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RECOVERY Version 2.0, A Mathematical Model to Predict the Temporal Response of Surface Water to Contaminated Sediments

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January 2001

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RECOVERY Version 2.0, A Mathematical Model to Predict the Temporal Response of Surface Water to Contaminated Sediments

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Contents

Preface

The work reported herein was conducted as part of the Water Quality Research Program (WQRP), Work Unit 32989. The WQRP is sponsored by the Headquarters, U.S. Army Corps of Engineers (HQUSACE), and is assigned to the U.S. Army Engineer Research and Development Center (ERDC), under the purview of the Environmental Laboratory (EL), Vicksburg, MS. Funding was provided under Department of the Army Appropriation No. 96X3121, General Investigation. Dr. John W. Barko was Program Manager for the WQRP, and Mr. Robert C. Gunkel, Jr., was Assistant Manager. Program Monitor was Mr. Frederick B. Juhle, HQUSACE.

This report was prepared by Dr. Carlos E. Ruiz, Water Quality and Contaminant Modeling Branch (WQCMB), Environmental Processes and Effects Division (EPED), EL, ERDC, and Mr. Terry Gerald, AScI, Vicksburg.

The work was conducted under the general supervision of Dr. Mark S. Dortch, Chief, WQCMB, Dr. Richard E. Price, Chief, EPED, and Dr. John Keeley, Acting Director, EL.

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1 Introduction

Toxic substances are known to associate strongly with fine-grained particulate matter. Consequently, it is not surprising that toxicants tend to accumulate in the bottom sediments of natural waters. Important questions in environmental impact assessment are to what extent do these contaminated sediments influence overlying waters, and how can the impacts be minimized.

This report describes a modeling framework designed to assess the impact of contaminated bottom sediments on surface waters. The analysis is limited to cases where the overlying water is well-mixed. In addition, the contaminant is assumed to be organic and to follow reversible linear equilibrium sorption and first-order decay kinetics.

The framework is implemented via a personal computer software package--RECOVERY. The present version is called RECOVERY Version 2.0, and it will be referred to in this report as RECOVERY. It is designed for interactive implementation and is self-documented. RECOVERY allows the user to rapidly generate and analyze recovery scenarios for contaminated systems. The software includes graphical displays and can be run on IBM-PC compatible microcomputers. This report provides supplemental documentation that includes a mathematical description of the model and its computational algorithm. It also includes a user's guide.

2 Model Description

The present model is an application and extension of frameworks developed previously (Boyer et al. 1994, Chapra 1982, 1986, and Chapra and Reckhow 1983). As in Figures 1 and 2, the system is idealized as a well-mixed surface water layer underlain by a vertically stratified sediment column. The sediment is well-mixed horizontally but segmented vertically into a well-mixed surface layer and a deep sediment. The latter, in turn, is segmented into layers of user-defined thicknesses, porosities, and contaminant concentrations underlain by an uncontaminated region. The discretized sediment layer configuration is useful for capping scenarios and sites where contamination occurred over a long period of time; thus, contamination appears layered. The specification of a mixed surface layer is included, because an unconsolidated layer is often observed at the surface of sediments as a result of a number of processes, including bioturbation and mechanical mixing.

A list of assumptions used in the development of this model can be found in Table 1. Table 2 lists the features of RECOVERY (Version 2.0). Also, nomenclature used in this report is listed in Appendix A.

Contaminant Mass Balances

A mass balance for the contaminant in the water can be written as

$$\begin{aligned} V_w \frac{dc_w}{dt} &= Qc_i - Qc_w - k_w V_w c_w - k_v V_w c_w - v_s A_w F_{pw} c_w \\ &\quad + v_r A_m c_m + v_d A_m \left(F_{dp} c_m - F_{dw} c_w \right) + W \end{aligned} \tag{1}$$

Only single-component mass transfer is described. The movement of the contaminant is independent of the presence of other contaminants

where

V_w = volume of water body, m^3

c_w and c_m = concentrations of toxicant in water and mixed sediments, respectively, $\mu g/m^3$

c_i = inflow concentration, $\mu g/m^3$, which reflects both direct and tributary loadings

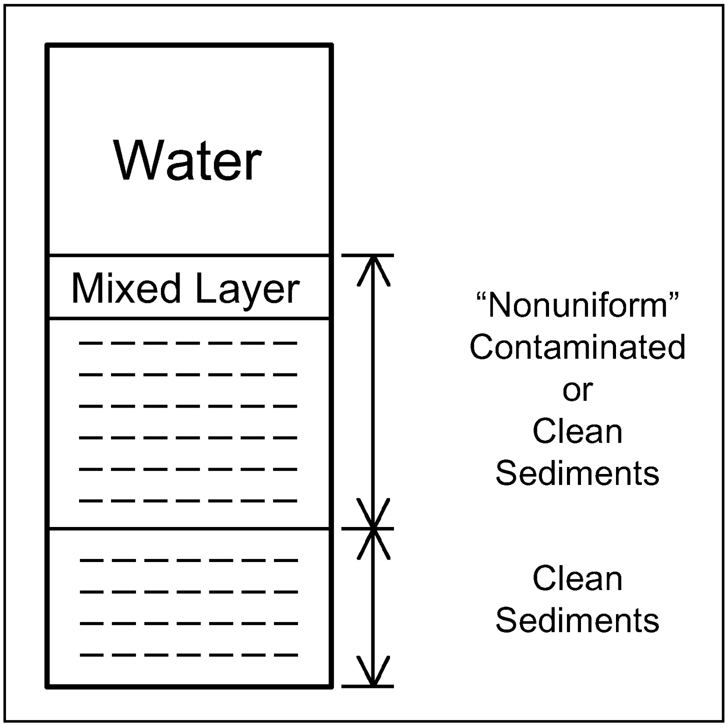

Figure 1. Physical configuration used in RECOVERY

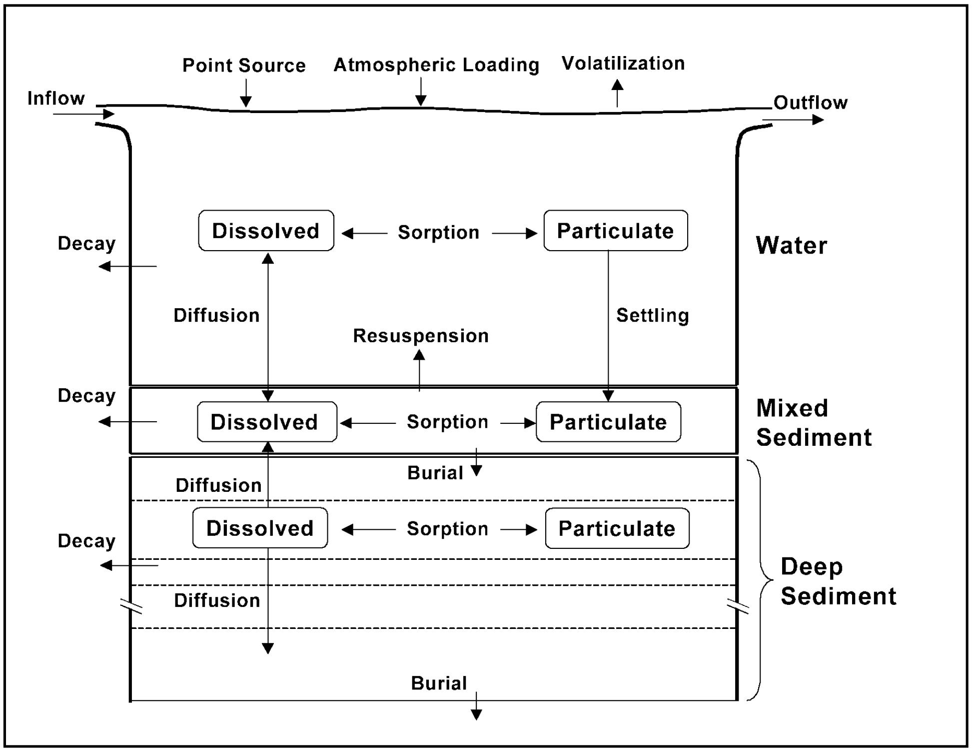

Figure 2. Schematic of the sediment-water system as modeled in RECOVERY

Table 1
List of Assumptions Used in the Development of RECOVERY Version 2.0

Contaminant is of organic nature.
The water body is well-mixed.
The mixed layer is well-mixed.
In the deep sediments, contaminant concentration varies in the vertical direction only.
The initial concentration of the contaminant in the region below the contaminated region is zero.
The contaminant follows a linear reversible equilibrium sorption mechanism.
The contaminant decays according to first-order kinetics.
There is no compaction in the sediments.
The system is isothermal.
The water body is at 25 °C.
Flowthrough is constant.
Only single-component mass transfer is described. The movement of the contaminant is independent of the presence of other contaminants.

Table 2
Features of RECOVERY Version 2.0

Allows for contaminant concentration associated with inflows
Allows for point sources
Allows for atmospheric loadings
Allows for nonuniform deep sediment layers of user-defined thicknesses, porosities, and contaminant concentrations

t = time, years

Q = flushing flow rate, m^3/yr

k_w = decay rate constant of the contaminant in the water, yr^{-1}

k_v = volatilization rate of contaminant, yr^{-1}

v_s = settling velocity of particulate matter, m/yr

A_w and A_m = surface areas of water and mixed sediment, respectively, m^2

F_{pw} = fraction of contaminant in particulate form in the water

v_r = resuspension velocity of sediments, m/yr

v_d = diffusion mass-transfer coefficient at the sediment-water interface, m/yr

F_{dp} = ratio of contaminant concentration in the sediment pore water to contaminant concentration in total sediment

F_{dw} = fraction of contaminant in the dissolved form in the water

W = external loads, µg/yr

The initial condition for Equation 1 at $t = 0$ is $c_w = c_{wo}$.

A mass balance for the mixed-sediment layer can be written as

$$V_m \frac{dc_m}{dt} = -k_m V_m c_m + v_s A_w F_{pw} c_w - v_r A_m c_m - v_b A_m c_m \\ + v_d A_m \left(F_{dw} c_w - F_{dp} c_m\right) + v_d A_m \left(F_{dp} c_s(0) - F_{dp} c_m\right) \tag{2}$$

where

V_m = volume of mixed layer, m^3

k_m = the decay rate constant of the contaminant in the mixed layer, yr^{-1}

v_b = the burial velocity, m/yr

$c_s(0)$ = the contaminant concentration at the top of the deep contaminated layer, $\mu g/m^3$

The initial condition for this equation at $t = 0$ is $c_m = c_{mo}$. Both the deep contaminated and clean sediments can be modeled with one-dimensional advection-diffusion-decay equations of the form

$$\frac{\partial c_s}{\partial t} = \phi F_{dp} D_s \frac{\partial^2 c_s}{\partial z^2} - v_b \frac{\partial c_s}{\partial z} - k_s c_s \tag{3}$$

where

c_s = the contaminant concentration in the deep sediments, $\mu g/m^3$

ϕ = the sediment porosity

D_s = diffusion rate in the sediment pore water, m^2/yr

z = depth into the sediment, m, where $z = 0$ at the top of the deep sediments

k_s = the decay rate constant of the contaminant in the deep sediments, yr^{-1}

The initial and boundary conditions for Equation 3 are:

IC: at $t = 0$, $c_s = c_{so}$ $(z_m<z<L)$

IC: at $t = 0$, $c_s = 0$ $(L<z<\infty)$

BC 1: at $z = z_m$, $J = J_{ms}$

BC 2: at $z = \infty$, $\frac{\partial c_s}{\partial z} = 0$

where

L = distance from the top of the mixed layer to the bottom of the contaminated layer, m

J = mass flux of the contaminant, g/m^2-yr

J_{ms} = mass flux of the contaminant from the mixed layer to the sediment layer, g/m^2-yr

The F variables in Equations 1 through 3 are dimensionless ratios that reflect how the contaminant partitions between solid matter and water assuming a linear sorption mechanism. Denoting the contaminant as A, they are defined as

$$F_{pw} = \frac{K_{dw} s_w}{1 + K_{dw} s_w} = \left(\frac{\dfrac{Mass\ of\ A\,(Particulate\ Form)}{Total\ Volume}}{\dfrac{Mass\ of\ A\,(Dissolved\ Form) + Mass\ of\ A\,(Particulate\ Form)}{Total\ Volume}} \right)_{water\ body} \tag{4}$$

$$F_{dw} = 1 - F_{pw} = \frac{1}{1 + K_{dw} S_w} = \left(\frac{\dfrac{Mass\ of\ A\,(Dissolved\ Form)}{Total\ Volume}}{\dfrac{Mass\ of\ A\,(Dissolved\ Form) + Mass\ of\ A\,(Particulate\ Form)}{Total\ Volume}} \right)_{Water\ Body} \tag{5}$$

$$F_{dp} = \frac{1}{\phi + K_{ds}\,(1 - \phi)\rho_p} = \left(\frac{\dfrac{Mass\ of\ A\,(Dissolved\ Form)}{Volume\ of\ Pore\ Water}}{\dfrac{Mass\ of\ A\,(Dissolved\ Form) + Mass\ of\ A\left(Particulate\ Form\right)}{Total\ Volume}} \right)_{Se\dim ent} \tag{6}$$

where

K_{dw} and K_{ds} = the contaminant partitioning coefficient in the water and sediments, respectively, m^3/g

ρ_p = density of sediment solids, g/m^3

S_w = suspended solids concentration in the water, g/m^3

Note that the model allows different values of this parameter to be employed in the mixed layer and the vertically segmented sediments (F_{dpm} and F_{dps}).

The decay rate constants, k_w, k_m, and k_s, represent all mechanisms for decay except volatilization, which is accounted for separately. These mechanisms include photolysis, hydrolysis, and bacterial degradation.

The mass transfer coefficient for diffusive sediment-water exchange is related to more fundamental parameters by

$$v_d = \frac{\phi D_s}{z'} \tag{7}$$

where

ϕ = sediment porosity

D_s = diffusion rate in the sediment pore water, m^2/yr

z' = characteristic length over which the gradient exists at the sediment-water interface, m

Note that a value of 1 cm is assumed for z' after Thomann and Mueller (1987). Also, D_s is related to molecular diffusivity D_m by the relation (Berner 1980, Manheim and Waterman 1974)

$$D_s = D_m \phi^2$$

Solids Budget

The velocity terms--v_s, v_r, and v_b--in Equations 1 and 2 are computed according to a steady-state mass balance for mixed-sediment layer solids as described by Chapra and Reckhow (1983). The mass balance is

$$0 = v_s A_w S_w - (v_r + v_b) A_m (1 - \phi) \rho_p \tag{8}$$

The framework assumes that suspended solids concentration, s_w, is given. Therefore, if two of the three velocities are specified, Equation 8 can be employed to calculate the third.

In addition to these transfer velocities, the other facet of the model related to the solids budget is the sediment porosity. Different porosities are allowed for the mixed layer and the deep sediments. Within the layers of the deep sediment region, porosity can vary from layer to layer but is assumed constant over time. This means that compaction is not included. The same discretization applies to particle density.

Default Parameters

Several parameters in the above framework are provided by the software as default values. These are suggested values that represent first estimates. They can be easily modified by the user.

