An Aquatic Pathways Model to Predict the Fate of Phenolic Compounds

Appendixes A Through D

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April 1983

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PREFACE

This volume contains details of a preliminary aquatic model and a brief review of other available aquatic models. The Aquatic Pathways Model (APM) developed for the synfuels program can be used to estimate the potential environmental transport, fate, and resulting coal liquid product concentrations available to man from releases to the aquatic environment. More general information is found in the main text of PNL-4202.

This effort is part of the Ecological Effects of Coal Conversion project managed by Dr. John A. Strand of Pacific Northwest Laboratory (PNL). The overall program is managed by Dr. F. J. Wobber of the Department of Energy, Office of Health and Environmental Research, Ecological Research Division.

Experimental data being developed at PNL and scientific judgments will continue to be incorporated into the model as they are obtained, and results will be compared through a sensitivity analysis. The effort will be aimed at prioritizing research needs and coordinating efforts of environmental chemistry and aquatic and terrestrial biology tasks.

ACKNOWLEDGMENTS

The principal investigator wishes to thank D. L. Strenge who reviewed other aquatic models and wrote Appendix A, and R. A. Peloquin who designed, programmed, and documented APM.

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SUMMARY

Organic materials released from energy-related activities could affect human health and the environment. To better assess possible impacts, we developed a model to predict the fate of spills or discharges of pollutants into flowing or static bodies of fresh water.

A computer code, Aquatic Pathways Model (APM), was written to implement the model. The computer programs use compartmental analysis to simulate aquatic ecosystems. The APM estimates the concentrations of chemicals in fish tissue, water and sediment, and is therefore useful for assessing exposure to humans through aquatic pathways.

The APM will consider any aquatic pathway for which the user has transport data. Additionally, APM will estimate transport rates from physical and chemical properties of chemicals between several key compartments. The major pathways considered are biodegradation, fish and sediment uptake, photolysis, and evaporation. The model has been implemented with parameters for distribution of phenols, an important class of compounds found in the water-soluble fractions of coal liquids.

In areas where additional information is required for the model to more accurately predict the fate of aqueous releases of complex organic mixtures, experiments have been suggested. The model was developed to estimate the fate of liquids derived from coal, but it could be applied to other chemical contaminants as well.

The structure of the model allows a great deal of flexibility in its application. The major restriction of the current model is the use of first order rate constants, which describe the exchange of material between compartments. The material exchanged could be any material for which transfer coefficients are known. The compartments could be any set of components of an aquatic ecosystem.

Validation of APM is needed to confirm or improve its capacity as a predictive tool. In addition, the data used to derive model parameters should be revised as more information becomes available.

Current modeling efforts show that, in comparison with many pesticides and polyaromatic hydrocarbons (PAH), the lighter phenolics (the cresols) are not persistent in the environment. The properties of heavier molecular weight phenolics (indanols, naphthols) are not well enough understood at this time to make similar judgments. For the twelve phenolics studied, biodegradation appears to be the major pathway for elimination from aquatic environments. A pond system simulation (using APM) of a spill of solvent refines coal (SRC-II) materials indicates that phenol, cresols, and other single cyclid phenolics are degraded to 16 to 25 percent of their original concentrations within 30 hours. Adsorption of these compounds into sediments and accumulation by fish was minor.

Results of a simulated spill of a coal liquid (SRC-II) into a pond show that APM predicted the allocation of 12 phenolic components among six compartments at 30 hours after a small spill.

The simulation indicated that most of the introduced phenolic compounds were biodegraded. No degradation was assumed for C5 phenol and the indanols, where insufficient information was available. Photolysis was estimated to be a minor degradation pathway for all pheolic compounds except resorcinol.

The phenolics remaining in the aquatic system partitioned according to their molecular weight and structure. A substantial amount was predicted to remain in the water, with less than 0.01% distributed in sediment or fish.

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APPENDIX A

AQUATIC ECOSYSTEM TRANSPORT MODELS

APPENDIX A

AQUATIC ECOSYSTEM TRANSPORT MODELS

Several models were reviewed to determine their applicability for incorporation into the aquatic pathways model. The models described below assess the environmental concentrations of chemicals released to aquatic ecosystems.

NEELY FISH POND MODEL

The aquatic ecosystem model developed by Neely (1979) is a compartmental model designed to predict the environmental concentration of neutral organic compounds. The model describes the transient behavior of compounds as they move through a simple aquatic ecosystem. The compartments of Neely's fish pond model are water, air, fish, and soil. Models of transfer and removal mechanisms are indicated in Figure A.1. Each of these transfer modes (e.g., K_0 , K_1) will be discussed briefly with respect to extension of the model to other types of compounds.

The rate of input (K_0) can be defined as a function of time or can be held constant. It is independent of chemical properties.

FIGURE A.1. Compartments and Modes of Transfer in Neely's Fish Pond Model

Neely considers the atmosphere to be a sink with transfer from water to the air defined by the evaporation rate constant (K1). An expression is given to estimate this rate constant as a function of molecular weight, temperature, solubility of the chemical in water, and atmospheric pressure. Careful consideration should be given to ensure that the chemical under study is represented by the given expression.

Water Phase Reactivity (K2) represents a sink for removal of the chemical by chemical reaction/degradation processes and must be defined for each chemical.

The fish intake rate (K3) is defined in terms of ml of water per gram of fish per hour. When multiplied by the water concentration the rate of accumulation in fish is found (grams per gram of fish per hour). The method suggested by Neely for estimating the fish uptake rate was developed for neutral organic compounds and is probably not applicable for polar compounds, ionic compounds, relatively soluble compounds or reactive compounds. The uptake rate should be based on experimental measurements or careful modification of Neely's expression considering the properties of the compound under study. The method given also assumes the uptake to be independent of the species of fish which may not be true of all chemical compounds.

The rate of excretion from the fish (K4) can be estimated from the bioaccumulation factor if it is assumed that the uptake and excretion rates are independent of concentration. An expression is given relating the bioaccumulation factor to solubility of the compound in water (Chiou et al. 1977). This expression applies in the solubility range of 10^{-3} to 10^{-4} ppm and is based on experimental data on a wide variety of chemicals including aliphatic and aromatic hydrocarbons, aromatic acids, organochlorine and organophosphate pesticides, and polychlorinated biphenyls. Examination of data on phenols may indicate if the expression is also applicable to phenols. Hamelink and Spacie (1977) have suggested that predicting bioaccumulation factors based on partition (or solubility) alone is risky, but that satisfactory results usually can be derived for an analogue series within a family chemicals. Perhaps the phenols can be considered as such a series for which a usable relation can be experimentally determined.

Metabolic degradation of the chemical (K5) may be significant and must be evaluated for each compound.

The transfer of chemical from water to soil or sediment (K6) is dependent of the dynamics of the aquatic system in addition to chemical properties of the compound and the soil. An evaluation must be made for each compound of interest. As a first approximation Neely assumed that the rate of uptake by soil is independent of the chemical and depends directly on the character of the soil. A value of 0.68 ml per gram per hour was used based on chlorpyrifos analysis.

Neely presents a method to estimate the soil release rate (K7) based on the soil uptake rate, the partition coefficient between soil organic matter and water, solubility and the percent of organic matter in the soil. The

method uses empirical equations which may not be applicable to relatively soluble compounds. As for the fish excretion rate constant, the method for estimating the soil release rate is based on equilibrium rate assumptions.

Reaction of the chemical with soil matter is not considered to be significant removal term for neutral organic compounds but may be of concern for reactive compounds.

Neely and Blau (1977) discuss experiments that can be used to measure values of the parameters for the pond model.

HICKS MATRIX MODEL

Hicks has described a general matrix method to determine the concentration of a material in a multi-compartment system (Hicks 1981). The method can be used to describe the time dependent transfer of a contaminant in the environment. The fish pond system of Neely can be described by this modeling technique. Hicks describes two methods of solution to the matrix equation: the Euler (rectangular) method and the Runge-Kutta method. The Euler method uses a linear extrapolation over each time increment based on parameter values at the start of the increment. The initial version of our aquatic model used this method. The Runge-Kutta method makes a more sophisticated estimate of the change in parameter values over the time increment. The Runge-Kutta method should be easy to implement in our model.

The model assumes all transfer rates to be linear functions of compartment concentrations. This is a limitation that we should not impose on our model. The numerical methods that we use must be able to accomodate non-linear relationships. The Runge-Kutta method can be applied to non-linear systems if used outside of the framework that Hicks suggests.

SANDIA FOODWEB MODEL

The Sandia FOODWEB model (Niemczyk 1980) was developed to simulate radionuclide migration through surface water pathways that result in exposure of man. The compartment model was designed to be applicable to fresh water and shallow marine ecosystems. The compartments of the ecosystem considered in the model are:

- Aquatic herbivores and carnivores
- Atmosphere
- Benthos
- Detritus suspended in the water column
- Detritus in the sediments
- Man
- Non-aquatic herbivores and carnivores
- Near-shore water
- Off-shore water
- Primary products

- Kelp
- Sediments

In applying the model to a particular site, it may not be appropriate to include compartments.

The main feature of FOODWEB that may be applicable to our aquatic model is the definition of material transfer rates into compartments that represent living organisms. Some organisms have an equilibrium concentration above which accumulation of a substance is negligible. When the concentration in the organisms approaches the equilibrium concentration, intake of material is slowed. The transfer rate for this situation is defined by:

$$f(i,j) = \max \{0, [CE(j)-C(j)]*M(j)T/(j)\}$$

where

- $f(i,j)$ = the rate constant for transfer of material X from compartment i into compartment j
- $CE(j)$ = the equilibrium concentration of X in compartment i
- $C(j)$ = the current concentration of X in compartment j
- $M(j)$ = the total biomass of compartment j
- $T(j)$ = the uptake time parameter (time required for j to consume some fixed fraction of its mass from i).

This representation of the transfer rate is useful when relatively high concentrations of a compound are expected for an organism. The compounds of interest for our work may not be in high enough concentrations for the equilibrium effect to be of concern.

The report of the FOODWEB model contains discussions on estimation of various parameters for the compartment model as applied to a freshwater lake, an estuary, and a coastal site. The discussion contains reference information that may be of use to us later for specific applications of our model.

EPA MODEL -- EXAMS

The EPA Exposure Analysis Modeling System (EXAMS) (Burns, Cline and Lassiter, 1982) is a multi-compartment model to describe the behavior of chemical pollutants in natural aquatic systems. The model has user-defined parameters to describe components of the system, reaction rates, and transfer rates.

The purpose of EXAMS is to generate information on three areas of interest:

1. Exposure -- the steady-state chemical concentration in each compartment of the aquatic system

2. Fate -- the ultimate distribution of the chemical in the system and fraction of the loadings that are consumed by each transport process
3. Persistence--the time required for effective purification of the system once the chemical loadings terminate.

The EXAMS computer program is essentially a large, general numerical processor that will accept user input in definition an aquatic environment and parameters related to behavior of a specific chemical pollutant. Our aquatic model can probably be described mathematically using the EXAMS program. There is little actual data associated with the EXAMS program, except for a few compounds used as a sample problem.

EXAMS couples the important characteristics of the environment with the properties of a given organic chemical through the use of process models appropriate to each aspect of chemical behavior. Processes may include the kinetics of volatilization, transport, direct photolysis, hydrolysis (specific-acid/base ad neutral), oxidation, and bacterial transformations in the water column and bottom sediments of the ecosystem, as well as equilibrium partitioning of the chemical into ionic species, each of which may occur as a dissolved, sediment-sorbed, or biosorbed molecule.

The transport aspects of the program are limited in that a compartment model may be a poor means of describing transport in a given system. The size of the compartments is critical in determining the adequacy of the system representation.

NRC PATH1 MODEL

The US Nuclear Regulatory commission (USNRC) PATH1 model (Helton and Kaestner 1981) was developed by Sandia National Laboratory for the NRC to be used in estimating environmental consequences of geologic disposal of radioactive wastes. There are two submodels in the program: an environmental transport model and a pathways-to-man model. The pathways-to-man model uses concentration ratios to estimate uptake through food chains. This is similar to several other models available (Napier et al., 1981; USNRC 1977) and will not be discussed further. The environmental transport model is of interest.

The system to be studied is assumed to receive contamination from groundwater from an underground repository. The system is defined as a series of zones or compartments with surface water connections. Each zone is composed of four subcompartments: surface water, sediment, groundwater and soil. Input to the system can be to any subcompartment. Flow between zones is assumed to occur only between surface water subcompartments. Each of the four subcompartments is assumed to be composed of a water component and a solids component. Distribution of contaminant between the water and solids components is determined by distribution coefficients defined for each subcompartment. Additional information required includes volume or mass of each subcompartment and flow rates between compartments.

Based on input defined by the user, the program establishes a set of linear differential equations describing the system. The current version of the code includes a subroutine GEARB (Hindmarsh 1977) to solve the equations. The subroutine is designed to solve (numerically) systems of stiff banded differential equations. Other subroutines could be substituted to perform the solution.

SIMPLIFIED LAKE OR STREAM MODEL (SLSA)

The SLSA is a compartment model (Di Toro et al 1981) composed of suspended solids, sediment solids, and a water column with inflow and outflow. When a stream is being modeled, a series of water compartments is defined to represent downstream flow. The relevant reactions considered are hydrolysis, oxidation, biodegradation, photolysis, and volatilization. The adsorption-desorption transport process between water and solids is assumed to be at equilibrium. The pollutant distribution between water and solids is determined from the mass of the adsorbing solids and the partition coefficients in the water column and the sediments.

Transport from the water column to the sediment layer is determined by the settling velocity of adsorbing particles and their resuspension rate. Aqueous transport is determined by the flow rate of the water column and the velocity (for streams) or the hydraulic detention time (for lakes). This model is similar to the aquatic pathways model under development in the Environmental Analysis Section at Pacific Northwest Laboratory. Some submodels of SLSA may be worth considering for inclusion into the Aquatic Pathways Model.

FATE OF AROMATICS MODEL (FOAM)

The Fate of Aromatics Model (FOAM) (Bartell et al. 1981) was constructed to predict transport and fate of polycyclic aromatic hydrocarbons (PAH). Parameters describing transport, degradation, and accumulation are estimated from regression equations using molecular weight, melting point, octanol-water partition coefficient, and light absorbance spectrum. Model processes include dissolution, photolysis volatilization, sorption onto suspended particulate matter and sediments, and accumulation by rooted aquatic vegetation, zooplankton, and benthic invertebrates. FOAM predicts time-varying concentration in these system components and simulates seasonal changes in biomass of all food web components. The model has been used in conjunction with an effects model to extrapolate to risks of indirect effects on higher trophic levels (Bartell, O'Neill and Gardner 1982).

FOAM uses quantitative structure-activity relationships (QSARS) for PAHs to predict fate of these compounds. The methods may be extended to other organics if appropriate structure-activity relationships can be determined. The biological production submodel includes producer and consumer biomass, photosynthesis, respiration, consumption, excretion, mortality, sinking losses, egestion losses, direct uptake, and metabolic degradation of PAH. Compartments such as these may be useful additions to the fate modeling effort.

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APPENDIX B

AQUATIC PATHWAYS MODEL SYSTEM AND MODEL DESCRIPTION

APPENDIX B

AQUATIC PATHWAYS MODEL SYSTEM AND MODEL DESCRIPTION

The Aquatic Pathways Model and APM code are described in detail in this Appendix. The information will be most useful to a programmer who may need to install or modify the code. Although knowledge of this information is not necessary to adequately execute APM, it will assist the user in understanding the code.

This Appendix is divided into 5 main sections. Section 1, "Computer Code Structure," describes the relationships and hierarchy between the various codes and data bases. The user's interaction with the codes is also outlined. Section 2, "File Descriptions" details the function and organization of the data bases and information files used by APM. Section 3, "Code Descriptions," outlines the functions of each the codes in the APM package. Section 4, "Code Logic," contains charts of the logic structures that comprise each of the codes. Section 5 "Variable descriptions" will be an aid to the user modifying the code. It contains the definition of all variables used in the APM package.

INTRODUCTION

The computer codes presented here were developed to implement models of the spill of coal-liquids into either a static or flowing body of water. The simulation is divided into two phases. The first phase will calculate the amount of each of the chemicals under consideration in a spill of a given size. This part generates input files for each of the chemicals which are used in the second phase to simulate the behavior of each chemical selected aquatic environment.

The first phase of the computer code is named Aquatic Pathways Model of a Coal-Liquid Spill (APMSPILL). It is a separate program which functions as a superstructure to the second phase, known as the Aquatic Pathways Model of toxic chemicals (APM). This partitioning of the code package (APM) is less specific and its application is not limited to coal-liquids.

APMSPILL prints a report of the amount of selected chemicals that would occur in a coal-liquid spill of a given size. The chemicals currently considered by APMSPILL are phenol, o-cresol, p-cresol, m-cresol, C2-phenol, C3-phenol, C4-phenol, C5-phenol, 5-indanol, C1-indanol, resorcinol, and naphthol. A file for each of these chemicals is created by APMSPILL for the particular environment that the user specifies. This file is the input to the APM code.

APM simulates the fate of a chemical in a static or flowing body of water. The aquatic ecosystem is partitioned into user-selected compartments which are assumed to have uniform transport and transformation characteristics.

Instantaneous mixing of the chemical is assumed for all compartments. The partitioning of the chemical into the various compartments is followed for the given time period.

The user may select any of the following compartments to represent the system: water, sediment, fish, air, hydrolysis, biodegradation, metabolism (by fish), and photolysis. Additional compartments can be added without code modification because all such specific parameters are stored in data bases separate from the code. The user selects the sizes of each compartment in the system. The system is closed in that some of the compartments serve only as sinks to chart the amount of chemical leaving the system through various processes (e.g., hydrolysis).

The system to be modeled can be either a static (as a pond or lake) or flowing (as a river). Minor modifications to the code would allow simulating a pond or lake with streams flowing in or out of the system. The river model is divided into a number of user-selected lengths referred to as reaches. The chemical flowing out of each reach during each time period is input to the next reach during the corresponding time period. This allows the tracking of the chemical as it flows downstream.

The pathway diagram of the current version of APM is depicted in Figure B.1. Each compartment of the system is represented by a box. The flow of chemical between the compartments is signified by arrows. The arrows show the direction of the flow and are classified by two numbers. The first number indicates which compartment is the receiver, and the second number indicates which compartment is the source. The computer code allows for the transfer of chemical between any of the compartments in the system. If the user stores the rate constant between any two compartments in the chemical data base, the code will automatically consider the flow between those compartments whenever those two components are selected for a case.

