvelocities (0=do not print; 1=print for first time step; 2=print for all time steps).

	57-60	I4	NPNTD	Option for printing computed dispersion equation coefficients (0=do not print; 1=print for first time step; 2=print for all time steps).
	61-64	I4	NPDELC	Option for printing computed changes in concentration (0=do not print; 1=print).
	65-68	I4	NPNCHV	Option to punch velocity data (0=do not punch; 1 =punch the node velocities on unit 7).
	69-72	I4	NREACT	Option for retardation and decay (0=retardation factor is equal to 1 and no decay; 1=retardation factor > 1 and/or decay).
3	1-5	G5.0	PINT	Pumping period in years (0.01..99.99).
	6-10	G6.0	TOL	Convergence criteria in ADIP (usually < 0.01).
	11-15	G5.0	POROS	Effective porosity (0.01..1).
	16-20	G5.0	BETA	Characteristic length (longitudinal dispersivity) in feet (0.01..99.99)
	21-25	G5.0	S	Storage coefficient (set S=0 for steady flow problems).
	26-30	G5.0	TIMX	Time increment multiplier for transient flow problems (0.01..99.99). TIMX is disregarded if S=0.
	31-35	G5.0	TINIT	Size of initial time step in seconds (0...). TINIT is disregarded if S=0.
	36-40	G5.0	XDEL	Width of finite difference cell in the x direction in feet (0.1..999.9).
	41-45	G5.0	YDEL	Width of finite difference cell in the y direction in feet (0.1..999.9).
	46-50	G5.0	DLTRAT	Ratio of transverse to longitudinal dispersivity (0.001..1).
	51-55	G5.0	CELDIS	Maximum cell distance perparticle move (0.001..1).
	56-60	G5.0	ANFCTR	Ratio of T_{yy} to T_{xx} (0.001..9.999)

4	Free Format (separated by spaces or commas)	DK RHOB THALF DEC1 DEC2	Distribution coefficient (L^3/M). Bulk density of the solid (M/L^3). Half-life of the solute (seconds). Anaerobic decay coefficient (day^{-1}). Reaeration coefficient (day^{-1}).

Data Set	Number Format of Lines	Variable	Definition	
1	NUMOBS	2I2	IXOBS, IYOBS	Coordinates of observation points. This data set is not used if NUMOBS=0.
2	NREC	2I2,3G8.2	IX,IY	Coordinates of pumping (+) or injection (-) wells for contaminant or oxygenated water
			REC	Pumping/injection rate in cfs
			CNRECH	Concentration of injected contaminated water
			CNRECO	Concentration of injected oxygenated water
3	1 or NY	I1	INPUT	Parameter card for transmissivity (0=constant transmissivity is defined by FCTR; 1=transmissivity is read from following array).
		G10.0	FCTR	Constant transmissivity in ft^2/s OR factor to multiply transmissivity array.
		20G4. 1	VPRM	Array for temporary storage of transmissivity data in ft^2/s. For an anisotropic array, enter the values of T_{xx} and the values for T_{yy} will be computed by multiplying by ANFCTR.
4	1 or NY	I1	INPUT	Parameter card for thickness (0=constant thickness is def ined by FCTR; 1=thickness is read from following array).
		G10.0	FCTR	Constant thickness in feet, OR factor to multiply thickness array.
		20G3.0	THCK	Array of saturated thickness in feet.

Data Set	Number of Lines	Format	Variable	Definition
5	1 or NY	I1	INPUT	Parameter card for recharge (0=constant recharge is defined by FCTR; 1=recharge is read from following array).
		G10.0	FCTR	Constant diffuse recharge (-) or discharge (+) in ft/s OR factor to multiply recharge array.
		20G4.1	RECH	Array of diffuse recharge (-) or discharge (+) in ft/s.
6	1 or NY	I1	INPUT	Parameter card for node identification (0=all nodes identified by FCTR; 1=node identifications in following array)
		G10.0	FCTR	Node identification OR factor to multiply node identification array.
		20I1	NODEID	Node identification matrix (used to define constant-head nodes or other boundary conditions and stresses).
7	NCODES	I2	ICODE	Instructions for using the NODEID array. When NODEID= ICODE. then the following factors are set. Otherwise, the values remain set as they were previously.
		4G10.2	FCTR 1	Leakance
			FCTR2	Concentration of contaminated water
			FCTR4	Concentration of oxygenated water
			FCTR3	Diffuse recharge (-) or discharge (+)

Data Set	Number of Lines	Format	Variable	Definition
7		I2	OVERRD	If OVERRD=0, then the value of RECH is not changed. If OVERRD is nonzero, then the value of RECH is set to FCTR3.
8	1 or NY	I1	INPUT	Parameter card for water table (0=constant water table defined by FCTR; 1=water table is read from following array).
		G10.0	FCTR	Initial water table, potentiometric elevation, or constant head in stream or source bed in feet OR factor to multiply water table array.
		20G4.0	WT	Array of initial water table, potentiometric elevation, or constant head in stream or source bed in feet.
9	1 or NY	I1	INPUT	Parameter card for initial contaminant concentration (0=constant concentration def ined by FCTR; 1=contaminant concentration is read from following array).
		G10.0	FCTR	Initial contaminant concentration in aquifer OR factor to multiply contaminant concentration array.
		20G4.0	CONC	Array of initial contaminant concentration in aquifer.
10	1 or NY	I1	INPUT	Parameter card for initial oxygen concentration (0=constant concentration defined by FCTR; 1=oxygen concentration is read from following array).
		G10.0	FCTR	Initial oxygen concentration in aquifer OR factor to multiply oxygen concentration array.
		20G4.0	CONC1	Array of initial oxygen concentration in aquifer.

11	1	I1	I CHK	Parameter to check whether any revisions are desired (1=revision is desired, more data to follow; 0=no revision desired, end of data set). This data set allows 13 timing, printing, and pumping variables to be revised for each pumping period. Data set 11 can only be used if NPMP > 1. The sequence of cards in this data set must be repeated NPMP-1 times (for each pumping period after the first).
	1	10I4, 3G5.0	NTIM NPNT, NITP, ITMAX, NREC, NPNTMV, NPNTVL, NPNTD, NPDELC, NPNCHV, PINT, Tl MX, Tl N I T	Previously defined variables for cards 2 and 3 which will be revised for the next pumping period. This card is used only if ICHK= 1.
	NREC	2I2, 3G8.2	IX,IY,REC, CNRECH, CNRECO	Previously defined variables for data set 2 which will be revised for the next pumping period. This card is used only if ICHK= 1 and NREC > 0.

APPENDIX B: Output Data for Test Problem #1

BIOPLUME II
CONTAMINANT TRANSPORT UNDER THE INFLUENCE OF OXYGEN LIMITED BIODEGRADATION

TEST PROBLEM #l - NATURAL BIODEGRADATION

I N P U T D A T A

GRID DESCRIPTORS

NX (NUMBER OF COLUMNS)	=	11
NY (NUMBER OF ROWS)	=	20
XDEL (X-DISTANCE IN FEET)	=	50.0
YDEL (Y-DISTANCE IN FEET)	=	50.0

TIME PARAMETERS

NTIM (MAX. NO. OF TIME STEPS)	=	1
NPMP (NO. OF PUMPING PERIODS)	=	1
PINT (PUMPING PERIOD IN YEARS)	=	6.000
TIMX (TIME INCREMENT MULTIPLIER)	=	0.00
TINIT (INITIAL TIME STEP IN SEC.)	=	0.

HYDROLOGIC AND CHEMICAL PARAMETERS

S (STORAGE COEFFICIENT)	=	0.000000
POROS (EFFECTIVE POROSITY)	=	0.300
BETA (LONGITUDINAL DISPERSIVITY)	=	10.0
DLTRAT (RATIO OF TRANSVERSE TO LONGITUDINAL DISPERSIVITY)	=	0.10
ANFCTR (RATIO OF T-YY TO T-XX)	=	1.000000

EXECUTION PARAMETERS

NITP (NO. OF ITERATION PARAMETERS)	=	7
TOL (CONVERGENCE CRITERIA - ADIP)	=	0.0010
ITMAX (MAX.NO.OF ITERATIONS - ADIP)	=	100
CELDIS (MAX.CELL DISTANCE PER MOVE OF PARTICLES - M.O.C.)	=	0.500
NPMAX (MAX. NO. OF PARTICLES)	=	2000
NPTPND (NO. PARTICLES PER NODE)	=	9

OUTPUT DATA FOR TEST PROBLEM #1

PROGRAM OPTIONS

NPNT (TIME STEP INTERVAL FOR COMPLETE PRINTOUT)	=	1
NPNTMV (MOVE INTERVAL FOR CHEM. CONCENTRATION PRINTOUT)	=	0
NPNTVL (PRINT OPTION-VELOCITY 0=NO; 1=FIRST TIME STEP; 2=ALL TIME STEPS)	=	0
NPNTD (PRINT OPTION-DISP.COEF. 0=NO; 1=FIRST TIME STEP; 2=ALL TIME STEPS)	=	0
NUMOBS (NO. OF OBSERVATION WELLS FOR HYDROGRAPH PRINTOUT)	=	1
NREC (NO. OF PUMPING WELLS)	=	1
NCODES (FOR NODE IDENT.)	=	1
NPNCHV (PUNCH VELOCITIES)	=	0
NPDELC (PRINT OPT.-CONC. CHANGE)	=	0

REACTION TERMS

DK (DISTRIBUTION COEFFICIENT)	=	0.00000E+00
RHOB (BULK DENSITY OF SOLIDS)	=	0.00000E+00
RF (RETARDATION FACTOR)	=	0.10000E+01
THALF (HALF LIFE OF DECAY,IN SEC)	=	0.00000E+00
DECAY (DECAY CONSTANT=LN 2/THALF)	=	0.00000E+00

DECAY TERMS

DEC1 (ANAEROBIC DECAY COEFF.)	=	0.00000E+00
DEC2 (REAERATION DECAY COEFF.)	=	0.00000E+00

OUTPUT DATA FOR TEST PROBLEM #1

STEADY-STATE FLOW

TIME INTERVAL (IN SEC) FOR SOLUTE-TRANSPORT SIMULATION = 0.18935E+09

LOCATION OF OBSERVATION WELLS

NO.	X	Y
1	5	10

LOCATION OF PUMPING WELLS

X	Y	RATE(IN CFS)	CONC.	CONC(02)
6	6	-0.0002	100.00	0.00

AREA OF ONE CELL = 2500.

X-Y SPACING:
50.000
50.000

OUTPUT DATA FOR TEST PROBLEM

TRANSMISSIVITY MAP (FT*Ft/SEC)

0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
0.00E+00	2.50E-03	2.50E-03	2.50E-03	2.50E-03	2.50E-03	2.50E-03	2.50E-03	2.50E-03	2.50E-03	0.00E+00
0.00E+00	2.50E-03	2.50E-03	2.50E-03	2.50E-03	2.50E-03	2.50E-03	2.50E-03	2.50E-03	2.50E-03	0.00E+00
0.00E+00	2.50E-03	2.50E-03	2.50E-03	2.50E-03	2.50E-03	2.50E-03	2.50E-03	2.50E-03	2.50E-03	0.00E+00
0.00E+00	2.50E-03	2.50E-03	2.50E-03	2.50E-03	2.50E-03	2.50E-03	2.50E-03	2.50E-03	2.50E-03	0.00E+00
0.00E+00	2.50E-03	2.50E-03	2.50E-03	2.50E-03	2.50E-03	2.50E-03	2.50E-03	2.50E-03	2.50E-03	0.00E+00
0.00E+00	2.50E-03	2.50E-03	2.50E-03	2.50E-03	2.50E-03	2.50E-03	2.50E-03	2.50E-03	2.50E-03	0.00E+00
0.00E+00	2.50E-03	2.50E-03	2.50E-03	2.50E-03	2.50E-03	2.50E-03	2.50E-03	2.50E-03	2.50E-03	0.00E+00
0.00E+00	2.50E-03	2.50E-03	2.50E-03	2.50E-03	2.50E-03	2.50E-03	2.50E-03	2.50E-03	2.50E-03	0.00E+00
0.00E+00	2.50E-03	2.50E-03	2.50E-03	2.50E-03	2.50E-03	2.50E-03	2.50E-03	2.50E-03	2.50E-03	0.00E+00
0.00E+00	2.50E-03	2.50E-03	2.50E-03	2.50E-03	2.50E-03	2.50E-03	2.50E-03	2.50E-03	2.50E-03	0.00E+00
0.00E+00	2.50E-03	2.50E-03	2.50E-03	2.50E-03	2.50E-03	2.50E-03	2.50E-03	2.50E-03	2.50E-03	0.00E+00
0.00E+00	2.50E-03	2.50E-03	2.50E-03	2.50E-03	2.50E-03	2.50E-03	2.50E-03	2.50E-03	2.50E-03	0.00E+00
0.00E+00	2.50E-03	2.50E-03	2.50E-03	2.50E-03	2.50E-03	2.50E-03	2.50E-03	2.50E-03	2.50E-03	0.00E+00
0.00E+00	2.50E-03	2.50E-03	2.50E-03	2.50E-03	2.50E-03	2.50E-03	2.50E-03	2.50E-03	2.50E-03	0.00E+00
0.00E+00	2.50E-03	2.50E-03	2.50E-03	2.50E-03	2.50E-03	2.50E-03	2.50E-03	2.50E-03	2.50E-03	0.00E+00
0.00E+00	2.50E-03	2.50E-03	2.50E-03	2.50E-03	2.50E-03	2.50E-03	2.50E-03	2.50E-03	2.50E-03	0.00E+00
0.00E+00	2.50E-03	2.50E-03	2.50E-03	2.50E-03	2.50E-03	2.50E-03	2.50E-03	2.50E-03	2.50E-03	0.00E+00
0.00E+00	2.50E-03	2.50E-03	2.50E-03	2.50E-03	2.50E-03	2.50E-03	2.50E-03	2.50E-03	2.50E-03	0.00E+00
0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00

OUTPUT DATA FOR TEST PROBLEM #1

AQUIFER THICKNESS (FT)

0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.0	25.0	25.0	25.0	25.0	25.0	25.0	25.0	25.0	25.0	0.0
0.0	25.0	25.0	25.0	25.0	25.0	25.0	25.0	25.0	25.0	0.0
0.0	25.0	25.0	25.0	25.0	25.0	25.0	25.0	25.0	25.0	0.0
0.0	25.0	25.0	25.0	25.0	25.0	25.0	25.0	25.0	25.0	0.0
0.0	25.0	25.0	25.0	25.0	25.0	25.0	25.0	25.0	25.0	0.0
0.0	25.0	25.0	25.0	25.0	25.0	25.0	25.0	25.0	25.0	0.0
0.0	25.0	25.0	25.0	25.0	25.0	25.0	25.0	25.0	25.0	0.0
0.0	25.0	25.0	25.0	25.0	25.0	25.0	25.0	25.0	25.0	0.0
0.0	25.0	25.0	25.0	25.0	25.0	25.0	25.0	25.0	25.0	0.0
0.0	25.0	25.0	25.0	25.0	25.0	25.0	25.0	25.0	25.0	0.0
0.0	25.0	25.0	25.0	25.0	25.0	25.0	25.0	25.0	25.0	0.0
0.0	25.0	25.0	25.0	25.0	25.0	25.0	25.0	25.0	25.0	0.0
0.0	25.0	25.0	25.0	25.0	25.0	25.0	25.0	25.0	25.0	0.0
0.0	25.0	25.0	25.0	25.0	25.0	25.0	25.0	25.0	25.0	0.0
0.0	25.0	25.0	25.0	25.0	25.0	25.0	25.0	25.0	25.0	0.0
0.0	25.0	25.0	25.0	25.0	25.0	25.0	25.0	25.0	25.0	0.0
0.0	25.0	25.0	25.0	25.0	25.0	25.0	25.0	25.0	25.0	0.0
0.0	25.0	25.0	25.0	25.0	25.0	25.0	25.0	25.0	25.0	0.0
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