Volatilization rate

The volatilization rate is computed by

$$k_v = F_{dw} \frac{v_v}{z_w} \tag{9}$$

where

v_v = a volatilization transfer coefficient, m/yr

z_w = depth of the water column, m

The volatilization transfer coefficient can be computed according to the Whitman two-film theory as

$$v_v = \frac{K_1 K_g H_e}{K_g H_e + K_1} \tag{10}$$

where H_e = a dimensionless Henry's coefficient which is related to the common form, H'_e, atm m^3/mole, by

$$H_e = \frac{H'_e}{RT} \tag{11}$$

where

R = the universal gas constant = 8.206 × 10^{-5} atm m^3/(mole °K)

T = absolute temperature, °K

A temperature of 298 °K (25 °C) is assumed in the model.

The parameter K_g is a gas-film mass transfer coefficient, m/yr, which can be related to wind speed, U_w m/s, and molecular weight, MW g/gmole, by (Mills et al. 1982)

$$K_g = 61{,}320\left(\frac{18}{MW}\right)^{0.25} U_w \tag{12}$$

The parameter K_l is a liquid-film mass transfer coefficient, m/yr, which can be related to wind speed, U_w m/s, and molecular weight, MW g/gmole, by (Mills et al. 1982, Banks 1975, Banks and Herrera 1977)

$$K_1 = 365\left(\frac{32}{Mw}\right)^{0.25} \left(0.728U_w^{0.5} - 0.317U_w + 0.0372U_w^2\right) \tag{13}$$

Partitioning coefficient

The partitioning coefficient for organic contaminants is computed via (Karichhoff, Brown, and Scott 1979)

$$K_d = 0.617\, f_{oc} K_{ow} \tag{14}$$

where

k_d = equilibrium partitioning coefficient, L/kg

f_{oc} = the weight fraction of organic carbon in the solid matter, g-orgC/g

k_{ow} = octanol-water partitioning coefficient, (mg/m^3-octanol)/(mg/m^3-water)

Note that the model assumes a default of 0.05 for f_{oc}. Different values for f_{oc} are allowed for the water column, mixed layer, and the deep sediments. Analogous to other physico-chemical characteristics of the sediments, the f_{oc} can vary with depth (layers) in the deep sediments.

Numerical Methods

The coupled set of differential equations is solved numerically. The two first-order ordinary differential equations are solved using an adaptive-step-size, fourth-order Runge-Kutta method (Press et al. 1986). The partial differential equation is solved using the Crank-Nicolson technique (Chapra and Canale 1988).

The total number of years for which the model is run is determined by approximating the time required for the contaminant concentration in the water to decrease to 10 percent of the maximum value achieved. This is determined by using an analytical solution for the case where only the water and a single well-mixed layer are considered. This procedure has been effective in approximating the total time.

3 User's Guide

Use of RECOVERY Version 2.0 is described in this section. Two files are required to run this program (see Program Features) RECOVERY.EXE and RECOVERY.DBI. RECOVERY.DBI contains the chemical database information and is analogous to CORPCOMP.DAT in Version 1.0. The other files included on the distribution disk are only required for specific hardware systems and to set up the environment variables of the program. Source code, although not included for typical requests, can be obtained, if requested. (See Model Source.) Do not run RECOVERY from a write-protected disk as this will result in an error.

To start the program, move to the directory that contains the software, and type RECOVERY at the DOS prompt. The first two screens are title screens. Press ENTER to view the introduction screen, which follows. Press ENTER again, and choose between creating a new file and retrieving data from an existing data file. If the second selection is made, any files ending in .REC and the subdirectories located in the current directory are displayed. The .REC files are the data files that are created after saving a run made by RECOVERY. (This will be discussed later). If the file is not located in the current directory or in one of the listed subdirectories, press ESC to return to the previous screen and then press ALT D and specify the path name to the file(s). The .REC file(s) should then be displayed. After a file is chosen, you can either view and/or change the input file or just run the model using that data file. If 'create a new file' is chosen, a list of compounds is displayed. The properties of 18 compounds are included in the original database, the new database contains “194” compounds. If the compound under consideration is not listed, press ENTER under the COMPOUND NOT LISTED entry. The selection is made by moving the cursor to the desired selection using the arrow keys and pressing ENTER.

If a new compound is selected, the database modification screen appears. The user has three choices: (1) a new compound to run RECOVERY, (2) modify RECOVERY’s existing database, and/or (3) add a new compound to RECOVERY’s database. After the selection, a screen appears to enter the name of the compound. As the user types, the name will appear in the highlighted area. Corrections can be made by using the BACKSPACE or DELETE keys. After the name has been typed in, press ENTER to enter the name and advance to the next screen.

The next five screens are used to enter or change input values. After typing in a cell, the user must press ENTER before proceeding to the next cell. The first morphometry and hydrology screen should be displayed. The new compound name should appear in this first screen, at the "Initial Concentration of" entry. The user may change or leave the water initial concentration, the input concentration, and the external loadings at the default value of zero. Three of the next four values need to be entered. Press F9 to calculate the fourth and its value will be displayed. When all the data are entered, press F10 to store the values and advance to the next screen. If invalid values are entered, a message will appear; if help is needed, press the F1 key; ESC brings the user back one screen; and ALT X exits the program.

The next screen is for the contaminated sediments layer. If nothing is changed, the default values will be used; nonzero values are needed in this screen. The user has the option of selecting constant (FIXED) concentration and properties for the deep sediments or discretizing the deep sediments (VARIABLE). Press F10 to continue. System properties are listed on the next screen. Default values or zero are listed for the first eight variables. These values can be changed as described above. Since the three velocity values are interrelated, two of the three values should be entered. Typical values are listed in the center column. After entering two values, press F9 to calculate the third value. It will appear near the bottom of the screen. Press F10 to store the data and proceed.

The next two screens list contaminant properties. Default values or zeros are listed in the far right column and will be specific to the selected compound if it is in the database. These values will be used unless the user changed them in the center column (values must be nonzero, except for degradation coefficients). The second screen also contains intermediate values calculated from the previously entered data (e.g., F_{dw}, K_{dw}). Press F10 to store and advance.

To return to a previous screen in the input process described above, the user can press ESCAPE (ESC) until the desired screen appears. The next screen serves as a check to see if the entered data are correct and if not, the user can return to the input screens. Selecting the third option starts the model. The user receives the "running model" message. After the run is finished, the user is in the RECOVERY Output Screen.

The model's completion status can be viewed. One of the parameters in the completions status screen is total number of years; the value is calculated internally as the approximate time when the water concentration decreases to 10 percent of its maximum value.

Another option is the View Plot Menu screen, with five options available. Four of the options are analogous to the original version, and the fifth option is the concentration profile in the deep sediments. Since the numerical method uses an adaptive-step-size, the time between profile displays will not be even. Options 1 through 4 are graphics plots. The first two plots are graphs of the contaminant concentration in the water layer and the mixed layer, respectively, versus time. The third plot shows the flux of the contaminant from the sediments to the water versus time. A graph of the volatilization rate of the contaminant will be displayed if option 4 is selected. These results can be printed by selecting the Write Output Option in the Output screen (4).

Selection 3 allows the user to estimate the Total Bioaccumulation Potential for the given contaminant and a selected target organism. Selection 4 is for printing or plotting results. The user can select a table of results on the printer or save the results to file or similar options for hard copy plots. Selection 5 will make modifications to the existing run and Selection 6 should be chosen to return to the beginning of the program. Selection 7 will save the existing run. The user will be prompted for a file name to be used to store the results. Selection 8 will result in exiting the program.

Changing Chemical Database

RECOVERY.DBI is the name of the file that RECOVERY will recognize as the chemical database, which currently has 194 chemicals. This file can be changed and enlarged to include more compounds. The file is a text file, and the format is one that RECOVERY can input (READ). Thus, if using a text editor to make changes, make sure that the modifications do not alter the tabular nature of the file. The file can be changed within the RECOVERY execution by selecting new compound in RECOVERY as discussed in the previous section. The data required for any chemical compound to be included in the database are:

- Name
- Molecular Weight
- Octanol-Water Partition Coefficient
- Henry's Constant
- Molecular Diffusivity
- Decay Constants -
    - water, dissolved phase
    - water, particulate phase
    - mixed layer, dissolved phase
    - mixed layer, particulate phase
    - deep sediments, dissolved phase
    - deep sediments, particulate phase

Additions and changes are made by altering or adding data statements to the file RECOVERY.DBI. RECOVERY.DBI is the file on disk with the default database.

Model Source

RECOVERY Version 2.0 is written in FORTRAN 77; the Graphical User Interface (GUI) is written in C. To modify the model's source code, the user needs a FORTRAN Compiler. However, the modifications will not be implemented in the linked GUI and model (RECOVERY). The user can use the GUI for creating the input data set and for visualization of the results (PLOT.EXE), but the executable file produced from recompiling the source code cannot be linked to the original RECOVERY executable file. PLOT.EXE is provided for graphical visualization of the results and for hard copies of the run plots. The FORTRAN source code that can be obtained by request are the files:

COMMON.INC
BASIC_IN.FOR
RECOV.FOR
DERIVS.FOR
DRIVER.FOR
FLUX_TER.FOR
GET_INPU.FOR
SETUP_OD.FOR
SETUP_PD.FOR

Program Features

A list of data required to run this program can be found in Table 3. Since the compound properties for several contaminants are included in the provided database, the user must provide compound properties only if the contaminant under consideration is not one that is in the database. The values in the database that comes with the distribution disk are listed in Table 4 (RECOVERY.DBI). Appendix B contains a listing of compounds with their common names. The data file can be changed as described in Chapter 3.

These data are entered on a series of input screens with editing capabilities. The user can easily page forward and backward through the screens while entering data. On-line help is also available. If any of the entered data are invalid, an error message appears instructing the user to reenter these data.

A new feature of the RECOVERY program is the option to discretize the contaminant concentration and physico-chemical properties in the deep sediments (Table 3). The user can specify variable (layered) concentration in the vertical direction (depth), deep sediment porosity, deep sediment particle density, and the fraction of organic carbon. The convention is to specify the concentration or physico-chemical property from the bottom of the layer.

The final results are displayed as plots on the screen and can be printed on a printer or saved to disk by selecting the proper form of output from the Model Output Screen. Numerical results can be dumped to the printer or disk also. The plots are:

a. Contaminant Concentration in the Water versus Time

b. Contaminant Concentration in the Mixed Layer versus Time

c. Flux of the Contaminant from the Sediments into the Water versus Time

d. Volatilization Losses of the Contaminant from the Water versus Time

e. Deep Sediment Concentration Profile over Time

The input data can be stored on a disk and retrieved for later use. The user can also easily return to the input screens to make modifications. Appendix C gives a sequential example of the screens in running the RECOVERY model.

Table 3
Input Data for RECOVERY Model

- Water Column Morphometry/Hydrology: (3 specified, 4th computed)
    - Flow through (m^3/yr)
    - Residence time (yr)
    - Surface area (m^2)
    - Water depth (m)

- Water Layer:
- Initial concentration (μg/m^3)
    - Inflow concentration (μg/m^3)
    - External loadings (kg/yr)

- Contaminated Sediments:
    - Depth of contaminated sediment layer (m)
    - Depth of mixed layer (m)
    - Mixed layer surface area (m^2)
    - Initial concentrations (μg/m^3)
        - Mixed layer
        - Deep contaminated sediments
            - Constant
                - Deep sediment initial concentration (μg/m^3)
            - Variable
                - Depth (m)
                - Deep sediment initial concentration (μg/m^3)
                - Deep sediment particle density (g/m^3)
                - Deep sediment fraction organic carbon (g-orgC/g-dry wt solids)

- System Properties:
    - Suspended solids concentration in water (g/m^3)
    - Mixed layer porosity
    - Deep sediment porosity
    - Sediment particle density (g/m^3)
    - Wind speed (m/s)
    - Fraction organic carbon (g-orgC/g-dry wt solids)
        - Water layer
        - Mixed layer
        - Deep contaminated sediments
    - Two of the following three velocities:
        - Resuspension velocity (m/s)
        - Burial velocity (m/s)
        - Settling velocity (m/s)

- Compound Properties:
    - Molecular diffusivity (cm^2/sec)
    - Decay coefficients (yr^{-1}): Particulate - water
        - Dissolved - water
        - Particulate - mixed layer
        - Dissolved - mixed layer
        - Particulate - deep sediments
        - Dissolved - deep sediments
    - Henry's constant (atm-m^3/gmole)
    - Octanol-water partition coefficient
    - Molecular weight (g/gmole)

Table 4
Compound Properties (RECOVERY.DBI)

Compound Name	Molecular Weight g/gmole	Kow	Log Kow	Henry's Constant @ 25 ^{3}C atm m3/gmole
1,1 DICHLOROETHY	96.9	6.92E+01	1.84	1.60E-01
1,1,1,2-TETRACHL	168.0	1.07E+03	3.03	4.89E-04
1,1,1-TRICHLOROE	133.0	3.16E+02	2.50	4.92E-03
1,1,2,2-TETRACLO	168.0	2.45E+02	2.39	3.81E-04
1,1,2-TRICHLOROE	133.0	2.95E+02	2.47	1.17E-03
1,1-DICHLOROETHA	99.0	6.17E+01	1.79	5.43E-03
1,2 DICHLOROBENZ	147.0	4.00E+03	3.60	1.93E-03
1,2 DICHLOROETHA	99.0	3.02E+01	1.48	9.78E-04
1,2 DICHLOROETHY	96.9	3.02E+00	0.48	6.90E-02
1,2,3TRICHLOROPR	147.0	3.72E+04	4.57	3.12E-04
1,2,4,5-TETRACHL	216.0	4.68E+04	4.67	2.37E-03
1,2,4TRICHLOROBE	181.0	2.00E+04	4.30	2.31E-03
1,2-DIBROMO-3-CH	236.0	1.95E+02	2.29	3.11E-04
1,3-CIS-DICHLORO	111.0	1.00E+02	2.00	1.30E-03
1,3-DICHLOROBENZ	147.0	3.98E+03	3.60	2.63E-03
1,4-DICHLOROBENZ	147.0	3.98E+03	3.60	2.89E-03
1-NAPHTHYLAMINE	143.0	1.17E+02	2.07	5.21E-09
2(METHYLTHIO)PRO	90.2	7.59E+01	1.88	1.37E-03
2,3,4,6,-TETRACH	232.0	1.26E+04	4.10	3.07E-07
2,3,7,8TCDD DIOX	322.0	5.25E+06	6.72	1.60E-05
2,4,5-TRICHLOROP	197.0	5.25E+03	3.72	2.18E-04
2,4,6-TRICHLOROP	197.0	7.41E+03	3.87	3.90E-06
2,4,6-TRIMETHYLP	136.0	2.63E+03	3.42	3.34E-05
2,4-D	221.0	6.46E+02	2.81	1.88E-04
2,4-DICHLOROPHEN	163.0	7.94E+02	2.90	2.75E-06
2,4-DIMETHYLPHEN	122.0	6.46E+02	2.81	1.75E-05
2,4-DINITROPHENO	184.0	3.16E+01	1.50	6.50E-10
2,4-DINITROTOLUE	182.0	1.00E+02	2.00	5.09E-06
2,6-DICHLOROPHEN	163.0	4.37E+00	0.64	6.63E-05
2-CHLOR-1,3-BUTA	88.5	6.03E+01	1.78	8.18E-03
2-CHLORONAPHTHAL	162.0	1.00E+04	4.00	5.40E-04
2-CHLOROPHENOL	129.0	1.51E+02	2.18	1.03E-05
2-METHYLNAPHTHAL	142.0	7.24E+03	3.86	3.10E-04
2-SEC-BUTYL-4,6-	240.0	4.57E+03	3.66	2.40E-11
3,3′-DIMETHOXYBE	244.0	1.91E+01	1.28	3.50E-11
3,3′-DIMETHYLBEN	212.0	1.19E+02	2.08	2.40E-10
3,3-DICHLOROBENZ	253.0	3.16E+03	3.50	8.33E-07
3-CHLOROPROPENE()	76.5	6.61E+00	0.82	3.42E-01
4,4′-METHYLENE-B	267.0	8.71E+03	3.94	6.70E-10
4,6-DINITRO-O-CR	198.0	5.01E+02	2.70	1.40E-06
4-CHLORO PH PH E	205.0	1.20E+04	4.08	2.67E-04
4-METHYLPHENOL(P)	108.0	8.51E+01	1.93	2.38E-07
4-NITROPHENOL	139.0	8.13E+01	1.91	2.95E-04
5-NITRO-O-TOLUID	152.0	9.12E+01	1.96	3.91E-07
ACETONITRILE	41.0	4.60E-01	-0.34	4.00E-06
ACRYLONITRILE	53.0	1.78E+00	0.25	8.84E-05
ALDRIN	365.0	2.00E+05	5.30	5.00E-04