FIGURE B.1. Pathway Diagram of the Aquatic Pathways Model

DEFINITION OF RATE CONSTANTS

To simulate an ecosystem using compartmental analysis, it is essential to know the rate of transfer of chemical between significant compartments. When discussing chemical transfer, it is important to distinguish between the rate constants and turnover rates. The authors are adhering to the terminology suggested by Robertson (1957) and advocated by Atkins (1969). Rate Constant is used for units of inverse time. Turnover Rate is used for units in mass time. Both types of rates are used in APM. The chemical data base can store any known transfer rate for a particular chemical. It is the users responsibility to ensure that input values have the proper units as defined in Figure B.2.

The model attempts to calculate turnover rates between some of the key compartments based on the physical properties of the chemical. These estimates are then used in the simulation if no rates are input from the chemical data base. These equations need continuing study and verification and can be easily modified to reflect the test findings. The properties currently used by APM are water solubility, vapor pressure, molecular weight, and the temperature at which these properties apply.

The APM currently calculates the turnover rates from water to air and from water to fish using these properties. The computer code model will also calculate the octanol-water partition coefficient (K_{ow}) from these properties if it is unknown. The octanol-water partition coefficient is used to calculate turnover rates from the water to the fish, from the water to the sediment, and from fish back to the water. An estimation of the soil organic matter-water partition coefficient (K_{oc}) is also based on the K_{ow} . The K_{oc} is used to calculate the turnover rate of the chemical between water and the sediments.

It was noted early in this work that the correlation being used to estimate K_{ows} did not appear to hold for the higher range of solubilities of many of the phenolic compounds. We did not attempt to establish a new correlation with the more highly water-soluble chemicals because the octanol-water partition coefficient can be estimated by other means and stored in the chemical data base.

If experimental rate constants are known they can be input into chemical data base. The program will use rates from the chemical data base instead of the rates it generates whenever those rates are available. Turnover rates must be converted to rate constants before the simulation takes place. The code automatically calculates rate constants from the turnover rates after the system has been defined.

The equations currently used in APM to calculate transfer rates between the various compartments of the system are listed in the "Code Logic" section of this Appendix. Many of the equations are from the works of W. B. Neely (1979a, b). The equations can be modified and additional ones included as new correlations are discovered.

FIGURE B.2. Structure of APM package

CODE DESIGN AND STRUCTURE

The APM computer code was designed for

- convenience to the user,
- ease of modification to reflect new research
- and cost effectiveness.

Frequently, computer codes are so user-unfriendly that only a few persons become familiar enough with the codes to actually execute them. The APM code package has attempted to overcome this barrier by using interactive interfaces that ask the user for all input data in plain English.

This code package is designed to allow for easy modification, so development work can proceed rapidly. This has been accomplished by creating generalized modular subroutines. APM stores most of the system-specific parameters outside of the code in data bases where they can easily be changed and modified.

Development of computer codes and execution of cases with long running times can be costly. The APM code package was designed to be executed on a microcomputer using only 65 kilobytes of memory. This eliminates the need to pay the time-sharing costs of a large mainframe. Because the code was developed and runs under the CPM (Control Program Monitor) operating system, it is extremely portable and consequently usable to a greater number of people.

COMPUTER CODE STRUCTURE

The Aquatic Pathways Model package is comprised of the following elements:

1. Chemical data base (CHEMRATE)
2. Compartment data base (APMCMPRT)
3. Parameters description data base (APMVAR)
4. Compartment model code package:
 - a. User interface (APM)
 - b. Edit case file program (APMED - not completed)
 - c. Simulation program (APMCALC)
 - i. Read input file module
 - ii. Print report for quality assurance module
 - iii. Simulation module
 - iv. Detailed graphic output module
 - v. Summary output module
5. Coal-liquid spill simulation Input Generator (APMSPILL)
6. Multi-Reach River Input Generator (APMREACH)
7. Maintenance program for chemical data base (CHEMMOD)
8. General purpose maintenance program for data bases (RFC)

The functions of each element, the interrelationships of the elements, and the user interactions with the elements are described in Figure B.2. The file names associated with each code, input file, and output file are also depicted.

The user has several options in preparing input for the simulation (Figure B.2). Let us assume that the user wishes to simulate a spill of coal-liquids into a river. Running the APMSPILL program (initiated by typing "APMSPILL") will create all necessary input for the simulation. The user will be queried for all necessary information such as the length of simulation, compartments to be considered, sizes, and other needed information about each compartment. When finished, a report on the chemical composition of this particular spill and file names used will be output on the printer. Additionally, twelve on-line input files will have been created. The APMREACH code is a time saver when the user wants to follow the flow of a chemical through many reaches of a river. Instructions on how to use APMREACH are produced in Appendix C.

During normal execution, it should not be necessary to update the data bases. Any updating or compartment modifications can easily be accomplished by the user through the appropriate support code without modifying the actual code.

After the input files have been created the user can execute each case. This is initiated by typing "APM." The code will solicit the user's choices on input and output options. The user will be asked for the input file name (printed on the report from APMSPILL) and asked to select a name for the output file. The user has been given the task of executing the individual cases to allow greater flexibility. There will be numerous instances when it will not be necessary or desirable to execute all twelve cases. This allows the user to select which cases to run and the order to run them in.

Hierarchy charts are presented for each code in Figures B.3 and B.4. The charts show the organization of the modules within each code.

FIGURE B.3. Organization of APM Modules APMSPILL, APMREACH, APM and CHEMMOD

MODULE STRUCTURE - APMCALC

FIGURE B.4. Organization of APMCALC Module

FILE DESCRIPTIONS

The APM Package uses random and sequential files whenever possible to store specific information. This greatly simplifies modifying APM. In addition, the reduced core storage requirements allows the code to be executed on a smaller machine. All data stored in files are in ASCII format for the convenience of file maintenance. A summary of file usage for APM is given in Table B.1. Each file, its organization, use, and its present contents are described in this section.

APMOPT

APMOPT is a sequential file which contains program-specific information for the user. The file is used by APM for introductory information for the user. The file is comprised of 23-line "pages" for display on the video monitor at the user's terminal. Each page of the file is displayed in Figure C.4 of that users guide (Appendix C).

APMCMPRT

APMCMPRT is a MBASIC random file that stores data for each compartment which may be considered by APM. Random files are particularly useful because information stored in them is directly retrievable by the operating system. This translates into speed. Each compartment is assigned a number which indicates its position in the file and, in the case of APM, becomes its index

TABLE B.1. Aquatic Pathways Model of Toxic Chemicals File Usage

<u>File No.</u>	<u>Name</u>	<u>Organization</u>	<u>Description</u>
1	CHEMRATE	Random	Data base of transfer coefficients of chemicals
2	(input)	Sequential	Old input file name
3	(input)	Sequential	New input file name
4	(input)	Sequential	Output file name
5	APMDFLT	Sequential	Default input parameters, corresponds to file 2
6	APMOPT	Sequential	Descriptive instructions file
7	APMVAR	Random	Variable description file
8	APMCMPRT	Random	Compartment data base

number. APMCMPRT must be defined before the APMVAR and CHEMRATE are set up because these data bases as well as all the codes utilize the indexing of compartments defined in this data base. There is one record (128 bytes) for each compartment. Data are stored in the file as ASCII strings for ease of verifying and changing. Each record has nine fields (Table B.2).

Default values for the various compartments have not yet been defined. They can be inserted directly into the data base when they are established. The default values will be used by APMED to assist the user in setting up simulations.

The file, as it is currently utilized by APM, is depicted in Figure B.5 and in Appendix D, "Data Base and Code Listing".

APMVAR

APMVAR is a random organized file that stores descriptive information on each variable in APM. The variables must be input by the user. APMVAR is used to create input files (by APMSPILL, APMREACH, and APMED) and print reports. Each record contains a description of the variable and the appropriate units. This design has several advantages. First, new compartments may be added to APM without modifying the code. Second, the parameter definitions can be more descriptive because they are not stored

TABLE B.2. Description of APM Compartment Data Records

<u>Field</u>	<u>Beginning Position</u>	<u>No. of Char.</u>	<u>Description</u>
1	1	10	Compartment number. Same as record location, included for quality assurance.
2	11	10	Compartment name. Used for descriptive input and output.
3	21	10	Number of variables associated with this compartment. The range of acceptable values is 0 to 6
4	31	10	Default value of Parameter No. 1
5	41	10	Default value of Parameter No. 2
6	51	10	Default value of Parameter No. 3
7	61	10	Default value of Parameter No. 4
8	71	10	Default value of Parameter No. 5
9	81	10	Default value of Parameter No. 6

Record No.	Compartment Name	No. of Variables	Default 1	Default 2	Default 3	Default 4	Default 5	Default 6
1	Water	5						
2	Sediment	2						
3	Fish	2						
4	Air	0						
5	Hydrolysis	0						
6	Biodegradation	0						
7	Metabolism	0						
8	Photolysis	0						

FIGURE B.5. APMCMPRT (Aquatic Pathways Model Compartment Data Base)

in core. And finally, because the variables can be stored separately they can easily be retrieved, verified, listed in reports and manipulated by other means.

Each record in APMVAR can consist of up to 128 characters of descriptive information. Units for the parameters should be included in each record. Each record should be terminated by a colon (:). APM looks for the colon to determine the actual length of the record for formatting purposes.

The record locations in the APMVAR file are related to the APMCMPRT file. The records are divided into groups of six which are associated with each of the compartments as described in the APMCMPRT file. The first two groups (twelve records) are reserved for general parameter descriptions. One group of six records is reserved for each of the compartments. This allows for easy indexing through the files by the code. The parameters will be stored in a two dimensional array when they are read into the program. This enables easy modification of the code. (The file as it is currently utilized is depicted in Appendix D, "Data and Code Listings," Figure D.2)

CHEMRATE

The chemical data base stores information about the physical properties of the chemical as well as a matrix of aquatic rate transfers. The data base, named CHEMRATE, is divided into two sections and its organization follows the compartment organization of the APMCMPRT file.

A group of 17 records is reserved for each chemical. The first record in each group contains data on the physical properties of the chemical. The other 16 records, each have 16 fields, which allows for the storage of a 16 x 16 matrix of transfer rates. The rate constant matrix corresponds to the compartments described in the APMCMPRT file.

The value stored in this data base may be either a turnover rate or a rate constant. The distinction between these two rates is discussed in the beginning of this Appendix ("System and Model Descriptions").

A utility program has been written to aid the user in maintaining the data base, which should be updated as new information on chemicals becomes available. This program, CHEMMOD, will be discussed in the next section, "Code Descriptions."

The CHEMRATE data base is organized as follows. The first record stores information about the physical properties of the chemical; as shown in Table B.3.

The next sixteen records of the group comprise a matrix of rate constants and turnover rates between the various compartments of the system. Because we have currently only defined eight compartments, we will define our discussion to an 8 x 8 matrix. The indexing system is based on the APMCMPRT data base. The worksheet for the CHEMRATE data base, shown in Figure B.5, portrays the organization of the file. Each record in the file stores a column of the matrix, and each field is allotted eight positions. The user need not be

TABLE B.3. Description of CHEMRATE Data Records

Field	Beginning Position	No. of Char.	Description
1	1	4	Chemical number. Same as record location; included for quality assurance.
2	5	12	Molecular formula
3	17	8	Molecular weight
4	25	20	Name of chemical
5	45	20	Chemical is also known by this name
6	65	8	Water solubility of the chemical ($\mu\text{g/g}$)
7	73	8	Vapor pressure of the chemical ($\mu\text{g/g}$)
8	81	8	Temperature at which the water solubility and vapor pressure listed above apply (degrees centigrade)
9	89	8	Log octanol-water partition coefficient
10	97	8	Log soil organic matter-water partition coefficient
11	105	8	Ultra-violet adsorption coefficient. Currently not utilized but may be used in future versions.
12	113	8	Dissociation constant. Not used at present.

concerned about these details, because the utility program, CHEMMOD, will assist the user in creating and maintaining new records. The units in Figure B.6 refer to the current version of APM and indicate either rate constants (per hour units) or turnover rates (other than per hour). It is the user's responsibility to adjust input transfer rates to these units before their inclusion into the file.

CHEMRATE

chemical data base worksheet for APM

Index no. of chemical: _____

Molecular formula: _____

Molecular weight: _____

Chemical name: _____

Second name: _____

Solubility: _____ $\mu\text{g/g}$

Vapor pressure: _____ mm Hg

Temperature (solubility & vapor pressure): _____ degrees C

Log octanol-water partition coefficient: _____

Log soil organic matter-water partition coefficient: _____

Ultra-violet adsorption coefficient: _____

Dissociation constant: _____

Rate constants and flow rates:

From compartment:

	1 Water	2 Sediment	3 Fish	4 Air	5 Hydrolysis	6 Biodegrade	7 Metabolism	8 Photolysis
1	X	1/hr	1/hr					
2	mL/(g-hr)	X						
3	mL/(g-hr)		X					
4	cm/hr			X				
5	1/hr				X			
6	1/hr	1/hr				X		
7			1/hr				X	
8	1/hr							X

FIGURE B.6. Chemical Data Base Worksheet for APM

CODE DESCRIPTIONS

Code descriptions are provided for the input file generators (APMSPILL and APMREACH), the simulation code package (APM), and the file maintenance codes (CHEMMOD and RFC). The APM code package consists of two chained MBASIC® compiled programs: APM and APMCACL. A third program in the package (APMED), which is not ready for implementation, would allow the user to edit an input file before executing the case.

APMSPILL

APMSPILL is an interactive program that creates the input files for APM to simulate a spill of coal-liquids into an aquatic ecosystem. The user is queried for the size of the spill, the compartments that the user wishes to consider, the sizes of the selected compartments, the time period to consider, and whether the system is best modeled as a pond or a river. Input files, one for each of 12 chemical components of coal-liquids, are created from the above information. In addition, a report is printed listing the amount of each chemical in the spill and the names of the corresponding input files.

APMREACH

There will be occasions when a chemical is to be followed many reaches down a river. Input of specific information on each compartment for many reaches becomes quite laborious. If the assumptions can be made that all compartment sizes will remain the same for each reach. Then APMREACH can be used to create the lengthy input files. APMREACH is an interactive program and is similar to APMSPILL in structure.

APM

APM is the input-output interfacier with the user for the APM code package. The user invokes the APM code when a simulation is to be executed. The APM performs the following functions:

1. APM solicits input and output file names from the user. APM checks if the names are valid (i.e., the input file must have been created and reside on the specified device).
2. APM allows the operator create a new case, run a previously created case, or edit a previously created case. (Note: only the second is currently functional. The input file would have been created by APMSPILL or APMREACH.)
3. APM queries for the user's report selection, which is either a detailed report of each reach or a summary report of a river.
4. APM calls the appropriate code corresponding to the user's selection.

APMCALC

This program is the main simulation of the Aquatic Pathways model of Toxic Chemicals. The code is modular in design and could easily be divided into separate codes performing each major activity. APMCALC performs the following functions:

1. APMCALC reads the input file and data bases and prints the quality assurance report.
2. APMCALC calculates, inputs, adjusts and prints rate constants as needed.
3. APMCALC calculates the amount of chemical in each compartment for each time-step of the simulation.
4. APMCALC prints a report of the results of the simulation.

Functions 2, 3, and 4 are performed for each reach of a river. It is necessary to re-calculate rate constants for each reach because the flow rates are dependent upon the sizes of the compartments which may change for each reach.

APMCALC calculates turnover rates between selected compartments if the physical properties of the chemical are stored in the chemical data base and a correlation has been made with the physical properties. APMCALC then reads in the rate constants and turnover rates stored in the chemical data base. Any known values from the data base will be used instead of the calculated rate constants and flow rates. APMCALC adjusts the turnover rates to rate constants. Definitions of turnover rate and rate constants are found in the "System and Model Description" at the beginning of this Appendix.

The capability to handle chronic input of the chemical to any of the compartments is included in the simulation routine. This feature, however, has not been brought out to the input-output level.

The Runge-Kutta method is used to find a numerical solution of the differential equations used in the simulation of the APM code. The code implementation is based on the work of Hicks (1981). The logic of the algorithm as it is implemented in the code is depicted in the Chapin chart of the simulation subroutine (Figure B.16).

In the river simulation, the amount of chemical leaving the reach during each time step is stored in an array so that it can be input into the next reach (uniform mixing presumed) during the corresponding time step.

Either a detailed graphic report or a one-line summary is printed for each reach of a river. The user selects this option when running the code. The summary option should be selected in multi-reach river simulations unless the user has particular need of the extensive output.

The detailed report consists of:

1. The selected compartments and their sizes
2. The rate constants between the compartments and their sources
3. A table of the amount of chemical in each compartment during each of ten equally-spaced time steps
4. The percent of chemical in each compartment at the end of the simulation
5. The concentration in $\mu\text{g/g}$ of this chemical in the water, sediment, and fish compartments.^(a)
6. The bioconcentration factor of this chemical in the sediments and in the fish.^(b)
7. A graph of the amount of this chemical in each compartment versus time.

The summary report assumes that all reaches of the river are uniform. Consequently, compartment and rate data are printed only once. The summary report contains the following information:

1. A report of selected compartments and compartment sizes
2. A list of rate constants
3. A table of the amount of chemical in each reach of the river as well as the amount of chemical in each compartment at the end of the simulation in that reach
4. The total amount of chemical in the river system and the total amount of chemical in each compartment for all reaches divided by the total chemical in the river system
5. The percent of the total amount of chemical in each compartment at the end of the time period
6. The average concentration in $\mu\text{g/g}$. This value is the total amount of chemical in each compartment for all reaches divided by the total amount of chemical in the river system.^(c)

(a) This calculation assumes that, in the input case, Compartments 1 through 3 will be defined as water, sediment, and air, respectively.

(b) This calculation assumes that, in the input case, Compartments 1 through 3 will be defined as water, sediment, and air, respectively.

(c) This calculation assumes that, in the input case, Compartments 1 through 3 will be defined as water, sediment, and air, respectively.

7. The amount of chemical flowing out of the river system. (This amount plus the total chemical in the system should equal the amount of chemical spilled.)