OUTPUT DATA FOR TEST PROBLEM #1

DIFFUSE RECHARGE AND DISCHARGE (FT/SEC)

0.00E+00 0. 00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E100 0.00E+00 0.00E+00 0.00E+00 0.00E+00
0.00E+00
0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E-00 0.00E+00 0.00E+00 0.00E+00 0.00E-00 0.00E+00
0.00E+00
0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00
0.00E+00
0.00E+00 0.00E-00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00
0.00E+00
0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00
0.00E+00
0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00
0.00E+00
0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00
0.00E+00
0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00
0.00E+00
0.00E+00 0.00E+00 0.00E+00 0.00E100 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00
0.00E+00
0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00
0.00E+00
0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00
0.00E+00
0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00
0.00E+00
0.00E+00 0.00E+00 0.00E-00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00
0.00E+00
0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00
0.00E+00
0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00
0.00E+00
0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00
0.00E+00
0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00
0.00E+00
0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00
0.00E+00
0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00
0.00E+00
0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00
0.00E+00

PERMEABILTY MAP (FT/SEC)

0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00
0.00E+00
0.00E+00 1.00E-04 1.00E-04 1.00E-04 1.00E-04 1.00E-04 1.00E-04 1.00E-04 1.00E-04 1.00E-04
0.00E+00
0.00E+00 l.00E-04 1.00E-04 1.00E-04 1.00E-04 1.00E-04 1.00E-04 1.00E-04 1.00E-04 1.00E-04
0.00E+00
0.00E+00 l.00E-04 1.00E-04 1.00E-04 1.00E-04 1.00E-04 1.00E-04 1.00E-04 1.00E-04 1.00E-04
0.00E+00
0.00E+00 l.00E-04 1.00E-04 1.00E-04 1.00E-04 1.00E-04 1.00E-04 1.00E-04 1.00E-04 1.00E-04

OUTPUT DATA FOR TEST PROBLEM #1

```
0.00E+00
0.00E+00  1.00E-04  1.00E-04  1.00E-04  1.00E-04  1.00E-04  1.00E-04  1.00E-04  1.00E-04  1.00E-04
0.00E+00
0.00E+00  1.00E-04  1.00E-04  1.00E-04  1.00E-04  1.00E-04  1.00E-04  1.00E-04  1.00E-04  1.00E-04
0.00E+00
0.00E+00  1.00E-04  1.00E-04  1.00E-04  1.00E-04  1.00E-04  1.00E-04  1.00E-04  1.00E-04  1.00E-04
0.00E+00
0.00E-00  1.00E-04  1.00E-04  1.00E-04  1.00E-04  1.00E-04  1.00E-04  1.00E-04  1.00E-04  1.00E-04
0.00E+00
0.00E+00  1.00E-04  1.00E-04  1.00E-04  1.00E-04  1.00E-04  1.00E-04  1.00E-04  1.00E-04  1.00E-04
0.00E+.00
0.00E+00  1.00E-04  1.00E-04  1.00E-04  1.00E-04  1.00E-04  1.00E-04  1.00E-04  1.00E-04  1.00E-04
0.00E+00
0.00E+00  1.00E-04  1.00E-04  1.00E-04  1.00E-04  1.00E-04  1.00E-04  1.00E-04  1.00E-04  1.00E-04
0.00E+00
0.00E+00  1.00E-04  1.00E-04  1.00E-04  1.00E-04  1.00E-04  1.00E-04  1.00E-04  1.00E-04  1.00E-04
0.00E+00
0.00E+00  1.00E-04  1.00E-04  1.00E-04  1.00E-04  1.00E-04  1.00E-04  1.00E-04  1.00E-04  1.00E-04
0.00E+00
0.00E+00  1.00E-04  1.00E-04  1.00E-04  1.00E-04  1.00E-04  1.00E-04  1.00E-04  1.00E-04  1.00E-04
0.00E+00
0.00E+00  1.00E-04  1.00E-04  1.00E-04  1.00E-04  1.00E-04  1.00E-04  1.00E-04  1.00E-04  1.00E-04
0.00E+00
0.00E+00  1.00E-04  1.00E-04  1.00E-04  1.00E-04  1.00E-04  1.00E-04  1.00E-04  1.00E-04  1.00E-04
0.00E+00
0.00E+00  1.00E-04  1.00E-04  1.00E-04  1.00E-04  l.00E-04  1.00E-04  1.00E-04  1.00E-04  1.00E-04
0.00E+00
0.00E+00  1.00E-04  1.00E-04  1.00E-04  1.00E-04  1.00E-04  1.00E-04  1.00E-04  1.00E-04  1.00E-04
0.00E+00
0.00E+00 0.00E+00  0.00E+00  0.00E+00  0.00E+00  0.00E+00  0.00E+00  0.00E+00  0.00E+00  0.00E+00
0.00E+00
                    NO. OF FINITE-DIFFERENCE CELLS IN AQUIFER     =  162
                    AREA OF AQUIFER IN MODEL                      = 0.40500E+06   SQ. FT.

                    NZCRIT   (MAX. NO. OF CELLS THAT CAN BE VOID OF
                              PARTICLES;  IF EXCEEDED, PARTICLES ARE REGENERATED)   =    3
```

OUTPUT DATA FOR TEST PROBLEM #1

NODE IDENTIFICATION MAP

0	0	0	0	0	0	0	0	0	0	0
0	1	1	1	1	1	1	1	1	1	0
0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0
0	1	1	1	1	1	1	1	1	1	0
0	0	0	0	0	0	0	0	0	0	0

NO. OF NODE IDENT. CODES SPECIFIED = 1

THE FOLLOWING ASSIGNMENTS HAVE BEEN MADE:

CODE NO.	LEAKANCE	SOURCE CONC.	02 CONC	RECHARGE
1	0.100E+01	0.00	8.00	

OUTPUT DATA FOR TEST PROBLEM #1

VERTICAL PERMEABILITY/THICKNESS (FT/(FT*SEC))

0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
0.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	0.00E+00
0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E-00	0.00E+00	0.00E+00	0.00E+00
0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
0.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00	0.00E+00
0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00

OUTPUT DATA EOR TEST PROBLEM # 1

WATER TABLE

0.	0.	0.	0.	0.	0.	0.	0.	0.
0.	0.							
0.	100.	100.	100.	100.	100.	100.	100.	100.
100.	0.							
0.	0.	0.	0.	0.	0.	0.	0.	0.
0.	0.							
0.	0.	0.	0.	0.	0.	0.	0.	0.
0.	0.							
0.	0.	0.	0.	0.	0.	0.	0.	0.
0.	0.							
0.	0.	0.	0.	0.	0.	0.	0.	0.
0.	0.							
0.	0.	0.	0.	0.	0.	0.	0.	0.
0.	0.							
0.	0.	0.	0.	0.	0.	0.	0.	0.
0.	0.							
0.	0.	0.	0.	0.	0.	0.	0.	0.
0.	0.							
0.	0.	0.	0.	0.	0.	0.	0.	0.
0.	0.							
0.	0.	0.	0.	0.	0.	0.	0.	0.
0.	0.							
0.	0.	0.	0.	0.	0.	0.	0.	0.
0.	0.							
0.	0.	0.	0.	0.	0.	0.	0.	0.
0.	0.							
0.	0.	0.	0.	0.	0.	0.	0.	0.
0.	0.							
0.	0.	0.	0.	0.	0.	0.	0.	0.
0.	0.							
0.	0.	0.	0.	0.	0.	0.	0.	0.
0.	0.							
0.	0.	0.	0.	0.	0.	0.	0.	0.
0.	0.							
0.	0.	0.	0.	0.	0.	0.	0.	0.
0.	0.							
0.	97.	97.	97.	97.	97.	97.	97.	97.
97.	0.							
0.	0.	0.	0.	0.	0.	0.	0.	0.
0.	0.							

OUTPUT DATA FOR TEST PROBLEM #1

HEAD DISTRIBUTION - ROW

NUMBER OF TIME STEPS = 0

TIME(SECONDS) = 0.00000E+00

TIME(DAYS) = 0.00000E+00

TIME(VEARS) = 0.00000E+00

0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
0.0000000	0.0000000	0.0000000					
0.0000000	100.0000000	100.0000000	100.0000000	100.0000000	100.0000000	100.0000000	100.0000000
100.0000000	100.0000000	0.0000000					
0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
0.0000000	0.0000000	0.0000000					
0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
0.0000000	0.0000000	0.0000000					
0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
0.0000000	0.0000000	0.0000000					
0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
0.0000000	0.0000000	0.0000000					
0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
0.0000000	0.0000000	0.0000000					
0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
0.0000000	0.0000000	0.0000000					
0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
0.0000000	0.0000000	0.0000000					
0.0000000	0.0000000	0.000.0000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
0.0000000	0.0000000	0.0000000					
0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
0.0000000	0.0000000	0.0000000					
0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
0.0000000	0.0000000	0.0000000					
0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
0.0000000	0.0000000	0.0000000					
0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
0.0000000	0.0000000	0.0000000					
0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
0.0000000	0.0000000	0.0000000					
0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
0.0000000	0.0000000	0.0000000					
0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
0.0000000	0.0000000	0.0000000					
0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
0.0000000	0.0000000	0.0000000					
0.0000000	97.0000000	97.0000000	97.0000000	97.0000000	97.0000000	97.0000000	97.0000000
97.0000000	97.0000000	0.0000000					
0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000	0.0000000
0.0000000	0.0000000	0.0000000					

OUTPUT DATA FOR TEST PROBLEM #1

ITERATION PARAMETERS

0.616850E-02
0.144040E-01
0.336346E-01
0.785398E-01
0.183397
0.428249
1.00000
0.000000E+00
0.000000E+00
0.000000E+00
0.000000E+00
0.000000E+00
0.000000E+00
0.000000E+00
0.000000E+00
0.000000E+00
0.000000E+00
0.000000E+00
0.000000E+00
0.000000E+00
0.000000E+00

OUTPUT DATA FOR TEST PROBLEM #1

CONCENTRATION OF CONTAMINANT

NUMBER OF TIME STEPS	=	0
TIME(SECONDS)	=	0.00000E+00
CHEM.TIME(SECONDS)	=	0.00000E+00
CHEM.TIME(DAYS)	=	0.00000E+00
TIME(YEARS)	=	0.00000E+00
CHEM.TIME(YEARS)	=	0.00000E+00
NO. MOVES COMPLETED	=	0

0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0

OUTPUT DATA FOR TEST PROBLEM #1

CONCENTRATION OF OXYGEN

NUMBER OF TIME STEPS = 0

TIME(SECONDS) = 0.00000E+00
CHEM.TIME(SECONDS) = 0.00000E+00
CHEM.TIME(DAVS) = 0.00000E+00
TIME(YEARS) = 0.00000E+00
CHEM.TIME(VEARS) = 0.00000E+00
NO. MOVES COMPLETED = 0

0	0	0	0	0	0	0	0	0	0	0
0	8	8	8	8	8	8	8	8	8	0
0	8	8	8	8	8	8	8	8	8	0
0	8	8	8	8	8	8	8	8	8	0
0	8	8	8	8	8	8	8	8	8	0
0	8	8	8	8	8	8	8	8	8	0
0	8	8	8	8	8	8	8	8	8	0
0	8	8	8	8	8	8	8	8	8	0
0	8	8	8	8	8	8	8	8	8	0
0	8	8	8	8	8	8	8	8	8	0
0	8	8	8	8	8	8	8	8	8	0
0	8	8	8	8	8	8	8	8	8	0
0	8	8	8	8	8	8	8	8	8	0
0	8	8	8	8	8	8	8	8	8	0
0	8	8	8	8	8	8	8	8	8	0
0	8	8	8	8	8	8	8	8	8	0
0	8	8	8	8	8	8	8	8	8	0
0	8	8	8	8	8	8	8	8	8	0
0	8	8	8	8	8	8	8	8	8	0
0	0	0	0	0	0	0	0	0	0	0

N = 1
NUMBER OF ITERATIONS = 20

OUTPUT DATA FOR TEST PROBLEM #1

HEAD DISTRIBUTION - ROW
NUMBER OF TIME STEPS = 1
TIME(SECONDS) = 0.18935E+09
TIME(DAYS) = 0.21915E+04
TIME(YEARS) = 0.60000E+01

0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000
0.0000000 0.0000000 0.0000000
0.0000000 99.9999998 99.9999998 99.9999998 99.9999998 99.9999998 99.9999998 99.9999998
99.9999998 99.9999998 0.0000000
0.0000000 99.8291477 99.8294635 99.8302416 99.8310992 99.8315824 99.8310992 99.8302416
99.8294635 99.8291477 0.0000000
0.0000000 99.6586734 99.6595657 99.6612187 99.6633789 99.6649445 99.6633789 99.6612187
99.6595657 99.6586734 0.0000000
0.0000000 99.4866865 99.4880365 99.4909366 99.4955451 99.5007236 99.4955451 99.4909366
99.4880365 99.4866865 0.0000000
0.0000000 99.3131983 99.3147908 99.3187861 99.3270257 99.3467482 99.3270257 99.3187861
99.3147908 99.3131983 0.0000000
0.0000000 99.1386046 99.1399849 99.1429669 99.1476276 99.1528277 99.1476276 99.1429669
99.1399849 99.1386046 0.0000000
0.0000000 98.9622862 98.9632029 98.9650297 98.9673115 98.9689244 98.9673115 98.9650297
98.9632029 98.9622862 0.0000000
0.0000000 98.7848457 98.7853475 98.7863989 98.7874966 98.7880871 98.7874966 98.7863989
98.7853475 98.7848457 0.0000000
0.0000000 98.6071305 98.607,4165 98.6079959 98.6085203 98.6087643 98.6085203 98.6079959
98.6074165 98.6071305 0.0000000
0.0000000 98.4289299 98.4290704 98.4293942 98.4296452 98.4297534 98.4296452 98.4293942
98.4290704 98.4289299 0.0000000
0.0000000 98.2503905 98.2504197 98.2506138 98.2507353 98.2507850 98.2507353 98.2506138
98.2504197 98.2503905 0.0000000
0.0000000 98.0720432 98.0720689 98.0721733 98.0722224 98.0722427 98.0722224 98.0721733
98.0720689 98.0720432 0.0000000
0.0000000 97.8934704 97.8934850 97.8935556 97.8935769 97.8935868 97.8935769 97.8935556
97.8934850 97.8934704 0.0000000
0.0000000 97.7145462 97.7144821 97.7145573 97.7145736 97.7145774 97.7145736 97.7145573
97.7144821 97.7145462 0.0000000
0.0000000 97.5361558 97.5361572 97.5361729 97.5361670 97.5361656 97.5361670 97.5361729
97.5361572 97.5361558 0.0000000
0.0000000 97.3576164 97.3576574 97.3576539 97.3576438 97.3576428 97.3576438 97.3576539
97.3576574 97.3576164 0.0000000
0.0000000 97.1784342 97.1783588 97.1784118 97.1784250 97.1784260 97.1784250 97.1784118
97.1783588 97.1784342 0.0000000
0.0000000 97.0000002 97.0000002 97.0000002 97.0000002 97.0000002 97.0000002 97.0000002
97.0000002 97.0000002 0.0000000
0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000
0.0000000 0.0000000 0.0000000