(Sheet 1 of 4)

Table 4 (Continued)

Compound Name	Molecular Weight g/gmole	Kow	Log Kow	Henry's Constant @ 25 ^{3}C atm m3/gmole
ALPHA-HEXACHLORO	291.0	7.94E+03	3.90	5.87E-06
ANILINE	93.1	8.71E+00	0.94	1.08E-06
ANTHRACENE	178.0	2.82E+04	4.45	1.90E-05
AROCLOR 1016 (PC)	258.0	3.80E+05	5.58	3.30E-04
AROCLOR 1221 (PC)	201.0	1.20E+04	4.08	1.70E-04
AROCLOR 1232 (PC)	232.0	1.59E+03	3.20	1.13E-05
AROCLOR 1242 (PC)	267.0	1.29E+04	4.11	1.98E-03
AROCLOR 1248 (PB)	300.0	5.75E+05	5.76	3.60E-03
AROCLOR 1254 (PC)	328.0	1.10E+06	6.04	8.30E-03
AROCLOR 1260 (PC)	376.0	1.41E+07	7.15	1.70E-04
BENZENE	78.0	1.32E+02	2.12	5.59E-03
BENZIDINE	184.0	2.00E+01	1.30	3.03E-07
BENZO(A)ANTHRACE	228.0	3.98E+05	5.60	1.16E-06
BENZO(A)PYRENE	252.0	1.15E+06	6.06	1.55E-06
BENZO(B)FLUORANT	252.0	1.15E+06	6.06	1.19E-05
BENZO(K)FLUORANT	252.0	1.15E+06	6.06	3.94E-05
BENZYL ALCOHOL	108.0	1.26E+01	1.10	3.91E-07
BETA – HCCH	291.0	7.94E+03	3.90	4.47E-07
BIS(2-CHLOROETHY)	143.0	3.16E+01	1.50	1.31E-05
BIS(2-CHLOROISOP)	171.0	1.26E+02	2.10	1.13E-04
BIS(2ET-HEXYL)PH	391.0	4.10E+00	0.61	4.40E-07
BROMODICHLOROMET	164.0	1.74E+02	2.24	2.12E-03
BROMOMETHANE	94.9	1.55E+01	1.19	1.16E-01
CARBON TETRACHLO	154.0	4.36E+02	2.64	3.02E-02
CHLORDANE	410.0	6.03E+04	4.78	5.00E-05
CHLOROBENZENE	113.0	6.92E+02	2.84	3.72E-03
CHLOROBENZILATE	325.0	3.24E+04	4.51	2.34E-08
CHLORODIBROMOMET	208.0	1.23E+02	2.09	9.95E-04
CHLOROETHANE	64.5	2.69E+01	1.43	1.48E-02
CHLOROFORM	119.0	9.33E+01	1.97	2.87E-03
CHLOROMETHANE(ME)	50.5	8.91E+00	0.95	4.42E-02
CHRYSENE	228.0	4.07E+05	5.61	9.46E-07
CYCLOHEXANE	84.2	2.75E+03	3.44	2.51E-01
DDD	320.0	1.58E+06	6.20	7.96E-06
DDE	218.0	1.00E+07	7.00	6.80E-05
DDT	355.0	1.55E+06	6.19	5.13E-04
DELTA-HCCH	291.0	1.26E+04	4.10	2.07E-07
DI-N-BUTYL PHTHA	278.0	4.00E+05	5.60	2.82E-07
DI-N-OCTYLPHTHAL	391.0	7.41E+09	9.87	5.50E-06
DIAZINON	304.0	6.46E+03	3.81	1.25E-01
DIBENZO(A,H)ANTR	278.0	4.07E+05	5.61	2.61E-09
DIBROMOMETHANE	174.0	1.66E+01	1.22	2.38E-03
DICHLORODIFLUORO	121.0	1.45E+02	2.16	1.01E-04
DIELDRIN	381.0	3.16E+03	3.50	5.80E-05
DIETHYL PHTHALAT	222.0	2.88E+02	2.46	2.00E-08
DIMETHYL ETHER	46.1	1.26E+00	0.10	4.90E-04
DIMETHYLAMINE (D)	45.1	4.20E-01	-0.38	1.50E-04
DIMETHYLPHTHALAT	194.0	3.63E+01	1.56	1.10E-06

(Sheet 2 of 4)

Table 4 (Continued)

Compound Name	Molecular Weight g/gmole	Kow	Log Kow	Henry's Constant @ 25 ^{3}C atm m3/gmole
DIESEL FUEL	142.0	7.24E+03	3.86	2.90E-04
DIURON	233.0	6.30E+02	2.80	8.70E-03
ENDOSULFAN I (AL)	407.0	3.55E+03	3.55	1.00E-05
ENDOSULFAN II (B)	407.0	4.17E+03	3.62	1.91E-05
ENDRIN	381.0	3.98E+05	5.60	1.00E-01
ETHYL METHACRYLA	114.0	8.71E+01	1.94	5.53E-04
ETHYLBENZENE	106.0	1.41E+03	3.15	6.43E-03
FLUORANTHENE	202.0	7.94E+04	4.90	1.02E-05
FLUORENE	166.0	1.58E+04	4.20	1.17E-04
FORMALDEHYDE	30.0	2.24E+00	0.35	3.72E-03
FUEL OIL #2	142.0	7.24E+03	3.86	2.90E-04
FURAN	68.1	2.19E+01	1.34	6.06E-03
GAMMA-HCCH (LIND)	291.0	7.94E+03	3.90	7.85E-06
GLYPHOSATE	169.0	1.00E-03	-3.00	1.50E-06
HEPTACHLOR	374.0	2.51E+04	4.40	2.90E-03
HEPTACHLOR EPOXI	389.0	5.10E+02	2.71	4.39E-04
HEXACHLOROBENZEN	285.0	1.70E+05	5.23	6.81E-04
HEXACHLOROBUTADI	261.0	6.03E+04	4.78	1.00E-02
HEXACHLOROCYCLOP	273.0	1.00E+04	4.00	2.75E-02
HEXACHLORODIBENZ	375.0	5.00E+06	6.70	3.60E-03
HEXACHLORODIBENZ	391.0	5.25E+06	6.72	3.60E-03
HEXACHLOROETHANE	237.0	3.98E+04	4.60	9.85E-03
HEXACHLOROPHENE	407.0	3.47E+07	7.54	8.30E-10
HMX (H-NO2 TETZO)	296.0	3.90E+00	0.59	3.53E-06
INDENO(1,2,3-CD)	276.0	3.16E+06	6.50	6.86E-08
JP4	142.0	7.24E+03	3.86	2.90E-04
KEPONE	491.0	1.00E+02	2.00	4.90E-11
M-DINITROBENZENE	168.0	4.17E+01	1.62	5.84E-08
m-XYLENE	106.0	1.82E+03	3.26	1.07E-02
METHAPYRILENE	261.0	7.41E+02	2.87	1.61E-09
METHOXYCHLOR	346.0	2.00E+04	4.30	2.48E-08
METHYLCYCLOHEXAN	98.2	7.41E+03	3.87	3.15E-01
METHYLCYCLOPENTA	84.2	2.06E+03	3.31	1.81E-01
METHYLENE CHLORI	84.9	2.00E+01	1.30	2.03E-03
N-NITROSODI-N-BU	158.0	8.32E+01	1.92	7.52E-03
N-NITROSODIETHYL	102.0	3.02E+00	0.48	7.90E-06
N-NITROSODIMETHY	74.1	2.09E-01	-0.68	7.90E-07
N-NITROSODIPHNYL	198.0	1.35E+03	3.13	6.60E-04
N-NITROSODIPROPY	130.0	3.09E+01	1.49	6.30E-06
N-NITROSOMORPHOL	116.0	3.63E-01	-0.44	2.65E-04
N-NITROSOPIPERID	114.0	3.24E-01	-0.49	1.11E-08
N-NITROSOPYRROLI	100.0	8.71E-02	-1.06	2.07E-09
N-PHENYL BENZENA	169.0	3.16E+03	3.50	3.70E-07
NAPHTHALENE	128.0	1.70E+03	3.23	7.20E-04
NITROBENZENE	123.0	7.08E+01	1.85	2.40E-05
O-NITROANILINE	138.0	6.17E+01	1.79	2.25E-05
o-XYLENE	106.0	8.91E+02	2.95	7.97E-03
P-BENZOQUINONE	108.0	1.58E+00	0.20	1.47E-06

(Sheet 3 of 4)

Table 4 (Concluded)

Compound Name	Molecular Weight g/gmole	Kow	Log Kow	Henry's Constant @ 25 ^{3}C atm m3/gmole
P-CHLORO-M-CRESO	143.0	1.26E+03	3.10	4.31E-07
P-CHLOROANILINE	128.0	6.76E+01	1.83	9..68E-07
P-DIMETHLAMINOAZ	225.0	5.25E+03	3.72	7.19E-09
P-NITROANILINE	138.0	2.45E+01	1.39	3.75E-07
P-XYLENE	106.0	1.41E+03	3.15	7.40E-03
PARATHION	291.0	6.46E+03	3.81	1.22E-06
PCBs (GENERAL)	328.0	1.10E+06	6.04	2.60E-03
PENTACHLOROBENZE	250.0	1.55E+05	5.19	1.77E-02
PENTACHLOROETHAN	202.0	4.68E+03	3.67	1.34E-02
PENTACHLORONITRO	295.0	2.82E+05	5.45	6.18E-04
PENTACHLOROPHENO	266.0	1.00E+05	5.00	2.75E-06
PENTAERYTHRITOL	316.0	3.89E+00	0.59	3.53E-06
PHENACETIN	179.0	3.72E+01	1.57	1.08E-03
PHENANTHRENE	178.0	2.88E+04	4.46	2.30E-05
PHENOL	94.1	2.88E+01	1.46	1.30E-06
PICLORAM	281.0	2.27E+02	2.36	3.19E-10
PICOLINE	93.1	1.29E+01	1.11	4.21E-05
POLYACRYLAMIDE	1000.0	1.00E+03	3.00	1.00E-04
POLYCHLORNTED FU	322.0	5.30E+06	6.72	3.60E-03
PRINCEP 80W	202.0	1.51E+02	2.18	1.91E-09
PYRENE	202.0	2.09E+05	5.32	5.04E-06
PYRIDINE	79.1	4.57E+00	0.66	2.29E-06
RDX 6H-3NO2-TRIA	222.0	1.91E+03	3.28	8.30E-06
SILVEX	270.0	8.51E+03	3.93	8.40E-11
STRYENE-BUTADIEN	158.0	1.19E+04	4.08	4.09E-04
STYRENE	104.0	8.91E+02	2.95	4.71E-03
TETRACHLOROETHYL	166.0	3.98E+02	2.60	2.59E-02
TETRAETHYLDITHIO	322.0	8.90E+03	3.95	1.76E-06
TNT 3NO2-TOLUENE	227.0	7.76E+01	1.89	1.37E-04
TOLUENE	92.2	5.37E+02	2.73	6.37E-03
TOLUENE DIISOCYA	174.0	4.14E+03	3.62	3.56E+00
TOXAPHENE	414.0	2.00E+03	3.30	4.90E-03
TRANS-1,3-DICHLO	111.0	1.00E+02	2.00	1.30E-03
TRANS-1,4-DICHLO	125.0	5.00E-01	-0.30	1.01E-04
TREFLEN	335.0	2.40E+05	5.38	1.70E-08
TRIBROMEMETHANE	253.0	2.51E+02	2.40	5.52E-04
TRICHLOROETHYLEN	131.0	2.40E+02	2.38	9.10E-03
TRICHLOROMETHANE	151.0	3.39E+02	2.53	8.09E-04
TRICHLOROMONOFLU	137.0	3.39E+02	2.53	5.83E-02
TRICL-HEPTAF-BUT	287.0	5.75E+03	3.76	2.13E-01
TRIETHANOLAMINE	149.0	1.78E-02	-1.75	3.77E-13
TRIETHYLENE GLYC	150.0	8.32E-03	-2.08	1.34E-10
TRIMETHYLBENZENE	120.0	2.63E+03	3.42	3.70E-01
TRIS(2,3-DIBROMO)	698.0	1.32E+04	4.12	1.45E-06
VINYL ACETATE	86.1	2.95E+00	0.47	3.76E-04
VINYL CHLORIDE	62.5	2.40E+01	1.38	8.19E-02
XYLENE (MIXED)	106.0	1.82E+03	3.26	7.04E-03

(Sheet 4 of 4)

This program and GUI were complied in Watcom^R C and Watcom^R FORTRAN and have been written for the following combinations of graphic adapters and displays:

CGA and Color Display
EGA and Monochrome Display
EGA and Color Display
EGA and Enhanced Color Display
VGA and Monochrome Display
VGA and Color Display

A math coprocessor is not required to run RECOVERY. The use of one, however, will decrease the computation time.

System Specific Issues

The following list describes procedures that are specific to particular hardware systems. If you have problems running RECOVERY, please consult the list below.

a. *Run setup.* If your system has problems displaying the GUI, run the SETUP program and select the proper environment definition variables. The first environment variable is the location of the directory where RECOVERY.EXE is in your hard drive. The user selects the specific printer driver and computer output port from the selection in SETUP.

b. *Strange sediment profile results.* If your system has all of the following characteristics, you may have floating-point math problems.

   (1) Uses MS-DOS Version 3.20.

   (2) Boots from a hard drive.

   (3) Has a math coprocessor (for instance, an 8087 chip).

These problems can be avoided by booting the computer from a floppy disk drive instead of the hard drive.

WARNING: If you have floating-point math problems, the model information will not be correct. This should be evident by the graphical results.

4 Conclusions and Recommendations

RECOVERY is designed for interactive implementation via a personal computer. The program allows the user to rapidly generate and analyze recovery scenarios for contaminated sediments and cap evaluations. The software includes graphical displays and is self-documented. The intent of this report is to document the model and its user's guide.