CHEMMOD

CHEMMOD allows for the easy maintenance of the chemical data base. It is necessary for the user to know the data base index number of a chemical to view or modify information on that chemical. Alternately the user can "page" through the file by index number until the chemical in question is encountered. If any changes are made to the file, the date, time, and user's name are stored in the title for quality assurance

CODE LOGIC

Logic diagrams for each module of the codes are presented in this section. The logic diagrams use flow charting techniques described by Chapin (1974) and are referred to as Chapin charts. The basic logic constructs used in the diagrams are indicated in Figure B.7. The relationships of the modules and their hierarchy is presented in Figure B.1 in the introduction of this Appendix ("Computer Code Structure").

Logic diagrams are presented for the following modules:

APMSPILL	Figure B.8
APMREACH	Figure B.9
APM	Figure B.10
INPUT-TEST subroutine	Figure B.11
APMCALC	Figure B.12
QUALITY ASSURANCE subroutine	Figure B.13
READ COMPARTMENTS subroutine	Figure B.14
RATE CONSTANTS subroutine	Figure B.15
SIMULATION subroutine	Figure B.16
DETAIL REPORT subroutine	Figure B.17
SUMMARY REPORT subroutine	Figure B.18
SUMMARY REPORT TRAILER subroutine	Figure B.19
CHEMMOD	Figure B.20
MODIFY PARAMETER subroutine	Figure B.21

The information in this section is not needed by the user who wishes only to execute the code. For those who wish to modify the code or adapt it to a different application, the information will be helpful.

Sequential Block of Code

Conditional

Do While Loop

Do Until Loop

Abnormal Transfer

Abnormal Termination

FIGURE B.7. Chapin Chart Logic Constructs

APMSPILL - Logic Diagram

FIGURE B.8. APMSPILL Logic Diagram

End

FIGURE B.8. (contd)

Apmreach Logic Diagram

FIGURE B.9. APMREACH Logic Diagram

FIGURE B.9. (contd)

APM Logic Diagram

Print heading (page 4)				
Input date and time				
Open files				
Print page 2 of option file				
	Query for selected option			
	Input option			
Repeat until valid option is input				
Print page 3 of option file				
Then	If edit or old case option selected		Else	
Clear 3-chances flag				
Do while flag < 3				
Input selected file name				
Then	If file not found			Else
Increment 3-chance flag		Set 3-chance flag to 99		
Then	If 3-chance flag < 99		Else	
Point error message; Stop			Null	Null
Then	If create or edit option selected			Else
Clear 3-chance flag				Set new file name
Do while flag < 3				

FIGURE B.10. APM Logic Diagram

Input selected file name		equal to old file- name	
Then	If file already exists		Else
Increment 3-chance flag			Set 3-chance flag to 99
Then			If 3-chance flag < 99
Print error message; stop		Null	
Clear 3-chances flag			
Do while flag < 3			
Input selected file name			
Then	If file already exists	Else	
Increment 3-chance flag		Set 3-chance flag to 99	
Then	If 3-chance flag < 99	Else	
Print error message; stop		Null	
Print page-4 of option file			
Query for selected option			
Input option			
Repeat until valid option selected			
Then	If create or edit option selected	Else	
Chain "APMED" program		Chain "APMCALC" program	

End

FIGURE B.10. (Contd)

Input-Test Subroutine (APM, APMSPIII, APMREACH)

Adjust description line					
Clear screen					
On type of parameter: Integer (subroutine)			Real (subroutine)		String (sub)
Print L\$			Print L\$		
Input value			Input value		
Test limits?			Test limits?		Print L\$
Yes	No		Yes	No	
Outside limits?			Outside limits?		Input value
Yes	No		Yes	No	
Repeat		Null Null	Repeat		Null Null

FIGURE B.11. Input-Test Subroutine (APM, APMSPIII, APMREACH)

APMCALC Logic Diagram

End

FIGURE B.12. APMCALC Logic Diagram

APMCALC - Print Quality Assurance Report Subroutine

Print file names		
Print title of case, date and time		
Print time information		
Print chemical loading information		
Print chemical data		
Print type of environment		
Then	If river model	Else
Print number of reaches		Null
Print flow rate of water		

Return

FIGURE B.13. APMCALC Quality Assurance Report Subroutine

APMCALC - Read Compartment Information Subroutine

Return

FIGURE B.14. APMCALC Read Compartment Information Subroutine

			Print description value		
		Query if any of this column need modification			
		Yes	Modify any this column?	No	
		For each rate constant		Null	
		Print description, value			
		Modify parameter (subroutine)			
				Null	
Do until exit requested					
Then	If data base has been modified			Else	
Update file header with date, time user's name				Null	
Close files					

End

FIGURE B.14. (Contd)

APMCALC - Rate Constants Subroutine

FIGURE B.15. APMCALC Rate Constants Subroutine

Then	If water and sediment compartments considered?		Else
Calculate water to sediment rate			Null
Then	If water and fish compartments considered?		Else
Calculate water to fish rate from flow rate			Null
Then	If water and air compartments considered?		Else
Calculate water to air rate from flow rate			Null
Then	If sediment and water compartments considered?		Else
Then	If flowrate was not supplied in chemrate		Else
Then	If KOC is unknown	Else	
Estimate KOC		Null	
Estimate sediment to water flow rate		Null	
Calculate sediment to water rate from flow rate		Null	
Then	If water and fish compartments considered?		Else
Then	If transfer rate was not supplied in chemrate		Else
Estimate fish to water flow rate		Null	Null
Calculate fish to water transfer rate			
Then	If detail report or first reach of summary report		Else
Print report of rate constants (subroutine)			Null

Return

FIGURE B.15. (Contd)

APMCALC - Simulation Subroutine

FIGURE B.16. APMCALC Simulation Subroutine

For each column of matrix		
Initialize partitioning accumulator for this point		
For each row position of matrix		
Then	If transfer rate is non-zero	Else
Calculate dx/dt at P		Null
Add dx to receiving compartment		
Subtract dx from donor compartment		
For each compartment		
Make estimate of state Q at time $IJ-1/2$		
For each column of matrix		
Initialize partitioning accumulator for this point		
For each row position of matrix		
Then	If transfer rate is non-zero	Else
Calculate dx/dt at Q		Null
Add dx to receiving compartment		
Subtract dx from donor compartment		
For each compartment		
Make estimate of state R at time J		

FIGURE B.16. (Contd)

For each column of matrix	
Initialize partitioning accumulator for this point	
For each row position of matrix	
Then	If transfer rate is non-zero
Calculate dx/dt at R	
Add dx to receiving compartment	
Subtract dx from donor compartment	
Else	
Null	
For each compartment	
Take weighted average of estimates for state at time J	
Calculate mass of chemical flowing out of reach during this time step	
Subtract amount of chemical leaving this reach from water compartment	
Store compartment masses for this time step in permanent array	
Then	If doing a river simulation
Calculate total of chemical flowing out of this reach (subroutine)	
Else	
Null	

Return

FIGURE B.16.

AMPCALC-Detail Report Subroutine

FIGURE B.17. APMCALC Detail Report Subroutine

APMCALC - Summary Report Subroutine

Then	If first reach of river	Else
	Print heading	Null
	Set chemical flowing into system equal to initial loading	
	Calculate and print amount of chemical in the system for this reach	
	For each compartment	
	Print amount of chemical for this reach	
	Accumulate total of chemical in all reaches for this compartment	

Return

FIGURE B.18. APMCALC Summary Report Subroutine

APMCALC - Summary Report Trailer Subroutine

Return

FIGURE B.19. APMCALC Summary Report Trailer Subroutine

Chemmod Logic Diagram

FIGURE B.20. CHEMMOD Logic Diagram

Return

FIGURE B.21. CHEMMOD Modify Parameter Subroutine

VARIABLE DESCRIPTIONS

This section consists of a list of variables used in the APM. Variable names including dimensions are listed alphabetically in the column headed "Parameter". The type of variable (integer, real, r string) is given in the "Type" column. The presence of the variable in common is denoted by an asterisk in the "Common" column. A description of each variable including units and option flag definitions is given in the "Description" column.

Parameter	Type	Common	Description
A(16,16)	real	*	compartment-specific parameter storage array
AX(16)	real		temporary storage of mass of chemical in each compartment for first point within each time step. Used by Runge-Kutta integration method.
B(16,1)	real		matrix of rate coefficients of chemical to each compartment from outside the system. For use with chronic spills; not currently utilized.
CS	string		name of selected chemical
CS(16)	string		input array for rate constants from data base
C2\$	string		secondary name for chemical
CN(16)	integer		index numbers of selected compartments in data base
CN	integer		temporary index number of compartment
CNS(16)	string	*	names of each selected compartment
CON!(3)	real		final (pond) or average final (river) concentration of the chemical in 1-water, 2-sediment, and 3-fish
DATS	string	*	date of execution
DC	real		dissociation constant of the chemical
DT	real	*	change of time for each integration time-step $DT = 1 / KK$
DUMP	real		amount of chemical (grams) loaded into the water compartment
DUMP(16)	real		amount of chemical (grams) loaded into each compartment
E	real		intermediate fish uptake rate parameter

Parameter	Type	Common	Description
E(16,16)	real		error associated with each rate constant. Not presently utilized.
EG	real		intermediate result - evaporation rate (gas)
EL	real		intermediate result - evaporation rate (liquid)
EOX	real		fraction of oxygen transferred across the gill surface of fish
F\$	string		general purpose filename string
F1\$ -- F9\$	string	*	file names; correspond to assigned file number
FR	real		flow rate of the river in cubic meters per hour
H	real		intermediate result - evaporation rate constant
I	integer		looping index (usually first level)
I(16,16)	integer		index of quality of each rate constant; not currently installed
IJK	integer		looping index for river reaches
J	integer		looping index (usually second level)
J1 -- J2	integer		cross-index subscript to match rate constants with appropriate compartments
JJ	integer		looping index for iterations within each time step
K	integer		looping index (usually third level)
KK	integer	*	number of iterations performed for each time-step of integration
KOC!	real		log soil organic material / water partitioning coefficient
KOW!	real		log octanol / water partitioning coefficient

Parameter	Type	Common	Description
L	integer		temporary storage
LS	string		general I/O string
L1\$ -- L9\$	string		general purpose I/O
MCOX	real		intermediate result - fish uptake rate
MFS	string		molecular formula string
MW	real		molecular weight of chemical
N	integer		temporary index number
NS	string		general purpose string of looping index
N1	integer	*	number of reaches in river
N2	integer		number of compartments in system
N3	integer		number of variables associated with this compartment
N4	integer	*	a) number of chemicals in data base, b) index number of selected chemical in data base
N5	integer		number of inputs to each compartment from outside the system. Assumed to be one for this level of program development.
N6	integer		temporary
NLINE	integer		number of rows in graph
NCOL	integer		number of columns in graph
P1	integer	*	option selection flag: 1 - create new case 2 - run a previously created case 3 - edit a previously created case
P2	integer		temporary flag

Parameter	Type	Common	Description
P3	integer		parameter type flag: 1 - integer 2 - real 3 - string
P4	integer		test flag for CHANGE-INPUT-TEST subroutine: >0 - test if input is within limits for this variable 0 - no action <0 - no changes allowed for this variable
P5	integer		environment classification: 1 - pond 2 - river
P6(16,16)	integer	*	rate constant source index: 1 - calculated in APM 2 - from the chemical data base
P7	integer		if set, the rate constant between the two considered compartments needs adjusting. Returned from testing subroutine.
P8	integer	*	report option flag: 0 - detail report for each reach of river. This option always used for pond or lake. 1 - summary report selected, first reach 2 - set to repress printing of input parameters after first reach.
P9	integer		if set, this compartment is being considered this case. Returned from testing subroutine.
Q	real		intermediate result - fish uptake equation
Q(100,16)	real	*	mass of chemical in each compartment (16) at the end of each of 100 time intervals
QI(16)	real		mass of chemical available for direct input into each compartment from outside the system. Not utilized at this time.

Parameter	Type	Common	Description
QR(100)	real		mass of chemical flowing out of water compartment of this reach during each time period
QUAL\$(10)	string		rate constant source descriptive string: 1 - calculated in APM 2 - from the chemical data base
R(16,16)	real	*	matrix of rate constants between up to 16 compartments
RS(3)	string		printing array for rate constants
R1\$ -- R9\$	string		field string for rate constant random file buffer
RCS(16)	string		rate constant input field string array
RIN	real		total amount of chemical entering reach (grams)
RL%	integer		record location within random file considered
ROUT	real		total amount of chemical flowing out of reach (grams)
RSYS	real		total amount of chemical in the system (grams)
S	real		water solubility of chemical in ug per gram
SRC	real		amount of coal-liquid spilled into the water in liters
STOT	real		total of chemical in all reaches (grams)
STOT(16)	real		total of chemical in all reaches for each compartment (grams)
T	real		temperature (degrees Centigrade) that solubility and vapor pressure apply for this chemical
TEMP	real		temporary parameter
TIME	real		total time period evaluated (hours)
TIT\$	string		descriptive title for this case

Parameter	Type	Common	Description
TK	real		length of each of 100 time steps in hours
TOD\$	string	*	time-of-day string for printing and quality assurance
TOT	real		accumulator for a) amount of chemical in the system, b) amount of chemical flowing out of the system
UVA	real		ultra-violet absorption factor of this chemical. Stored, but not utilized at this time.
VP	real		vapor pressure of this chemical (mm Hg)
V1\$ -- V9\$	string		program identification
W\$	string		input string and C-I-T subroutine passing parameter
W1%	integer		C-I-T subroutine passing parameter
W1M%	integer		C-I-T minimum allowable input integer value
W1X%	integer		C-I-T maximum allowable input integer value
W2	real		C-I-T subroutine passing parameter
W2M	real		C-I-T minimum allowable input real value
W2X	real		C-I-T maximum allowable input real value
X(16)	real		mass of chemical in each compartment for the previous time-step
XD(16)	real		dX/dt at time J-1 for each compartment
XP(16)	real		dX/dt at time P for each compartment
XQ(16)	real		dX/dt at time Q for each compartment
XR(16)	real		dX/dt at time R for each compartment

Parameter	Type	Common	Description
Y(4)	real		temporary general purpose array
Z\$	string		field string for random buffers
Z1\$ -- Z9\$	string		fields string for random buffers

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APPENDIX C

APM USER'S GUIDE

APPENDIX C

APM USER'S GUIDE

This guide contains instructions on how to use APM. It includes a demonstration showing how to execute a simulation.

There are two ways to create input files to run APM cases. APMSPILL is the general spill simulation. It is used to designate characteristics of each compartment of either a pond or river, which may have reaches of differing characteristics. It currently creates 12 files, one for each chemical considered. APMREACH is used to create an input file for a specific chemical for a river that has many identical reaches.

APMSPILL

The interactive input file generator, APMSPILL, should be used to simulate the unit coal-liquid spill into a body of water. To successfully simulate the spill, the user must know:

1. The time period to be simulated (There are one hundred time-steps built into APM--enter the length of each of the 100 time-steps.)
2. The size of the spill (liters)
3. The compartments of the environment which are of interest
4. Physical characteristics of those compartments.

APMSPILL will query the user for all needed information. To activate this code, it is only necessary to type: APMSPILL. The user will be asked to supply a file name prefix, which will identify this case. Upon termination, 12 input files, one for each chemical considered, will have been created. In addition, a report on the spill will have been printed. An example of the interactive input session is given in Figure C.1. The sample case involves a river with two reaches having different characteristics. User responses are underlined in the text for clarity. A sample of the input files created by this example are shown in Figure C.2. The printer report from this session is displayed in Figure C.3.

The printer report will give the file name for the input file of each chemical. To run a simulation of any of the chemicals, the user then types: APM. The code will ask for the date and time, and then query for the user's execution option. Because the input files have already been created by APMSPILL, the user selection Option 2 (Run an old case). APM then asks for the user's choice of an output file name. Figure C.4 shows the interactive session used to execute one of the sample files created by the sample run shown in Figure C.1.