OUTPUT DATA FOR TEST PROBLEM #1

HEAD DISTRIBUTION - ROW
NUMBER OF TIME STEPS = 1
TIME(SECONDS) = 0.18935E+09
TIME(DAYS) = 0.21915E+04
TIME(YEARS) = 0.60000E+01

0	0	0	0	0	0	0	0	0	0	0
0	100	100	100	100	100	100	100	100	100	0
0	100	100	100	100	100	100	100	100	100	0
0	100	100	100	100	100	100	100	100	100	0
0	99	99	99	99	100	99	99	99	99	0
0	99	99	99	99	99	99	99	99	99	0
0	99	99	99	99	99	99	99	99	99	0
0	99	99	99	99	99	99	99	99	99	0
0	99	99	99	99	99	99	99	99	99	0
0	99	99	99	99	99	99	99	99	99	0
0	98	98	98	98	98	98	98	98	98	0
0	98	98	98	98	98	98	98	98	98	0
0	98	98	98	98	98	98	98	98	98	0
0	98	98	98	98	98	98	98	98	98	0
0	98	98	98	98	98	98	98	98	98	0
0	98	98	98	98	98	98	98	98	98	0
0	97	97	97	97	97	97	97	97	97	0
0	97	97	97	97	97	97	97	97	97	0
0	97	97	97	97	97	97	97	97	97	0
0	0	0	0	0	0	0	0	0	0	0

OUTPUT DATA FOR TEST PROBLEM #1

DRAWDOWN

0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0
0	-99	-99	-99	-99	-99	-99	-99	-99	-99	0
0	-99	-99	-99	-99	-99	-99	-99	-99	-99	0
0	-98	-98	-98	-98	-99	-98	-98	-98	-98	0
0	-98	-98	-98	-98	-98	-98	-98	-98	-98	0
0	-98	-98	-98	-98	-98	-98	-98	-98	-98	0
0	-98	-98	-98	-98	-98	-98	-98	-98	-98	0
0	-98	-98	-98	-98	-98	-98	-98	-98	-98	0
0	-98	-98	-98	-98	-98	-98	-98	-98	-98	0
0	-97	-97	-97	-97	-97	-97	-97	-97	-97	0
0	-97	-97	-97	-97	-97	-97	-97	-97	-97	0
0	-97	-97	-97	-97	-97	-97	-97	-97	-97	0
0	-97	-97	-97	-97	-97	-97	-97	-97	-97	0
0	-97	-97	-97	-97	-97	-97	-97	-97	-97	0
0	-97	-97	-97	-97	-97	-97	-97	-97	-97	0
0	-96	-96	-96	-96	-96	-96	-96	-96	-96	0
0	-96	-96	-96	-96	-96	-96	-96	-96	-96	0
0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0

CUMULATIVE MASS BALANCE -- (IN FT**3)

RECHARGE AND INJECTION	=	-0.37869E+05
PUMPAGE AND E-T WITHDRAWAL	=	0.00000E+00
CUMULATIVE NET PUMPAGE	=	-0.37869E+05
WATER RELEASE FROM STORAGE	=	0.00000E+00
LEAKAGE INTO AQUIFER	=	0.72354E+06
LEAKAGE OUT OF AQUIFER	=	-0.76007E+06
CUMULATIVE NET LEAKAGE	=	-0.36531E+05
MASS BALANCE RESIDUAL	=	1338.4
ERROR (AS PERCENT)	=	0.17594

RATE MASS BALANCE -- (IN C.F.S.)

LEAKAGE INTO AQUIFER	=	0.38213E-02
LEAKAGE OUT OF AQUIFER	=	-0.40142E-02
NET LEAKAGE (QNET)	=	-0.19293E-03
RECHARGE AND INJECTION	=	-0.20000E-03
PUMPAGE AND E-T WITHDRAWAL	=	0.00000E+00
NET WITHDRAWAL (TPUM)	=	-0.20000E-03

OUTPUT DATA FOR TEST PROBLEM #1

STABILITY CRITERIA --- M.O.C.

FLUID VELOCITIES
VMAX = 9.32E-08 VMAY = 1.26E-06
VMXBD= 1.31E-07 VMYBD= 1.29E-06

TMV (MAX. INJ.) = 0.43898E+08
TIMV (CELDIS) = 0.19338E+08

TIMV = 1.93E+07 NTIMV = 9 NMOV = 10

TIM (N) = 0.18935E+09
TIMEVELO = 0.18935E+08
TIMEDISP = 0.87852E+08

TIMV = 1.89E+07 NTIMD = 2 NMOV = 10

THE LIMITING STABILITY CRITERION IS CELDIS
NO. OF PARTICLE MOVES REQUIRED TO COMPLETE THIS TIME STEP = 10

NP	=	1709	IMOV	=	1		
TIM(N)	=	0.18935E+09	TIMV	=	0.18935E+08	SUMTCH =	0.18935E+08
NP1	=	1709	IMOV(02)	=	1		
TIM(N)	=	0.18935E+09	TIMV	=	0.18935E+08	SUMTCH =	0.18935E+08
NP	=	1715	IMOV	=	2		
TIM(N)	=	0.18935E+09	TIMV	=	0.18935E+08	SUMTCH =	0.37869E+08
NP1	=	1715	IMOV(02)	=	2		
TIM(N)	=	0.18935E+09	TIMV	=	0.18935E+08	SUMTCH =	0.37869E+08
NP	=	1715	IMOV	=	3		
TIM(N)	=	0.18935E+09	TIMV	=	0.18935E+08	SUMTCH =	0.56804E+08
NP1	=	1715	IMOV(02)	=	3		
TIM(N)	=	0.18935E+09	TIMV	=	0.18935E+08	SUMTCH =	0.56804E+08
NP	=	1724	IMOV	=	4		
TIM(N)	=	0.18935E+09	TIMV	=	0.18935E+08	SUMTCH =	0.75738E+08
NPI	=	1724	IMOV(02)	=	4		
TIM(N)	=	0.18935E+09	TIMV	=	0.18935E+08	SUMTCH =	0.75738E+08
NP	=	1740	IMOV	=	5		
TIM(N)	=	0.18935E+09	TIMV	=	0.18935E+08	SUMTCH =	0.94673E+08
NPI	=	1740	IMOV(02)	=	5		
TIM(N)	=	0.18935E+09	TIMV	=	0.18935E+08	SUMTCH =	0.94673E+08
NP	=	1748	IMOV	=	6		
TIM(N)	=	0.18935E+09	TIMV	=	0.18935E+08	SUMTCH =	0.11361E+09
NPI	=	1748	IMOV(02)	=	6		
TIM(N)	=	0.18935E+09	TIMV	=	0.18935E+08	SUMTCH =	0.11361E+09
NP	=	1757	IMOV	=	7		
TIM(N)	=	0.18935E+09	TIMV	=	0.18935E+08	SUMTCH =	0.13254E+09
NPI	=	1757	IMOV(02)	=	7		
TIM(N)	=	0.18935E+09	TIMV	=	0.18935E+08	SUMTCH =	0.13254E+09
NP	=	1757	IMOV	=	8		
TIM(N)	=	0.18935E+09	TIMV	=	0.18935E+08	SUMTCH =	0.15148E+09
NPI	=	1757	IMOV(02)	=	8		
TIM(N)	=	0.18935E+09	TIMV	=	0.18935E+08	SUMTCH =	0.15148E+09
NP	=	1760	IMOV	=	9		
TIM(N)	=	0.18935E+09	TIMV	=	0.18935E+08	SUMTCH =	0.17041E+09

NP1	=	1760	IMOV(02)	=	9		
TIM(N)	=	0.18935E+09	TIMV	=	0.18935E+08	SUMTCH =	0.17041E+09
NP	=	1764	IMOV	=	10		
TIM(N)	=	0.18935E+09	TIMV	=	0.18935E+08	SUMTCH =	0.18935E+09
NPI	=	1764	IMOV(02)	=	10		
TIM(N)	=	0.18935E+09	TIMV	=	0.18935E+08	SUMTCH =	0.18935E+09

OUTPUT DATA FOR TEST PROBLEM #1

CONCENTRATION OF CONTAMINANT

NUMBER OF TIME STEPS	=	1
DELTA T	=	0.18935E+09
TIME(SECONDS)	=	0.18935E+09
CHEM.TIME(SECONDS)	=	0.18935E+09
CHEM.TIME(DAYS)	=	0.21915E+04
TIME(YEARS)	=	0.60000E+01
CHEM.TIME(YEARS)	=	0.60000E+01
NO. MOVES COMPLETED	=	10

0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	1	0	0	0	0	0
0	0	0	0	0	30	0	0	0	0	0
0	0	0	0	0	35	0	0	0	0	0
0	0	0	0	6	30	6	0	0	0	0
0	0	0	0	5	26	5	0	0	0	0
0	0	0	0	0	18	0	0	0	0	0
0	0	0	0	0	9	0	0	0	0	0
0	0	0	0	0	1	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0

CHEMICAL MASS BALANCE

MASS IN BOUNDARIES	=	0.00000E+00
MASS OUT BOUNDARIES	=	-0.82522E-03
MASS PUMPED IN	=	0.37869E+07
MASS PUMPED OUT	=	0.00000E+00
MASS LOST W. BIODEG.	=	0.78974E+06
MASS LOST BY RADIO. DCY	=	0.00000E+00
MASS LOST BY ANAER. DCY	=	0.00000E+00
MASS LOST RY REAER. DCY	=	0.00000E+00
MASS ADSORBED ON SOLIDS	=	0.00000E+00
INITIAL MASS ADSORBED	=	0.00000E+00
INFLOW MINUS OUTFLOW	=	0.37869E+07
INITIAL MASS DISSOLVED	=	0.00000E+00
PRESENT MASS DISSOLVED	=	0.32135E+07
CHANGE MASS DISSOLVED	=	0.40033E+07
CHANGE TOTL.MASS STORED	=	0.40033E+07

COMPARE RESIDUAL WITH NET FLUX AND MASS ACCUMULATION:

MASS BALANCE RESIDUAL	=	-0.21635E+06
ERROR (AS PERCENT)	=	-0.57130E+01

OUTPUT DATA FOR TEST PROBLEM #1

CONCENTRATION OF OXYGEN

NUM8ER OF TIME STEPS	=	1
DELTA T	=	0.18935E+09
TIME(SECONDS)	=	0.18935E+09
CHEM.TIME(SECONDS)	=	0.18935E+09
CHEM.TIME(DAYS)	=	0.21915E+04
TIME(YEARS)	=	0.60000E+01
CHEM.TIME(YEARS)	=	0.60000E+01
NO. MOVES COMPLETED	=	10

0	0	0	0	0	0	0	0	0	0	0
0	8	8	8	8	8	8	8	8	8	0
0	8	8	8	8	8	8	8	8	8	0
0	8	8	8	8	7	8	8	8	8	0
0	8	8	8	8	0	8	8	8	8	0
0	8	8	8	7	0	7	8	8	8	0
0	8	8	8	2	0	2	8	8	8	0
0	8	8	8	0	0	0	8	8	8	0
0	8	8	8	0	0	0	8	8	8	0
0	8	8	8	1	0	1	8	8	8	0
0	8	8	8	5	0	5	8	8	8	0
0	8	8	8	7	0	7	8	8	8	0
0	8	8	8	8	6	8	8	8	8	0
0	8	8	8	8	8	8	8	8	8	0
0	8	8	8	8	8	8	8	8	8	0
0	8	8	8	8	8	8	8	8	8	0
0	8	8	8	8	8	8	8	8	8	0
0	8	8	8	8	8	8	8	8	8	0
0	0	0	0	0	0	0	0	0	0	0

CHEMICAL MASS BALANCE FOR OXYGEN

MASS IN BOUDARIES	=	0.57883E+07
MASS OUT BOUNDARIES	=	-0.60805E+07
MASS PUMPED IN	=	0.00000E+00
MASS PUMPED OUT	=	0.00000E+00
MASS LOST W. BIODEG.	=	0.23692E+07
INFLOW MINUS OUTFLOW	=	-0.29222E+06
INITIAL MASS DISSOLVED	=	0.24300E+08
PRESENT MASS DISSOLVED	=	0.21721E+08
CHANGE MASS DISSOLVED	=	-0.20981E+06
CHANGE TOTL.MASS STORED	=	-0.20981E+06

COMPARE RESIDUAL WITH NET FLUX AND MASS ACCUMULATION FOR OXVGEN:

MASS BALANCE RESIDUAL	=	-0.82416E+05
ERROR (AS PERCENT)	=	-0.14238E+01

COMPARE INITIAL MASS STORED WITH CHANGE IN MASS STORED FOR OXYGEN:

ERROR (AS PERCENT)	=	0.33513E+00

OUTPUT DATA FOR TEST PROBLEM #1

TEST PROBLEM #1 - NATURAL BIODEGRADATION

TIME VERSUS HEAD AND CONCENTRATION AT SELECTED OBSERVATION POINTS
PUMPING PERIOD NO. 1

STEADY-STATE SOLUTION

OBS.WELL NO.	X	Y	N	HEAD (FT)	CONC.(MG/L)	TIME (YEARS)
1	5	10				
			0	0.0	0.0	0.000
			1	98.6	0.0	0.600
			2	98.6	0.0	1.200
			3	98.6	0.0	1.800
			4	98.6	0.0	2.400
			5	98.6	0.0	3.000
			6	98.6	0.0	3.600
			7	98.6	0.0	4.200
			8	98.6	0.0	4.800
			9	98.6	0.0	5.400
			10	98.6	0.0	6.000

OUTPUT DATA FOR TEST PROBLEM #1

TEST PROBLEM #1 - NATURAL BIODEGRADATION

TIME VERSUS HEAD AND CONCENTRATION(0_2) AT SELECTED OBSERVATION POINTS

PUMPING PERIOD NO. 1

STEADY-STATE SOLUTION FOR OXYGEN

OBS.WELL NO.	X	Y	N	HEAD (FT)	CONC.(MG/L)	TIME (YEARS)
1	5	10				
			0	0.0	8.0	0.000
			1	98.6	8.0	0.600
			2	98.6	8.0	1.200
			3	98.6	8.0	1.800
			4	98.6	8.0	2.400
			5	98.6	7.9	3.000
			6	98.6	7.8	3.600
			7	98.6	7.2	4.200
			8	98.6	6.2	4.800
			9	98.6	4.3	5.400
			10	98.6	0.9	6.000

OUTPUT DATA FOR TEST PROBLEM # I

Non-biodegraded contaminant Plume for Test Problem #1

0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	3	0	0	0	0	0
0	0	0	0	0	32	0	0	0	0	0
0	0	0	0	2	37	2	0	0	0	0
0	0	0	0	8	31	8	0	0	0	0
0	0	0	0	8	28	8	0	0	0	0
0	0	0	0	2	20	2	0	0	0	0
0	0	0	0	1	11	1	0	0	0	0
0	0	0	0	0	4	0	0	0	0	0
0	0	0	0	0	1	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0