RECOVERY Version 1.0 was confirmed against the quarry experiments (Di Toro and Paquin 1983 and Waybrant 1973). The confirmation shows the ability of the program to simulate behavior of organics in a real system with a limited amount of data. Results are similar to those predicted by another model and, thus, appear to demonstrate the validity of the algorithms used to describe the fate and transport of organics.

One problem found in the original confirmation exercise was the simulation of the initial part of the quarry experiment where an initial organic load was applied to the pond. The current formulation of the model assumes loadings associated with the inflow and, thus, is more applicable than Version 1.0.

The RECOVERY model can be applied in a variety of scenarios including lakes, embayments, harbors, estuaries, and ocean parcels as long as the assumption of a completely mixed water body is acceptable along with other assumptions listed in Table 1. Average yearly flushing would be needed in any of the previous applications, in addition to the other chemical and physical parameters for a well-defined simulation.

Mechanistic and/or modular improvements addressed in RECOVERY Version 2.0 are the following:

a. Allows external contaminant loadings from point and nonpoint sources.

b. Allows atmospheric contaminant loads, such as dry or wet deposition.

c. Allows the variation of physical and chemical properties in the contaminated sediment.

A major improvement recommended for RECOVERY is to be able to assess the impact on surface waters from bottom sediments contaminated with heavy metals. The above recommendation would involve substantial effort since metal specialization and associated equilibrium and kinetic chemistry are involved.

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Appendix A
Nomenclature

A_m	Mixed layer surface area, m^2
A_w	Water surface area, m^2
C_i	Contaminant concentration in the inlet to the water body, $\mu g/m^3$
C_m	Contaminant concentration in the mixed layer, $\mu g/m^3$
C_s	Contaminant concentration in the deep sediments, $\mu g/m^3$
$C_s(0)$	Contaminant concentration at the top of the deep sediments, $\mu g/m^3$
C_w	Contaminant concentration in the water, $\mu g/m^3$
D_s	Molecular diffusivity, m^2/s
D_m	Diffusion coefficient in the sediment pore water, m^2/s
F_{dpm}	Ratio of contaminant concentration in the mixed layer pore water to concentration in the total mixed layer, dimensionless
F_{dps}	Ratio of contaminant concentration in the deep sediment pore water to concentration in the total deep sediments, dimensionless
F_{dw}	Fraction of contaminant in particulate form in the water, dimensionless
f_{oc}	Weight fraction of organic carbon in the solid matter, g-orgC/g-solid
F_{pw}	Fraction of contaminant in dissolved form in the water, dimensionless
H_e	Henry's law constant, dimensionless
H_e'	Henry's law constant, atm-m^3/gmole
J	Flux of the contaminant, g/(m^2-year)
J_{ms}	Flux of the contaminant from the mixed layer to the deep sediments, g/(m^2-year)

K_{dw}	Contaminant partition coefficient in the water, m^3/g
K_{ds}	Contaminant partition coefficient in the sediments, m^3/g
K_g	Gas-film mass transfer coefficient, m/year
K_l	Liquid-film mass transfer coefficient, m/year
k_m	Decay rate constant of the contaminant in the mixed layer, $year^{-1}$
K_{ow}	Octanol-water partition coefficient, $(mg/m^3$-Octanol)/$(mg.m^3$-water)
k_s	Decay rate constant of the contaminant in the deep sediments, $year^{-1}$
k_v	Volatilization rate of the contaminant, $year^{-1}$
k_w	Decay rate constant of the contaminant in the water, $year^{-1}$
MW	Molecular weight of the contaminant, g/gmole
Q	Flow rate into and out of the water body, m^3
R	Universal gas constant, atm-m^3/(gmole-kelvins)
S_w	Suspended solids concentration in the water, g/m^3
t	Time, years
T	Absolute temperature, kelvins
v_b	Burial velocity, m/year
v_d	Diffusive mass transfer coefficient, m/year
V_m	Volume of the mixed layer, m^3
v_r	Resuspension velocity of the sediments into the water, m/year
v_s	Settling velocity of the particulate matter from the water to the sediments, m/year
v_v	Volatilization transfer coefficient, m/year
V_w	Volume of the water, m^3
U_w	Wind speed, m/year
z'	Length over which the concentration gradient exists at the sediment/water interface, m
z_m	Depth of the mixed layer, m

ρ	Density of the sediment solids, g/m3
φ	Porosity

Appendix B
Chemical Common Names

Table B1
Common Names

Compound	Common Name
1,1 DICHLOROETHYLEN	1,1 dichloroethylene, Vinylidine chloride
1,1,1,2-TETRACHLORO	1,1,1,2-Tetrachloroethane
1,1,1-TRICHLOROETHA	1,1,1-Trichloroethane, Methyl chloroform
1,1,2,2-TETRACLOROE	1,1,2,2-Tetracloroethane, Cellow
1,1,2-TRICHLOROETHA	1,1,2-Trichloroethane, Vinyl trichloride
1,1-DICHLOROETHANE	1,1-Dichloroethane, Chlorure
1,2 DICHLOROBENZENE	1,2 Dichlorobenzene, Dowtherm E
1,2 DICHLOROETHANE	1,2-Dichloroethane, Ethylene dichloride
1,2 DICHLOROETHYLEN	Trans-1,2-Dichloroethylene, Trans-acetylene dichloride
1,2,3 TRICHLOROPRPAN	1,2,3-Trichloropropane, NCI-C60220
1,2,4,5-TETRACHLORO	1,2,4,5-Tetrachlorobenzene
1,2,4 TRICHLOROBENZN	1,2,4-Trichlorobenzene, unsym-Trichlorobenzene
1,2-DIBROMO-3-CHLOR	1,2-dibrom-3-chlor-propane, Fumazone
1,3-CIS-DICHLOROPRO	1,3-cis-dichloropropene, 1-propene,1,3-dichloro-(1)-(9CI)
1,3-DICHLOROBENZENE	1,3-Dichlorobenzene
1,4-DICHLOROBENZENE	1,4-Dichlorobenzene, Paracide, PDB
1-NAPHTHYLAMINE	1-Naphthylamine, Fast garnet base B
2(METHYLTHIO)PROPAN	2-Methyl-2-propanethiol
2,3,4,6-TETRACHLOR	2,3,4,6-Tetrachlorophenol, Dowicide 6
2,3,7,8 TCDD DIOXIN	2,3,7,8-Tetrachlorodibrnzo-p-Dioxin, TCDD
2,4,5-TRICHLOROPHEN	2,4,5-Trichlorophenol, Nurelle
2,4,6-TRICHLOROPHEN	2,4,6-Trichlorophenol, Omal
2,4,6-TRIMETHYLPHEN	2,4,6-Trimethylphenol
2,4-D	2,4-D, Amidox, Estone, Fernesta
2,4-DICHLOROPHENOL	2,4-Dichlorophenol, DCP, NCI-C55345
2,4-DIMETHYLPHENOL	2,4-Dimethylphenol, 1-hydroxy-2,4-dimethylbenzene
2,4-DINITROPHENOL	2,4-Dinitrophenol, Nitro kleenup, Solfo black B
2,4-DINITROTOLUENE	2,4-Dinitrotoluene, DNT
2,6-DICHLOROPHENOL	2,6-Dichlorophenol, NCI-C55345
2-CHLOR-1,3-BUTADIE	2-chloro-1,3-butadiene, Chloroprene, Neoprene
2-CHLORONAPHTHALENE	2-Chloronaphthalene
2-CHLOROPHENOL	2-Chlorophenol, Phenol
2-METHYLNAPHTHALENE	Methylnaphthalene, Methylanftalen
2-SEC-BUTYL-4,5-DIN	2-sec-butyl-4,6-dintrophenol, Dinoseb, DNBP, Spurge
3,3'-DIMETHOXYBENZI	3,3'-Dimethoxybenzidine, Diacel navy DC
3,3'-DIMETHYLBENZID	3,3'-Dimethylbenzidine, o-Tolidine
3,3-DICHLOROBENZIDI	3,3'-Dichlorobenzidine, 4,4-Diamine
3-CHLOROPROPENE(ALL)	3-Chloropropene, Chlorallylene
4,4'-METHYLENE-BIS( )	4,4'-Methylenebis (2-chloroaniline), Bis amine, MOCA
4,6-DINOTRO-O-CRESO	4,6-Dinitro-O-cresol, Krenite, Lipan

(Sheet 1 of 5)

Table B1 (Continued)

Compound	Common Name
4-CHLORO PH PH ETHE	4-Chlorophenyl phenyl ether
4-METHYLPHENOL(P-CR)	4-Methylphenol, p-Cresol
4-NITROHENOL	4-Notrophenol, Ncl-C55992
5-NITRO-O-TOLUIDINE	5-Nitro-o-toluidine, NCI-C01843
ACETONITRILE	Acetonitrile, methyl cyanide
ACRYLONITRILE	Acrylonitrile, Propenenitrile, Vinyl cyanide
ALDRIN	Aldrin, HHDN, Octalene, Aldrex
ALPHA-HEXACHLOROCYC	Alpha-hexachlorocyclohexane, Alpha-lindane
ANILINE	Aniline, Aminobenzene, Phenylamine
ANTHRACENE	Antjracene, Paranaphthalene
AROCLOR 1016 (PCB)	Aroclor 1016, PCB 1016
AROCLOR 1221 (PCB)	Aroclor 1221, Chlorodiphenyl (21% Cl), PCB 1021
AROCLOR 1232 (PCB)	Aroclor 1232, Chlorodiphenyl (32% Cl), PCB 1232
AROCLOR 1242 (PCB)	Aroclor 1242, PCB 1242
AROCLOR 1248 (PBC)	Aroclor 1248, Chlorodiphenyl (48% Cl), PCB 1248
AROCLOR 1254 (PCB)	Aroclor 1254, PCB 1254
AROCLOR 1260 (PCB)	Aroclor 1260, PCB 1260
BENZENE	Benzene, Penzol, Benzolene, Mineral naphtha
BENZIDINE	Benzidine, 4,4'-diaminobiphenyl
BENZO(A)ANTHRACENE	Benzo(a)anthracene, 1,2-benzanthracene
BENZO(A)PYRENE	Benzo(a)pyrene, 3,4-benzopyrene, B(a)p
BENZO(B)FLUORANTHEN	Benzo(b)fluoranthene, Benz(3)acephenanthrylene
BENZO(K)FLUORANTHEN	Benzo(k)flouranthene, 11,12-benzo(k)flouranthene
BENZYL ALCOHOL	Benzyl Alcohol
BETA – HCCH	Beta-hexachlorocyclohezane, Beta-HCH, Beta-BHC, Beta-Lin
BIS(2-CHLOROETHYL)	Bis(2-chloroethyl ether), Chloroethyl ether, BCEE
BIS(2-CHLOROISOPROP	Bis(2-chloroisopropyl)ether, 2,2'-dichloroisopropyl ether
BIS(2RY-HEXYL)PHTHL	Bis(2-ethylhexyl phthalate), DEPHP, DOP
BROMODICHLOROMETHAN	Bromodichloromethane, Dichlorobromomethane
BROMOMETHANE	Bromomethane, Methyl bromide, MB, MBX, MEBR
CARBON TETRACHLORID	Carbon tetrachloride, Freon 10, Tetrachloromethane
CHLORDANE	Chlordane, BELT, Ortho-klor, Velsicol 1968
CHLOROBENZENE	Chlorobenzene, Phenyl chloride
CHLOROBENZILATE	Chlorobenzilate, 4,4'-dichlorobenzilic acid ethyl ester
CHLORODIBROMOMETHAN	Chlorodibromomethane, Dibromochloromethane
CHLOROETHANE	Chloroethane, Ethyl chloride
CHLOROFORM	Chloroform, Trichloromethane, Freon 20
CHLOROMETHANE(METHY)	Chloromethane, Methyl chloride
CHRYSENE	Chrysene, Benz(a)phenanthrene
CYCLOHEXANE	Cyclohexane, Hexahydrobenzene
DDD	DDD, Rhothane
DDE	DDE, Dichloroethylene
	(Sheet 2 of 5)

Table B1 (Continued)

Compound	Common Name
DDT	DDT, Kopsol, Dicophane
DELTA-HCCH	Delta-hexachlorocyclohexane, Delta-HCH, Delta-BHC, Delta
DI-N-BUTYL-PHTHALAT	Di-n-butyl Phthalate, Elaol, DBP
DI-N-OCTYLPHTHALATE	Di-n-octylphalate
DIAZINON	Diazinon
DIBENZO(A,H)ANTRAC	Dibenzo(a,h)anthracene, 1,2,5,6-DBA
DIBROMOMETHANE	Dibromomethane, Methylene bromide
DICHLORODIFLUOROMET	Dichlorodifluoromethane, Halon
DIELDRIN	Dieldrin, Octalox, Heod, Quintox
DIETHYL PHTHALATE	Diethyl phthalate, Neantine, Solvanol
DIMETHYL ETHER	Dimethyl ether, methyl ether, wood ether
DIMETHYLAMINE (DMA)	Dimethylamine, DMA
DIMETHYLPHTHALATE	Dimethyl phthalate, Solvarone
DIESEL FUEL	Diesel fuel, Fuel Oil, Diesel Oil
DIURON	Diuron, Dichlorfenidim, Vonduron
ENDOSULFAN I (ALPHA)	Endosulfan, Thiomul, Malix
ENDOSULFAN II (BETA)	Endosulfan, Thiomul, Malix
ENDRIN	Endrin, Hezadrin
ETHYL METHACRYLATE	Ethyl methacrylate, Ethyl ester
ETHYLBENZENE	Ethyl benzene, Phenylethane
FLUORANTHENE	Flouranthene, IDRYL
FLUORENE	Fluorene
FORMALDEHYDE	Formaldehyde, Methanal, Formic aldehyde, Formalin
FUEL OIL #2	Fuel oil
FURAN	Furan, furfuran, oxacyclopentadiene
GAMMA-HCCH (LINDANE)	Famma-hexachlorocyclohexane, Lindane, Gamma-BHC, Gamma-H
GLYPHOSATE	Glyphosate, N-(Phosphonomethyl) Glycine, MON0573
HEPTACHLOR	Heptachlor, Rhodiachlor, Drinox
HEPTACHLOR EPOXIDE	Heptachlor epoxide
HEXACHLOROBENZENE	Hexachlorobenzene
HEXACHLOROBUTADIENE	Hexachlorobutadiene, HCBD, Dolen-pur
HEXACHLOROCYCLOPENT	Hexachlorocyclopentadiene, C-56
HEXACHLORODIBENZO-P	Hexachlorodibenzo-p-dioxin
HEXACHLORODIBENZOFU	Hexachlorodibenzofurans
HEXACHLOROETHANE	Hexachloroethane, Phenohep
HEXACHLOROPHENE	Hexachlorophene
HMX (H-NO2 TETZOCIN	1,3,5,7-Tetrazocine, Octahydro-1,3,5,7-tetranitro, Octag
INDENO(1,2,3-CD)PYR	Indeno(1,2,3-CD)pryene, IP
JP4	JP-4 Jet Fuel, Aviation Fuel
KEPONE	Kepone, Merex, CIBA 8514
M-DINITROBENZENE	m-Dinitrobenzene, Dinitrobenzene
m-XYLENE	m-Xylene, 1,3-Dimethylbenzene

(Sheet 3 of 5)

