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Project Summary

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; Preprocessor Source Code Version 1.0; Source Code Version 1.0)

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This manual presents a two-dimensional computer model, BIOPLUME II,that simulates the transport of dissolved hydrocarbons under the influence of oxygen-limited biodegradation. BIOPLUME II 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 II.

BIOPLUME II 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 II 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 II 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.

This Project Summary was developed by EPA's Robert S. Kerr Environ-mental Research Laboratory, Ada, OK, to announce key findings of the research project that is fully documented in a separate report of the same title (see Project Report ordering information at back).

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 II 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 II, 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 mass units of O_2 are required to completely biodegrade 1 mass unit of HC).

BIOPLUME II 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 II 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.

System Requirements

To run BIOPLUME II, 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 Hercules)[3]
7. SURFER supported graphics print plotter (see Appendix D of SUR manual)

System Setup

In order to run the programs, following command must be includ the file CONFIG.SYS on your sy disk:

DEVICE = ANSI.SYS

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

Overview of the Model

Description of the Program

The purpose of this section describe the overall structure o program and to present a de description of the model's capabi This section is not intended to di the numerical methods and techr used to solve the flow and trar equations since these method discussed in detail in the USGS r (Konikow and Bredehoeft, 197 should be noted, however, that numerical limitations of the USGS apply to BIOPLUME II and the needs to be aware of these limit The user also needs to be aware limitations of the method of ch teristics for solving the tran equation.

The major steps in the calcu procedure are summarized in Fig which presents a simplified flow c the overall structure of the con program. The flow chart illustrate two independent sets of particle tracer particles and HC tracer pa are generated. Since the tracer pa may have to be moved more thar to complete a given time step a reaction between O_2 and HC is as instantaneous, the O_2 and HC particles are moved independentl their subsequent concentrations a computed independently. The re two plumes (HC and O_2) are cor after every particle move time s simulate the reaction between C HC. In this version of the mode

Note. Specific mention of equation, page or section numbers herein refer to the final reports which are available from the National Technical Information Service, as described on the last page of this Project Summary

[1] A minimum of 605K 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)

