BIO1D

Overview

BIO1D, developed by P. Srinivasan and J.W. Mercer is a one-dimensional modeling code which simulates biodegradation and sorption in contaminant transport. The objective was to provide an interactive, user-friendly microcomputer software package to serve as an educational tool for understanding the relative importance of various physicochemical and biochemical processes.

Applications

BIO1D may be applied to solute transport problems involving a reactive substrate. The reactions may include aerobic and anaerobic degradation and/or adsorption described by a linear, Freundlich or Langmuir isotherm. Figure 1 shows the simulation of organic transport involving aerobic biodegradation at a waste site in Conroe, Texas, and is based on an earlier study by Borden, *et al.* (1984).

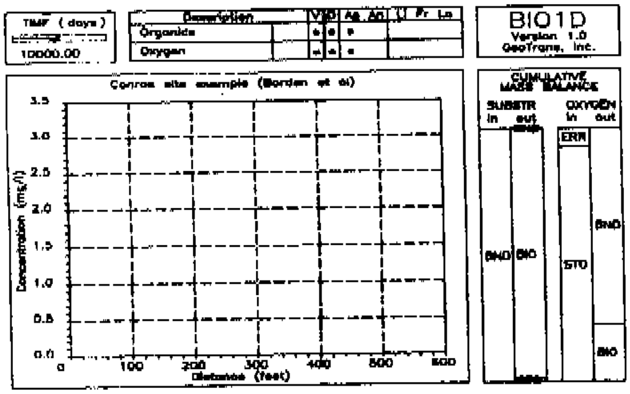


Figure 1. Simulation of aerobic biodegradation at Conroe site, Texas

The code may be used in a conceptualization mode for many applications to help determine the importance of transport processes. The applications can involve a number of reactive substrates such as organic solvents and petroleum products. In addition, because anaerobic radionuclides with decay can be simulated. The code will be especially useful for analyzing laboratory data from column experiments.

Model Features

- Advective and dispersive transport of a hydrocarbon and an electron acceptor (e.g. oxygen)
- Aerobic biodegradation using modified Monod function
- Anaerobic biodegradation using Michaelis-Menten kinetics
- First-order degradation for both substances
- Linear, Freundlich, and Langmuir adsorption isotherms for both substances
- Dirichlet, Neumann, and Cauchy boundary conditions modified to include first-order degradation
- Cumulative mass balance report

Limitations

- Transport is one-dimensional.
- The flow field is uniform (constant velocity).
- Material properties of both substances are uniform throughout the medium.
- Only one reactive substrate is considered per simulation.
- Microbial density is assumed constant.

Governing Equations

A summary of the equations solved in BIO1D is presented below.

$$D\frac{\partial^2 S}{\partial x^2} - V\frac{\partial S}{\partial x} - B(S,O) - \{1+A(S)\}\frac{\partial S}{\partial t} = 0 \qquad (1)$$

$$D\frac{\partial^2 O}{\partial x^2} - V\frac{\partial O}{\partial x} - F.B(S,O) - \{1+A(O)\}\frac{\partial O}{\partial t} = 0 \qquad (2)$$

where

S substrate concentration in the pore fluid (ML^{-3});
O oxygen concentration in the pore fluid (ML^{-3});
D longitudinal hydrodynamic dispersion coefficient (L^2T^{-1});

V	interstitial fluid velocity (LT^{-1}), assumed uniform;
$B(S,O)$	biodegradation term ($ML^{-3}T^{-1}$), expressed as a function of the dependent variables S and O;
F	ratio of oxygen to substrate consumed;
$A(S)$	substrate adsorption term;
$A(O)$	oxygen adsorption term; and
t	time (T).

Aerobic Biodegradation (Monod function)

$$B(S,O) = Mk \frac{S}{k_S + S} \frac{O}{k_O + O} \frac{S - S_{min}}{S} \qquad (3)$$
$$= 0 \text{ for } S \le S_{min} \text{ or } O \le O_{min}$$

where

$B(S,O)$	aerobic biodegradation term, a function of substrate and oxygen concentration ($ML^{-3}T^{-1}$);
M	microbial mass (ML^{-3}) assumed constant;
k	maximum substrate utilization rate per unit mass of microorganisms (T^{-1});
k_S	substrate half-saturation constant (ML^{-3});
k_O	oxygen half-saturation constant (ML^{-3});
S_{min}	minimum substrate concentration that limits growth and decay (ML^{-3}); and
O_{min}	minimum oxygen concentration that limits growth and decay (ML^{-3}).