APPENDIX C: Selected Output for Test Problem #2

CONCENTRATION OF CONTAMINANT

NUMBER OF TIME STEPS	=	1
DELTA T	=	0.18935E+09
TIME(SECONDS)	=	0.18935E+09
CHEM.TIME(SECONDS)	=	0.18935E+09
CHEM.TIME(DAYS)	=	0.21915E+04
TIME(YEARS)	=	0.60000E+01
CHEM.TIME(YEARS)	=	0.60000E+01
NO. MOVES COMPLETED	=	10

0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	28	0	0	0	0	0
0	0	0	0	0	30	0	0	0	0	0
0	0	0	0	4	22	4	0	0	0	0
0	0	0	0	3	18	3	0	0	0	0
0	0	0	0	0	11	0	0	0	0	0
0	0	0	0	0	5	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0

CHEMICAL MASS BALANCE

MASS IN BOUNDARIES	=	0.00000E+00
MASS OUT BOUNDARIES	=	-0.64388E-03
MASS PUMPED IN	=	0.37869E+07
MASS PUMPED OUT	=	0.00000E+00
MASS LOST W. BIODEG.	=	0.72548E+06
MASS LOST 8Y RADIO. DCY	=	0.00000E+00
MASS LOST BY ANAER. DCY	=	0.00000E+00
MASS LOST BY REAER. DCY	=	-0.82054E+06
MASS ADSORBED ON SOLIDS	=	0.00000E+00
INITIAL MASS ADSOR8ED	=	0.00000E+00
INFLOW MINUS OUTFLOW	=	0.37869E+07
INITIAL MASS DISSOLVED	=	0.00000E+00
PRESENT MASS DISSOLVED	=	0.23741E+07
CHANGE MASS DISSOLVED	=	0.30996E+07
CHANGE TOTL.MASS STORED	=	0.30996E+07
COMPARE RESIDUAL WITH NET FLUX AND MASS ACCUMULATION:		
MASS BALANCE RESIDUAL	=	-0.13322E+06
ERROR (AS PERCENT)	=	-0.35180E+01

SELECTED OUTPUT FOR TEST PR0BLEM #2

CONCENTRATION OF OXYGEN

NUMBER OF TIME STEPS =
DELTA T = 0.18935E+09
TIME(SECONDS) = 0.18935E+09
CHEM.TIME(SECONDS) = 0.18935E+09
CHEM.TIME(DAYS) = 0.21915E+04
TIME(YEARS) = 0.60000E+01
CHEM.TIME(YEARS) = 0.60000E+01
NO. MOVES COMPLETED = 10

0	0	0	0	0	0	0	0	0	0	0
0	8	8	8	8	8	8	8	8	8	0
0	8	8	8	8	8	8	8	8	8	0
0	8	8	8	8	7	8	8	8	8	0
0	8	8	8	8	0	8	8	8	8	0
0	8	8	8	7	0	7	8	8	8	0
0	8	8	8	3	0	3	8	8	8	0
0	8	8	8	0	0	0	8	8	8	0
0	8	8	8	0	0	0	8	8	8	0
0	8	8	8	3	0	3	8	8	8	0
0	8	8	8	6	0	6	8	8	8	0
0	8	8	8	7	0	7	8	8	8	0
0	8	8	8	8	6	8	8	8	8	0
0	8	8	8	8	8	8	8	8	8	0
0	8	8	8	8	8	8	8	8	8	0
0	8	8	8	8	8	8	8	8	8	0
0	8	8	8	8	8	8	8	8	8	0
0	8	8	8	8	8	8	8	8	8	0
0	0	0	0	0	0	0	0	0	0	0

CHEMICAL MASS BALANCE FOR OXYGEN

MASS IN BOUDARIES = 0.57883E+07
MASS OUT BOUNDARIES = -0.60805E+07
MASS PUMPED IN = 0.00000E+00
MASS PUMPED OUT = 0.00000E+00
MASS LOST W. BIODEG. = 0.21764E+07
INFLOW MINUS OUTFLOW = -0.29222E+06
INITIAL MASS DISSOLVED = 0.24300E+08
PRESENT MASS DISSOLVED = 0.21915E+08
CHANGE MASS DISSOLVED = -0.20890E+06
CHANGE TOTL.MASS STORED = -0.20890E+06
COMPARE RESIDUAL WITH NET FLUX AND MASS ACCUMULATION FOR OXYGEN:
MASS BALANCE RESIDUAL = -0.83328E+05
ERROR (AS PERCENT) = -0.14396E+01
COMPARE INITIAL MASS STORED WITH CHANGE IN MASS STORED FOR OXYGEN:
ERROR (AS PERCENT) = 0.33884E+00

SELECTED OUTPUT FOR TEST PROBLEM #2

TEST PROBLEM #2 - NATURAL BIODEGRADATION WITH REAERATION

TIME VERSUS HEAD AND CONCENTRATION AT SELECTED 085ERVATION POINTS
PUMPING PERIOD NO. 1

STEADY-STATE SOLUTION

OBS.WELL NO.	X	Y	N	HEAD (FT)	CONC.(MG/L)	TIME (YEARS)
1	5	10				
			0	0.0	0.0	0.000
			1	98.6	0.0	0.600
			2	98.6	0.0	1.200
			3	98.6	0.0	1.800
			4	98.6	0.0	2.400
			5	98.6	0.0	3.000
			6	98.6	0.0	3.600
			7	98.6	0.0	4.200
			8	98.6	0.0	4.800
			9	98.6	0.0	5.400
			10	98.6	0.0	6.000

SELECTED OUTPUT FOR TEST PROBLEM #2

TEST PROBLEM #2 - NATURAL BI0DEGRADATION WITH REAERATION

TIME VERSUS HEAD AND CONCENTRATION(02) AT SELECTED OBSERVATION POINTS

PUMPING PERIOD NO. I

STEADY-STATE SOLUTION FOR OXYGEN

OBS.WELL NO.	X	Y	N	HEAD (FT)	CONC.(MG/L)	TIME (YEARS)
1	5	10				
			0	0.0	8.0	0.000
			1	98.6	8.0	0.600
			2	98.6	8.0	1.200
			3	98.6	8.0	1.800
			4	98.6	8.0	2.400
			5	98.6	7.9	3 000
			6	98.6	7.8	3.600
			7	98.6	7.4	4.200
			8	98.6	6.6	4.800
			9	98.6	5.3	5 400
			10	98.6	3.1	6.000

Appendix D: Selected Output for Test Problem #3

CONCENTRATION OF CONTAMINANT

NUM8ER OF TIME STEPS	=	1
DELTA T	=	0.18935E+09
TIME(SECONDS)	=	0.18935E+09
CHEM.TIME(SECONDS)	=	0.18935E+09
CHEM.TIME(DAYS)	=	0.21915E+04
TIME(YEARS)	=	0.60000E+01
CHEM.TIME(YEARS)	=	0.60000E+01
NO. MOVES COMPLETED	=	18

0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	5	0	0	0	0	0
0	0	0	0	0	4	0	0	0	0	0
0	0	0	0	0	1	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0

CHEMICAL MASS BALANCE

MASS IN BOUNDARIES	=	0.00000E+00
MASS OUT BOUNDARIES	=	-0.27496E+02
MASS PUMPED IN	=	0.00000E+00
MASS PUMPED OUT	=	-0.30089E+07
MASS LOST W. BIODEG.	=	0.50875E+06
MASS LOST BY RADIO. DCY	=	0.00000E+00
MASS LOST BY ANAER. DCY	=	0.00000E+00
MASS LOST BY REAER. DCY	=	0.00000E+00
MASS ADSORBED ON SOLIDS	=	0.00000E+00
INITIAL MASS ADSORBED	=	0.00000E+00
INFLOW MINUS OUTFLOW	=	-0.30089E+07
INITIAL MASS DISSOLVED	=	0.32250E+07
PRESENT MASS DISSOLVED	=	0.19133E+06
CHANGE MASS DISSOLVED	=	-0.25249E+07
CHANGE TOTL.MASS STORED	=	-0.25249E+07

SELECTED OUTPUT FOR TEST PROBLEM #3

```
COMPARE RESIDUAL WITH NET FLUX AND MASS ACCUMULATION:
  MASS BALANCE RESIDUAL              =        -0.48396E+06
  ERROR  (AS PERCENT)                =         0.00000E+00
COMPARE INITIAL MASS STORED WITH CHANGE IN MASS STORED:
  ERROR  (AS PERCENT)                =         0.77633E+01
```

SELECTED OUTPUT FOR TEST PROBLEM #3

CONCENTRATION OF OXYGEN

NUMBER OF TIME STEPS	=	1
DELTA T	=	0.18935E+09
TIME(SECONDS)	=	0.18935E+09
CHEM.TIME(SECONDS)	=	0.18935E+09
CHEM.TIME(DAYS)	=	0.21915E+04
TIME(YEARS)	=	0.60000E+01
CHEM.TIME(YEARS)	=	0.60000E+01
NO. MOVES COMPLETED	=	18

0	0	0	0	0	0	0	0	0	0	0
0	8	8	8	8	8	8	8	8	8	0
0	8	8	8	8	8	8	8	8	8	0
0	8	8	8	8	8	8	8	8	8	0
0	8	8	8	8	8	8	8	8	8	0
0	8	8	8	8	8	8	8	8	8	0
0	8	8	8	8	8	8	8	8	8	0
0	8	8	8	8	7	8	8	8	8	0
0	8	8	8	6	6	6	8	8	8	0
0	8	8	8	5	3	5	8	8	8	0
0	8	8	7	3	1	3	7	8	8	0
0	8	8	7	5	0	5	7	8	8	0
0	8	8	7	6	0	6	7	8	8	0
0	8	8	8	7	0	7	8	8	8	0
0	8	8	8	7	2	7	8	8	8	0
0	8	8	8	7	3	7	8	8	8	0
0	8	8	8	8	6	8	8	8	8	0
0	8	8	8	8	7	8	8	8	8	0
0	8	8	8	8	8	8	8	8	8	0
0	0	0	0	0	0	0	0	0	0	0

CHEMICAL MASS BALANCE FOR OXYGEN

MASS IN BOUNDARIES	=	0.51645E+07
MASS OUT BOUNDARIES	=	-0.51519E+07
MASS PUMPED IN	=	0.24236E+07
MASS PUMPED OUT	=	-0.46651E+06
MASS LOST W. BIODEG.	=	0.15262E+07
INFLOW MINUS OUTFLOW	=	0.19698E+07
INITIAL MASS DISSOLVED	=	0.21769E+08
PRESENT MASS DISSOLVED	=	0.22443E+08
CHANGE MASS DISSOLVED	=	0.22001E+07
CHANGE TOTL.MASS STORED	=	0.22001E+07

COMPARE RESIDUAL WITH NET FLUX AND MASS ACCUMULATION FOR OXYGEN:

MASS BALANCE RESIDUAL	=	-0.23036E+06
ERROR (AS PERCENT)	=	-0.30357E+01

COMPARE INITIAL MASS STORED WITH CHANGE IN MASS STORED FOR OXYGEN:

ERROR (AS PERCENT)	=	0.11635E+01

SELECTED OUTPUT FOR TEST PROBLEM #3

TEST PROBLEM #3 - IN-SITU BIORESTORATION

TIME VERSUS HEAD AND CONCENTRATION AT SELECTED OBSERVATION POINTS

PUMPING PERIOD NO. 1

STEADY-STATE SOLUTION

OBS.WELL NO.	X	Y	N	HEAD (FT)	CONC.(MG/L)	TIME (YEARS)
1	5	10				
			0	0.0	0.0	0.000
			1	98.4	1.8	0.333
			2	98.4	3.5	0.667
			3	98.4	4.9	1.000
			4	98.4	4.8	1.333
			5	98.4	4.8	1.667
			6	98.4	5.0	2.000
			7	98.4	3.3	2.333
			8	98.4	2.5	2.667
			9	98.4	2.1	3.000
			10	98.4	1.7	3.333
			11	98.4	3.1	3.667
			12	98.4	0.0	4.000
			13	98.4	0.0	4.333
			14	98.4	0.0	4.667
			15	98.4	0.0	5.000
			16	98.4	0.0	5.333
			17	98.4	0.0	5.667
			18	98.4	0.0	6.000

SELECTED OUTPUT FOR TEST PR0BLEM #3

TEST PROBLEM #3 - IN-SITU BI0RESTORATION

TIME VERSUS HEAD AND CONCENTPATION(02) AT SELECTED 0BSERVATION POINTS

PUMPING PERIOD NO. 1

STEADY-STATE SOLUTION FOR OXYGEN

0BS.WELL NO.	X	Y	N	HEAD (FT)	CONC.(MG/L)	TIME (YEARS)
1	5	10				
			0	0.0	1.0	0.000
			1	98.4	0.0	0.333
			2	98.4	0.0	0.667
			3	98.4	0.0	1.000
			4	98.4	0.0	1.333
			5	98.4	0.0	1.667
			6	98.4	0.0	2.000
			7	98.4	0.0	2.333
			8	98.4	0.0	2.667
			9	98.4	0.0	3.000
			10	98.4	0.0	3.333
			11	98.4	0.0	3.667
			12	98.4	1.8	4.000
			13	98.4	2.2	4.333
			14	98.4	0.8	4.667
			16	98.4	1.3	4.000
			16	98.4	2.3	5.333
			17	98.4	4.4	5.667
			18	98.4	0.0	6.000