Table B1 (Continued)	
Compound	**Common Name**
METHAPYRILENE	Methapyrilene, Tenalin, Restryl
METHOXYCHLOR	Methoxychlor, Metox, DMDT
METHYLCYCLOHEXANE	Methylcyclohexane, Hexahydrotoluene, UN2296
METHYLCYCLOPENTANE	Methylcyclopentane, UN2298
METHYLENE CHLORIDE	Methylene chloride, Dichloromethane, DCM, Freon 30
N-NITROSODI-N-BUTYL	N-Nitro-di-n-butylamine, DBN
N-NITROSODIETHYLAMI	N-Nitrosodiethylamine, DANA
N-NITROSODIMETHYLAM	N-Nitrosodimethylamine, DMNA
N-NITROSODIPHNYLAMN	N-Nitrodosiphenylamine, REDAX
N-NITROSODIPROPYLAM	N-Nitrosodipropylamine, N-nitroso-1-propyl-1-propanamine
N-NITROSOMORPHOLINE	N-Nitrosomorpholine, 4-Nitrosomorpholine, NMOR
N-NITROSOPIPERIDINE	N-Nitrosopoperidine, NPIP
N-NITROSOPYRROLIDIN	N-Nitrosopyrrolidine, NPYR
N-PHENYL BENZENAMIN	N-phenyl benzenamine, Diphenylamine, N,N'-diphenylamine
NAPHTHALENE	Naphthalene, Naphthalin
NITROBENZENE	Nitrobenzene, Nitrobenzol (liquid)
O-NITROANILINE	O-Nitroaniline, Devol orange B
o-XYLENE	o-Xylene, 1,2-Dimethylbenzene
P-BENZOQUINONE	P-benzoquinone, 2,5-cyclohexadiene-1,4-diene
P-CHLORO-M-CRESOL	P-chloro-m-cresol, 4-chlor-m-creosol
P-CHLOROANILINE	P-chloroaniline, 1-amino-4-chlorobenzene
P-DIMETHLAMINOAZOBE	P-Dimethlaminoazobenzene, Dimethyl yellow
P-NITROANILINE	P-nitroaniline, Paranitroaniline (solid)
P-XYLENE	P-Xylene, 1,4-Dimethylbenzene
PARATHION	Parathion, Pethion, Alleron
PCBs (GENERAL)	Arocior, PCB (General Classification), Therminal, Poylch
PENTACHLOROBENZENE	Pentachlorobenzene, PCB
PENTACHLOROETHANE	Pentachloroethane, Pentalin
PENTACHLORONITROBEN	Pentachloronitrobenzene, Tritisan
PENTACHLOROPHENOL	Pentachlorophenol, Permite, EP 30
PENTAERYTHRITOL-4N	Initiating explosive pentaerythrite tetranitrate, PETN
PHENACETIN	Phenacetin, Fenia, Kalmin
PHENANTHRENE	Phenanthrene
PHENOL	Phenol, Carbolic acid, Ocybenzene
PICLORAM	Tordon 22K, 4-amino-3,5,6-trichloro-Piccolinic acid K-sal
PICOLINE	Picoline, 2-Picoline, alpha-Picoline, 2-Methylpyridine
POLYACRYLAMIDE	Polyacrylamide
POLYCHLORNTED FURAN	Polychlorinated furans
PRINCEP 80W	Princep 80W, 2-chloro-4,6-bix(ethylamino)-s-triazine, Si
PYRENE	Pyrene, Benzo(def)phenanthrene
PYRIDINE	Pyridine, Azine, Azabenzene
RDX 6H-3NO2-TRIAZIN	RDX, Hexahydro-1,3,4-Trinito-1,3,5-Triazine
	(Sheet 4 of 5)

Table B1 (Concluded)

Compound	Common Name
SILVEX	Silvex, Propon, Aqua-vex
STRYENE-BUTADIENE	Styrene-butadiene co-polymer
STYRENE	Styrene, Cinnamene, Styron
TETRACHLOROETHYLENE	Tetrachloroethylene, Ankilostin, PCE
TETRAETHYLDITHIOPYR	Tetraetyl dithio pyrophosphate, Pirofos
TNT 3NO2-TOLUENE	TNT, Trinitrotoluene (dry)
TOLUENE	Toluene, Toluol
TOLUENE DIISOCYUANAT	Toluene diisocyanate, Hylenet
TOXAPHENE	Toxaphene, Phenacide, Motox
TRANS-1,3-DICHLOROP	Trans-1,3-Dichloropropene, (E)-1,3-dichloropropene
TRANS-1,4-DICHLORO-	Trans-1,4-dichlorobutene-2, 2-Butylene dichloride
TREFLAN	Treflan a,a,a-trifluoro-2,6-dinitro-N-N'-dipropyl-p-tolu
TRIBROMOMETHANE	Tribromomethane, Bromoform
TRICHLOROETHYLENE	Trichloroethylene, Vitran, TCE
TRICHLOROMETHANETHI	Trichloromethanethiol, Perchloro-methyl mercaptan, Clair
TRICHLOROMONOFLUORO	Trichloromonofluoromethane, Arcton 9, Freon 11
TRICL-HEPTAF-BUTANE	Trichloroheptafluorobutane
TRIETHANOLAMINE	Triethanolamine, 2,2',2"-Nitrilotriethanol
TRIETHYLENE GLYCOL	Triethylene Glycol, 2,2'-Ethylenedioxy)diethanol
TRIMETHYLBENZENE	Trimethylbenzene (mixed isomers)
TRIS(2,3-DIBROMOPRO)	Tris(2,3-Dibromopropyl)phosphate, Flacavon R
VINYL ACETATE	Vinyl acetate, 1-Acetoxyethylene
VINYL CHLORIDE	Vinyl chloride, Monochloroethylene
XYLENE (MIXED)	Xylene, Benzene (dimethyl)

(Sheet 5 of 5)

Appendix C
Screens

```
                              »» RECOVERY 2.0 ««

          A Decision Support Model for Screening the Fate of In-Place
               Contaminated Sediments in Aquatic Environments
                                October, 1995

          Model Written By:    Jean M. Boyer and Steven C. Chapra
                               Center for Advanced Decision Support
                               in Water and Environmental Systems
                               University of Colorado
                               Boulder, CO  80309-0428

                               Carlos E. Ruiz
                               USAE Waterways Experiment Station
                               Water Quality and Contaminant Modeling Branch
                               Vicksburg, MS  39180-6199

          Interface By:        Benjamin J. Riley and Terry Gerald
                               USAE Waterways Experiment Station
                               Vicksburg, MS  39180-6199

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                                press any key...
```
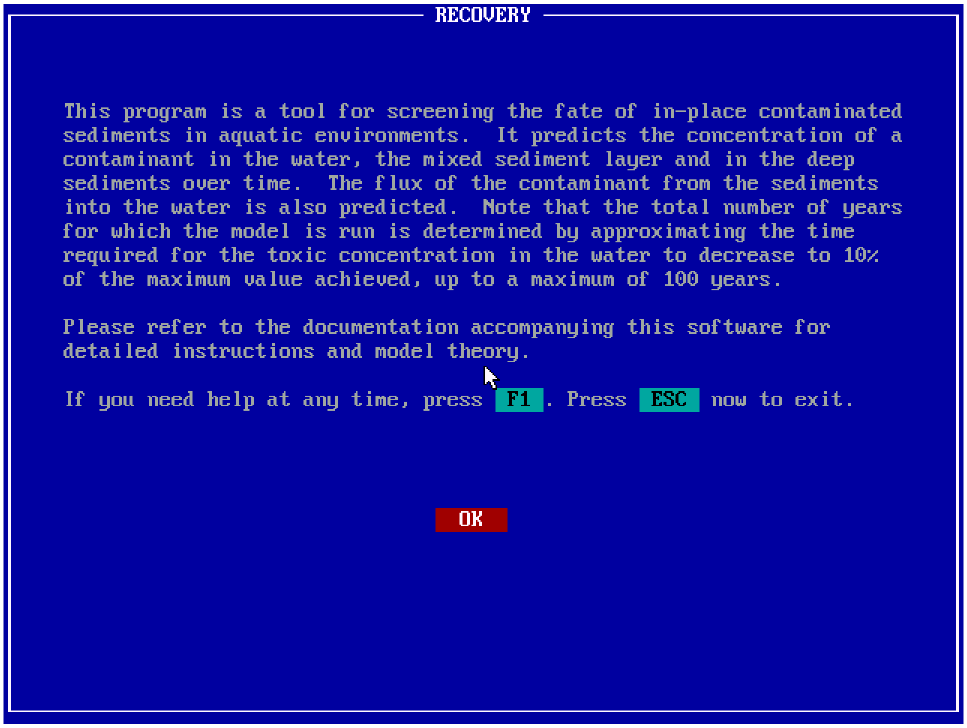

Screen 1

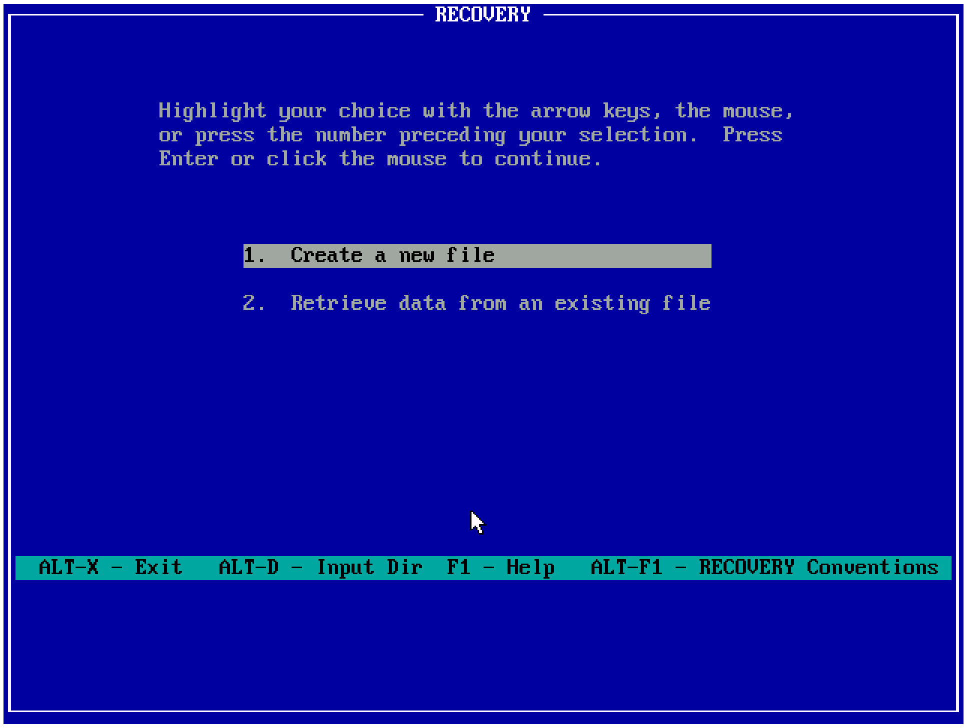


This program is a tool for screening the fate of in-place contaminated sediments in aquatic environments. It predicts the concentration of a contaminant in the water, the mixed sediment layer and in the deep sediments over time. The flux of the contaminant from the sediments into the water is also predicted. Note that the total number of years for which the model is run is determined by approximating the time required for the toxic concentration in the water to decrease to 10% of the maximum value achieved, up to a maximum of 100 years.

Please refer to the documentation accompanying this software for detailed instructions and model theory.

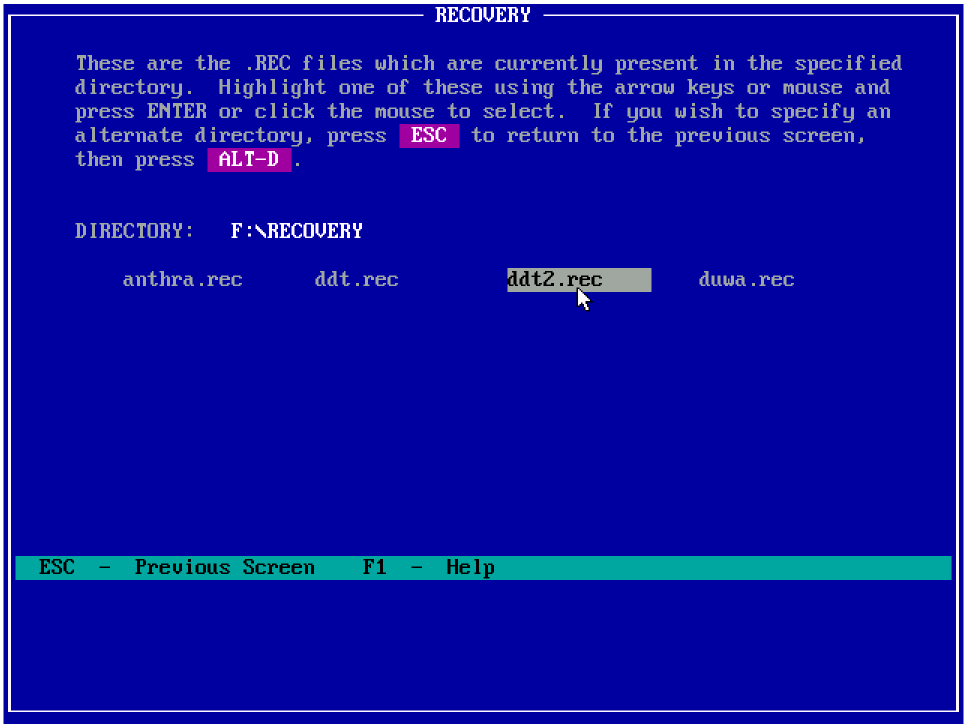
If you need help at any time, press F1. Press ESC now to exit.

Screen 2



Highlight your choice with the arrow keys, the mouse, or press the number preceding your selection. Press Enter or click the mouse to continue.

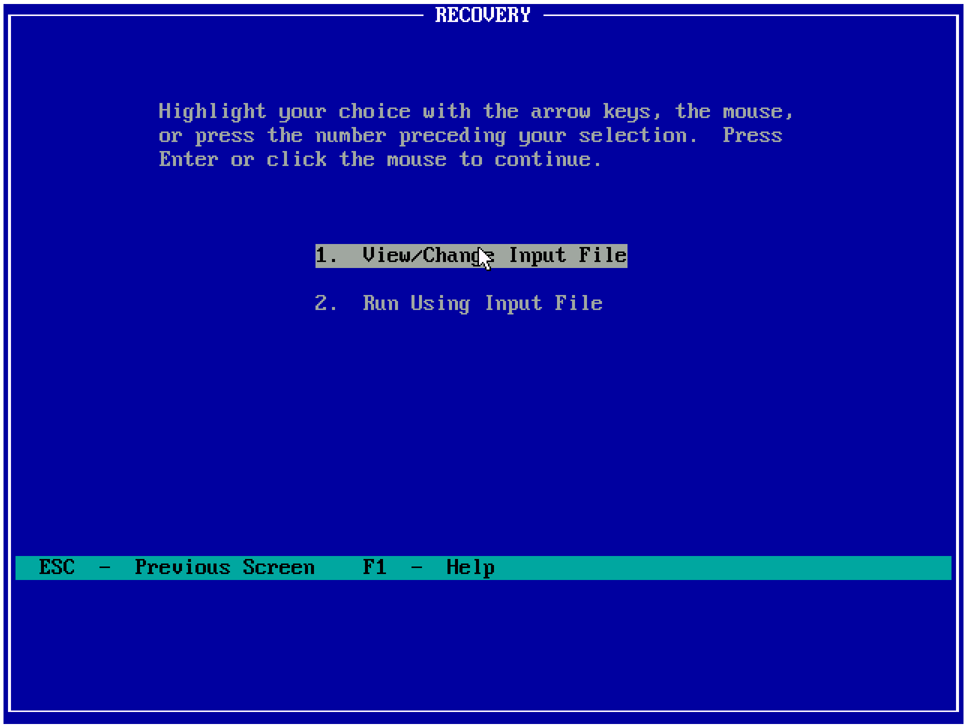
Screen 3



These are the .REC files which are currently present in the specified directory. Highlight one of these using the arrow keys or mouse and press ENTER or click the mouse to select. If you wish to specify an alternate directory, press ESC to return to the previous screen, then press ALT-D.