Anaerobic Biodegradation (Michaelis-Menten kinetics)

$$B(S) = M_n K_n \frac{S}{k_{Sn} + S} \frac{S - S_{min}}{S} \qquad (4)$$

where the terms, M_n, k_n, and k_{Sn} are counterparts of M, k and k_S under anaerobic conditions. As a special case, M_n, k_n, and k_{Sn} may be set equal to M, k and k_S, respectively.

First-Order Decay

$$B(S) = \mu_S S \qquad (5)$$

where μ_S is a first-order degradation coefficient (T^{-1}).

Linear Adsorption Isotherm

$$A(S) = \rho_b K_d / \phi \qquad (6)$$

where

ρ_b	bulk mass density of the porous medium (ML^{-3});
ϕ	effective porosity; and
K_d	distribution coefficient (L^3M^{-1}).

Freundlich Adsorption Isotherm

$$A(S) = \rho_b n K_f / \phi \ \ S^{n-1} \qquad (7)$$

where

K_f	rate constant; and
n	Freundlich isotherm exponent

Langmuir Adsorption Isotherm

$$A(S) = \frac{bK}{\phi(1 + bS)^2} \qquad (8)$$

where

b	constant; and
K	maximum sorption capacity of solid.

Uncoupled Simulation Option

When the biodegradation option is not used, the equations (1) and (2) are uncoupled and may be solved simultaneously. Two sets of input values are used for all parameters except those defining the grid and time steps. This permits a wide range of possible comparison studies. Some are listed below.

- Different velocities. This is an indirect way of comparing the effect of two hydraulic conductivity values. Figure 2 illustrates a field application of BIO1D where the predicted breakthrough curves are bracketed with two estimates of clay permeability. Similarly, hydraulic gradients may also be used for comparison.

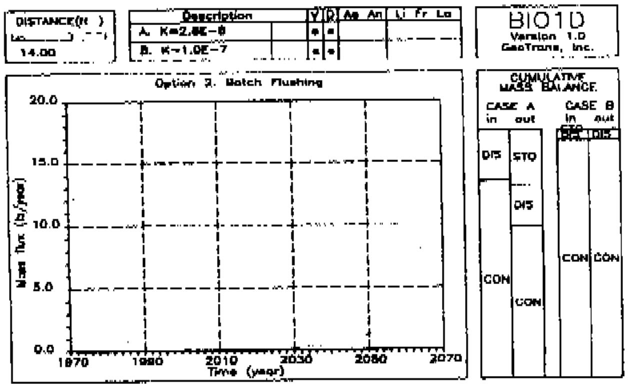


Figure 2. Varying clay permeability.

- Different dispersion coefficients.
- Different adsorption rates. BIO1D is an excellent tool for comparing two isotherms, or varying coefficients of the same isotherm. Figure 3 illustrates a study on varying Freundlich isotherm exponent.
- Different first-order decay rates. As a special case, one of the decay rates may be set to zero.
- Different boundary conditions. Three types of boundary conditions with built-in first-order degradations are available. In field situations, boundary conditions are not always clearly understood. Thus the importance of assumptions made at the boundary may be studied.

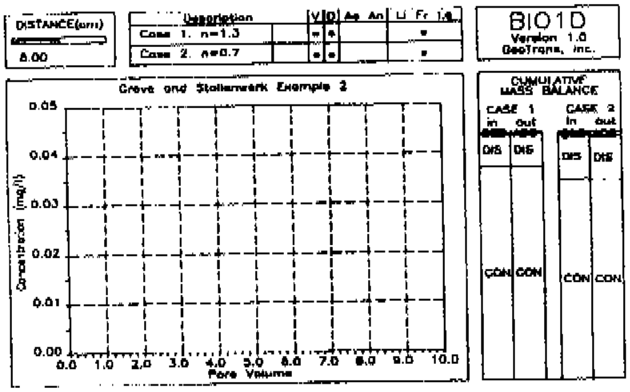


Figure 3. Uncoupled simulation option: Varying Freundlich isotherm exponent.