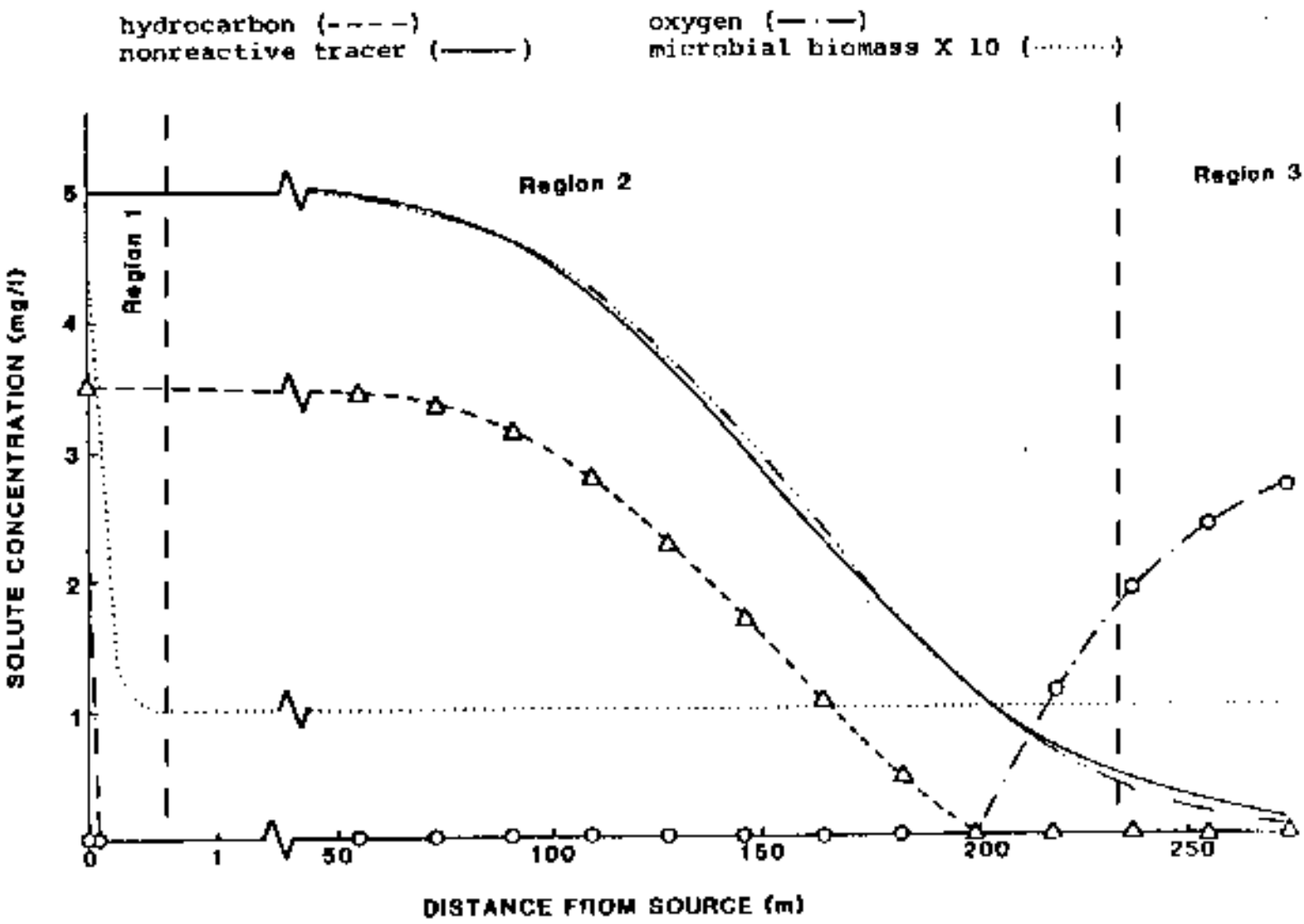


Figure 1.1 - Process Control Regions

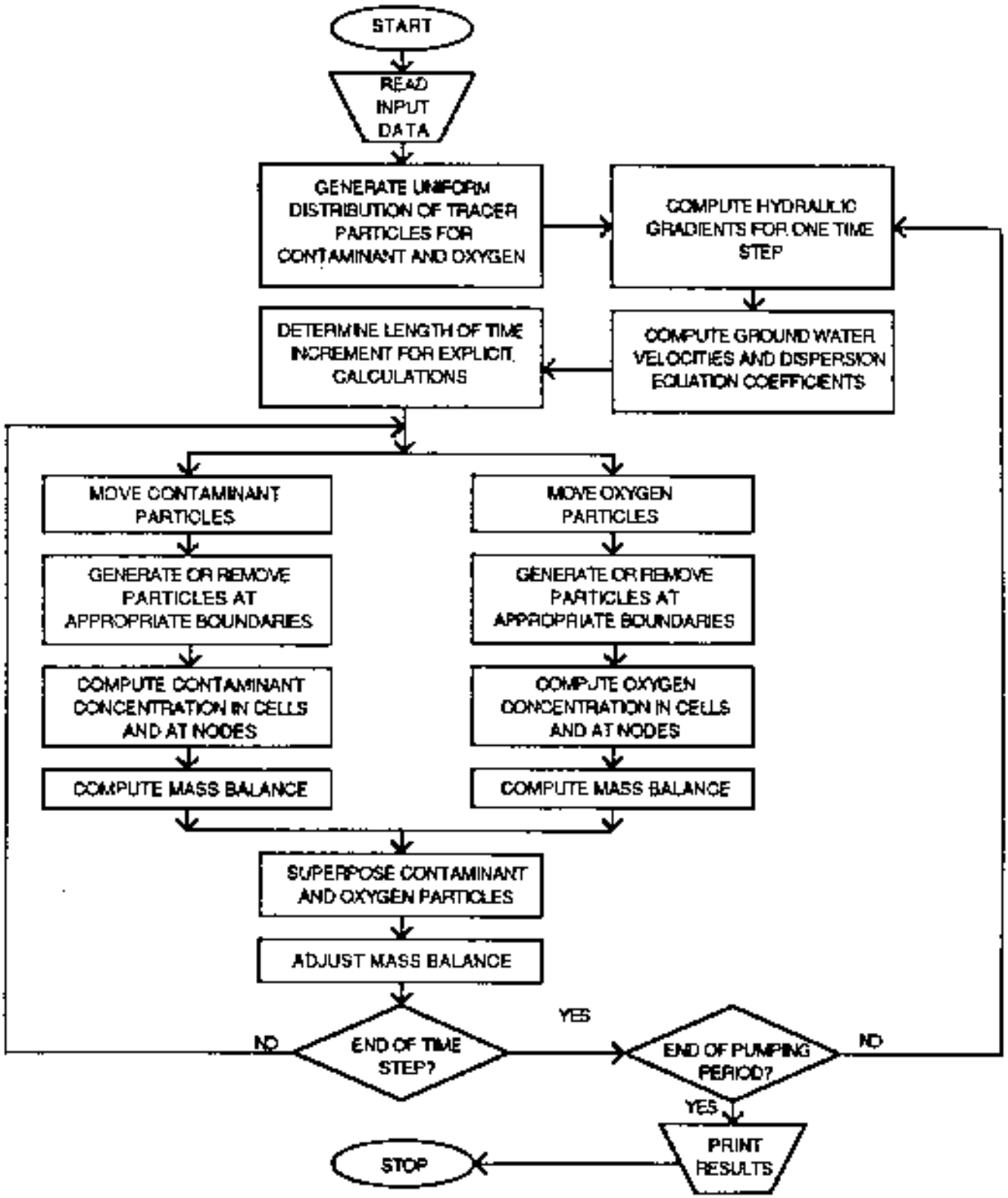
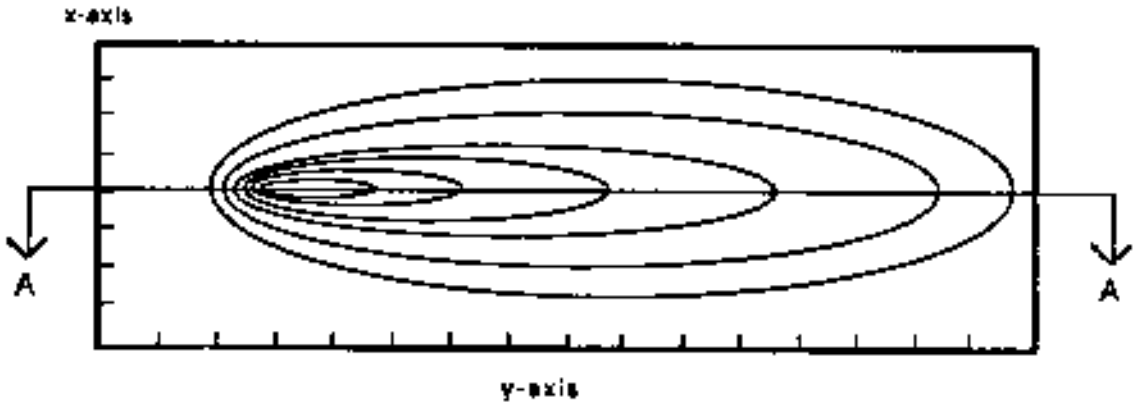
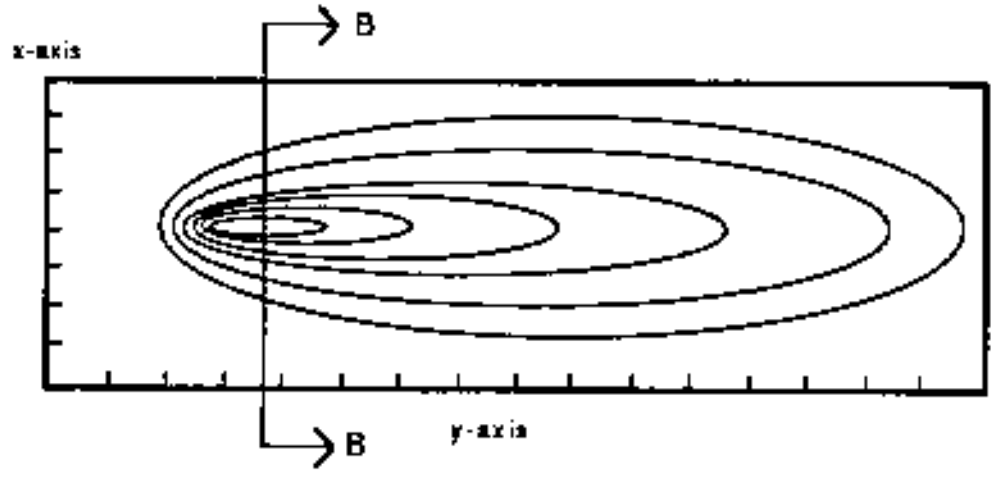


FIGURE 2.1 - Simplified Flowchart of BIOPLUME II

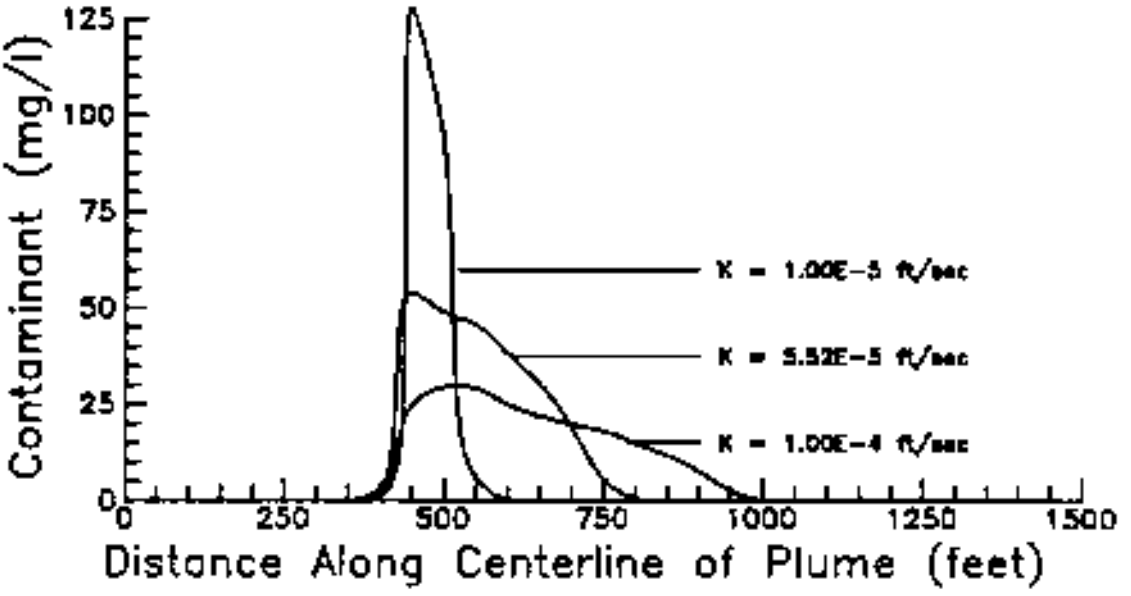


Section A-A is the Centerline of the Plume



Section B-B is the Transverse Section of the Plume

FIGURE 2.2 - Schematic of the Centerline and Transverse Section of a Plume



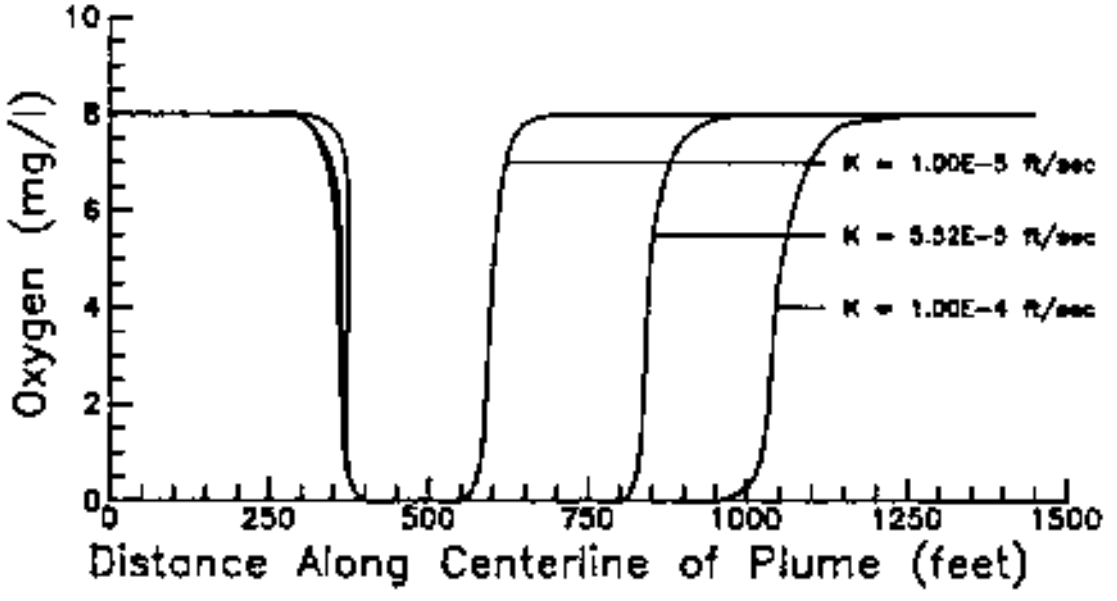


Figure 2.3 – Concentration Distributions for Various Values of Hydraulic Conductivity