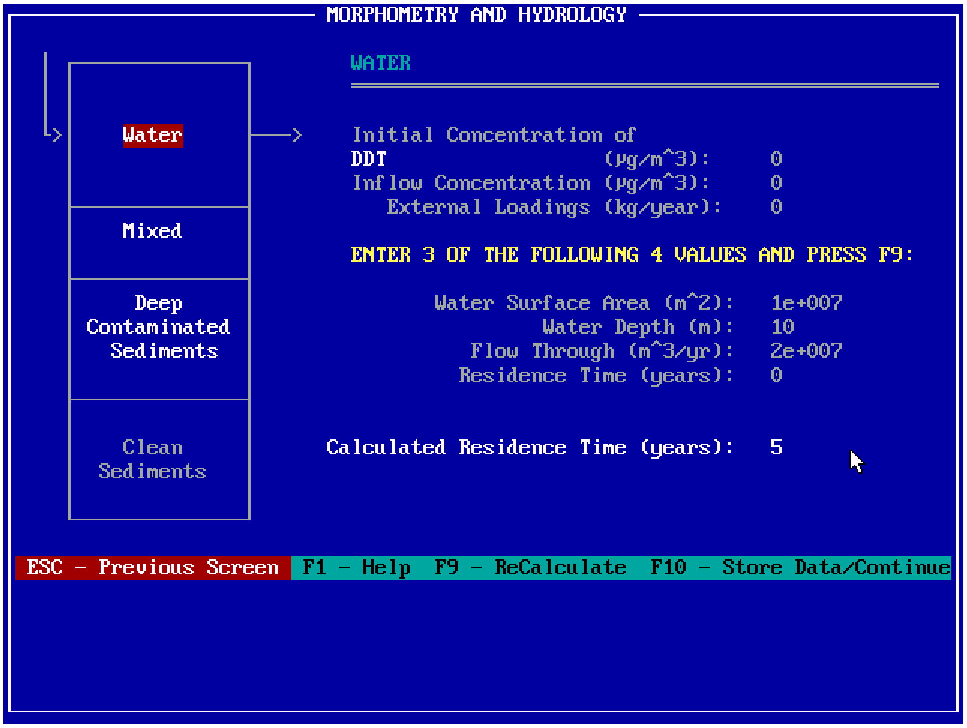
DIRECTORY: F:\RECOVERY

Screen 4



Highlight your choice with the arrow keys, the mouse, or press the number preceding your selection. Press Enter or click the mouse to continue.

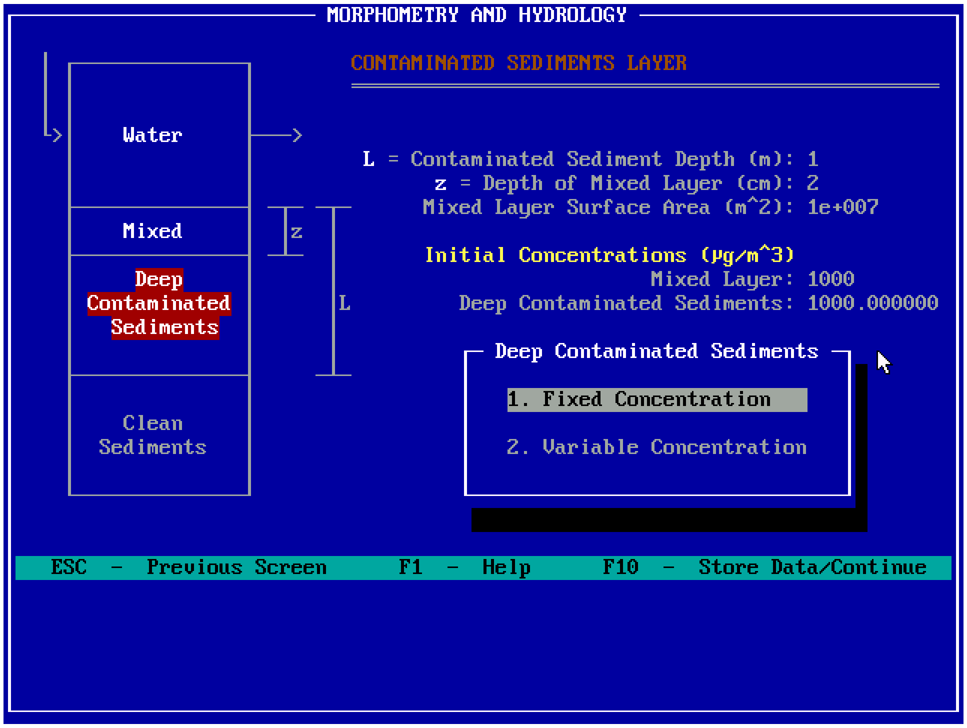
Screen 5



WATER

```
Initial Concentration of
DDT                  (µg/m^3):     0
Inflow Concentration (µg/m^3):     0
   External Loadings (kg/year):    0

ENTER 3 OF THE FOLLOWING 4 VALUES AND PRESS F9:

       Water Surface Area (m^2):   1e+007
              Water Depth (m):     10
          Flow Through (m^3/yr):   2e+007
         Residence Time (years):   0

Calculated Residence Time (years):  5
```

Screen 6



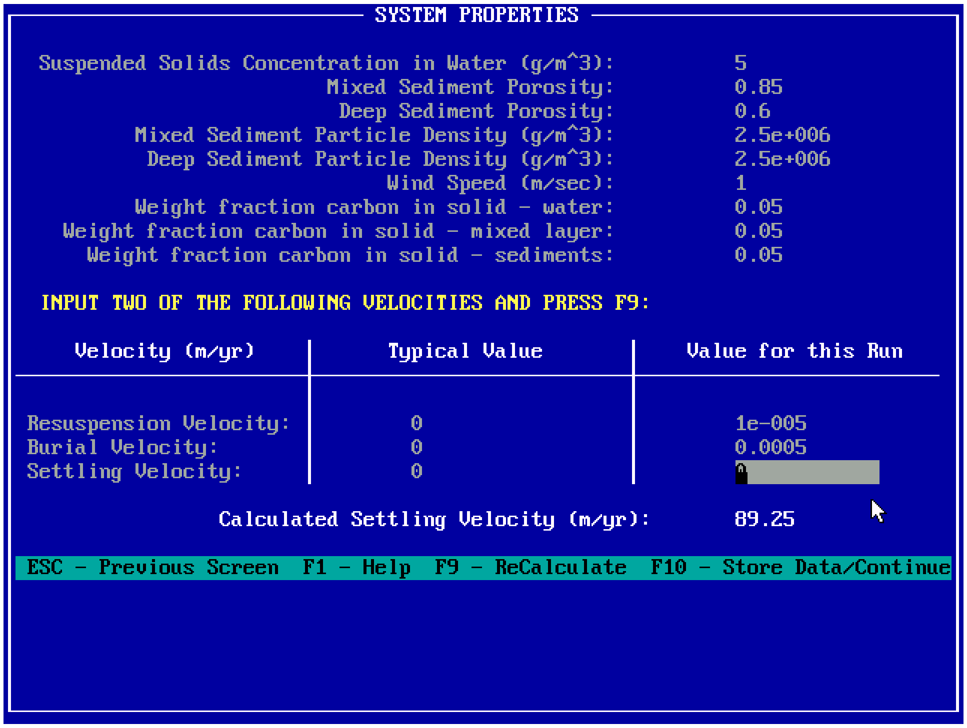
MORPHOMETRY AND HYDROLOGY

CONTAMINATED SEDIMENTS LAYER

L = Contaminated Sediment Depth (m): 1
z = Depth of Mixed Layer (cm): 2
Mixed Layer Surface Area (m^2): 1e+007

Initial Concentrations (µg/m^3)
Mixed Layer: 1000
Deep Contaminated Sediments: 1000.000000

Screen 7



SYSTEM PROPERTIES

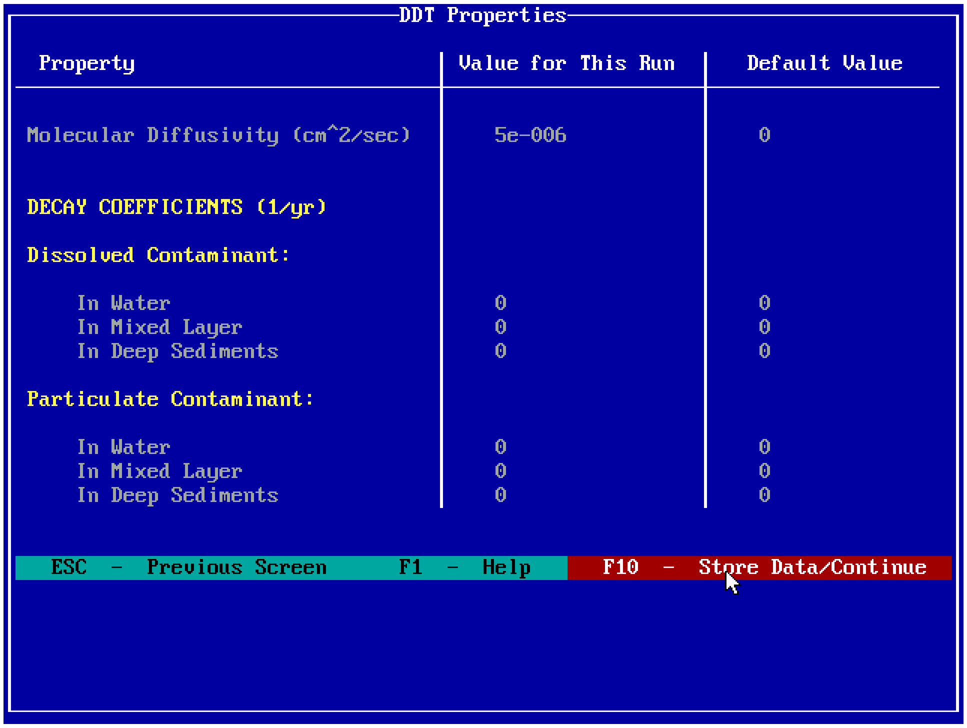
Suspended Solids Concentration in Water (g/m^3): 5
Mixed Sediment Porosity: 0.85
Deep Sediment Porosity: 0.6
Mixed Sediment Particle Density (g/m^3): 2.5e+006
Deep Sediment Particle Density (g/m^3): 2.5e+006
Wind Speed (m/sec): 1
Weight fraction carbon in solid - water: 0.05
Weight fraction carbon in solid - mixed layer: 0.05
Weight fraction carbon in solid - sediments: 0.05

INPUT TWO OF THE FOLLOWING VELOCITIES AND PRESS F9:

Velocity (m/yr)	Typical Value	Value for this Run
Resuspension Velocity:	0	1e-005
Burial Velocity:	0	0.0005
Settling Velocity:	0	0

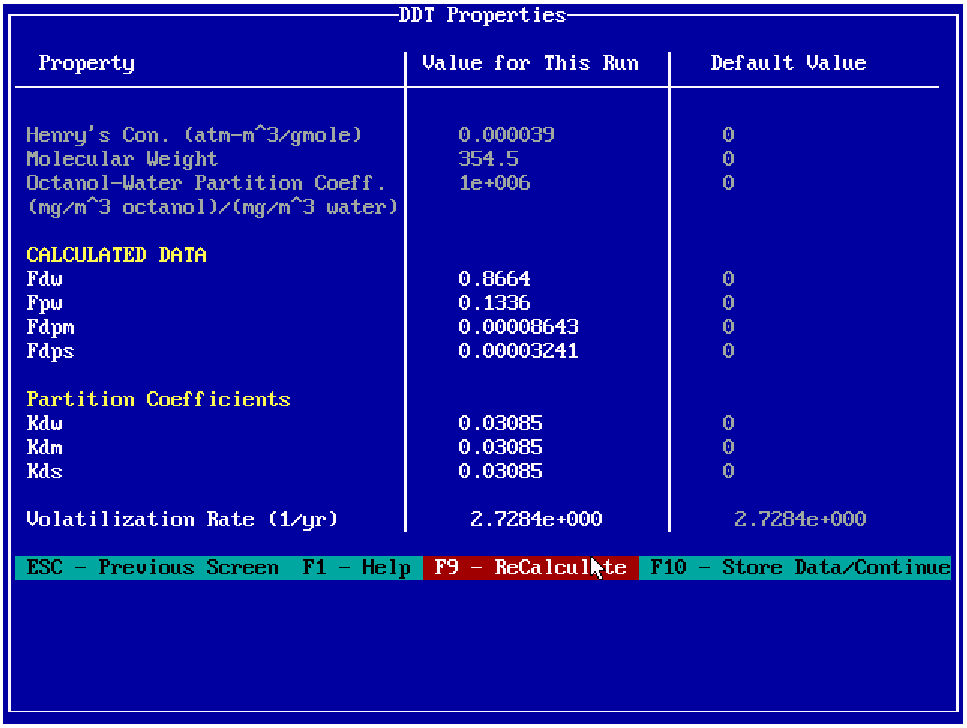
Calculated Settling Velocity (m/yr): 89.25