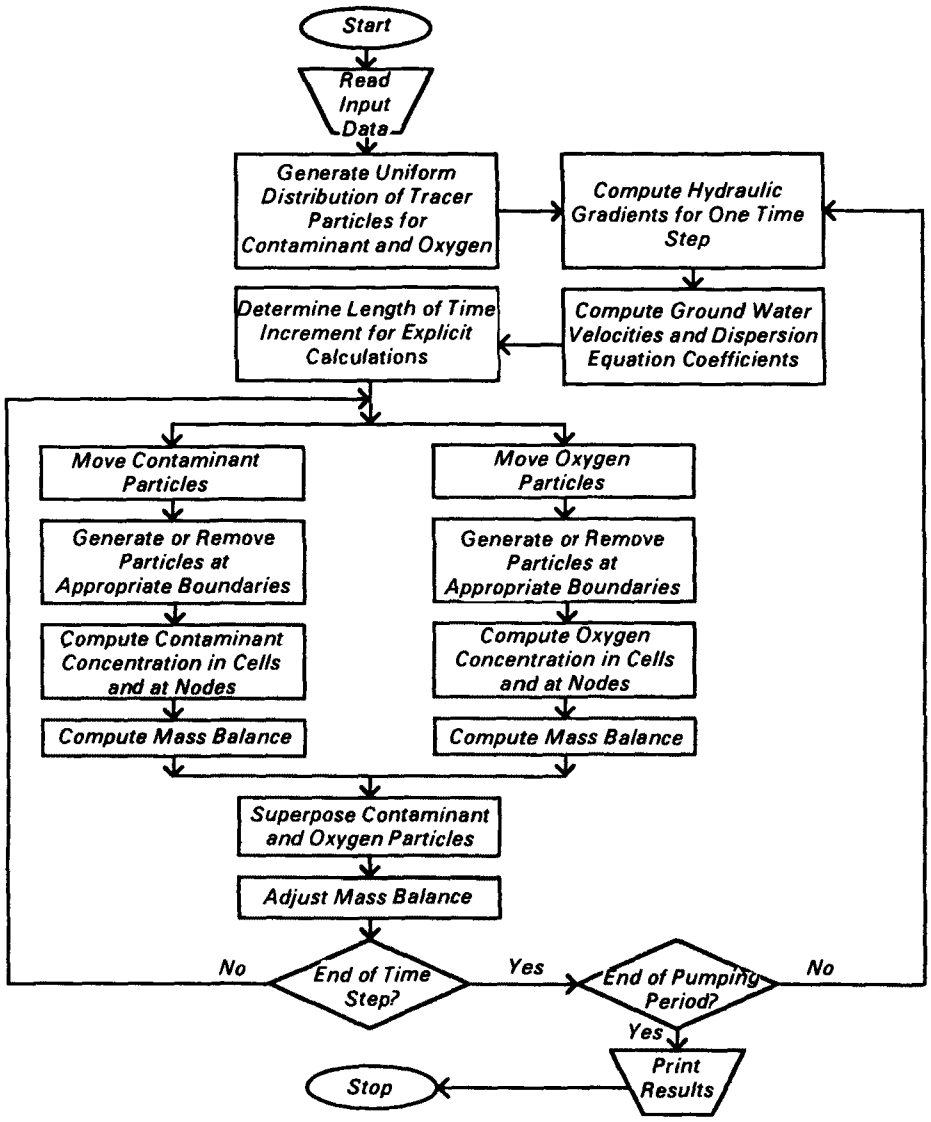

Figure 1. *Simplified Flowchart of BIOPLUME II.*

assumed that three mass units of oxygen are required to completely mineralize one mass 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 biodegrada-tion 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 ensure 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.

Use of the Preprocessor

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

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menu
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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

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

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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.

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. 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

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

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. T can be a file which was created using Edit/Create option or by some ot means. If the file does not exist, program will display a message tel you that the file does not exist and rep the prompt for the input file nai (Remember that CTRL C will return to the main menu.) If the file does e: the program will prompt:

Enter name of output file...

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

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

If an error occurs, you can disc where it occurred by looking at the ou data file. The DOS editor EDLIN or other text editor may be used to exa the output file. (See your DOS manu more information on EDLIN.) Find point at which the program stoppe any input variable which was not properly. Check the input data fil make sure that it contains the pr data. If you cannot locate the sour the error, call the phone number list the front of the manual or send ir preaddressed card at the back witl problem described in as much det possible.

Option 3: Prepare Graphics Files

Option 3 is used to convert the c from BIOPLUME II into files which c plotted using SURFER (Golden Soft 1987). The format for SURFER co of three columns of data. This data form X, Y, Z and could be used wit other plotting package which use format.

BIOPLUME II automatically v output data to three files n HEADS.BIO, HPLUME.BIO OPLUME.BIO. The file HEDS contains the array of computed values at the end of each time HPLUME.BIO and OPLUME.BIO c the HC and O_2 plumes, respectivel

The first line of the file HPLUM contains the variables NTIM, NPM NY, NPNT, and NPNTMV. This read before converting any of th from the files HEADS.BIO, HPLUM and OPLUME.BIO into the graphic

format. It informs the program how often he 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.

Option 4: QUIT

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

Summary

BIOPLUME II 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 occurring 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 II: (1) dissolved oxygen in the aquifer; (2) natural recharge, and; (3) oxygen exchange from 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 in press. The model provided a good match to field conditions at both sites. BIOPLUME II 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.

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The complete report consists of paper copy and software, entitled, "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; Preprocessor Source Code Version 1.0; Source Code Version 1.0),"

Paper Copy (Order No. PB 89-151 120/AS; Cost: $28.95)

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The above items will be available only from: (costsubject to change)

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