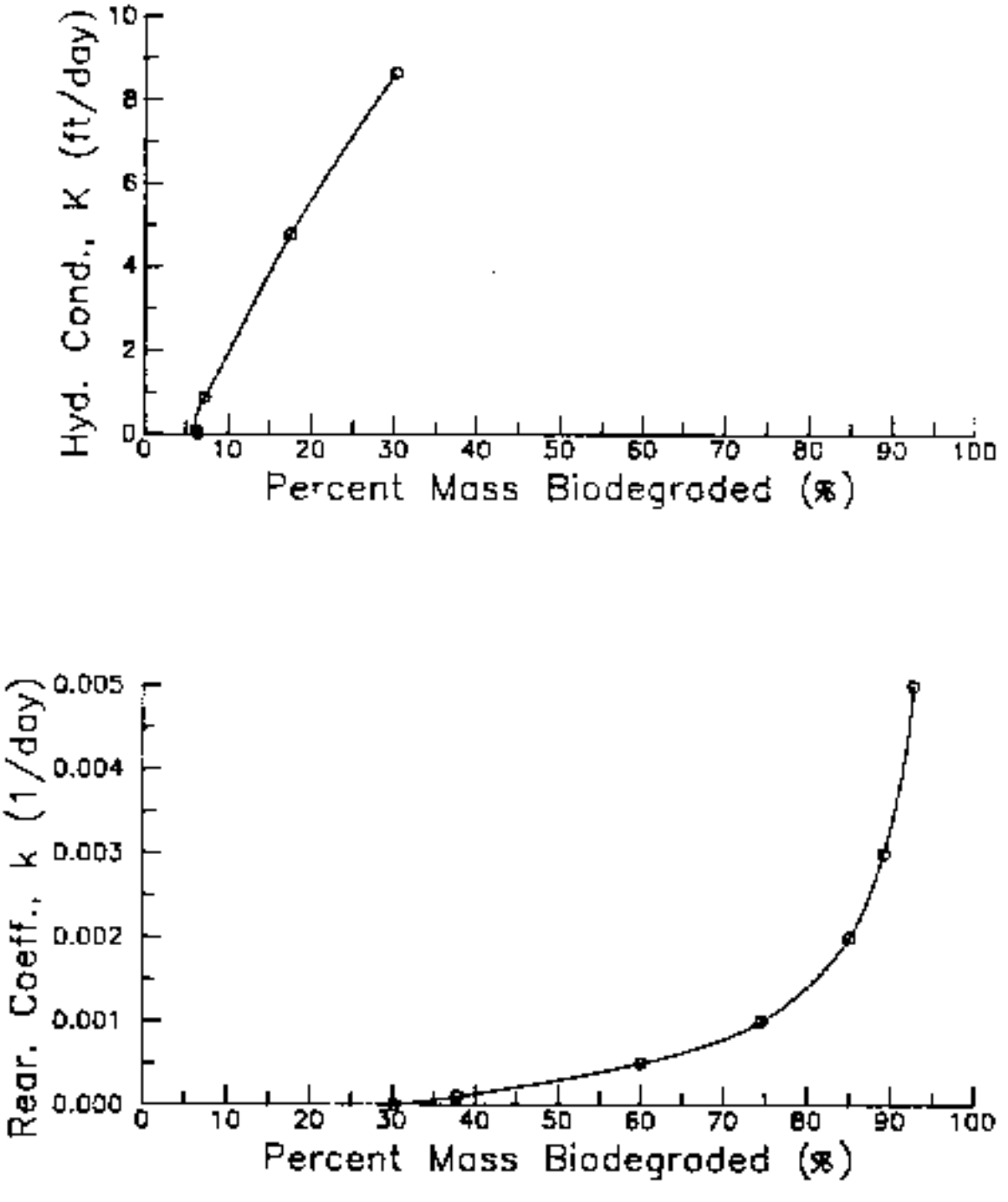
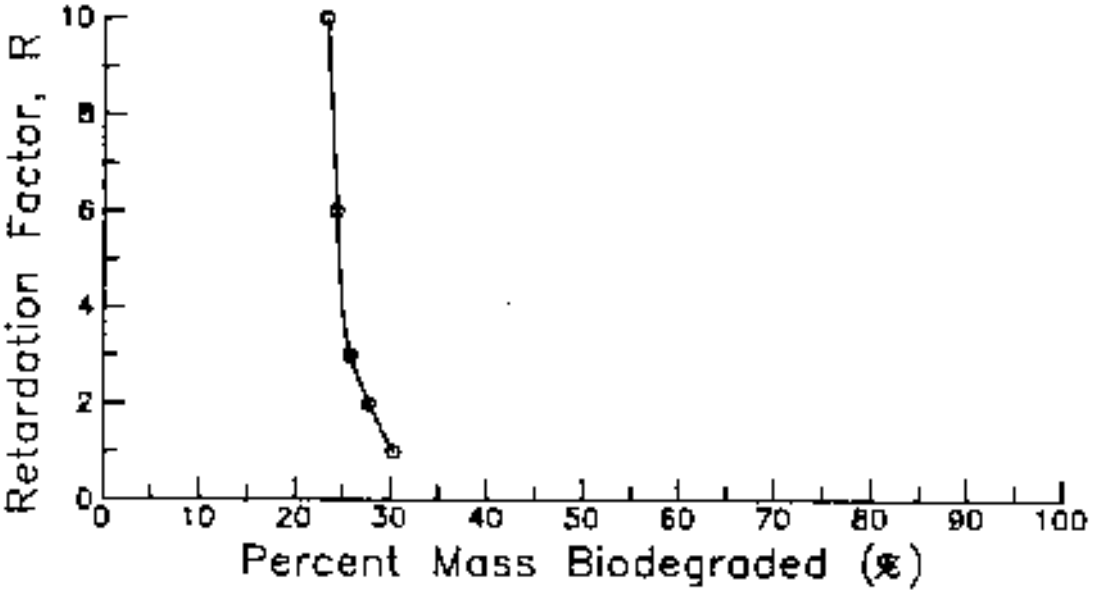


Figure 2.4a – Variation of Biodegraded Mass with Various Parameters



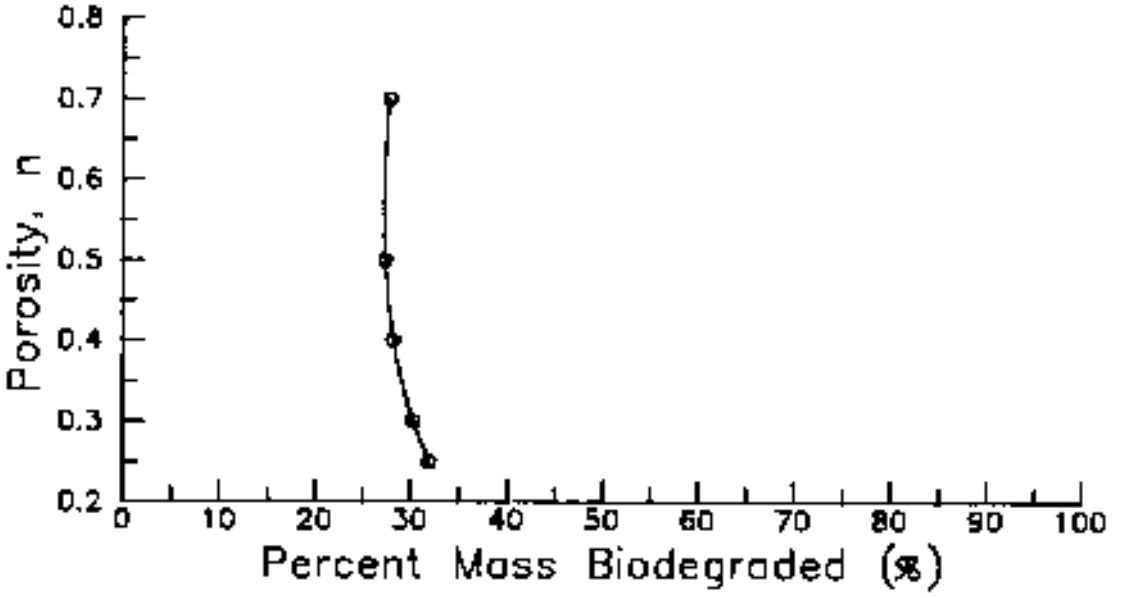


Figure 2.4b – Variation of Biodegraded Mass with Various Parameters

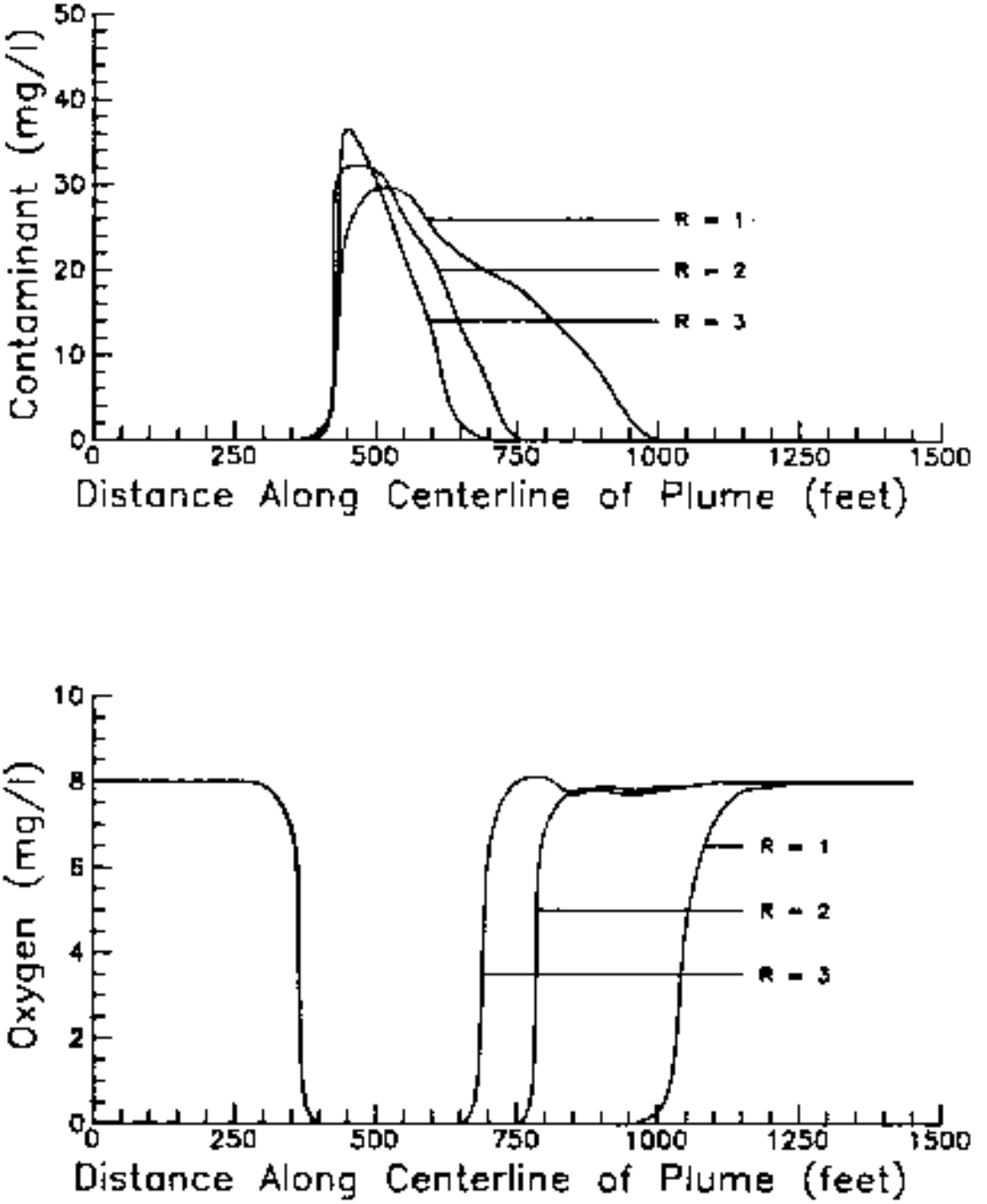
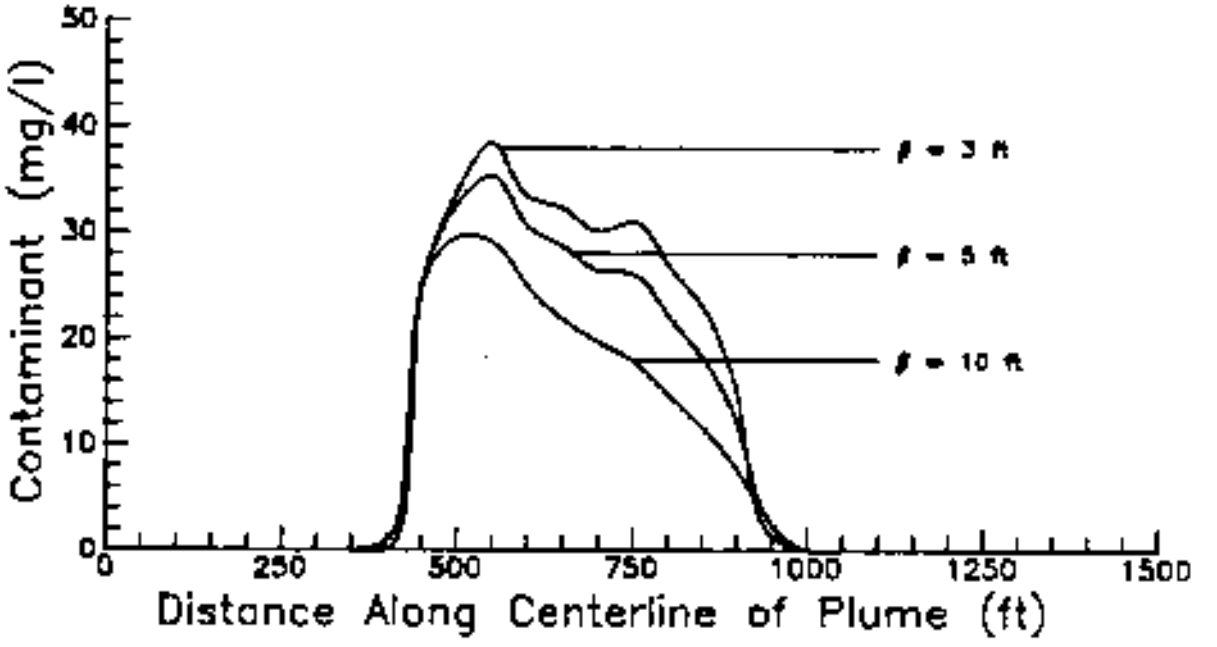


Figure 2.5 – Concentration Distributions for Various Values of Retardation



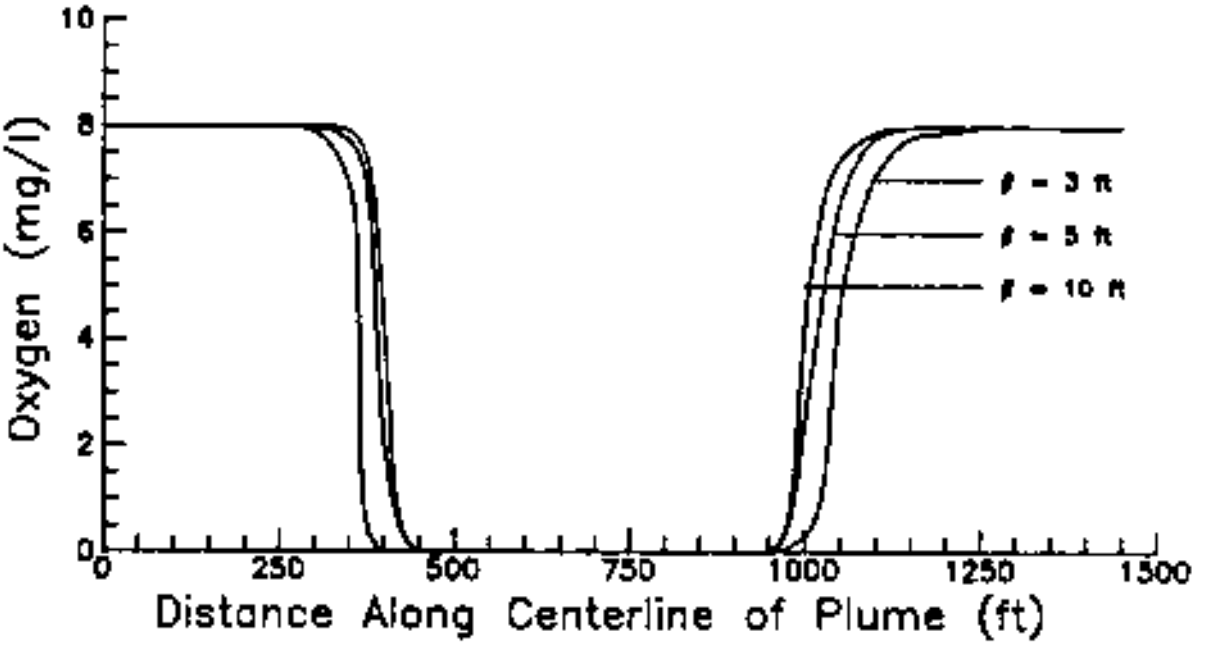
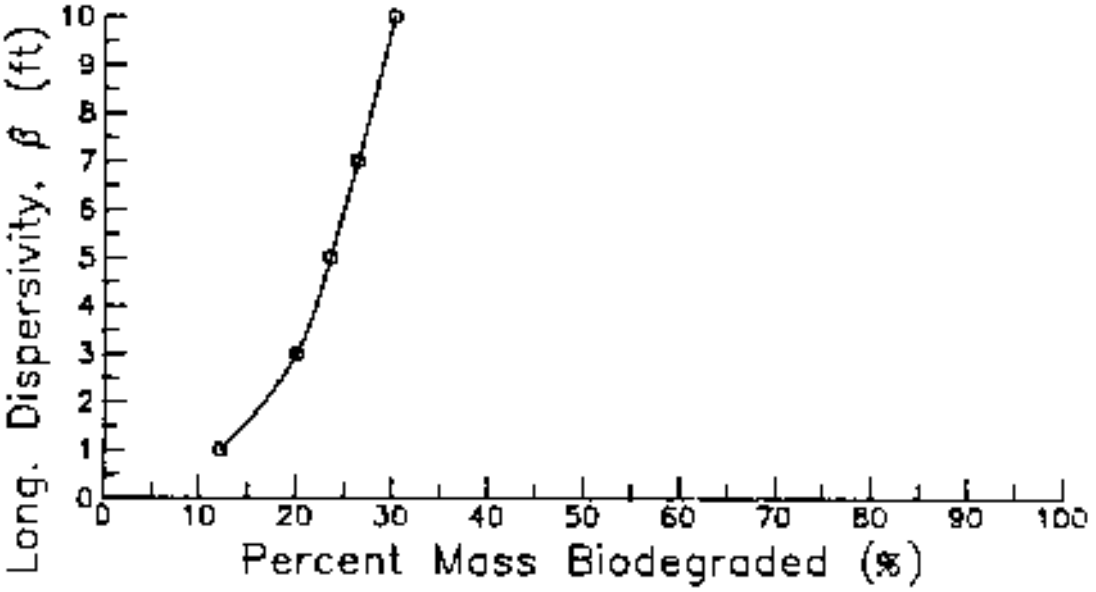