Screen 8



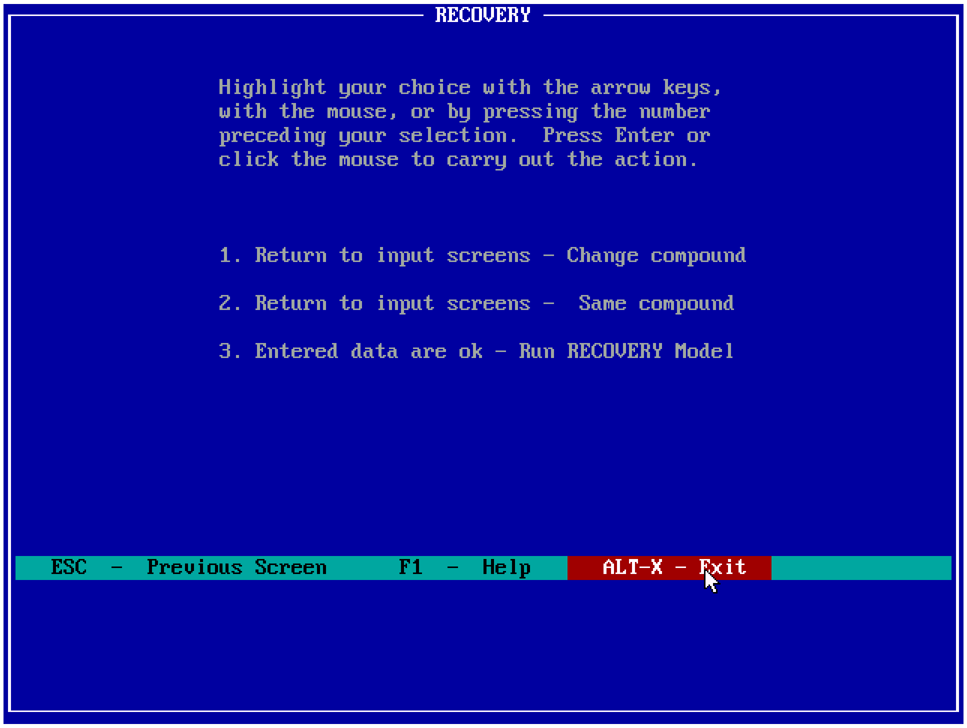
```
Property                              | Value for This Run | Default Value
---------------------------------------------------------------------------
Molecular Diffusivity (cm^2/sec)      |    5e-006          |   0
                                      |                    |
DECAY COEFFICIENTS (1/yr)             |                    |
                                      |                    |
Dissolved Contaminant:                |                    |
                                      |                    |
    In Water                          |    0               |   0
    In Mixed Layer                    |    0               |   0
    In Deep Sediments                 |    0               |   0
                                      |                    |
Particulate Contaminant:              |                    |
                                      |                    |
    In Water                          |    0               |   0
    In Mixed Layer                    |    0               |   0
    In Deep Sediments                 |    0               |   0
```

Screen 9



```
Property                              | Value for This Run | Default Value
---------------------------------------------------------------------------
Henry's Con. (atm-m^3/gmole)          |  0.000039          |  0
Molecular Weight                      |  354.5             |  0
Octanol-Water Partition Coeff.        |  1e+006            |  0
(mg/m^3 octanol)/(mg/m^3 water)       |                    |
                                      |                    |
CALCULATED DATA                       |                    |
Fdw                                   |  0.8664            |  0
Fpw                                   |  0.1336            |  0
Fdpm                                  |  0.00008643        |  0
Fdps                                  |  0.00003241        |  0
                                      |                    |
Partition Coefficients                |                    |
Kdw                                   |  0.03085           |  0
Kdm                                   |  0.03085           |  0
Kds                                   |  0.03085           |  0
                                      |                    |
Volatilization Rate (1/yr)            |   2.7284e+000      |   2.7284e+000
```

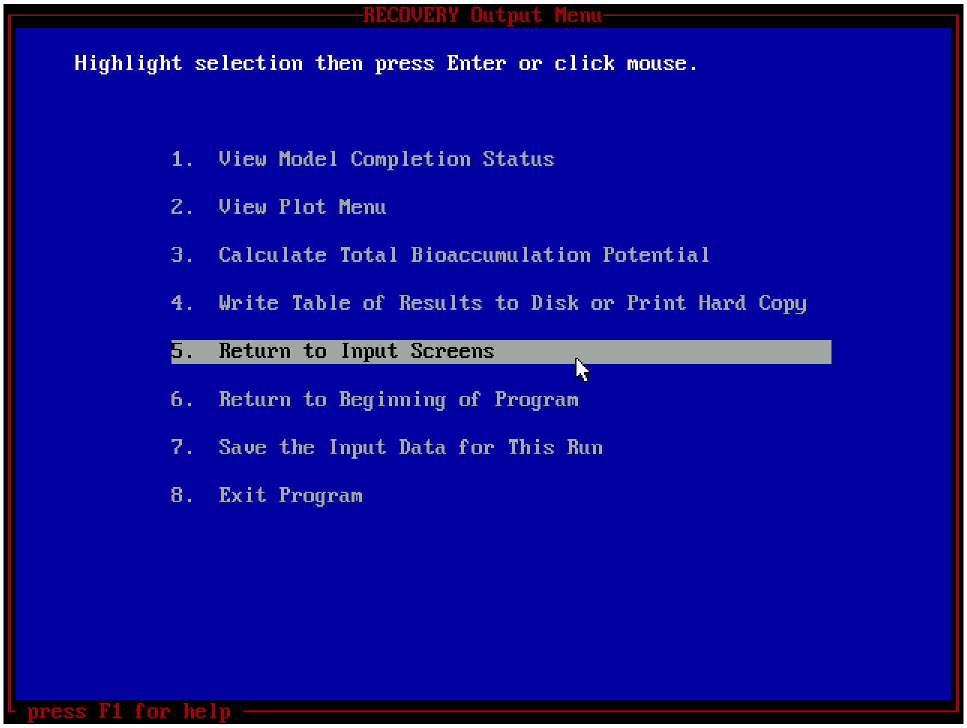
Screen 10



Highlight your choice with the arrow keys, with the mouse, or by pressing the number preceding your selection. Press Enter or click the mouse to carry out the action.

1. Return to input screens - Change compound
2. Return to input screens - Same compound
3. Entered data are ok - Run RECOVERY Model

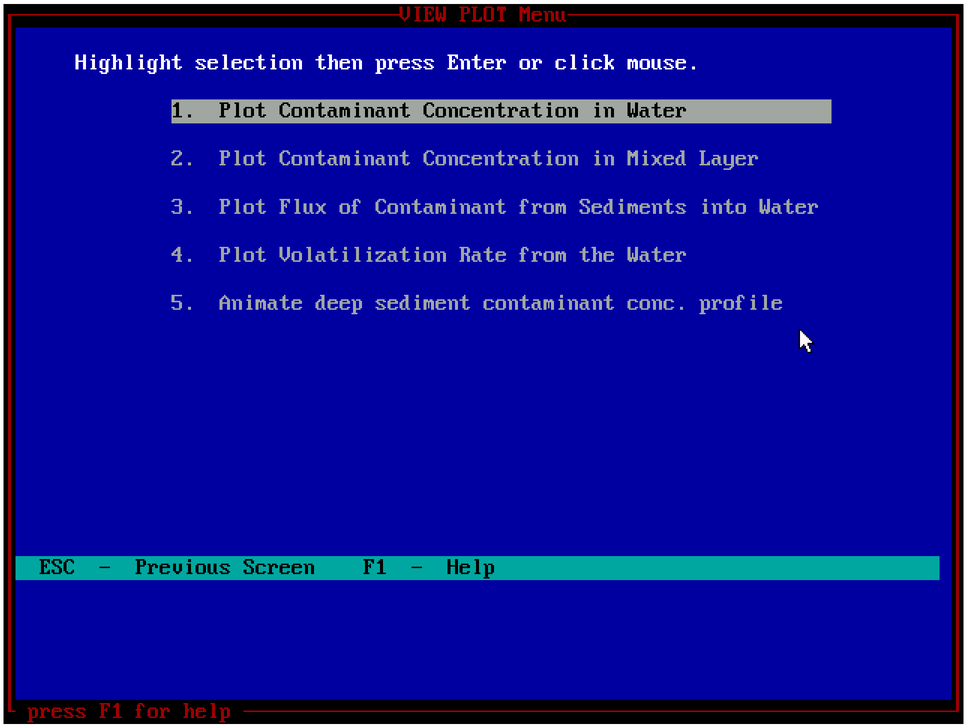
Screen 11



Highlight selection then press Enter or click mouse.

1. View Model Completion Status
2. View Plot Menu
3. Calculate Total Bioaccumulation Potential
4. Write Table of Results to Disk or Print Hard Copy
5. Return to Input Screens
6. Return to Beginning of Program
7. Save the Input Data for This Run
8. Exit Program

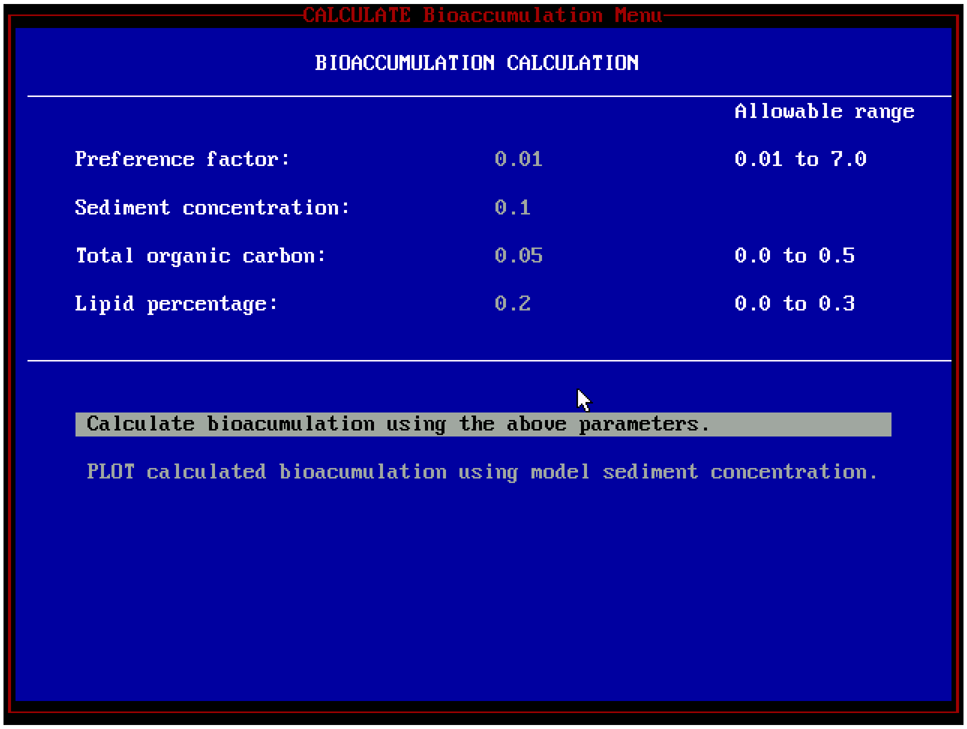
Screen 12



Highlight selection then press Enter or click mouse.

1. Plot Contaminant Concentration in Water
2. Plot Contaminant Concentration in Mixed Layer
3. Plot Flux of Contaminant from Sediments into Water
4. Plot Volatilization Rate from the Water
5. Animate deep sediment contaminant conc. profile

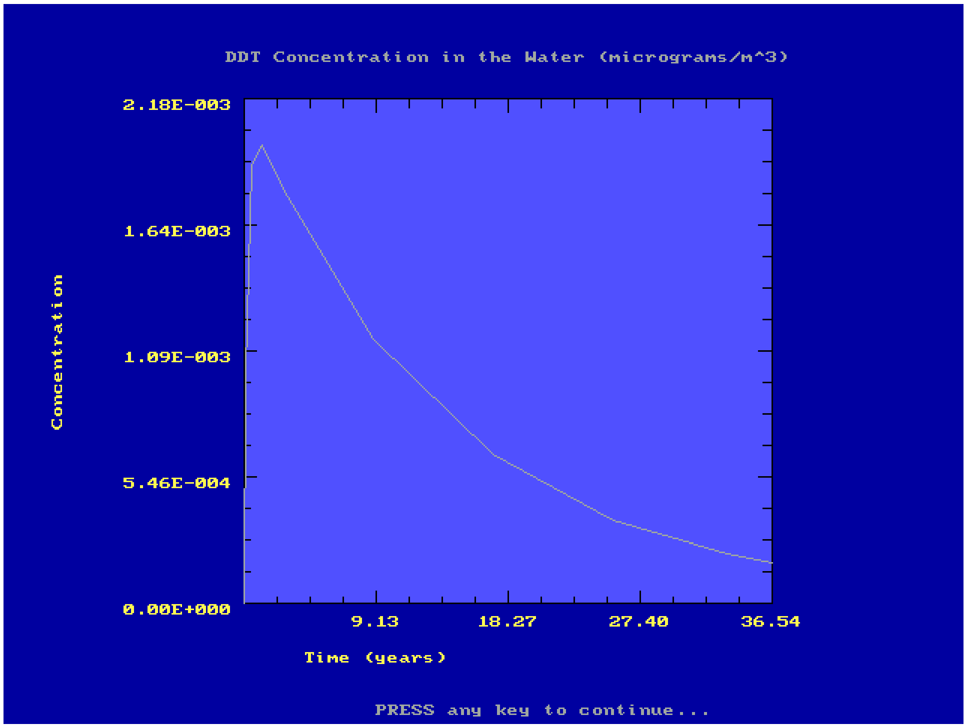
Screen 13



BIOACCUMULATION CALCULATION

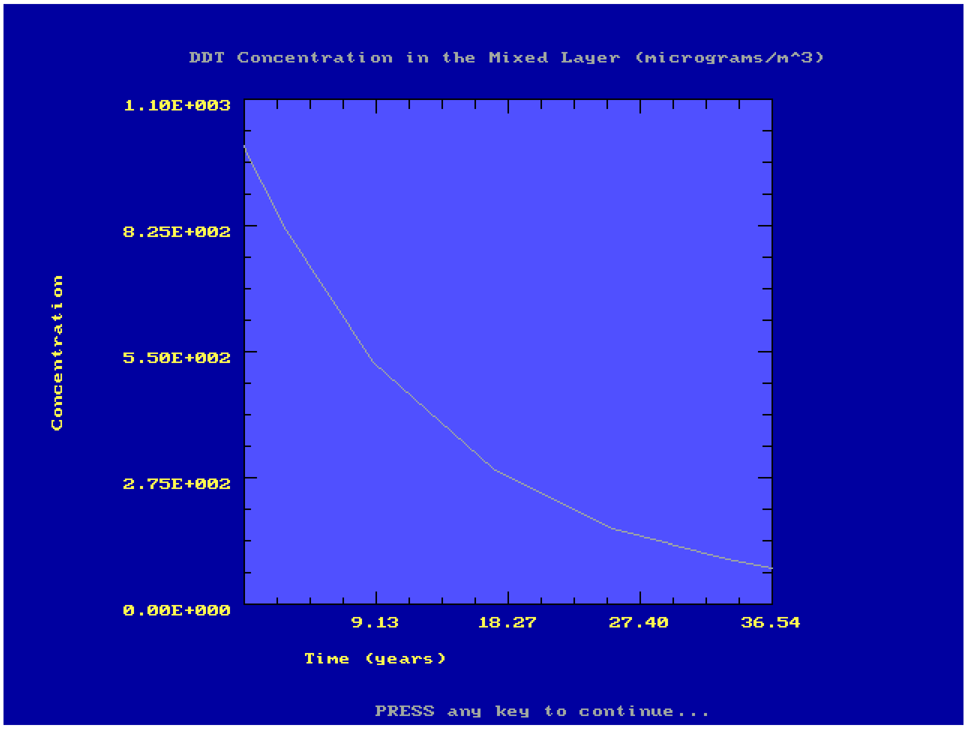
		Allowable range
Preference factor:	0.01	0.01 to 7.0
Sediment concentration:	0.1	
Total organic carbon:	0.05	0.0 to 0.5
Lipid percentage:	0.2	0.0 to 0.3

Screen 14



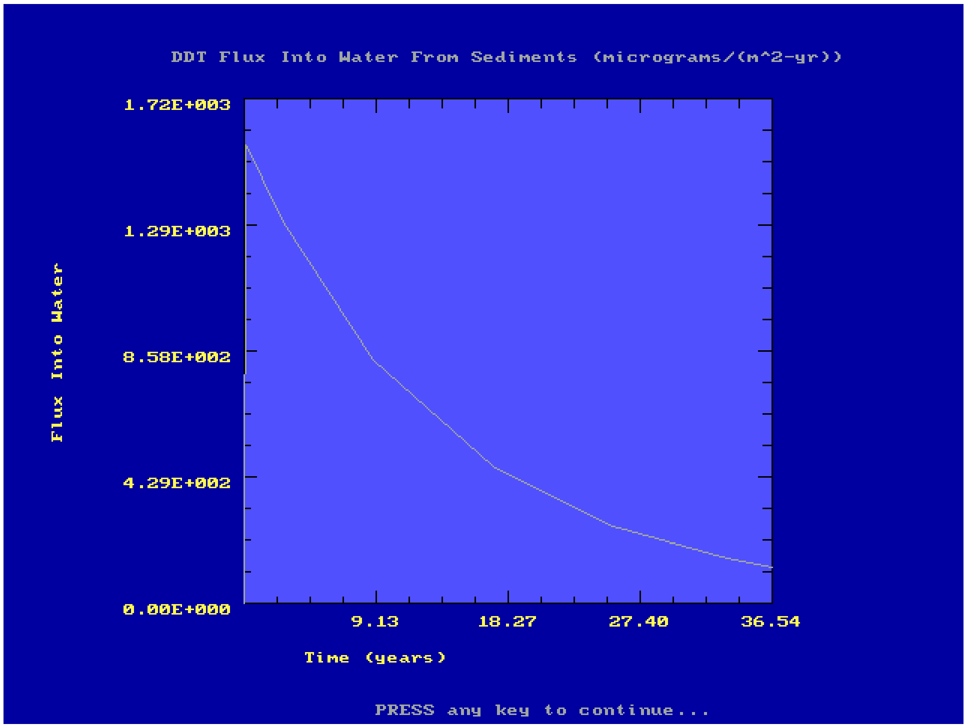
PRESS any key to continue...