A>APMSPILL

Aquatic Pathways Model of a Solvent-refined Coal Unit Spill
Version of December 21, 1981

Enter date: SEP 21, 1982

Enter time: 14:30

Enter input file name prefix (up to 8 letters): ? SAMPLE

Title: ? SAMPLE TWO REACH RIVER CASE

Length of each time unit in hours: ? .3

No. of iterations performed in each time step: ? 1

Enter amount of solvent-refined coal liquid spilled
into the water (liter): ? 100

Type of environment (1-pond, 2-river): ? 2

No. of reaches in flowing stream: ? 2

Flow rate of river (m^3/hr): ? 1E5

Number of compartments: ? 5

Compartment choices:

- 1 - WATER
- 2 - SEDIMENT
- 3 - FISH
- 4 - AIR
- 5 - HYDROLYSIS
- 6 - BIODEGRADE
- 7 - METABOLISM
- 8 - PHOTOLYSIS

FIGURE C.1. Interactive Input Session for APMSPILL

Compartment No: ? 1

Volume of water in compartment (liters): ? 3E10

Surface area of water (m²): ? 1.5E7

Average depth of water (m): ? 2

Compartment choices:

- 1 - WATER
- 2 - SEDIMENT
- 3 - FISH
- 4 - AIR
- 5 - HYDROLYSIS
- 6 - BIODEGRADE
- 7 - METABOLISM
- 8 - PHOTOLYSIS

Compartment No: ? 2

Total weight of sediment (kg): ? 7.5E5

Percent of organic matter in sediment: ? 1

Compartment choices:

- 1 - WATER
- 2 - SEDIMENT
- 3 - FISH
- 4 - AIR
- 5 - HYDROLYSIS
- 6 - BIODEGRADE
- 7 - METABOLISM
- 8 - PHOTOLYSIS

Compartment No: ? 3

Total weight of fish (kg): ? 30

Weight of average fish (g): ? 300

FIGURE C.1. (contd)

Compartment choices:

- 1 - WATER
- 2 - SEDIMENT
- 3 - FISH
- 4 - AIR
- 5 - HYDROLYSIS
- 6 - BIODEGRADE
- 7 - METABOLISM
- 8 - PHOTOLYSIS

Compartment No: ? 4

Compartment choices:

- 1 - WATER
- 2 - SEDIMENT
- 3 - FISH
- 4 - AIR
- 5 - HYDROLYSIS
- 6 - BIODEGRADE
- 7 - METABOLISM
- 8 - PHOTOLYSIS

Compartment No: ? 6

Number of compartments: ? 5

Compartment choices:

- 1 - WATER
- 2 - SEDIMENT
- 3 - FISH
- 4 - AIR
- 5 - HYDROLYSIS
- 6 - BIODEGRADE
- 7 - METABOLISM
- 8 - PHOTOLYSIS

Compartment No: ? 1

FIGURE C.1. (contd)

Volume of water in compartment (liters): ? 2E10

Surface area of water (m²): ? 1E7

Average depth of water (m): ? 2

Compartment choices:

- 1 - WATER
- 2 - SEDIMENT
- 3 - FISH
- 4 - AIR
- 5 - HYDROLYSIS
- 6 - BIODEGRADE
- 7 - METABOLISM
- 8 - PHOTOLYSIS

Compartment No: ? 2

Total weight of sediment (kg): ? 5E5

Percent of organic matter in sediment: ? 1

Compartment choices:

- 1 - WATER
- 2 - SEDIMENT
- 3 - FISH
- 4 - AIR
- 5 - HYDROLYSIS
- 6 - BIODEGRADE
- 7 - METABOLISM
- 8 - PHOTOLYSIS

Compartment No: ? 3

Total weight of fish (kg): ? 20

Weight of average fish (g): ? 300

FIGURE C.1. (contd)

Compartment choices:

- 1 - WATER
- 2 - SEDIMENT
- 3 - FISH
- 4 - AIR
- 5 - HYDROLYSIS
- 6 - BIODEGRADE
- 7 - METABOLISM
- 8 - PHOTOLYSIS

Compartment No: ? 4

Compartment choices:

- 1 - WATER
- 2 - SEDIMENT
- 3 - FISH
- 4 - AIR
- 5 - HYDROLYSIS
- 6 - BIODEGRADE
- 7 - METABOLISM
- 8 - PHOTOLYSIS

Compartment No: ? 6

FIGURE C.1. (contd)

SAMPLE TWO REACH RIVER CASE # SEP 21, 1982 14:20

.3

1

1690

1 PHENOL

2

2

100000

5

1	WATER	3	0.30E+11	0.30E+08	0.10E+01	0.00E+00	0.00E+00	0.00E+00
2	SEDIMENT	2	0.75E+06	0.10E+01	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3	FISH	2	0.30E+02	0.30E+03	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4	AIR	0	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
6	BIODEGRADE	0	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00

5

1	WATER	3	0.20E+11	0.10E+08	0.20E+01	0.00E+00	0.00E+00	0.00E+00
2	SEDIMENT	2	0.50E+06	0.10E+01	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3	FISH	2	0.20E+02	0.30E+03	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4	AIR	0	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
6	BIODEGRADE	0	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00

A>

FIGURE C.2. Input Files Created by Sample Run of APMSPILL

Aquatic Pathways Model of a Solvent-refined Coal Unit Spill
Version of December 21, 1981

Case title: SAMPLE TWO REACH RIVER CASE # SEP 21, 1982 14:20
Amount of coal-liquid spilled: 100 liters

----- Chemical -----	----- Chemical (g) per liter of liquid -----	----- Amount of Chemical (g) in this spill -----	----- APM input File name -----
PHENOL	16.90	0.17E+04	SAMPLE.1
O-CRESOL	8.10	0.81E+03	SAMPLE.2
P-CRESOL	16.90	0.17E+04	SAMPLE.3
M-CRESOL	12.40	0.12E+04	SAMPLE.4
C2-PHENOL	29.20	0.29E+04	SAMPLE.5
C3-PHENOL	9.60	0.96E+03	SAMPLE.6
C4-PHENOL	3.30	0.33E+03	SAMPLE.7
C5-PHENOL	0.30	0.30E+02	SAMPLE.8
5-INDANOL	5.30	0.53E+03	SAMPLE.9
C1-INDANOL	2.90	0.29E+03	SAMPLE.10
RESORCINOL	0.70	0.70E+02	SAMPLE.11
NAPHTHOL	0.40	0.40E+02	SAMPLE.12

FIGURE C.3. Printer Report Created by APMSPILL

Aquatic Pathways Model of Chemicals in the Environment

Version of January 6, 1982

Enter date: SEP 21, 1982

Enter time: 14:30

```
#####  
#  
#   Aquatic Pathways Model of Toxic Chemicals in the Environment   #  
#                                                                 #  
#####
```

You have the following options:

- 1 - Create a new case
- 2 - Run a previous case
- 3 - Edit a previous case and run

Enter selected option: ? 2

FIGURE C.4. Interactive Session to Execute APM

A filename consists of eight letters or numbers in any combination; a period and a three letter or number extension. The name may be prefixed by a device code followed by a colon.

MYFILE.001
MYFILE
A:MYFILE.001

The above are all examples of valid filenames.

Enter old filename: ? B:SAMPLE.1
Enter output filename: ? SAMPLE.OUT

There are two report options if you are modelling a river; a detailed report of each reach and a summary report listing only the totals of each compartment at the end of the simulation for each reach.

If you are not modelling a river, select the detail report.

OPTIONS:

- 0 - Detailed report
- 1 - Summary report

Enter selected option number: ? 0

FIGURE C.4. (Contd)

Upon completion of the run, an output file will be created on disk. This file can be viewed on the screen or spooled to the printer at the user's convenience. The report generated by APM for the sample input for the river simulation of Figure C.1 is given in Figure C.5. A printer report for a pond case simulation is shown in Figure C.6.

APMREACH

If a chemical is to be tracked through many similar reaches of a river, APMREACH may be used to quickly create the input file. APMREACH assumes that all reaches will have the same physical characteristics and that the same compartments will be considered for all reaches. APMREACH is an interactive input file generator which creates a file for a given chemical as opposed to a group of chemicals (APMSPILL). To execute APMREACH the user must provide:

1. The time period of the simulation
2. The number of the chemical in the CHEMRATE data base
3. The amount (liters) of chemical spilled into the aquatic system
4. The compartments which are to be considered
5. The physical characteristics of the selected compartments.

The code is initiated by typing: APMREACH

The interactive session will proceed similar to that of the APMSPILL session. The user will only be queried once for the characteristics of the chosen compartments. An example of the APMSPILL session is shown in Figure C.1.

To run the simulation of a selected chemical, the user types APM and proceeds as discussed in the previous section.

PROGRAM CONSIDERATIONS AND LIMITATIONS

At present, the input to the APM code can be generated by the APMSPILL code or the APMREACH code. The APMED program, which would build an input file for an individual chemical, has not been installed.

The first three compartments must be 1-water, 2-sediment, and 3-fish for the proper functioning of the concentration and bioaccumulation calculations. This restriction will be removed in later versions.

An entry on the selected chemical must be included in the CHEMRATE data base. If turnover rates are to be calculated in APM, the molecular weight, solubility, and vapor pressure of the chemical must be stored in CHEMRATE.

A>TYPE SAMPLE.OUT	
Input file name:	B: SAMPLE.1
Output file name:	SAMPLE.OUT
Title:	SAMPLE TWO REACH RIVER CASE
Executed on:	SEP 21, 1982 at: 14:30
Length of each time unit in hours:	.3
No. of iterations performed in each time step:	1
Total time of simulation (hrs)	30
Amount of chemical loaded into water compartment (g):	1690
Name and last update of chemical database:	
CHEMICAL AQUATIC RATE CONSTANT DATA BASE: 9-FEB-82 11:45 AM RAP	
Chemical:	PHENOL
Chemical also known as:	HYDROXYBENZENE
Molecular Formula:	C6H6O
Molecular Weight:	94.11
Solubility (ug/g):	91000
Vapor Pressure (mmHg):	.47
Temperature (solubility & VP - degrees C):	20
Log Octanol-water partition coefficient (KOW):	1.48
Log Soil organic matter-water partition coefficient:	0
Ultra-violet adsorption coefficient:	0
Dissociation constant (pKa):	9.89
Type of environment (1-pond, 2-river):	2
No. of reaches in flowing stream:	2
Flow rate of river (m ³ /hr):	100000
Number of compartments:	5
Compartment: WATER	
Volume of water in compartment (liters):	3E+10
Surface area of water (m ²):	3E+07
Average depth of water (m):	1
Compartment: SEDIMENT	
Total weight of sediment (kg):	750000
Percent of organic matter in sediment:	1
Compartment: FISH	
Total weight of fish (kg):	30
Weight of average fish (g):	300
Compartment: AIR	

FIGURE C.5. Printer Report for APM River Simulation

-----		-----	
The rate constant from:		per hour	
-----		-----	
SEDIMENT	to WATER	= 4.00153E-03	calculated in APM
FISH	to WATER	= .215286	calculated in APM
WATER	to SEDIMENT	= 1.47967E-08	calculated in APM
WATER	to FISH	= 1.81625E-09	calculated in APM
WATER	to AIR	= 3.48226E-04	calculated in APM
WATER	to BIODEGRADE	= .048	from CHEMRATE data base

Amount of chemical in each compartment for total time (grams):

-----	-----	-----	-----	-----	-----	-----
Reach No.	Chemical	WATER	SEDIMENT	FISH	AIR	BIODEGRADE
-----	-----	-----	-----	-----	-----	-----
1	0.16E+04	0.36E+03	0.35E-03	0.40E-05	0.90E+01	0.12E+04
2	0.81E+02	0.35E+02	0.13E-04	0.31E-06	0.17E+00	0.46E+02
-----	-----	-----	-----	-----	-----	-----
Total	0.17E+04	0.39E+03	0.37E-03	0.43E-05	0.91E+01	0.13E+04
% Total	1.00E+02	0.23E+02	0.22E-04	0.25E-06	0.54E+00	0.76E+02
Average						
Conc (ug/g)		0.98E-05	0.37E-06	0.11E-03		
-----	-----	-----	-----	-----	-----	-----

Chemical flowing out of system (g):

4.74069

A>

FIGURE C.5. (Contd)

Output file name:	OUTPOND.1
Title:	100 LITER COAL-LIQUID SPILL INTO POND # MAR 23, 1982 10:20
Executed on:	SEP 14, 1982 at: 7:35
Length of each time unit in hours:	.3
No. of iterations performed in each time step:	8
Total time of simulation (hrs)	30
Amount of chemical loaded into water compartment (g):	1700
Name and last update of chemical database:	
CHEMICAL AQUATIC RATE CONSTANT DATA BASE: 9-FEB-82 11:45 AM RAP	
Chemical:	PHENOL
Chemical also known as:	HYDROXYBENZENE
Molecular Formula:	C6H6O
Molecular Weight:	94.11
Solubility (ug/g):	91000
Vapor Pressure (mmHg):	.47
Temperature (solubility & VP - degrees C):	20
Log Octanol-water partition coefficient (KOW):	1.48
Log Soil organic matter-water partition coefficient:	0
Ultra-violet adsorption coefficient:	0
Dissociation constant (pKa):	9.89
Type of environment (1-pond, 2-river):	1
Number of compartments:	6
Compartment: WATER	
Volume of water in compartment (liters):	1E+08
Surface area of water (m ²):	100000
Average depth of water (m):	1
Compartment: SEDIMENT	
Total weight of sediment (kg):	2500
Percent of organic matter in sediment:	1
Compartment: FISH	
Total weight of fish (kg):	100
Weight of average fish (g):	100
Compartment: AIR	
Compartment: BIODEGRADE	
Compartment: PHOTOLYSIS	

FIGURE C.6. Printer Report for Pond Simulation

-----		-----	
The rate constant from:		per hour	
-----		-----	
SEDIMENT	to WATER	= 4.00153E-03	calculated in APM
FISH	to WATER	= .268189	calculated in APM
WATER	to SEDIMENT	= 1.47967E-08	calculated in APM
WATER	to FISH	= 2.26256E-06	calculated in APM
WATER	to AIR	= 3.48226E-04	calculated in APM
WATER	to BIODEGRADE	= .048	from CHEMRATE data base
WATER	to PHOTOLYSIS	= .00025	from CHEMRATE data base

Time (hr)	WATER	SEDIMENT	FISH	AIR	BIODEGRADE	PHOTOLYSIS	TOTAL
0.30E+00	0.17E+04	0.75E-05	0.11E-02	0.18E+00	0.24E+02	0.13E+00	0.17E+04
0.33E+01	0.14E+04	0.76E-04	0.77E-02	0.18E+01	0.25E+03	0.13E+01	0.17E+04
0.63E+01	0.13E+04	0.13E-03	0.97E-02	0.32E+01	0.44E+03	0.23E+01	0.17E+04
0.93E+01	0.11E+04	0.18E-03	0.97E-02	0.44E+01	0.61E+03	0.32E+01	0.17E+04
0.12E+02	0.94E+03	0.23E-03	0.90E-02	0.55E+01	0.76E+03	0.39E+01	0.17E+04
0.15E+02	0.81E+03	0.26E-03	0.80E-02	0.64E+01	0.88E+03	0.46E+01	0.17E+04
0.18E+02	0.70E+03	0.29E-03	0.71E-02	0.72E+01	0.99E+03	0.52E+01	0.17E+04
0.21E+02	0.60E+03	0.32E-03	0.62E-02	0.79E+01	0.11E+04	0.56E+01	0.17E+04
0.24E+02	0.52E+03	0.34E-03	0.54E-02	0.84E+01	0.12E+04	0.61E+01	0.17E+04
0.27E+02	0.45E+03	0.36E-03	0.46E-02	0.89E+01	0.12E+04	0.64E+01	0.17E+04
0.30E+02	0.40E+03	0.37E-03	0.41E-02	0.93E+01	0.13E+04	0.67E+01	0.17E+04
Final %	0.23E+02	0.22E-04	0.24E-03	0.55E+00	0.76E+02	0.39E+00	
Conc (ug/g)	0.40E-02	0.15E-03	0.41E-01				

FIGURE C.6. (contd)

A>

FIGURE C.6. (contd)

It is the user's responsibility to determine the validity of the time-step selection. This may require some trial and error testing. A simple test would be to halve the time step to see if this change has any effect on the simulation.

It is also the user's responsibility to select appropriately sized compartments in relation to other compartments and to the time-step selection. One area of concern is to size the compartments and the time step so that most of the chemical does not flow out of the system without its partitioning being tracked. This can quickly be checked using the following relationship:

$$\text{flow rate} * \frac{\text{length of time step}}{\text{no. of iterations}} * 1000 < \text{volume of water in reach}$$

Using program variables and units, the relationship can be stated as:

$$\frac{\text{FR m}^3}{\text{hr}} * \frac{\text{TK hr}}{\text{KK}} * \frac{1000 \text{ liters}}{\text{m}^3} < A(1,1) \text{ liters}$$

APPENDIX D

DATA BASE AND CODE LISTINGS

APPENDIX D

DATA BASE AND CODE LISTINGS

Listings of the data bases as they are currently used by APM are presented in this appendix. For information of the structure and organization of these files, refer to "File Descriptions" in Appendix B.

The contents of the following data bases are depicted: APMCMPRT (Figure D.1), APMVAR (Figure D.2), and CHEMRATE (Figure D.4). A directory of the CHEMRATE data base is presented, for the user's convenience, in Figure D.3. A listing of the entire APM code follows the listing of the data base.

Record No.	Compartment Name	No. of Variables	Default 1	Default 2	Default 3	Default 4	Default 5	Default 6
1	Water	5						
2	Sediment	2						
3	Fish	2						
4	Air	0						
5	Hydrolysis	0						
6	Biodegratio	0						
7	Metabolism	0						
8	Photolysis	0						

FIGURE D.1. APMCMPRT Aquatic Pathways Model Compartment Data Base

APMVAR
Aquatic Pathways Model variable data base

Compartment No.	Record No.	Text
	1	Title:
	2	Type of environment (1-pond, 2-river):
	3	No. of reaches in flowing stream:
	4	No. of compartments (1 to 16):
	5	Length of each time step in hours:
	6	No. of iterations performed in each time step:
	7	Amount of chemical loaded into water compartment (g):
	8	Flow rate of water (m ³ /hr):
	9	
	10	
	11	
	12	
1 (Water)	13	Volume of water in compartment (l):
	14	Surface area of water (m ²):
	15	Average depth of water (m):
	16	pH of water:
	17	Temperature of water (degrees C):
	18	
2 (Sediment)	19	Total weight of sediment (g):
	20	Percent of organic matter in sediment:
	21	
	22	
	23	
	24	
3 (Fish)	25	Total weight of fish (kg):
	26	Weight of average fish (g):
	27	
	28	
	29	
	30	

(Note: File continues for each compartment. There are no other variables stored in the file for APM.)