Figure 2.6 – Concentration Distributions for Various Values of Longitudinal Dispersivity



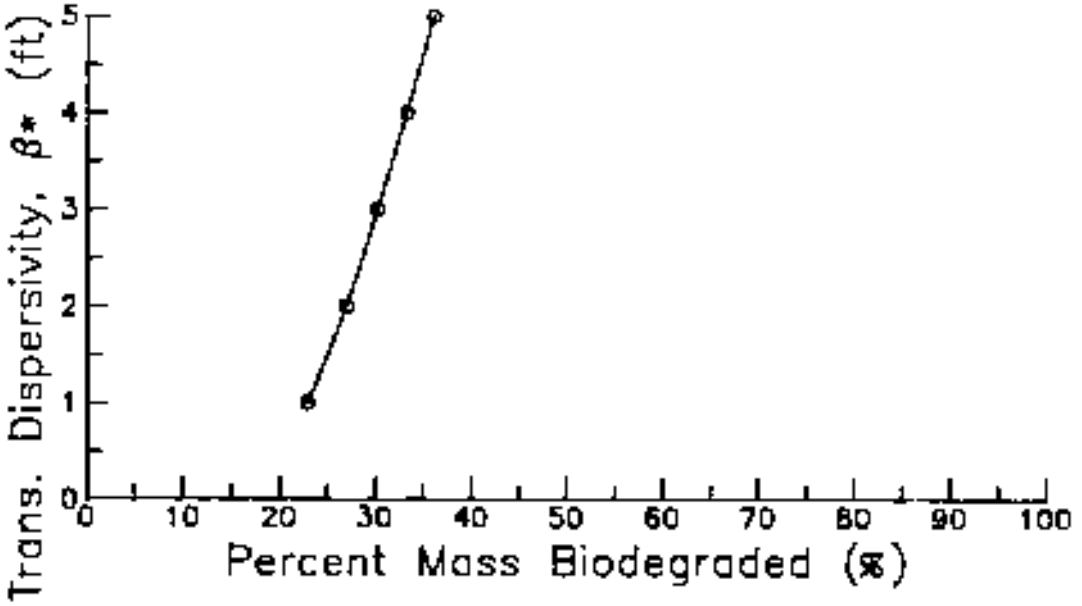
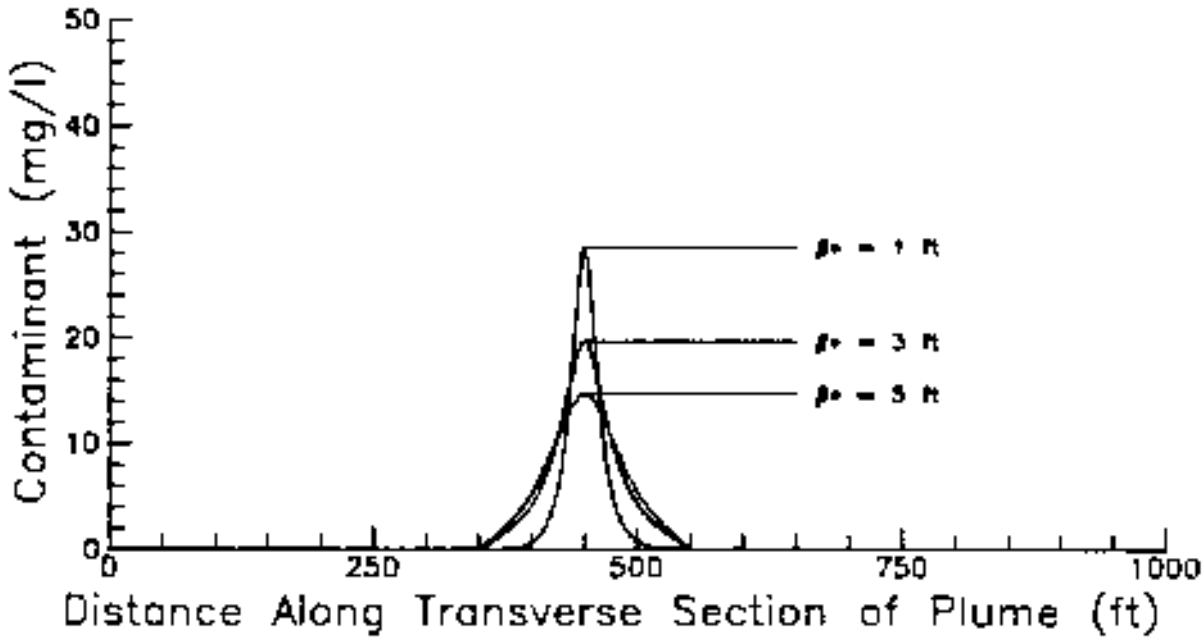


Figure 2.7 — Variation of Biodegraded Mass with Dispersivity



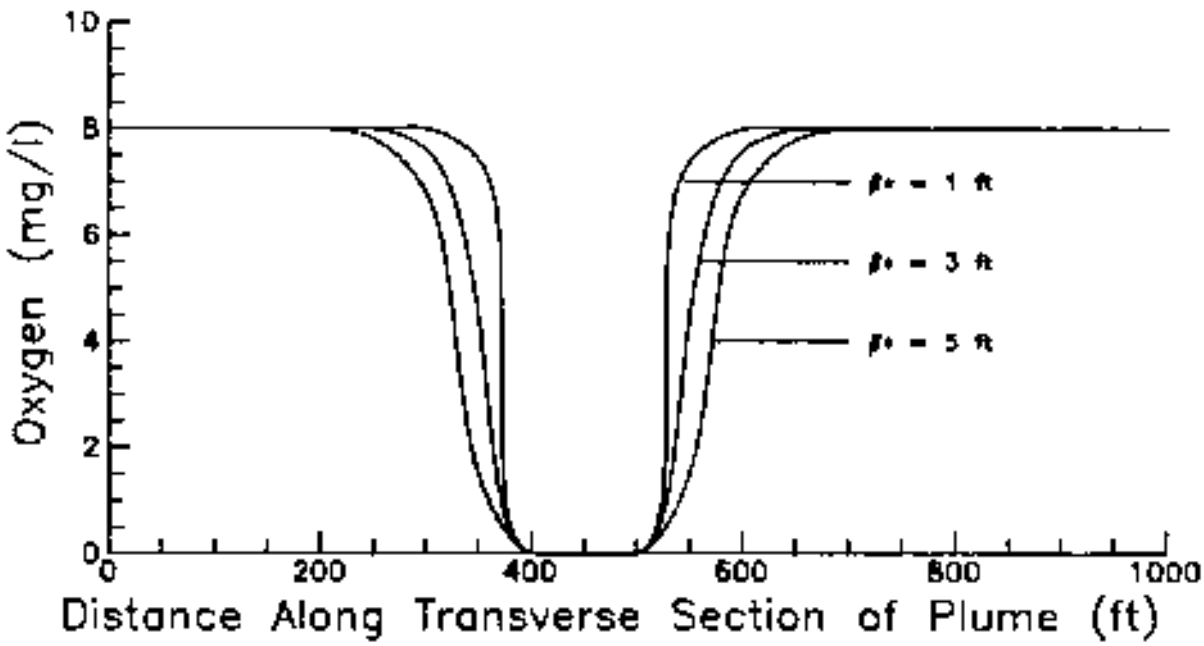
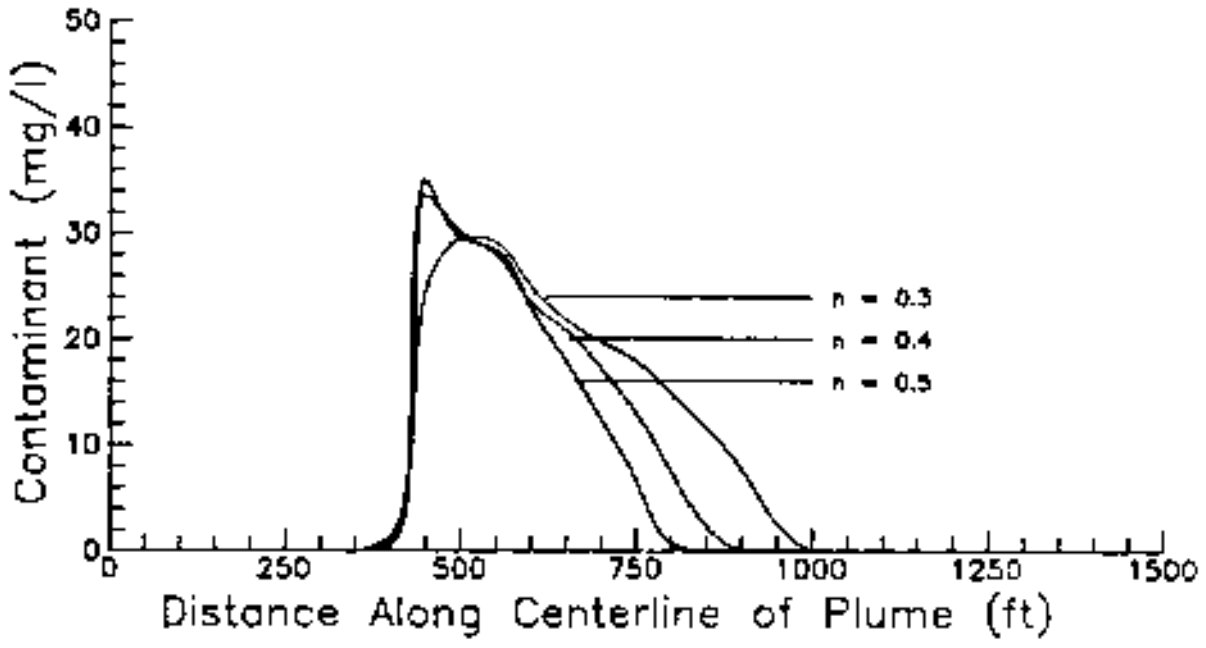


Figure 2.8 – Concentration Distributions for Various Values of Transverse Dispersivity



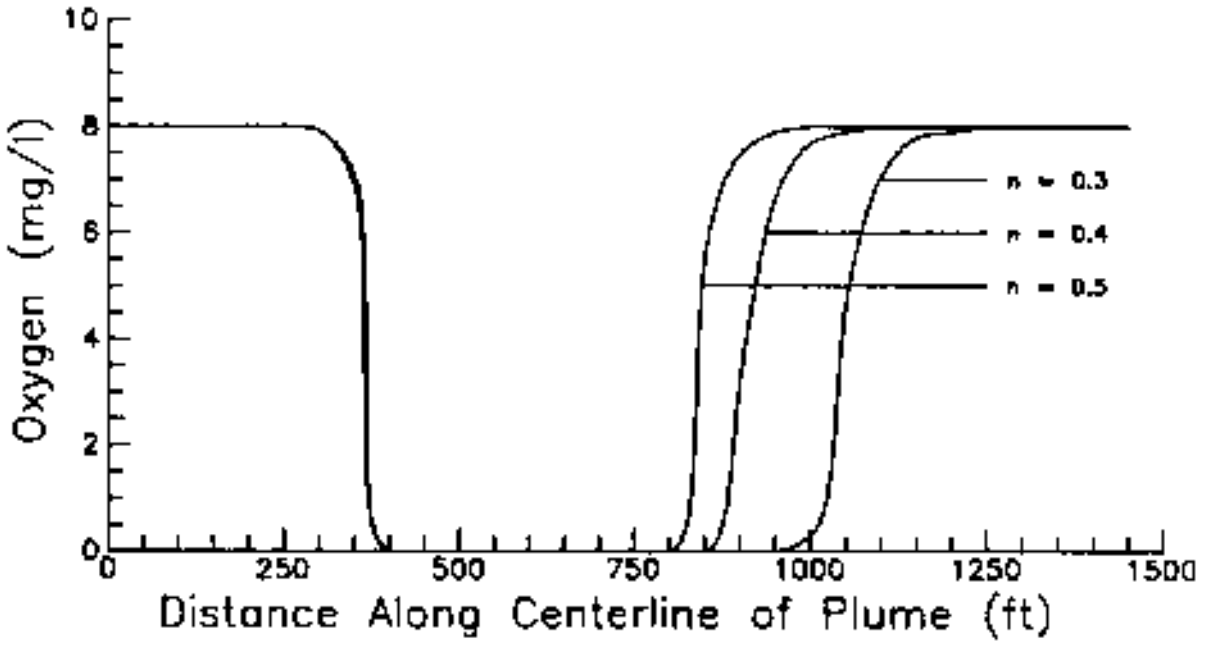
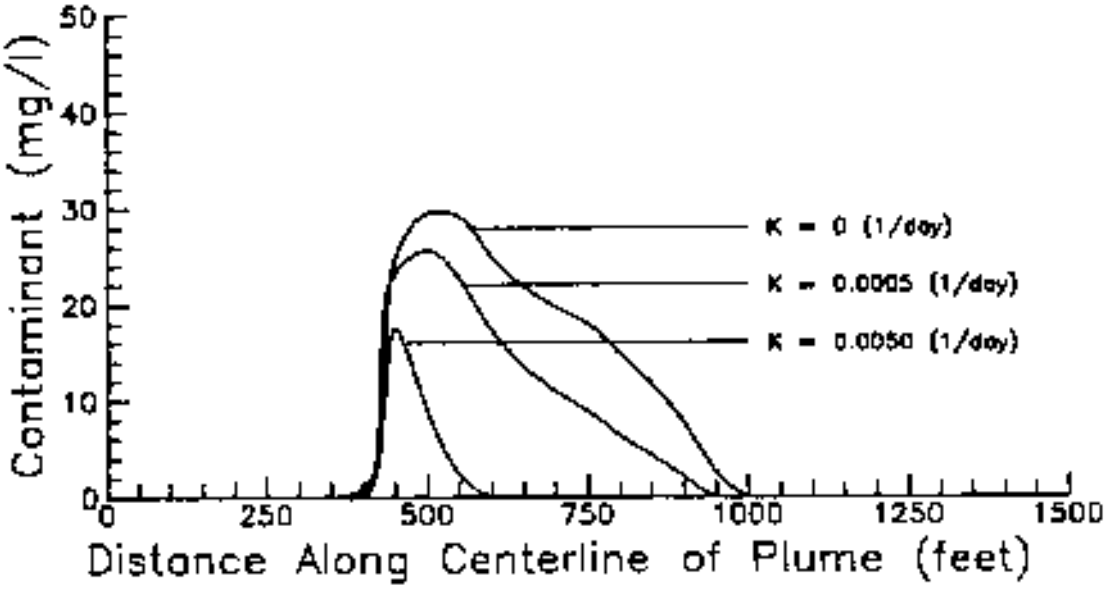