Screen 15

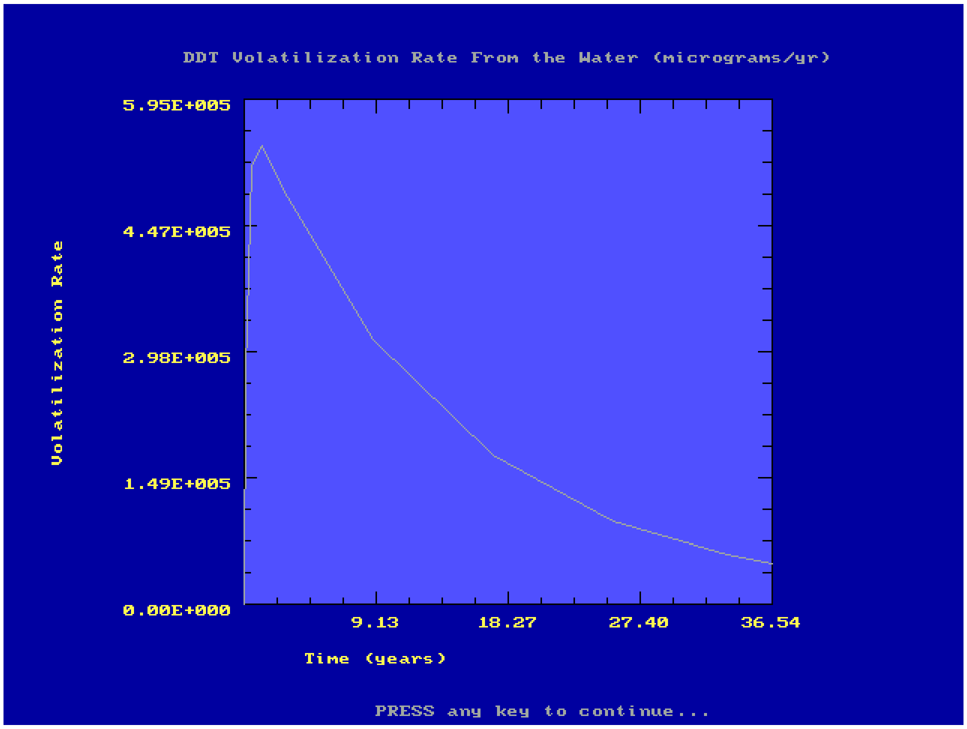


PRESS any key to continue...

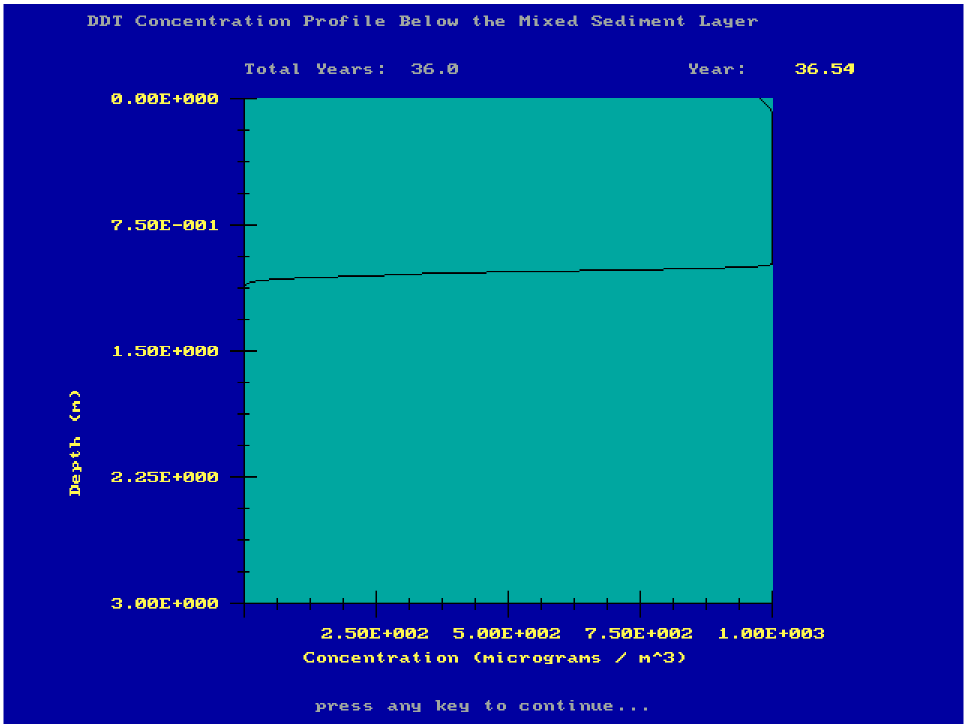
Screen 16



Screen 17



Screen 18

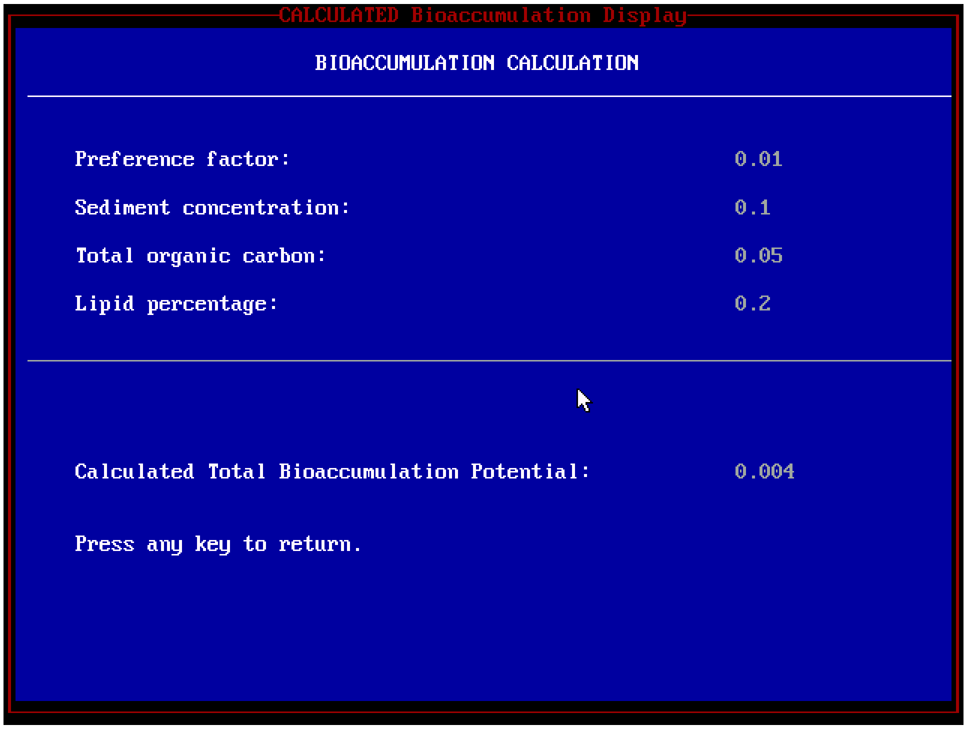


DDT Concentration Profile Below the Mixed Sediment Layer

Total Years: 36.0 Year: 36.54

press any key to continue...

Screen 19



CALCULATED Bioaccumulation Display

BIOACCUMULATION CALCULATION

Preference factor: 0.01

Sediment concentration: 0.1

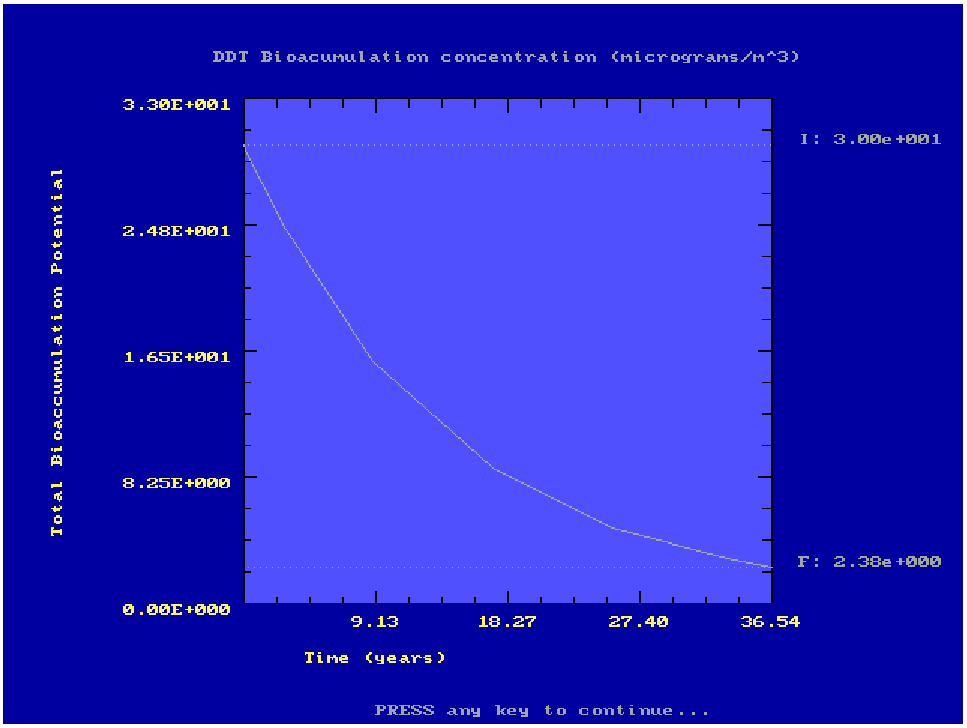
Total organic carbon: 0.05

Lipid percentage: 0.2

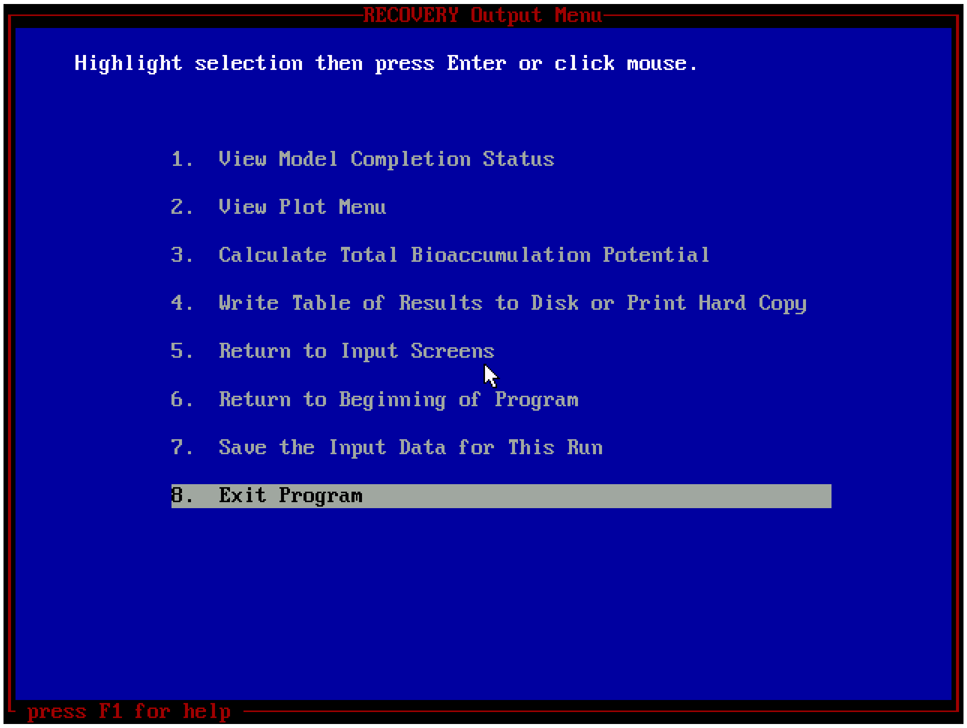
Calculated Total Bioaccumulation Potential: 0.004

Press any key to return.

Screen 20



Screen 21


RECOVERY Output Menu

Highlight selection then press Enter or click mouse.

1. View Model Completion Status
2. View Plot Menu
3. Calculate Total Bioaccumulation Potential
4. Write Table of Results to Disk or Print Hard Copy
5. Return to Input Screens
6. Return to Beginning of Program
7. Save the Input Data for This Run
8. Exit Program

press F1 for help

Screen 22

REPORT DOCUMENTATION PAGE

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12b. DISTRIBUTION CODE

13. ABSTRACT ***(Maximum 200 words)***

RECOVERY is a PC-based screening-level model to assess the impact of contaminated bottom sediments on surface waters. The analysis is limited to organic contaminants with the assumption that the water column is well-mixed. The contaminant is assumed to follow linear, reversible, equilibrium sorption, and first-order decay kinetics.

The physical representation of a system by RECOVERY consists of a well-mixed water column (i.e., zero-dimensional) underlain by a vertically stratified sediment column (i.e., one-dimensional). The sediment is well-mixed horizontally but segmented vertically into a well-mixed surface (active) layer and deep sediment. The deep sediment is segmented into contaminated and clean sediment regions.

Pathways incorporated in the RECOVERY model, in addition to sorption and decay, are volatilization, burial, resuspension, settling, advection, and pore-water diffusion.

RECOVERY is designed for interactive implementation via a personal computer. The program allows the user to rapidly generate and analyze recovery scenarios for contaminated sediments. The software includes graphical displays and is self-documented. A description of the mathematical description and computational algorithm of the model and a user's guide are included in this report.

14. SUBJECT TERMS

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Modeling	Sediment quality
Natural attenuation	Water quality

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