FIGURE D.2. APMVAR Aquatic Pathways Model Variable Data Base

CHEMRATE Directory

Chemical No.	Chemical Name
1	phenol
2	chlorpyrifos
3	resorcinol
4	1-naphthol
5	p-cresol
6	4-indanol
8	c2-phenol
9	c3-phenol
10	c4-phenol
12	o-cresol
13	m-cresol
14	hydroquinone
15	catechol
16	phenyl-phenol
17	2-naphthol
18	5-indanol
19	dimethyl resorcinol
20	c5-phenol
21	c1-indanol

FIGURE D.3. CHEMRATE Directory

CHEMICAL AQUATIC RATE CONSTANT DATA BASE: 9-FEB-82 11:45 AM RAP

CHEMRATE index no.	1
Chemical no. index:	
Molecular formula:	C6H6O
Molecular weight:	94.11
Chemical name:	PHENOL
Second chemical name:	HYDROXYBENZENE
Solubility (ug/g):	9.1E+4
Vapor pressure (mm Hg):	0.47
Temperature (degrees C):	20
Log octanol-water partition coef.	1.48
Log soil organic matter-water PC:	
Ultra-violet absorption:	
Dissociation constant:	9.89

The rate constant from WATER	to BIODEGRADE = .048	per hour
The rate constant from WATER	to PHOTOLYSIS = 2.5E-4	per hour

CHEMICAL AQUATIC RATE CONSTANT DATA BASE: 9-FEB-82 11:45 AM RAP

CHEMRATE index no.	2
Chemical no. index:	
Molecular formula:	
Molecular weight:	350
Chemical name:	CHLORPYRIFOS
Second chemical name:	
Solubility (ug/g):	2
Vapor pressure (mm Hg):	1.87E-5
Temperature (degrees C):	20
Log octanol-water partition coef.	4.81854
Log soil organic matter-water PC:	
Ultra-violet absorption:	
Dissociation constant:	

The rate constant from WATER	to SEDIMENT = .67	ml water/gm sediment/hr
The rate constant from WATER	to FISH = 55.5	ml water/gm fish/hr
The rate constant from WATER	to HYDROLYSIS = 9.6E-3	per hour
The rate constant from FISH	to METABOLISM = 7.8E-2	per hour

FIGURE D.4. Chemical Aquatic Rate Constant Data Base

CHEMICAL AQUATIC RATE CONSTANT DATA BASE: 9-FEB-82 11:45 AM RAP

CHEMRATE index no.	3
Chemical no. index:	
Molecular formula:	C6H6O2
Molecular weight:	110.11
Chemical name:	RESORCINOL
Second chemical name:	1-3 BENZENEDIOL
Solubility (ug/g):	1.23E+6
Vapor pressure (mm Hg):	.003
Temperature (degrees C):	20
Log octanol-water partition coef.	0.79
Log soil organic matter-water PC:	
Ultra-violet absorption:	
Dissociation constant:	9.81

The rate constant from WATER	to BIODGRADE = .016	per hour
The rate constant from WATER	to PHOTOLYSIS = 2.9E-3	per hour

CHEMICAL AQUATIC RATE CONSTANT DATA BASE: 9-FEB-82 11:45 AM RAP

CHEMRATE index no.	4
Chemical no. index:	
Molecular formula:	C10H8O1
Molecular weight:	144.19
Chemical name:	1-NAPHTHOL
Second chemical name:	1-HYDROXYNAPHTHALENE
Solubility (ug/g):	866
Vapor pressure (mm Hg):	.002
Temperature (degrees C):	20
Log octanol-water partition coef.	2.85
Log soil organic matter-water PC:	
Ultra-violet absorption:	
Dissociation constant:	9.34

The rate constant from WATER	to BIODGRADE = .01	per hour
The rate constant from SEDIMENT	to BIODGRADE = .01	per hour
The rate constant from WATER	to PHOTOLYSIS = 7.2E-4	per hour

FIGURE D.4. (Contd)

CHEMICAL AQUATIC RATE CONSTANT DATA BASE: 9-FEB-82 11:45 AM RAP

CHEMRATE index no. 5
 Chemical no. index:
 Molecular formula: C7H8O1
 Molecular weight: 108.15
 Chemical name: P-CRESOL
 Second chemical name: 4-HYDROXYTOLUENE
 Solubility (ug/g): 1.98E+4
 Vapor pressure (mm Hg): 0.17
 Temperature (degrees C): 20
 Log octanol-water partition coef. 1.93
 Log soil organic matter-water PC:
 Ultra-violet absorption:
 Dissociation constant: 10.17

The rate constant from WATER	to SEDIMENT	= 4.3E-3	ml water/gm sediment/hr
The rate constant from WATER	to AIR	= 4.E-3	cm water/hr
The rate constant from WATER	to BIODEGRADE	= .058	per hour
The rate constant from WATER	to PHOTOLYSIS	= 2.4E-3	per hour

CHEMICAL AQUATIC RATE CONSTANT DATA BASE: 9-FEB-82 11:45 AM RAP

CHEMRATE index no. 6
 Chemical no. index:
 Molecular formula: C9H10O1
 Molecular weight: 134.18
 Chemical name: 4-INDANOL
 Second chemical name: 4-HYDROXYINDAN
 Solubility (ug/g):
 Vapor pressure (mm Hg):
 Temperature (degrees C):
 Log octanol-water partition coef. 2.8
 Log soil organic matter-water PC:
 Ultra-violet absorption:
 Dissociation constant:

The rate constant from WATER	to PHOTOLYSIS	= 3.6E-4	per hour
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FIGURE D.4. (Contd)

CHEMICAL AQUATIC RATE CONSTANT DATA BASE: 9-FEB-82 11:45 AM RAP

CHEMRATE index no.	8
Chemical no. index:	
Molecular formula:	C8H10O1
Molecular weight:	122.17
Chemical name:	C2-PHENOL
Second chemical name:	
Solubility (ug/g):	
Vapor pressure (mm Hg):	.09
Temperature (degrees C):	20
Log octanol-water partition coef.	2.5
Log soil organic matter-water PC:	
Ultra-violet absorption:	
Dissociation constant:	

The rate constant from WATER	to BIODGRADE = .047	per hour
The rate constant from SEDIMENT	to BIODGRADE = .047	per hour

CHEMICAL AQUATIC RATE CONSTANT DATA BASE: 9-FEB-82 11:45 AM RAP

CHEMRATE index no.	9
Chemical no. index:	
Molecular formula:	C9H12O1
Molecular weight:	136.2
Chemical name:	C3-PHENOL
Second chemical name:	
Solubility (ug/g):	
Vapor pressure (mm Hg):	
Temperature (degrees C):	
Log octanol-water partition coef.	2.9
Log soil organic matter-water PC:	
Ultra-violet absorption:	
Dissociation constant:	

The rate constant from WATER	to BIODGRADE = .019	per hour
------------------------------	---------------------	----------

FIGURE D.4. (Contd)

CHEMICAL AQUATIC RATE CONSTANT DATA BASE: 9-FEB-82 11:45 AM RAP

CHEMRATE index no. 10
 Chemical no. index:
 Molecular formula: C10H14O1
 Molecular weight: 150.22
 Chemical name: C4-PHENOL
 Second chemical name:
 Solubility (ug/g):
 Vapor pressure (mm Hg):
 Temperature (degrees C):
 Log octanol-water partition coef. 3.25
 Log soil organic matter-water PC:
 Ultra-violet absorption:
 Dissociation constant:

The rate constant from WATER to BIODEGRADE = .009 per hour
 The rate constant from SEDIMENT to BIODEGRADE = .009 per hour

CHEMICAL AQUATIC RATE CONSTANT DATA BASE: 9-FEB-82 11:45 AM RAP

CHEMRATE index no. 12
 Chemical no. index:
 Molecular formula: C7H8O
 Molecular weight: 108.15
 Chemical name: O-CRESOL
 Second chemical name: 2 HYDROXY TOLUENE
 Solubility (ug/g): 2.5E+4
 Vapor pressure (mm Hg): .3
 Temperature (degrees C): 20
 Log octanol-water partition coef. 1.95
 Log soil organic matter-water PC:
 Ultra-violet absorption:
 Dissociation constant: 10.2

The rate constant from WATER to BIODEGRADE = .053 per hour
 The rate constant from WATER to PHOTOLYSIS = 8.E-4 per hour

FIGURE D.4. (Contd)

CHEMICAL AQUATIC RATE CONSTANT DATA BASE: 9-FEB-82 11:45 AM RAP

CHEMRATE index no.	13
Chemical no. index:	
Molecular formula:	C7H8O1
Molecular weight:	108.15
Chemical name:	M-CRESOL
Second chemical name:	3-HYDROXYTOLUENE
Solubility (ug/g):	2.23E+4
Vapor pressure (mm Hg):	.17
Temperature (degrees C):	20
Log octanol-water partition coef.	1.98
Log soil organic matter-water PC:	
Ultra-violet absorption:	
Dissociation constant:	10.01

The rate constant from WATER	to BIODEGRADE = .045	per hour
The rate constant from WATER	to PHOTOLYSIS = 8.E-4	per hour

CHEMICAL AQUATIC RATE CONSTANT DATA BASE: 9-FEB-82 11:45 AM RAP

CHEMRATE index no.	14
Chemical no. index:	
Molecular formula:	C6H6O2
Molecular weight:	110.11
Chemical name:	HYDROQUINONE
Second chemical name:	QUINOL
Solubility (ug/g):	7.18E+4
Vapor pressure (mm Hg):	.002
Temperature (degrees C):	20
Log octanol-water partition coef.	.54
Log soil organic matter-water PC:	
Ultra-violet absorption:	
Dissociation constant:	

The rate constant from WATER	to BIODEGRADE = .010	per hour
------------------------------	----------------------	----------

FIGURE D.4. (Contd)

CHEMICAL AQUATIC RATE CONSTANT DATA BASE: 9-FEB-82 11:45 AM RAP

CHEMRATE index no.	15
Chemical no. index:	
Molecular formula:	C6H6O2
Molecular weight:	110.11
Chemical name:	CATECHOL
Second chemical name:	1-2 BENZENEDIOL
Solubility (ug/g):	4.5E+5
Vapor pressure (mm Hg):	0.017
Temperature (degrees C):	20
Log octanol-water partition coef.	.95
Log soil organic matter-water PC:	
Ultra-violet absorption:	
Dissociation constant:	

The rate constant from WATER to BIODEGRADE = 0.039 per hour

CHEMICAL AQUATIC RATE CONSTANT DATA BASE: 9-FEB-82 11:45 AM RAP

CHEMRATE index no.	16
Chemical no. index:	
Molecular formula:	C12H10O
Molecular weight:	170.21
Chemical name:	PHENYL-PHENOL
Second chemical name:	
Solubility (ug/g):	
Vapor pressure (mm Hg):	
Temperature (degrees C):	
Log octanol-water partition coef.	3.4
Log soil organic matter-water PC:	
Ultra-violet absorption:	
Dissociation constant:	

FIGURE D.4. (Contd)

CHEMICAL AQUATIC RATE CONSTANT DATA BASE: 9-FEB-82 11:45 AM RAP

CHEMRATE index no.	17
Chemical no. index:	
Molecular formula:	C10H8O1
Molecular weight:	144.19
Chemical name:	2-NAPHTHOL
Second chemical name:	2-HYDROXYNAPHTHALENE
Solubility (ug/g):	626
Vapor pressure (mm Hg):	.001
Temperature (degrees C):	20
Log octanol-water partition coef.	2.84
Log soil organic matter-water PC:	
Ultra-violet absorption:	
Dissociation constant:	9.51

The rate constant from WATER	to BIODEGRADE = .01	per hour
The rate constant from SEDIMENT	to BIODEGRADE = .01	per hour
The rate constant from WATER	to PHOTOLYSIS = 7.2E-4	per hour

CHEMICAL AQUATIC RATE CONSTANT DATA BASE: 9-FEB-82 11:45 AM RAP

CHEMRATE index no.	18
Chemical no. index:	
Molecular formula:	C9H10O1
Molecular weight:	134.18
Chemical name:	5-INDANOL
Second chemical name:	5-HYDROXYINDAN
Solubility (ug/g):	
Vapor pressure (mm Hg):	
Temperature (degrees C):	
Log octanol-water partition coef.	2.7
Log soil organic matter-water PC:	
Ultra-violet absorption:	
Dissociation constant:	

The rate constant from WATER	to PHOTOLYSIS = 3.6E-4	per hour
------------------------------	------------------------	----------

FIGURE D.4. (Contd)

CHEMICAL AQUATIC RATE CONSTANT DATA BASE: 9-FEB-82 11:45 AM RAP

CHEMRATE index no.	19
Chemical no. index:	
Molecular formula:	C8H10O2
Molecular weight:	
Chemical name:	DIMETHYL RESORCINOL
Second chemical name:	
Solubility (ug/g):	
Vapor pressure (mm Hg):	
Temperature (degrees C):	
Log octanol-water partition coef.	1.6
Log soil organic matter-water PC:	
Ultra-violet absorption:	
Dissociation constant:	

The rate constant from WATER to PHOTOLYSIS = $2.9\text{E-}3$ per hour

CHEMICAL AQUATIC RATE CONSTANT DATA BASE: 9-FEB-82 11:45 AM RAP

CHEMRATE index no.	20
Chemical no. index:	
Molecular formula:	C11H16O1
Molecular weight:	164.25
Chemical name:	C5-PHENOL
Second chemical name:	BUTYL-METHYL
Solubility (ug/g):	
Vapor pressure (mm Hg):	
Temperature (degrees C):	
Log octanol-water partition coef.	3.55
Log soil organic matter-water PC:	
Ultra-violet absorption:	
Dissociation constant:	

FIGURE D.4. (Contd)

CHEMICAL AQUATIC RATE CONSTANT DATA BASE: 9-FEB-82 11:45 AM RAP

CHEMRATE index no.	21
Chemical no. index:	
Molecular formula:	C10H12O1
Molecular weight:	148.18
Chemical name:	C1-INDANOL
Second chemical name:	METHYLHYDROXYINDAN
Solubility (ug/g):	
Vapor pressure (mm Hg):	
Temperature (degrees C):	
Log octanol-water partition coef.	3.3
Log soil organic matter-water PC:	
Ultra-violet absorption:	
Dissociation constant:	

The rate constant from WATER to PHOTOLYSIS = $3.6E-4$ per hour

FIGURE D.4. (contd)

APMSPILL-1

```
1000 '----- Aquatic Pathways Model SRC Unit Spill Program -----
1005 '
1010 '--- written by R.A. Peloquin, P.J. Mellinger, D.A. Baker, R.L. Aaberg --
1020 '--- Pacific Northwest Laboratories, Battelle Northwest, Richland, WA ---
1030 '--- version of February 3, 1982
1032 '
1033 '--- This superstructure simulates a spill of solvent-refined coal -----
1034 '--- liquids into an aquatic environment.
1035 '
1036 '--- This module inputs spill and environmental information, creates in-
1037 '--- put files for each chemical for the Aquatic Pathways Model.
1038 '-----
1039 '
1040     DEFINT C, I-L, N-P
1042 '
1043     DIM CNS(16), A(16,6)
1044 '
1045     DIM CS(20), N4(20), DUMP(20), DPER(20)
1046 '
1049     N4 = 12                                'no of chemicals
1050     N4(1) = 1 : CS(1) = "PHENOL"           : DPER(1) = 16.9
1054     N4(2) = 12 : CS(2) = "O-CRESOL"       : DPER(2) = 8.1
1056     N4(3) = 5 : CS(3) = "P-CRESOL"       : DPER(3) = 16.9
1058     N4(4) = 13 : CS(4) = "M-CRESOL"       : DPER(4) = 12.4
1060     N4(5) = 8 : CS(5) = "C2-PHENOL"      : DPER(5) = 29.2
1062     N4(6) = 9 : CS(6) = "C3-PHENOL"      : DPER(6) = 9.6
1064     N4(7) = 10 : CS(7) = "C4-PHENOL"     : DPER(7) = 3.3
1066     N4(8) = 20 : CS(8) = "C5-PHENOL"     : DPER(8) = 0.3
1068     N4(9) = 18 : CS(9) = "5-INDANOL"     : DPER(9) = 5.3
1070     N4(10) = 21 : CS(10) = "C1-INDANOL"  : DPER(10) = 2.9
1072     N4(11) = 3 : CS(11) = "RESORCINOL"   : DPER(11) = 0.7
1073     N4(12) = 4 : CS(12) = "NAPHTHOL"    : DPER(12) = 0.4
1074 '
1076     I1$ = " ##### "
1078     I2$ = " #.##### "
1080     I3$ = " \          \"
1082     I4$ = "-----"
1088 '
1090     FOR I = 1 TO 20 : PRINT : NEXT I
1100     V1$ = "Aquatic Pathways Model of a Solvent-refined Coal Unit Spill"
1110     V2$ = "                Version of December 21, 1981"
1112     PRINT V1$ : PRINT V2$
1120     PRINT : PRINT : PRINT
1130 '
1140     PRINT "Enter date: "; : LINE INPUT DAT$
1150     PRINT
1160     PRINT "Enter time: "; : LINE INPUT TOD$
1170 '
1180     Set file names--
1200     F2$ = "SRC"
1210     F5$ = "APMDFLT"
1222     F7$ = "APMVAR"
```

APMSPILL-2

```
1224 F8$ = "APMCMPT"
1230 '
1235 OPEN "O", #2, F2$
1250 OPEN "R", #7, F7$
1260 OPEN "R", #8, F8$
1270 '
1272 FIELD #7, 128 AS Z$
1273 FIELD #8, 10 AS Z1$, 10 AS Z2$, 10 AS Z3$, 10 AS Z4$, 10 AS Z5$, 10 AS
1274 Z6$, 10 AS Z7$, 10 AS Z8$, 10 AS Z9$
1275 '
1275 Input input file prefix--
1276 PRINT : PRINT "Enter input file name prefix (up to 8 letters): ";
1277 INPUT F$
1278 '
1280 Input title of case--
1284 GET #7, 1 : L$ = Z$
1315 P3 = 3
1320 GOSUB 9000 ' C-I-T subroutine
1330 W$ = W$ + " # " + DAT$ + " " + TOD$
1335 T$ = W$
1340 PRINT #2, W$
1350 '
1352 Input length of each time step--
1354 GET #7, 5 : L$ = Z$ : P3 = 2
1356 GOSUB 9000
1358 PRINT #2, W2
1360 '
1362 Input no. of iterations for each time step--
1364 GET #7, 6 : L$ = Z$ : P3 = 1
1366 GOSUB 9000
1368 PRINT #2, W1%
1370 '
1372 PRINT : PRINT : PRINT
1374 PRINT "Enter amount of solvent-refined coal liquid spilled"
1376 PRINT "into the water (liter): ";
1378 INPUT SRC
1380 '
1382 Calculate amount of selected chemicals in SRC liquid--
1384 FOR I = 1 TO N4
1386 DUMP(I) = DPER(I) * SRC
1388 NEXT I
1390 '
1392 Input type of environment--
1394 GET #7, 2 : L$ = Z$
1396 W1M% = 1 : W1X% = 2 : P3 = 1
1400 GOSUB 9000 ' C-I-T subroutine
1410 P5 = W1%
1420 PRINT #2, P5
1440 '
1450 Input number of reaches for flowing model--
1480 IF W1% <> 2 THEN N1 = 1 : GOTO 1535
1490 GET #7, 3 : L$ = Z$
1510 W1M% = 1 : W1X% = 10 : P3 = 1
1520 GOSUB 9000 ' C-I-T subroutine
```