Interactive Preprocessor

A preprocessor has been built into BIO1D which enables the user to prepare input data interactively. The preparation includes features such as inputting new data and storing them in a disk file, or reading data from a disk file and editing them. The preprocessor has built-in error recovery procedures to forgive most input errors made by a user during interaction.

For first-order decay and linear, Freundlich, or Langmuir adsorption isotherms, definitions found in the literature are not always uniform. The preprocessor provides the user with alternative definitions, and the user may select the one that is most familiar. Figure 4 illustrates the definitions available for linear isotherm. The user may define the isotherm in terms of linear isotherm coefficient, distribution coefficient and bulk density, or retardation factor. Many such useful features may be found throughout the interaction.

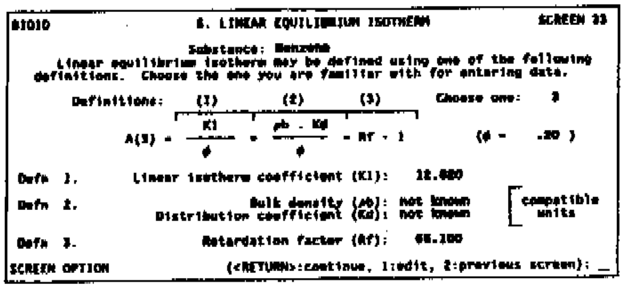

```
BIO1D              6. LINEAR EQUILIBRIUM ISOTHERM              SCREEN 33

                         Substance: Benzene
      Linear equilibrium isotherm may be defined using one of the following
    definitions.  Choose the one you are familiar with for entering data.

         Definitions:    (1)        (2)       (3)         Choose one:    3
                     ┌──────────┬──────────┬──────────┐
                          Kl         ρb · Kd
              A(3) =  ──────── =  ──────── = Rf - 1           (φ =    .20 )
                          φ          φ

 Defn  1.         Linear isotherm coefficient (Kl):   12.000

 Defn  2.                       Bulk density (ρb): not known     ┌compatible
                    Distribution coefficient (Kd): not known     └  units

 Defn  3.               Retardation factor (Rf):   65.100
SCREEN OPTION          (<RETURN>:continue, 1:edit, 2:previous screen): _
```

Figure 4. BIO1D data preparation:

Run-Time Options

Taking advantage of the single-user microcomputer environment, many simulation options are provided at run-time. A *run-time monitor* as illustrated in Figure 5 is displayed and updated constantly as the simulation progresses. The user may run the simulation for a certain time period, monitoring its behavior, and then choose a different set of run-time options for the rest of the simulation. The options include printing concentrations, cumulative mass balance information, and selecting plotting intervals. Advanced debugging options such as iteration information, nodal mass balance tables, displacement matrices, and matrix solver monitors are also available at run-time. These options can be useful when the processes simulated are highly nonlinear, or if the results of the simulation show unusual behavior.

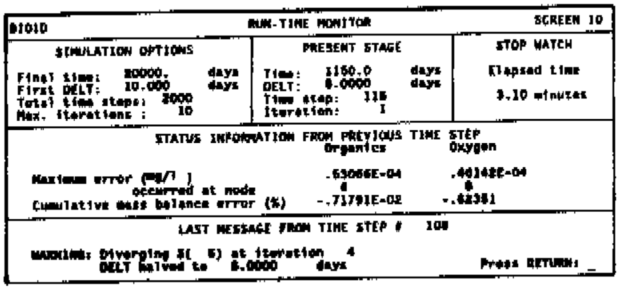

```
BIO1D                         RUN-TIME MONITOR                        SCREEN 10
     SIMULATION OPTIONS           PRESENT STAGE              STOP WATCH

Final time:      20000.    days   Time:   1160.0     days    Elapsed time
First DELT:      10.000    days   DELT:   8.0000     days
Total time steps:   2000          Time step:   118            3.10 minutes
Max. iterations :     10          Iteration:     1
                    STATUS INFORMATION FROM PREVIOUS TIME STEP
                                          Organics        Oxygen

  Maximum error (mg/l )                  .63066E-04      .40148E-04
                  occurred at node            4               8
  Cumulative mass balance error (%)     -.71791E-02     -.62381
                      LAST MESSAGE FROM TIME STEP #   108

  WARNING: Diverging S(  5) at iteration    4
           DELT halved to   8.0000      days                  Press RETURN: _
```

Figure 5. BIO1D run-time monitor.