Figure 2.9 — Concentration Distributions for Various Values of Porosity



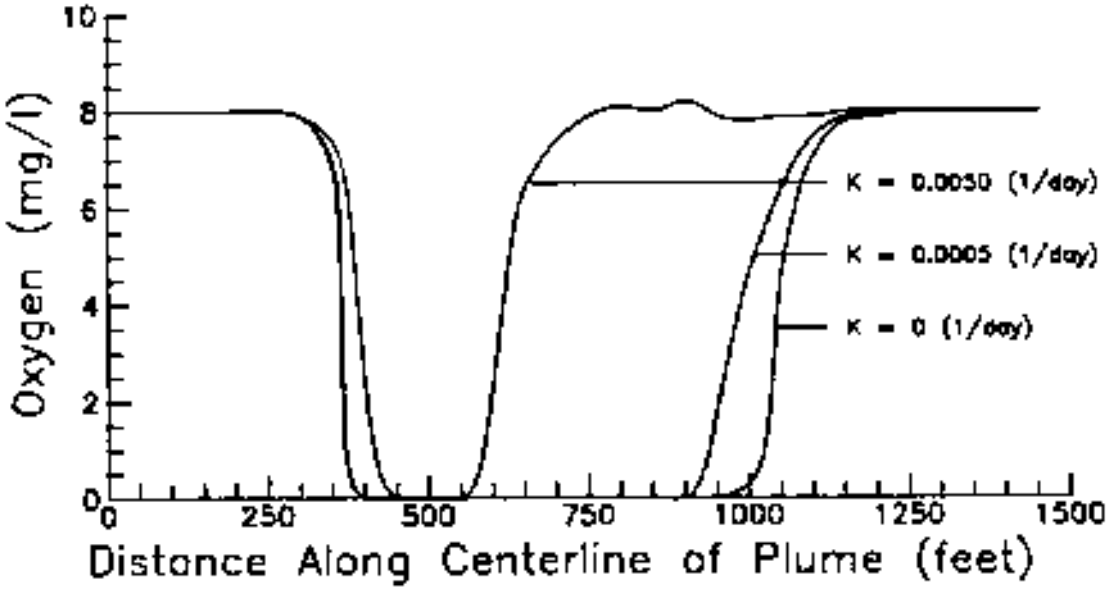
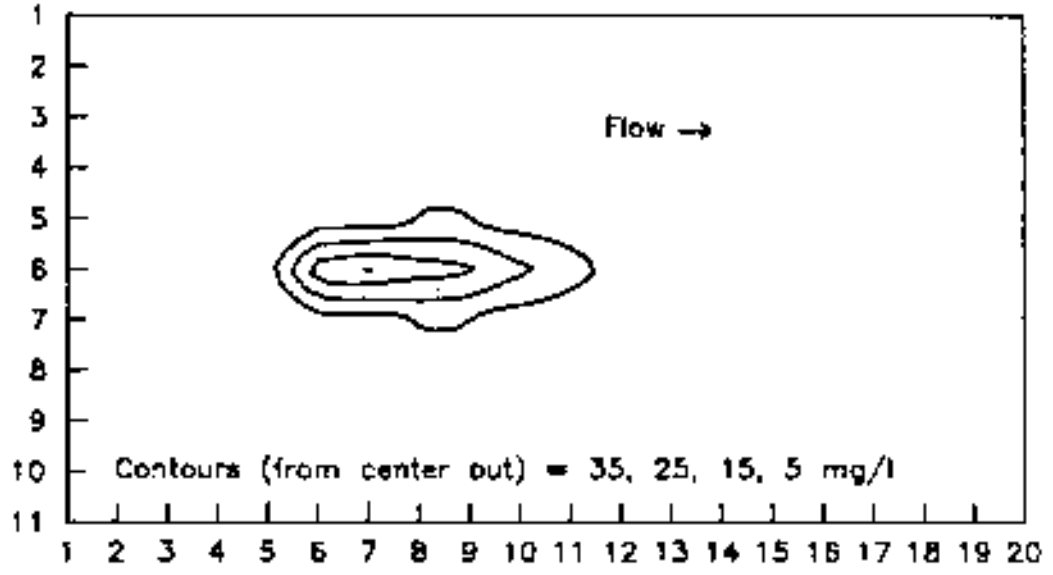
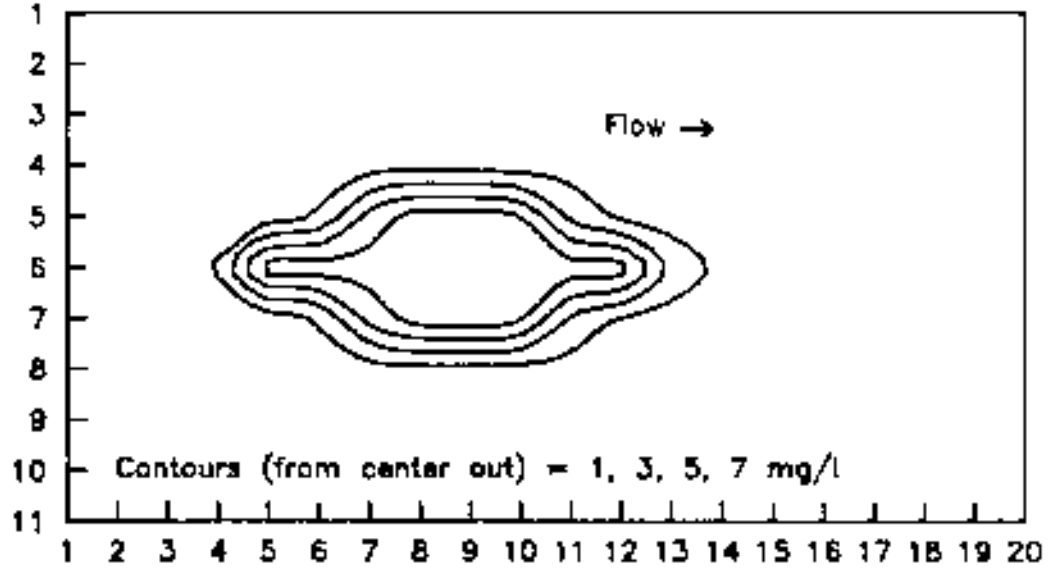


Figure 2.10 – Concentration Distributions for Various Values of the Reaeration Coefficient

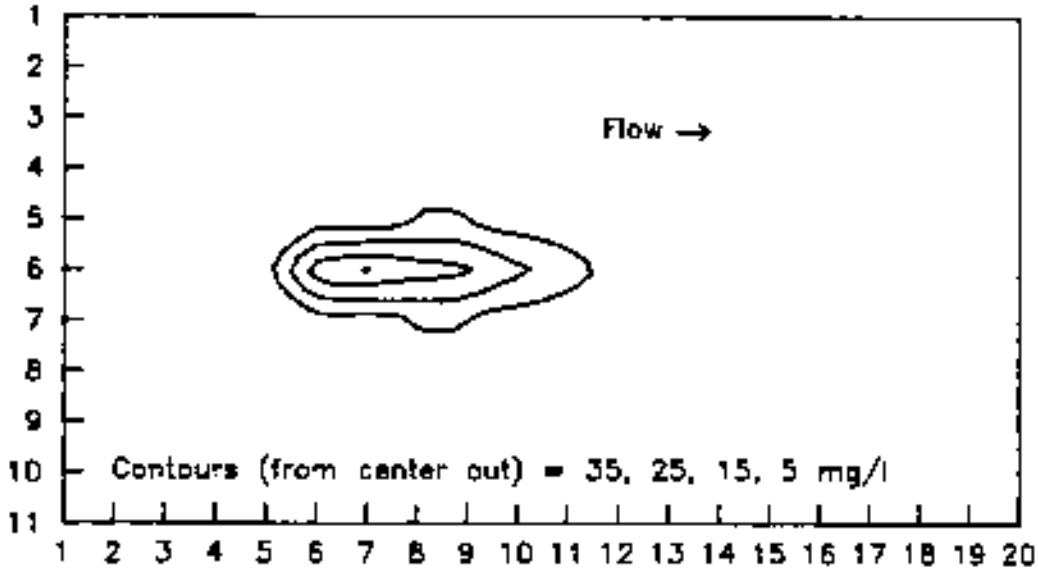


Biodegraded Contaminant Plume

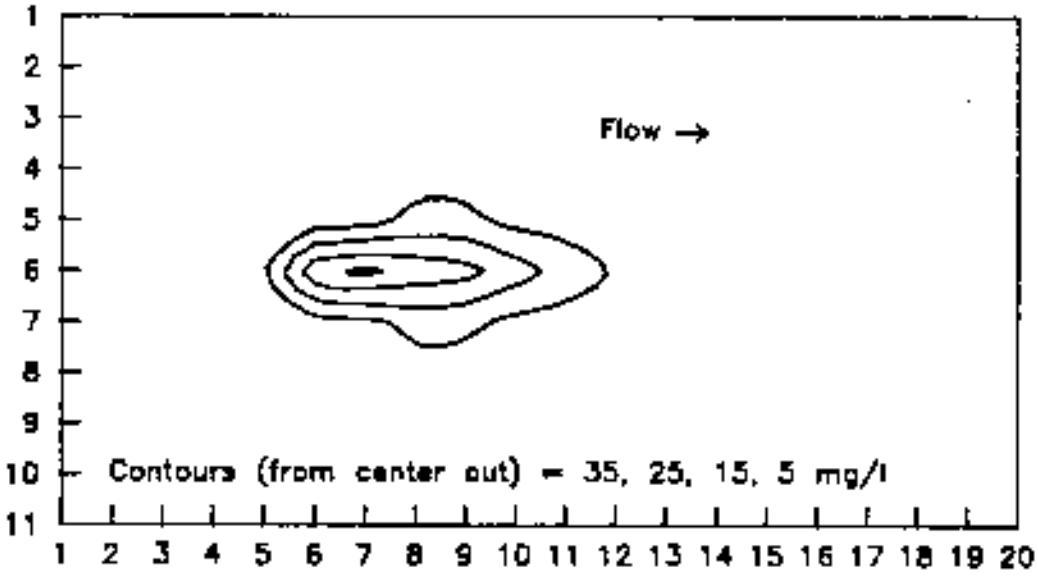


Oxygen Plume

FIGURE 4.1 — Contaminant and Oxygen Plumes for Test Problem #1

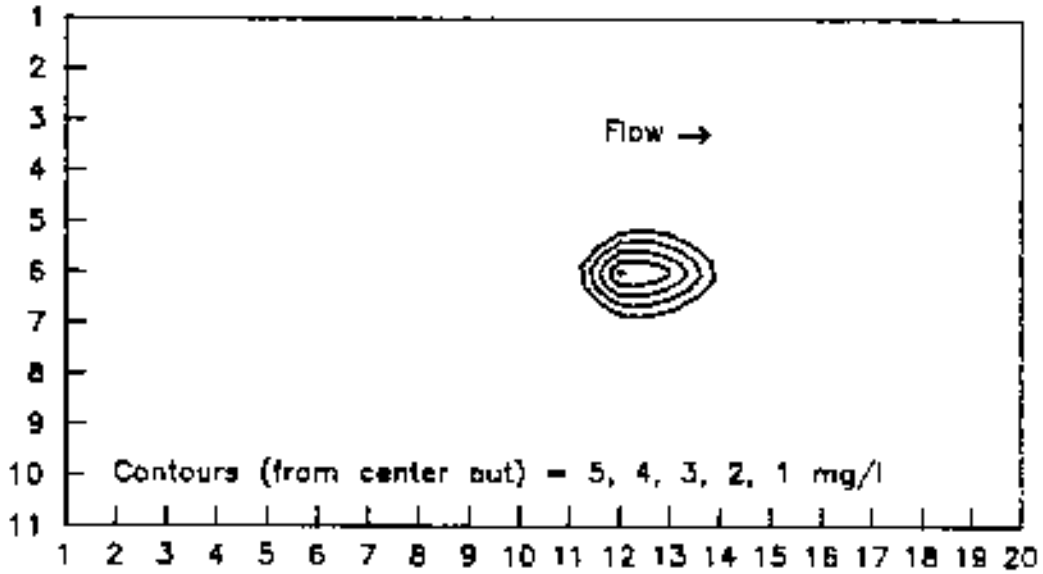


Biodegraded Contaminant Plume

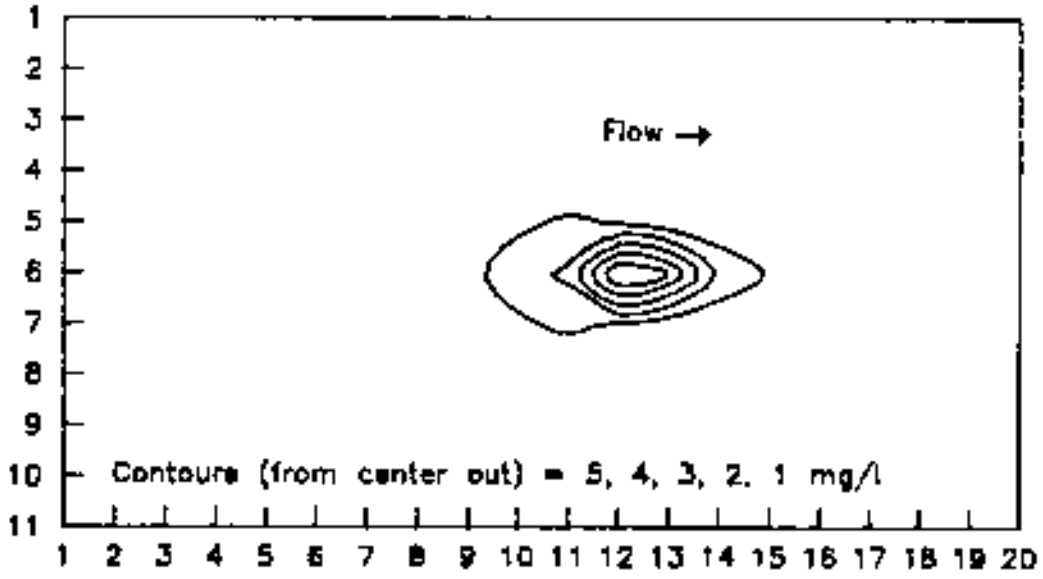


Non-Biodegraded Contaminant Plume

FIGURE 4.2 – Comparison of Biodegraded and Non-Biodegraded Plumes for Test Problem #1



Biodegraded Contaminant Plume



Non-Biodegraded Contaminant Plume

FIGURE 4.3 – Comparison of Biodegraded and Non-Biodegraded Plumes for Test Problem #3