APMSPILL-3

```
1530      N1 = W1%
1535      PRINT #2, N1
1540 '
1545 '      input flow rate if river--
1550      IF P5 <> 2 THEN FR = 0 : GOTO 1570
1555          GET #7, 8 : L$ = Z$
1560          P3 = 2 : GOSUB 9000
1565          FR = W2
1570      endif
1580      PRINT #2, FR
1590 '
1600      FOR I = 1 TO N1                                'For each reach--
1610 '
1620          GET #7, 4 : L$ = Z$
1640          W1M% = 1 : W1X% = 16 : P3 = 1
1650          GOSUB 9000                                    ' C-I-T subroutine
1660          N2 = W1%
1670          PRINT #2, N2
1680 '
1690          FOR J = 1 TO N2                                'For each compartment--
1700 '
1705              GOSUB 9300                                'display compartment choices
1710              PRINT "Compartment No: "; : INPUT CN(J)
1730              GET #8, CN(J)
1740              N3 = VAL (Z3$)
1745              C$$(J) = Z2$
1750 '
1810              A(CN(J),1) = VAL (Z4$)
1820              A(CN(J),2) = VAL (Z5$)
1830              A(CN(J),3) = VAL (Z6$)
1840              A(CN(J),4) = VAL (Z7$)
1845              A(CN(J),5) = VAL (Z8$)
1846              A(CN(J),5) = VAL (Z9$)
1850 '
2000              FOR K = 1 TO N3                            'For each variable
2010 '
2020                  GET #7, 6*CN(J)+6+K : L$ = Z$ : P3=2
2140                  GOSUB 9000                            ' C-I-T subroutine
2150                  A(CN(J),K) = W2
2160 '
2170              NEXT K
2180 '
2190              PRINT #2, USING I1$; CN(J);
2192              PRINT #2, USING I3$; C$$(J);
2194              PRINT #2, USING I1$; N3;
2195              PRINT #2, USING I2$; A(CN(J),1), A(CN(J),2), A(CN(J),3);
2196              PRINT #2, USING I2$; A(CN(J),4), A(CN(J),5), A(CN(J),6)
2200 '
2210          NEXT J
2220      NEXT I
2230 '
2240 '
2500      Create individual input files for each chemical--
```


APMSPILL-4

```
2505 '
2510     FOR I = 1 TO N4
2520         CLOSE
2530         OPEN "I", #2, F2$
2540         OPEN "O", #4, F$ + "." + MIDS(STR$(I),2)
2550 '
2560         LINE INPUT #2, LS
2570         LS = LS + CS
2580         PRINT #4, LS
2590 '
2592         FOR J = 1 TO 2
2593             LINE INPUT #2, LS
2594             PRINT #4, LS
2596         NEXT J
2598 '
2600         PRINT #4, DUMP(I)
2602         PRINT #4, USING " ### "; N4(I);
2604         PRINT #4, C$(I)
2606 '
2608         FOR J = 1 TO 32767
2610             IF EOF(2) THEN GOTO 2690
2612             LINE INPUT #2, LS
2620             PRINT #4, LS
2630         NEXT J
2640 '
2690     NEXT I
2700 '
2710 '
2720 '     Print report--
2730 '
2740     LPRINT TAB(21); V1$ : LPRINT TAB(21); V2$ : LPRINT : LPRINT
2750     LPRINT TAB(21); "Case title: "; T$
2760     LPRINT TAB(21); "Amount of coal-liquid spilled: "; SRC; " liters"
2765     LPRINT : LPRINT : LPRINT
2770     LPRINT TAB(21); I4$; TAB(41); I4$; TAB(61); I4$; TAB(81); I4$
2810     LPRINT TAB(41); "Chemical (g)          Amount of";
2820     LPRINT TAB(81); "APM input"
2830     LPRINT TAB(21); "Chemical"; TAB(41); "per liter";
2840     LPRINT TAB(61); "Chemical (g)";
2845     LPRINT TAB(81); "File name"
2847     LPRINT TAB(41); "of liquid"; TAB(61); "in this spill"
2850     LPRINT TAB(21); I4$; TAB(41); I4$; TAB(61); I4$; TAB(81); I4$
2880     LPRINT
2890 '
2894     FOR I = 1 TO N4
2900         LPRINT TAB(21); C$(I);
2905         LPRINT TAB(45);
2910         LPRINT USING "###.##"; DPER(I);
2915         LPRINT TAB(63);
2920         LPRINT USING "#.#####"; DUMP(I);
2930         LPRINT TAB(81); F$ + "." + MIDS(STR$(I),2)
2940     NEXT I
2950 '
2960     END
```

APMSPILL-5

```
2970 '
8040 '-----
8050 '
9000 '      Input-Test Subroutine
9010 '
9020 '      Parameters passed by this subroutine:
9030 '          P3      P4      LS      W$      W1%      W1M%      W1X%
9040 '          W2      W2M      W2X
9050 '
9060 '      Print description and parameter--
9062 '      P2 = INSTR (LS,":") : IF P2 < 1 THEN P2 = 80
9064 '      LS = MID$ (LS, 1, P2) + " "
9070 '      PRINT : PRINT : PRINT : PRINT : PRINT : PRINT : PRINT
9080 '      ON P3 GOSUB 9500, 9600, 9700
9090 '
9230 '      RETURN
9240 '-----
9250 '
9260 '
9300 '      Display compartment choices subroutine--
9310 '
9320 '      PRINT : PRINT : PRINT : PRINT "Compartment choices:" : PRINT
9330 '      FOR IJ = 1 TO 8
9340 '          GET #8, IJ : LS = Z2$
9350 '          PRINT IJ; " - "; LS
9360 '      NEXT IJ
9370 '      PRINT : PRINT
9380 '      RETURN
9390 '-----
9399 '
9400 '
9500 '      Integer input--
9510 '      PRINT LS; : INPUT W1%
9520 '      IF P4 > 0 THEN IF W1% < W1M% OR W1% > W1X% THEN GOTO 9510
9530 '      RETURN
9540 '
9550 '
9600 '      Real input--
9610 '      PRINT LS; : INPUT W2
9620 '      IF P4 > 0 THEN IF W2 < W2M OR W2 > W2X THEN GOTO 9610
9630 '      RETURN
9640 '
9650 '
9700 '      String input--
9710 '      PRINT LS; : INPUT W$
9720 '      RETURN
9730 '
9740 '-----
9850 '-----
```

APMREACH-1

```
1000 '----- Aquatic Pathways Model Multiple Reach File Generator -----
1005 '
1010 '--- written by R.A. Peloquin, P.J. Mellinger, D.A. Baker, R.L. Aaberg --
1020 '--- Pacific Northwest Laboratories, Battelle Northwest, Richland, WA ---
1030 '--- version of January 6, 1982
1032 '
1033 '--- This superstructure simulates a spill of a chemical into a multi---
1034 '--- reach river.
1035 '
1036 '--- This module inputs spill and environmental information and creates
1037 '--- the input file for the Aquatic Pathways Model.
1038 '-----
1039 '
1040     DEFINT C, I-L, N-P
1042 '
1043     DIM CNS(16), A(16,6)
1044 '
1045     DIM CS(10), N4(10), DUMP(10)
1046 '
1076     I1$ = " ##### "
1078     I2$ = " #.##^+++"
1080     I3$ = "\          \"
1082     I4$ = "-----"
1088 '
1090     FOR I = 1 TO 20 : PRINT : NEXT I
1100     V1$ = "Aquatic Pathways Model of a Chemical Spill into a Multi-reach Riv
er"
1102     V2$ = " All parameters in river reaches are assumed to be constant."
1110     V3$ = "          Version of January 6, 1982"
1112     PRINT V1$ : PRINT V2$ : PRINT V3$
1120     PRINT : PRINT : PRINT
1130 '
1140     PRINT "Enter date: "; : LINE INPUT DAT$
1150     PRINT
1160     PRINT "Enter time: "; : LINE INPUT TOD$
1170 '
1180     Set file names--
1200     F2$ = "REACH1"
1205     F3$ = "REACH2"
1210     F5$ = "APMDFLT"
1222     F7$ = "APMVAR"
1224     F8$ = "APMCMPT"
1230 '
1235     OPEN "O", #2, F2$
1250     OPEN "R", #7, F7$
1260     OPEN "R", #8, F8$
1270 '
1272     FIELD #7, 128 AS Z$
1273     FIELD #8, 10 AS Z1$, 10 AS Z2$, 10 AS Z3$, 10 AS Z4$, 10 AS Z5$, 10 AS
Z6$, 10 AS Z7$, 10 AS Z8$, 10 AS Z9$
1274 '
1275     Input input file prefix--
1276     PRINT : PRINT "Enter input file name (up to 8 letters): ";
```

APMREACH-2

```
1277 INPUT F$
1278 '
1280 ' Input title of case--
1284 GET #7, 1 : LS = Z$
1315 P3 = 3
1320 GOSUB 9000 ' C-I-T subroutine
1330 WS = WS + " # " + DAT$ + " " + TOD$
1335 TS = WS
1340 PRINT #2, WS
1350 '
1352 ' Input length of each time step--
1354 GET #7, 5 : LS = Z$ : P3 = 2
1356 GOSUB 9000
1358 PRINT #2, W2
1360 '
1362 ' Input no. of iterations for each time step--
1364 GET #7, 6 : LS = Z$ : P3 = 1
1366 GOSUB 9000
1368 PRINT #2, W1%
1370 '
1372 PRINT : PRINT : PRINT
1374 PRINT "Enter amount of chemical spilled into the water (gram): ";
1378 INPUT DUMP
1379 PRINT #2, DUMP
1380 '
1382 PRINT : PRINT : PRINT
1384 PRINT "Enter chemical number in CHEMRATE data base: ";
1386 INPUT CN
1388 PRINT #2, CN
1390 '
1392 ' Input type of environment--
1394 GET #7, 2 : LS = Z$
1396 W1M% = 1 : W1X% = 2 : P3 = 1
1400 GOSUB 9000 ' C-I-T subroutine
1410 P5 = W1%
1420 PRINT #2, P5
1440 '
1450 ' Input number of reaches for flowing model--
1480 IF W1% <> 2 THEN N1 = 1 : GOTO 1535
1490 GET #7, 3 : LS = Z$
1510 W1M% = 1 : W1X% = 10 : P3 = 1
1520 GOSUB 9000 ' I-T subroutine
1530 N1 = W1%
1535 PRINT #2, N1
1540 '
1545 ' Input flow rate if river--
1550 IF P5 <> 2 THEN FR = 0 : GOTO 1570
1555 GET #7, 8 : LS = Z$
1560 P3 = 2 : GOSUB 9000
1565 FR = W2
1570 ' endif
1580 PRINT #2, FR
1590 '

```

APMREACH-3

```
1595      CLOSE #2
1600      OPEN "O", #3, F3$
1610
1620          GET #7, 4 : L$ = Z$
1640          WIM% = 1 : WIX% = 16 : P3 = 1
1650          GOSUB 9000                                ' C-I-T subroutine
1660          N2 = W1%
1670          PRINT #3, N2
1680
1690          FOR J = 1 TO N2                            'For each compartment--
1700
1705              GOSUB 9300                            'display compartment choices
1710              PRINT "Compartment No: "; : INPUT CN(J)
1730              GET #8, CN(J)
1740              N3 = VAL (Z3$)
1745              CNS(J) = Z2$
1750
1810              A(CN(J),1) = VAL (Z4$)
1820              A(CN(J),2) = VAL (Z5$)
1830              A(CN(J),3) = VAL (Z6$)
1840              A(CN(J),4) = VAL (Z7$)
1845              A(CN(J),5) = VAL (Z8$)
1846              A(CN(J),5) = VAL (Z9$)
1850
2000          FOR K = 1 TO N3                            'For each variable
2010
2020              GET #7, 6*CN(J)+6+K : L$ = Z$ : P3=2
2140              GOSUB 9000                                ' C-I-T subroutine
2150              A(CN(J),K) = W2
2160
2170          NEXT K
2180
2190          PRINT #3, USING I1$; CN(J);
2192          PRINT #3, USING I3$; CNS(J);
2194          PRINT #3, USING I1$; N3;
2195          PRINT #3, USING I2$; A(CN(J),1), A(CN(J),2), A(CN(J),3);
2196          PRINT #3, USING I2$; A(CN(J),4), A(CN(J),5), A(CN(J),6)
2200
2210      NEXT J
2220      CLOSE #3
2230
2240
2500      Create individual input files for each chemical--
2505
2530          OPEN "I", #2, F2$
2540          OPEN "O", #4, F$
2550
2560          LINE INPUT #2, L$
2570          L$ = L$ + C$
2580          PRINT #4, L$
2590
2608          FOR J = 1 TO 32767
2610              IF EOF(2) THEN GOTO 2645
2612              LINE INPUT #2, L$
```

APMREACH-4

```
2620      PRINT #4, LS
2630      NEXT J
2640
2645      CLOSE #2
2650
2655      FOR I = 1 TO N1
2660          OPEN "I", #3, F3$
2665          FOR J = 1 TO 32767
2670              IF EOF(3) THEN GOTO 2690
2675              LINE INPUT #3, LS
2680              PRINT #4, LS
2685          NEXT J
2690          CLOSE #3
2695      NEXT I
2700
2710      CLOSE
2720
2960      END
2970
-----
8040
8050      Input-Test Subroutine
9000
9010      Parameters passed by this subroutine:
9020          P3      P4      LS      WS      W1%      W1M%      W1X%
9030          W2      W2M      W2X
9040
9050      Print description and parameter--
9060      P2 = INSTR (LS,":") : IF P2 < 1 THEN P2 = 80
9064      LS = MID$ (LS, 1, P2) + " "
9070      PRINT : PRINT : PRINT : PRINT : PRINT : PRINT : PRINT
9080      ON P3 GOSUB 9500, 9600, 9700
9090
9230      RETURN
9240
-----
9250
9260      Display compartment choices subroutine--
9300
9310      PRINT : PRINT : PRINT : PRINT "Compartment choices:" : PRINT
9320      FOR IJ = 1 TO 8
9330          GET #8, IJ : LS = Z2$
9340          PRINT IJ; " - "; LS
9350      NEXT IJ
9360      PRINT : PRINT
9370      RETURN
9380
9390
-----
9399
9400      Integer input--
9500      PRINT LS; : INPUT W1%
9510      IF P4 > 0 THEN IF W1% < W1M% OR W1% > W1X% THEN GOTO 9510
9520      RETURN
9530
```

APMREACH-6

```
9540 '  
9550 '  
9600 '      Real input--  
9610       PRINT LS; : INPUT W2  
9620       IF P4 > 0 THEN IF W2 < W2M OR W2 > W2X THEN GOTO 9610  
9630       RETURN  
9640 '  
9650 '  
9700 '      String input--  
9710       PRINT LS; : INPUT WS  
9720       RETURN  
9730 '  
9740 '  
9850 '-----
```

APM-1

```
1000 '----- Aquatic Pathways Model for Toxic Chemicals -----
1005 '
1010 '--- written by R.A. Pelouin, P.J. Mellinger, D.A. Baker, R.L. Aaberg --
1020 '--- Pacific Northwest Laboratories, Battelle Northwest, Richland, WA ---
1030 '--- version of January 14, 1982 for the ALTOS
1032 '
1033 '--- This is the first in a series of compiled BASIC-80 programs which --
1034 '--- comprise this package. See files APMDOCxx for program documentation.
1035 '
1036 '--- This module inputs operator run options and inputs and checks file -
1037 '--- names.
1038 '-----
1039 '
1040     DEFINT C, I-L, N-P
1042 '
1043     DIM Q(100,16), R(16,16), CNS(16), A(16,6), P6(16,16)
1044 '
1046     COMMON DAT$, TOD$, F1$, F2$, F3$, F4$, F7$, F8$, P1
1048     COMMON Q(), R(), CNS(), KK, DT, A(), P6(), N1, N4, P8
1050 '
1065     ON ERROR GOTO 8000                'error handling routine
1070 '
1072     DT = 0 : KK = 0 : N1 = 0 : N4 = 0
1074 '
1076     FOR I = 1 TO 20 : PRINT : NEXT I
1100     PRINT "Aquatic Pathways Model of Chemicals in the Environment"
1110     PRINT : PRINT "          Version of January 14, 1982"
1120     PRINT : PRINT : PRINT
1130 '
1140     PRINT "Enter date: "; : LINE INPUT DAT$
1150     PRINT
1160     PRINT "Enter time: "; : LINE INPUT TOD$
1170 '
1180     Set file names--
1190     F1$ = "CHEMRATE"
1200     F2$ = " "
1210     F5$ = "APMDFLT"
1220     F6$ = "APMOPT"
1222     F7$ = "APMVAR"
1224     F8$ = "APMCMPRT"
1230 '
1240     Print option message from file--
1250     OPEN "I", #6, F6$
1260     FOR I = 1 TO 23
1270         LINE INPUT #6, L$
1280         PRINT L$
1290     NEXT I
1300 '
1310     Query for selected option--
1320     WHILE P1 < 1 OR P1 > 3
```


APM-2

```
1330      PRINT , "Enter selected option: ";
1340      INPUT L$
1350      P1 = VAL (L$)
1360      WEND
1370
1380      Print filename message--
1390      FOR I = 1 TO 23
1400          LINE INPUT #6, L$
1410          PRINT L$
1420      NEXT I
1430
1440      Query for old filename if applicable--
1450      IF P1 = 1 THEN F2$ = F5$ : GOTO 1600
1460          P2 = 0
1470          WHILE P2 < 3                                'three tries allowed
1480              PRINT , "Enter old filename: ";
1490              INPUT F2$
1510              P2 = P2 + 1
1520              OPEN "I", #2, F2$                        'if error, try again
1530              P2 = 99                                    'set flag for success
1535          WEND
1540
1550          IF P2 = 99 THEN GOTO 1590
1560              PRINT "Execution abnormally terminated!"
1570              PRINT "Could not find old file."
1580              STOP
1590      endif
1600      endif
1610
1620      Query for new filename--
1630      P2 = 0
1640      IF P1 = 2 THEN F3$ = F2$ : GOTO 1780
1650          WHILE P2 < 3
1655              CLOSE #3
1660              PRINT , "Enter new filename: ";
1670              INPUT F3$
1680              P2 = P2 + 1
1690              OPEN "I", #3, F3$
1710          WEND
1720
1730          IF P2 = 99 THEN GOTO 1772
1740              PRINT "Execution abnormally terminated!"
1750              PRINT "New filename already exists on disk."
1760              STOP
1770      else
1772          OPEN "O", #3, F3$
1774      endif
1776
1780      endif
1790
1800      Query for output filename--
1810      P2 = 0
1820      WHILE P2 < 3
```