The advanced debugging options may also be used by students learning numerical methods. Every step of the nonlinear iterative solution scheme used in BIO1D may be monitored by the user. The *Peclet* and *Courant* stability numbers are displayed automatically during data preparation, and a *stop watch* (Figure 5) is activated to measure the CPU time during the simulation. These features are useful in understanding the effects of varying the input parameters such as, grid spacing, time step size, and convergence criteria which are associated with the numerical solution.

Plotted Results

Concentration vs. distance at a certain time, or concentration vs. time (or pore volume) at any node may be plotted. Concentration may be plotted in linear or log scale. Figures 1, 2 and 3 illustrate these options. Plots may be previewed on the screen and sent to any of the plotters listed under *Hardware* (page four). For comparative studies, hard copy plots from uncoupled simulation runs (eg. Figures 2 and 3) can be readily used in reports.

Verification Tests

The features available in BIO1D have been tested in a systematic manner. A variety of problems have been selected to test major options in biodegradation, adsorption, and boundary conditions. The data files for the above problems have also been carefully prepared to test many of the minor options (grid spacing, plotting, etc.) available in BIO1D. Table 1 shows the features tested by the problem sets A through F.

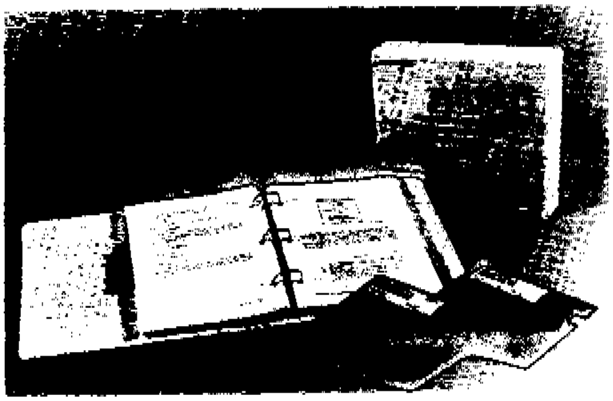
Table 1. BIO1D features tested.

FEATURES		PROBLEM SETS
advection/dispersion		A B C D E F
degradation	- *aerobic*	F
	- *anaerobic*	F
	- *first-order*	B F
uncoupled simulation		D
adsorption	- *linear*	B C
	- *Freundlich*	D
	- *Langmuir*	E
boundary (*: pulse)	- *Dirichlet*	A C* D* E* F
	- *Neumann*	
	- *Cauchy*	B*
solution	- *tridiagonal*	A B C E
	- *pentadiagonal*	D F
grid	- *uniform*	A B C D E
	- *variable*	F
plots	- *C vs. X*	A F
	- *C vs. T*	B
	- *C vs. PV*	C D E

Features that are not yet tested may also be identified from this table. A description of each test along with a complete list of corresponding input and output files of the BIO1D simulations are presented in the BIO1D documentation.

Documentation

The documentation for BIO1D is believed to be the most comprehensive ever for a groundwater code, setting new standards for the industry. It is divided into two major parts. The first part covers the theoretical aspects of BIO1D which include: derivation of the mathematical verification tests. The second part serves as the *user's manual* for the code. The sections included are: step-by-step installation instructions; three *guided tours* to familiarize the user with the data preparation, simulation, and plotting of the results; detailed input data instructions; interpretation of output; and error conditions and handling.



Hardware

BIO1D runs on an IBM PC, XT or AT compatible microcomputer with 640K memory. A numeric coprocessor (8087 or 80287) is required. CGA, Hercules monochrome or EGA graphics card is needed for screen graphics. HP 7440A, 7470A, 7475A, 7550A, 7580B, 7585B, 7586B plotters; HI DMP-51, 52, 56 plotters; Enter SP-600, 1200 plotters; EPSON FX, RX, MX, LQ, and JX series printers; IBM Proprinter, PC Graphics printer; Okidata ml 92/93, 182/192/193 printers; Centronics GLP printer; and HP Laserjet series laser printers are supported for hard copy plots. Examples shown in this brochure were made using the HP 7475A 6-pen plotter.

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