APM-3

```
1825 '      CLOSE #4
1830      PRINT , "Enter output filename: ";
1840      INPUT F4$
1850 '      P2 = P2 + 1
1860      OPEN "O", #4, F4$
1870 '      WEND
1880 '
1885      P2 = 99
1890      IF P2 = 99 THEN GOTO 1930
1900      PRINT "Execution abnormally terminated!"
1910      PRINT "Output file name already exists on disk."
1920      STOP
1930 '      endif
1940 '
1960 '
1970 '      Query for report option--
1980      FOR I = 1 TO 23
1990          LINE INPUT #6, L$
2000          PRINT L$
2010      NEXT I
2020 '
2030      PRINT , "Enter selected option number: ";
2040      INPUT P8$ : P8 = VAL (P8$)
2050      IF P8<0 OR P8>1 THEN GOTO 2030
2060 '
2070      CLOSE
2080      IF P1 = 2 THEN FS = "APMCALC.COM" ELSE FS = "APMED.COM"
2090      CHAIN FS
2100 '
2110 '-----
7999 '
8000 '      Error handling subroutine
8010 '
8020      IF ERR <> 53 THEN GOTO 8080
8030          IF ERL = 1520 THEN CLOSE #2 : GOTO 1480
8040          P2 = 99
8070          IF ERL = 1690 THEN GOTO 1710
8075          IF ERL = 1860 THEN GOTO 1870
8077          PRINT "Line No: "; ERL, "Error No: "; ERR
8080 '      endif
8090 '
8100      PRINT "Line No: "; ERL, "Error No: "; ERR
8110      STOP
8120 '
8130 '-----
```

APMCALC-1

```
1000 '--- Aquatic Pathways Model for Toxic Chemicals Calculation Program -----
1010 '
1020 '--- written by R.A. Peloquin, P.J. Mellinger, D.A. Baker, R.L. Aaberg --
1030 '--- Pacific Northwest Laboratories, Battelle Northwest, Richland, WA ---
1040 '--- version of SEPTEMBER 13, 1982.
1050 '
1060 '--- This is the third in a series of compiled BASIC-80 programs which
1070 '--- comprise this package. See files APMDOCxx for program documentation.
1080 '
1090 '--- This module reads information for each reach, calculates rate
1091 '--- constants and performs the mass balance calculations using the
1092 '--- Runge-Kutta method to solve the differential equations. A report
1094 '--- on each reach (or the lake or pond) is written to the report file.
1098 '
1100 '-----
1102 '
1104     DEFINT C, I-L, N-P
1110 '
1112     COMMON DAT$, TOD$, F1$, F2$, F3$, F4$, F7$, F8$, P1
1114 '
1148     DIM X(16), XD(16), AX(16), XP(16), XQ(16), XR(16)
1150     DIM R(16,16), A(16,6), Z%(50), CN(16), CNS(16), RS(3)
1160     DIM Q(100,16), B(16,1), QI(16,1), P6(16,16), RCS(16)
1165 '
1170     COMMON Q(), R(), CNS(), KK, DT, A(), P6 (), N1, N4, P8
1180 '
1190     DIM CON!(3), QUALS(10), QR(100), STOT(16), T2(16)
1192 '
1194     QUALS(1) = "calculated in APM"
1196     QUALS(2) = "from CHEMRATE data base"
1200 '
1205     DIM GRAPHS(40)                                'graph storage array
1210     NCOL = 100                                     'number of rows in graph
1215     NLINE = 40                                    'number of lines in graph
1220 '
1225     I5$ = " .## + + + + "
1230     I4$ = " .## ^ + + : "
1235 '
1240 '
1245     Open files--
1250     OPEN "I", #3, F3$
1255     OPEN "O", #4, F4$
1260     OPEN "R", #1, F1$
1265     OPEN "R", #7, F7$
1270     OPEN "R", #8, F8$
1272 '
1274     FIELD #7, 128 AS Z$
1276 '
1278     GOSUB 1320                                     'print QA report
1280 '
1281     FOR IJK = 1 TO N1                             'for each reach--
1282 '

```

APMCALC-2

```

1283      IF P5=2 AND P8=0 THEN GOSUB 9600      'print river reach heading
1284      GOSUB 1620                          'read input file
1285      GOSUB 2300                          'rate constants
1286      GOSUB 4000                          'simulation routine
1287      IF P8 >0 THEN GOSUB 7000 ELSE GOSUB 5000      'report
1288      IF P8 = 1 THEN P8 = 2                'set flag for summary report
1289
1290      NEXT IJK
1291
1292
1294      IF P8>0 THEN GOSUB 7200
1296      IF P5=2 THEN GOSUB 9700 : GOSUB 9750
1298      FOR I = 1 TO 10 : PRINT CHR$(7) : NEXT I      'ring bell
1300
1316      END
1318
1320      ----- Q A subroutine -----
1321
1322      Print file names--
1324      PRINT #4, "Input file name: "; TAB(60); F3$
1326      PRINT #4, "Output file name: "; TAB(60); F4$
1328
1330      Print title of case, date and time--
1332      RL% = 1 : GOSUB 9100
1334      LINE INPUT #3, W$
1336      PRINT #4, CHR$(13) : PRINT #4, CHR$(13) : PRINT #4, L$; TAB(60); W$
1338      PRINT #4, "Executed on: "; TAB(60); DAT$; " at: "; TOD$
1340
1342
1344      Print time information--
1346
1348      RL% = 5 : GOSUB 9100                  'length of time step
1350      LINE INPUT #3, W$
1352      TK = VAL (W$)
1354      TIME = TK * 100
1356      PRINT #4, CHR$(13) : PRINT #4, L$; TAB(60); TK
1358
1360      RL% = 6 : GOSUB 9100                  'no.of iterations for each time step
1362      LINE INPUT #3, W$ : KK = VAL (W$)
1364      PRINT #4, L$; TAB(60); W$
1365
1366      Print total time of simulation--
1367      PRINT #4, "Total time of simulation (hrs)"; TAB(60); TIME
1368
1369      Print loading information--
1370      RL% = 7 : GOSUB 9100
1372      LINE INPUT #3, W$ : DUMP = VAL (W$)
1374      PRINT #4, L$; TAB(60); DUMP
1376
1378      Print chemical information--
1380
1382      PRINT #4, CHR$(13) : PRINT #4, CHR$(13) : PRINT #4, CHR$(13)
1384
1386      FIELD #1, 128 AS R1$
1388      GET #1, 1 : L$ = R1$

```

APMCALC-3

```

1390 PRINT #4, "Name and last update of chemical database: "
1392 PRINT #4, TAB(10); LS
1394
1396 FIELD #1, 4 AS R2$, 12 AS R3$, 8 AS R4$, 20 AS R5$, 20 AS R6$, 8 AS R7$,
      8 AS R8$, 8 AS R9$, 8 AS R10$, 8 AS R11$, 8 AS R12$, 8 AS R13$
1400 LINE INPUT #3, WS
1402 N4 = VAL (MIDS (WS, 1, 4))
1404 GET #1, N4*17+1
1406 MF$ = R3$                                'molecular formula
1408 MW = VAL (R4$)                            'molecular weight
1410 CS = R5$                                'chemical name
1412 C2$ = R6$                                'second name for chemical
1414 S = VAL (R7$)                            'solubility
1416 VP = VAL (R8$)                          'vapor pressure
1418 T = VAL (R9$)                            'temperature at which S and VP apply
1420 KOW! = VAL (R10$)                        'octanol-water partition coefficient
1422 KOC! = VAL (R11$) 'soil organic matter-water partition coefficient
1424 UVA = VAL (R12$)                        'ultra-violet adsorption
1426 DC = VAL (R13$)                        'dissociation constant
1428
1429 PRINT #4, CHR$(13)
1430 PRINT #4, "Chemical: "; TAB(60); C$
1432 PRINT #4, CHR$(13)
1434 PRINT #4, " Chemical also known as: "; TAB(60); C2$
1436 PRINT #4, " Molecular Formula: "; TAB(60); MF$
1438 PRINT #4, " Molecular Weight: "; TAB(60); MW
1440 PRINT #4, " Solubility (ug/g): "; TAB(60); S
1442 PRINT #4, " Vapor Pressure (mmHg): "; TAB(60); VP
1444 PRINT #4, " Temperature (solubility & VP - degrees C): "; TAB(60); T
1446 PRINT #4, " Log Octanol-water partition coefficient (KOW): "; TAB(60); KOW!
1448 PRINT #4, " Log Soil organic matter-water partition coefficient: "; TAB(60); KOC!
1450 PRINT #4, " Ultra-violet adsorption coefficient: "; TAB(60); UVA
1452 PRINT #4, " Dissociation constant (pKa): "; TAB(60); DC
1454 PRINT #4, CHR$(13) : PRINT #4, CHR$(13)
1456
1458
1460 Print type of environment--
1462 RL% = 2 : GOSUB 9100
1464 LINE INPUT #3, WS
1466 PRINT #4, CHR$(13) : PRINT #4, CHR$(13) : PRINT #4, LS; TAB(60); WS
1468 P5 = VAL (WS)
1470
1472 Print number of reaches for flowing model--
1474 RL% = 3 : GOSUB 9100
1476 LINE INPUT #3, WS
1478 N1 = VAL (WS)
1482 IF P5 = 2 THEN PRINT #4, LS; TAB(60); N1
1484
1490 Print flow rate of water if river--
1500 RL% = 8 : GOSUB 9100
1510 LINE INPUT #3, WS
1520 FR = VAL (WS)
1530 IF P5=2 THEN PRINT #4, LS; TAB(60); FR

```

APMCALC-4

```

1540 '
1570 '
1580     RETURN
1616 '
1618 '-----
1619 '
1620 '   Input information specific to this reach--
1622 '
1625     RL% = 4 : GOSUB 9100
1630     LINE INPUT #3, WS                      'Input number of compartments
1660     N2 = VAL (WS)
1670     IF P8<2 THEN PRINT #4, L$; TAB(60); N2
1675     IF P8<2 THEN PRINT #4, CHR$(13) : PRINT #4, CHR$(13)
1680 '
1690     FOR J = 1 TO N2                          'For each compartment--
1700 '
1710         LINE INPUT #3, WS
1712         CN(J) = VAL (MID$(WS, 1, 10))
1714         CNS(J) = MID$(WS, 11, 10)
1716         N3 = VAL (MID$(WS, 21, 10))
1718 '
1720         IF P8<2 THEN PRINT #4, "Compartment: "; CNS(J)
1730 '
2000         FOR K = 1 TO N3                      'For each variable
2010 '
2120             RL% = (CN(J)+1) * 6 +K : GOSUB 9100
2130             A(CN(J),K) = VAL (MID$(WS,K*10+21,10)) 'parameter values
2140             IF P8<2 THEN PRINT #4, TAB(10); L$; TAB(60); A(CN(J),K)
2160 '
2170         NEXT K
2180 '
2190         IF P8<2 THEN PRINT #4, CHR$(13)
2210     NEXT J
2230     RETURN
2235 '
2242 '-----
2250 '
2260 '
2300     Rate constants subroutine--
2310 '
2500     FOR I = 1 TO N2                          'initialize rate constant array
2510         FOR J = 1 TO N2
2520             R(I,J) = 0!
2530         NEXT J
2540     NEXT I
2550 '
2555     IF T = 0 THEN T = 20
2556 '
2560     Calculate KOW if not known--
2570     IF KOW!=0 AND S>0 THEN KOW! = 5.0 - .67*(LOG (S*1000/MW) /LOG(10))
2712 '
2714     I1=3 : I2=1 : GOSUB 9300 : IF P7=0 THEN GOTO 2727
2718     EOX = .75

```

APMCALC-5

```

2720          E = .07 * KOW! - .02
2722          Q = .3 * A(3,2) + .8
2724          MCOX = 14.45 - .413 * T + .00556 * T 2
2726          R(J1,J2) = 1430! * E / A(3,2) * Q / EOX / MCOX      'water to fish
2727
2728          I1=4 : I2=1 : GOSUB 9300 : IF P7=0 THEN GOTO 2737
2729          IF VP = 0 OR S = 0 THEN GOTO 2737
2730          EL = 20! * (44! / MW) + .5
2732          EG = 3000! * (18! / MW) + .5
2734          H = (T + 273) * S / VP / MW / 16.04
2736          R(J1,J2) = 1 / ( 1 / EL + H / EG)                    'water to air
2737
2738          I1=2 : I2=1 : GOSUB 9300                                'water to sediment
2739          IF P7=1 THEN R(J1,J2) = 4.02E-05 * (KOW! + 6.86)
2740
2741          GOSUB 9500
2742
2743          Get experimental rate constants from file--
2744
2745          FIELD #1, 8 AS RC$(1), 8 AS RC$(2), 8 AS RC$(3), 8 AS RC$(4), 8 AS RC$(5),
2746                  8 AS RC$(6), 8 AS RC$(7), 8 AS RC$(8)
2747
2748          FOR I = 1 TO N2                                          'for each column of matrix
2749
2750              GET #1, N4 * 17 + 1 + CN(I)
2751
2752              FOR J = 1 TO N2
2753                  P6(I,J) = 1
2754                  FOR K = 1 TO 8
2755                      IF CN(J) <> K THEN GOTO 2802
2756                      IF VAL(RC$(K)) = 0 THEN GOTO 2804
2757                      R(I,J) = VAL (RC$(K))
2758                      P6(I,J) = 2
2759                  endif
2760              endif
2761              GOTO 2804
2762          NEXT K
2763          NEXT J
2764
2765          NEXT I
2766          GOSUB 9500
2767
2768          Adjust rate constants--
2769
2770          I1=2 : I2=1 : GOSUB 9300 : IF P7=0 THEN GOTO 2820
2771          R(J1,J2) = R(J1,J2) * A(2,1) / A(1,1)                'water to sedient
2772
2773          I1=3 : I2=1 : GOSUB 9300
2774          IF P7=1 THEN R(J1,J2) = R(J1,J2) * A(3,1) / A(1,1)    'water to fish
2775
2776          I1=4 : I2=1 : GOSUB 9300
2777          IF P7=1 THEN R(J1,J2) = R(J1,J2) * A(1,2) / A(1,1)*10. 'evaporation
2778
2779          I1=1 : I2=2 : GOSUB 9300 : IF P7=0 THEN GOTO 2836
2780          IF P6(I1,I2) > 1 THEN GOTO 2833

```

APMCALC-6

```

2831         IF KOC!=0! THEN KOC! = KOW! - 0.31
2832         R(I1,I2) = R(I2,I1) / 10 + KOC! / A(2,2) * 100.
2833     endif
2834         R(I1,I2) = R(I1,I2) / A(2,1) * A(1,1)           'sediment to water
2836     endif
2838
2839     I1=1: I2=3 : GOSUB 9300 : IF P7=0 THEN GOTO 2846
2840     IF P6(I1,I2) > 1 THEN GOTO 2846
2842         R(I1,I2) = R(I2,I1) / 10 + (.124 + .542 * KOW!)
2844         R(I1,I2) = R(I1,I2) / A(3,1) * A(1,1)           'fish to water
2846     endif
2848
2900     GOSUB 9500
3000     IF P8<2 THEN GOSUB 3500
3010
3020     RETURN
3030
3040 -----
3050
3500     Print rate constants for selected chemical (non-zero only)--
3502
3504     FOR IJ = 1 TO 3 : PRINT #4, CHR$(13) : NEXT IJ
3506     PRINT #4, "-----"; TAB(30); "-----"
3512     PRINT #4, "The rate constant from:"; TAB(32); "per hour"
3514     PRINT #4, "-----"; TAB(30); "-----"
3516
3520     FOR I = 1 TO N2                                     'for each row of matrix
3530         FOR J = 1 TO N2                                 'for each column of matrix
3540
3550             IF J = I THEN GOTO 3620
3560             IF R(I,J) = 0! THEN GOTO 3620
3590             L$ = C$(J)+" to "+C$(I)+" = "
3600             PRINT #4, L$; TAB(29); R(I,J); TAB(44); QUALS(P6(I,J))
3610
3620         NEXT J
3630     NEXT I
3640
3650     RETURN
3660
3670 -----
4000
4010     Simulation routine--
4015
4020     FOR J = 1 TO N2                                     'initialize temporary accumulators
4025         X(J) = 0.
4030     NEXT J
4035     IF IJK = 1 THEN X(1) = DUMP                         'initial chemical in H2O
4040
4045     FOR J = 1 TO N2                                     'initialize partitioning array
4050         FOR K = 1 TO 100
4052             Q(K,J) = 0.
4054         NEXT K
4056     NEXT J

```


APMCALC-7

```
4057 '
4058 IF P8>1 THEN GOSUB 9700 : RIN = TOT
4059 '
4060 FOR IJ = 1 TO 100                                'start simulation
4071 PRINT IJK, "IJ = "; IJ, "QR(IJ) = "; QR(IJ)
4080 '
4090 DT = 1 / KK * TK                                'delta T
4095 X(1) = X(1) + QR(IJ)
4100 '
4110 FOR JJ = 1 TO KK                                'start iterative integration loop
4120 '
4125 FOR I = 1 TO N2 'initialize intermediate total rate accumulators
4126 XD(I) = 0.
4127 XP(I) = 0.
4128 XO(I) = 0.
4129 XR(I) = 0.
4130 NEXT I
4131 '
4132 FOR I = 1 TO N2                                'compute dX/dt at time j-1
4135 '
4140 FOR J = 1 TO N2 : T2(J)=0. : NEXT J
4145 '
4170 FOR J = 1 TO N2
4172 IF R(J,I) = 0! THEN GOTO 4179
4175 TEMP = R(J,I) * X(I)
4176 T2(I) = T2(I) - TEMP
4177 T2(J) = TEMP
4179 NEXT J
4180 '
4181 T4 = T2(I) * DT/2.
4182 IF T4 + X(I) => 0. THEN GOTO 4188
4183 T3 = ABS (X(I) / T4)
4185 FOR J = 1 TO N2
4186 T2(J)=T2(J)*T3
4187 NEXT J
4188 endif
4189 '
4190 FOR J = 1 TO N2
4192 XD(J) = XD(J) + T2(J)
4194 NEXT J
4195 '
4210 FOR K = 1 TO N5 : XD(I) = XD(I) + B(I,K) * QI(K) : NEXT K
4250 NEXT I
4260 '
4280 FOR I = 1 TO N2                                '1st estimate of state (P) at time IJ-1/2
4290 AX(I) = X(I) + (DT/2) * XD(I)
4300 NEXT I
4310 '
4320 FOR I = 1 TO N2                                'compute dX/dt at P
4325 '
4340 FOR J = 1 TO N2 : T2(J)=0. : NEXT J
4345 '
4360 FOR J = 1 TO N2
```

APMCALC-8

```
4362         IF R(J,I) = 0! THEN GOTO 4368
4365         TEMP = R(J,I) * AX(I)
4366         T2(I) = T2(I) - TEMP
4367         T2(J) = TEMP
4368     NEXT J
4369 '
4370     T4 = DT/2 * T2(I)
4371     IF T4 + AX(I) => 0. THEN GOTO 4388
4372     T3 = ABS (AX(I) / T4)
4374     FOR J = 1 TO N2
4376         T2(J)=T2(J)*T3
4378     NEXT J
4388 'endif
4390 '
4392     FOR J = 1 TO N2
4394         XP(J) = XP(J) + T2(J)
4396     NEXT J
4398 '
4400     FOR K = 1 TO N5 : XP(I) = XP(I) + B(I,K) * QI(K) : NEXT K
4450 NEXT I
4460 '
4480     FOR I = 1 TO N2      '2nd estimate of state (Q) at time IJ-1/2
4490         AX(I) = X(I) + (DT/2) * XP(I)
4500     NEXT I
4510 '
4520 '
4530     FOR I = 1 TO N2      'compute dX/dt at Q
4535 '
4550         FOR J = 1 TO N2 : T2(J)=0. : NEXT J
4555 '
4570         FOR J = 1 TO N2
4572             IF R(J,I) = 0! THEN GOTO 4578
4575             TEMP = R(J,I) * AX(I)
4576             T2(I) = T2(I) - TEMP
4577             T2(J) = TEMP
4578         NEXT J
4579 '
4580         T4 = DT * T2(I)
4581         IF T4 + AX(I) => 0. THEN GOTO 4588
4582         T3 = ABS (AX(I) / T4)
4583         FOR J = 1 TO N2
4584             T2(J)=T2(J)*T3
4585         NEXT J
4588 'endif
4589 '
4590         FOR J = 1 TO N2
4592             XQ(J) = XQ(J) + T2(J)
4594         NEXT J
4596 '
4610         FOR K = 1 TO N5 : XQ(I) = XQ(I) + B(I,K) * QI(K) : NEXT K
4650 NEXT I
4660 '
4680     FOR I = 1 TO N2      'make estimate of state (R) at time J
4690         AX(I) = X(I) + DT * XQ(I)
```

APMCALC-9

```

4700      NEXT I
4710 '
4720 '
4730      FOR I = 1 TO N2                      'compute dX/dt at R
4735 '
4740          FOR J = 1 TO N2 : T2(J) = 0. : NEXT J
4742 '
4770          FOR J = 1 TO N2
4772              IF R(J,I) = 0! THEN GOTO 4778
4775              TEMP = R(J,I) * AX(I)
4776              T2(I) = T2(I) - TEMP
4777              T2(J) = TEMP
4778          NEXT J
4779 '
4780          T4 = DT * T2(I)
4781          IF T4 + AX(I) => 0. THEN GOTO 4786
4782          T3 = ABS (AX(I) / T4)
4783          FOR J = 1 TO N2
4784              T2(J) = T2(J) * T3
4785          NEXT J
4786          ENDIF
4788 '
4790          FOR J = 1 TO N2
4792              XR(J) = XR(J) + T2(J)
4794          NEXT J
4795 '
4810          FOR K = 1 TO N5 : XR(I) = XR(I) + B(I,K) * QI(K) : NEXT K
4850      NEXT I
4860 '
4880      FOR I = 1 TO N2                      'compute final values for state at time J
4900          X(I) = X(I) + DT * (XD(I)/6 + XP(I)/3 + XQ(I)/3 + XR(I)/6)
4920      NEXT I
4930 '
4940      NEXT JJ
4942 '
4944      QR(IJ) = FR * DT * X(1) / A(1,1) * 1000!
4945      X(1) = X(1) - QR(IJ)
4950 '
4955      FOR I = 1 TO N2                      'store compartment mases at time J in matrix
4960          Q(IJ,I) = X(I)
4965      NEXT I
4970 '
4975      NEXT IJ                              'end of iterative integration loop
4976 '
4977      IF P8>0 THEN GOSUB 9700 : ROUT = TOT
4980 '
4985      RETURN
4990 '
5000 -----
5010 '
5020      Report subroutine--
5710 '
5720      Print table of mass in each compartment at 10 times--

```

APMCALC-10

```

5730 '
5735 PRINT #4, CHR$(13) : PRINT #4, CHR$(13) : PRINT #4, CHR$(13)
5740 GOSUB 9000 'print heading
5750 PRINT #4, "Time (hr) ";
5760 FOR I = 1 TO N2
5770 PRINT #4, CNS(I); " ";
5790 NEXT I
5790 PRINT #4, "TOTAL"
5800 GOSUB 9000
5810 '
5820 FOR I = 1 TO 100 STEP 10
5830 GOSUB 9200 ' print detail line
5840 NEXT I
5850 I = 100 : GOSUB 9200 'print last time step info
5880 GOSUB 9000
5890 '
5900 Print percent of total in each compartment for final time step--
5902 PRINT #4, "Final % ";
5904 FOR J = 1 TO N2
5906 PRINT #4, USING I5$; Q(100,J) / TOT * 100!;
5908 NEXT J
5910 PRINT #4, CHR$(13)
5912 '
5914 CON!(1) = Q(100,1) * 1E3 / A(1,1) 'calculate concentrations
5916 CON!(2) = Q(100,2) * 1E3 / A(2,1)
5918 CON!(3) = Q(100,3) * 1E3 / A(3,1)
5920 GOSUB 8200
5946 '
5950 GOSUB 9000
6000 '
6010 Print graph of function--
6020 '
6025 PRINT #4, CHR$(13) : PRINT #4, CHR$(13) : PRINT #4, CHR$(13)
6030 PRINT #4, TAB(31); "Amount of "; C$; " in each compartment vs. time:"
6040 '
6050 QMAX = 0 'determine largest quantity in any compartment
6060 FOR I = 1 TO N2
6070 FOR J = 1 TO 100
6080 IF Q(J,I) > QMAX THEN QMAX = Q(J,I)
6090 NEXT J
6100 NEXT I
6110 '
6120 FOR I = 1 TO NLINE 'initialize graph array
6130 GRAPHS(I) = STRING$(NCOL, " ")
6140 NEXT I
6150 '
6160 YINC = QMAX / NLINE 'y-axis increment
6170 '
6180 FOR I = 1 TO N2 'store each value in graph array
6190 FOR J = 1 TO NCOL
6200 '
6210 K = NLINE - Q(J,I) / YINC
6220 IF K > NLINE THEN K = NLINE

```

APMCALC-11

```
6230         IF K < 1 THEN K = 1
6240
6250         X$ = MID$(GRAPH$(K), J, 1)
6260         IF X$ = " " THEN X$ = STR$(I) ELSE X$ = "*"
6270         X$ = RIGHT$(X$, 1)
6280
6290         MID$(GRAPH$(K), J, 1) = X$
6300
6310     NEXT J
6320 NEXT I
6330
6340     Print graph--
6350
6360     PRINT #4, USING I4$: QMAX; : PRINT #4, " "; STRING$(NCOL+2, "-")
6365
6370     FOR I = 1 TO N2                                     'print graph and legend
6380         PRINT #4, TAB(11); "!"; LEFT$(GRAPH$(I), NCOL); "!";
6390         PRINT #4, STR$(I); " - "; CN$(I)
6400     NEXT I
6410
6412     FOR I = N2+1 TO NLINE
6414         PRINT #4, TAB(11); "!"; LEFT$(GRAPH$(I), NCOL); "!"
6416     NEXT I
6418
6420     PRINT #4, TAB(11); STRING$(NCOL+2, "-"); " "; TIME; " hrs"
6430
6440
6450     RETURN
6460
6480 -----
6490
7000     Print summary report--
7010
7015     IF P8=1 THEN GOSUB 8000                               'heading
7020     IF P8=1 THEN RIN = DUMP
7025
7030     RSYS = RIN - ROUT
7035     STOT = STOT + RSYS
7040
7045     PRINT #4, USING " ###"; IJK;
7046     PRINT #4, " ";
7050     PRINT #4, USING I5$: RSYS;
7055
7060     FOR IJ = 1 TO N2
7065         PRINT #4, USING I5$: Q(100, IJ);
7070         STOT(IJ) = STOT(IJ) + Q(100, IJ)
7075     NEXT IJ
7080
7085     PRINT #4, CHR$(13)
7090     RETURN
7095
7096 -----
7097
7200     Print summary report tailer--
```

APMCALC-12

```
7210 '
7220     GOSUB 9000
7230 '
7240     PRINT #4, "Total      ";
7250     PRINT #4, USING I5$; STOT;
7260     FOR IJ = 1 TO N2
7270         PRINT #4, USING I5$; STOT(IJ);
7280     NEXT IJ
7290     PRINT #4, CHR$(13)
7300 '
7310     PRINT #4, "% Total      ";
7320     PRINT #4, USING I5$; STOT / DUMP * 100.;
7330     FOR IJ = 1 TO N2
7340         PRINT #4, USING I5$; STOT(IJ) / DUMP * 100.;
7350     NEXT IJ
7355     PRINT #4, CHR$(13)
7356 '
7358     CON!(1) = STOT(1) * 1E3 / A(1,1) / N1
7360     CON!(2) = STOT(2) * 1E3 / A(2,1) / N1
7362     CON!(3) = STOT(3) * 1E3 / A(3,1) / N1
7364     GOSUB 8200
7366     GOSUB 9000
7370 '
7380     RETURN
7390 '
7400 -----
7410 '
8000     Print summary report heading--
8010 '
8015     FOR IJ = 1 TO 4 : PRINT #4, CHR$(13) : NEXT IJ
8016     PRINT #4, "Amount of chemical in each compartment for total time";
8017     PRINT #4, " (grams): "
8018     PRINT #4, CHR$(13)
8020     GOSUB 9000
8030 '
8040     PRINT #4, "Reach No.   Chemical   ";
8050     FOR IJ = 1 TO N2
8060         PRINT #4, CNS(IJ); " ";
8070     NEXT IJ
8075     PRINT #4, CHR$(13)
8080 '
8090     GOSUB 9000
8100 '
8110     RETURN
8120 '
8130 -----
8140 '
8200     Print concentration in water, sediment, & fish compartments--
8210 '
8215     IF P8>0 THEN PRINT #4, "Average"
8220     PRINT #4, "Conc (ug/g) ";
8225     IF P8>0 THEN PRINT #4, STRING$(12, " ");
8230     FOR J = 1 TO 3
```

APMCALC-13

```
8250      PRINT #4, USING I5$; CON!(J);
8260      NEXT J
8270      PRINT #4, CHR$(13)
8275
8280      RETURN
8285
8290 -----
8295
8300      Print bioaccumulation factor for sediment, fish--
8305
8310      PRINT #4, "BCF";
8315      IF P8 > 0 THEN PRINT #4, STRINGS(12, " ");
8320      PRINT #4, USING I5$; CON!(2)/CON!(1); CON!(3)/CON!(1)
8330
8340      RETURN
8350
8360 -----
8370
9000      Heading border subroutine--
9010
9020      FOR I = 1 TO N2 + 2
9030          PRINT #4, "----- ";
9040      NEXT I
9050      PRINT #4, CHR$(13)
9060      RETURN
9070 -----
9080
9100      Read variable description file (#7)--
9110
9120      GET #7, RL% : L$ = Z$
9130      P2 = INSTR (L$, ":")
9140      IF P2 < 1 THEN P2 = 59
9150      L$ = LEFT$(L$, P2) + " "
9160      RETURN
9170
9180 -----
9190
9200      Print detail line subroutine--
9210
9220      TOT = 0!
9230      PRINT #4, USING I5$; I*TK;
9240      FOR J = 1 TO N2
9250          PRINT #4, USING I5$; Q(I,J);
9260          TOT = TOT + Q(I,J)
9270      NEXT J
9280      PRINT #4, USING I5$; TOT
9290      RETURN
9292
9294 -----
9296
9300      Test for index of compartment--
9310
9320      J1 = 0 : J2 = 0
```

APMCALC-14

```
9340 '
9350     FOR I = 1 TO N2
9360         IF CN(I) = I1 THEN J1 = I
9370         IF CN(I) = I2 THEN J2 = I
9380     NEXT I
9390 '
9400     IF J1 > 0 AND J2 > 0 THEN P7 = 1 ELSE P7 = 0
9405     IF J1 > 0 THEN P9 = 1 ELSE P9 = 0
9410 '
9420     RETURN
9430 '
9440 -----
9500 '
9515     Print rate constant matrix subroutine--
9520 '
9525     LPRINT : LPRINT : LPRINT DATS, TODS, "R(I,J)" : LPRINT
9530     FOR I = 1 TO N2
9535         FOR J = 1 TO N2
9540             LPRINT USING "#.##+ttt "; R(I,J);
9545         NEXT J
9550     LPRINT
9555     NEXT I
9560 '
9565     RETURN
9570 '
9575 -----
9580 '
9600     Print river reach heading subroutine--
9610 '
9620     FOR IJ = 1 TO 10 : PRINT #4, CHR$(13) : NEXT IJ
9630     PRINT #4, "River Reach No: "; IJK
9640     PRINT #4, CHR$(13) : PRINT #4, CHR$(13)
9650     RETURN
9660 '
9670 -----
9680 '
9700     Total amount of chemical flowing out of system--
9705 '
9710     TOT = 0.
9715     FOR IJ = 1 TO 100
9720         TOT = TOT + QR(IJ)
9725     NEXT IJ
9730 '
9735     RETURN
9740 '
9745 -----
9746 '
9750     Print amount of chemical flowing out of system--
9755 '
9760     FOR IJ = 1 TO 10 : PRINT #4, CHR$(13) : NEXT IJ
9765     PRINT #4, "Chemical flowing out of system (g):"; TAB(60); TOT
9770 '
9775     RETURN
9780 '
```


CHEMMOD-1

```
1000 '----- CHEMRATE data base modification program -----
1010 '--- written by R. A. Peloquin, Battelle PNL, Richland, WA -----
1020 '--- version of January 3, 1982 -----
1030 '
1040 '--- This programs allows data entry and modification of the CHEMRATE ---
1050 '--- data base which is used by the Pathways Model of Toxic Chemicals ---
1060 '--- program. -----
1070 '
1080 '-----
1090 '
2000 '      Initialize--
2010 '
2020 '      DEFINT A - Z
2030 '
2040 '      OPEN "R", #1, "CHEMRATE"
2045 '      OPEN "R", #2, "APMCMPT"
2050 '
2060 '      DIM FS(16), F(16,2)
2070 '      DIM F1$(16), R1$(16)
2080 '      DIM CNS(16)
2090 '
2100 '      FOR I = 1 TO 24 : PRINT : NEXT I
2110 '      PRINT ,, "CHEMMOD"
2120 '      PRINT , "This program modifies the CHEMRATE data base."
2130 '
2140 '      Input date and time--
2142 '      PRINT "Enter date: "; : INPUT DAT$
2144 '      PRINT "Enter time: "; : INPUT TIM$
2146 '      PRINT "Enter your name, please: " : INPUT INIS
2148 '
2200 '      Read in compartment names--
2210 '      FIELD #2, 128 AS Z$
2220 '
2230 '      FOR I = 1 TO 8
2240 '          GET #2, I
2250 '          LS = Z$
2260 '          CNS(I) = MIDS( LS, 11, 10)
2270 '      NEXT I
2280 '
2300 '      Input chemical number--
2310 '      PRINT : PRINT : PRINT
2320 '      PRINT "Enter chemical number: ";
2330 '      INPUT N
2340 '
2350 '      Initialize for chemical properties--
2360 '
2370 '      FS(1)="Chemical no.index:" :      F(1,1)= 1 : F(1,2)= 4
2380 '      FS(2)="Molecular formula:" :      F(2,1)= 5 : F(2,2)= 12
2390 '      FS(3)="Molecular weight:" :      F(3,1)= 17 : F(3,2)= 8
2400 '      FS(4)="Chemical name:" :      F(4,1)= 25 : F(4,2)= 20
2410 '      FS(5)="Second chemical name:" :      F(5,1)= 45 : F(5,2)= 20
```

CHEMMOD-2

```

2420      FS(6)="Solubility:" :           F(6,1)= 65 : F(6,2)= 8
2430      FS(7)="Vapor pressure:" :       F(7,1)= 73 : F(7,2)= 8
2440      FS(8)="Temperature:" :          F(8,1)= 81 : F(8,2)= 8
2450      FS(9)="Log octanol-water partition coef.":F(9,1)= 89 : F(9,2)= 8
2460      FS(10)="Soil organic matter - water PC:" :F(10,1)= 97 : F(10,2)= 8
2470      FS(11)="Ultra-violet adsorption:" : F(11,1)=105 : F(11,2)= 8
2480      FS(12)="Dissociation constant:" : F(12,1)=113 : F(12,2)= 8
2490
3000
3010      FIELD #1, 4 AS F1$(1), 12 AS F1$(2), 3 AS F1$(3), 20 AS F1$(4), 20 AS F1$(5), 8 AS F1$(6), 8 AS F1$(7), 8 AS F1$(8), 8 AS F1$(9), 8 AS F1$(10), 8 AS F1$(11), 8 AS F1$(12)
3020
3025      RN = 17 * N + 1
3030      GET #1, RN
3040
3050
3060      Print chemical properties--
3070      FOR I = 1 TO 12
3080          PRINT FS(I); TAB(50); F1$(I)
3090      NEXT I
3100
3190      PRINT : PRINT
3200      PRINT "Do you wish to modify any of these chemical properties? ";
3210      INPUT QS
3220      QS = LEFT$(QS,1)
3230      IF QS = "Y" OR QS = "y" THEN P1 = 1 ELSE P1 = 0
3240
3250      IF P1 = 0 THEN GOTO 3300
3260      FOR I = 1 TO 12
3265          PRINT : PRINT
3270          PRINT FS(I); TAB(50); F1$(I)
3275          K = I
3290          GOSUB 9000
3290      NEXT I
3300      endif
3310
3320
3325      PRINT : PRINT : PRINT : PRINT : PRINT : PRINT
3330      PRINT "Do you wish to modify any rate constants (Y or <cr>)? ";
3340      INPUT QS : QS = LEFT$(QS,1)
3350      IF QS = "Y" OR QS = "y" THEN P1 = 1 ELSE P1 = 0
3360      IF P1 = 0 THEN GOTO 4000
3370
3380
3400      Initialize F array for rate constants--
3410      FOR I = 1 TO 8
3420          F(I,1) = (I-1)*8 + 1
3430          F(I,2) = 8
3440      NEXT I
3450
3460      FIELD #1, 8 AS R1$(1), 8 AS R1$(2), 8 AS R1$(3), 8 AS R1$(4), 8 AS R1$(5), 8 AS R1$(6), 8 AS R1$(7), 8 AS R1$(8)
3470

```

CHEMMOD-3

```
3480 '
3500   FOR I = 1 TO 8
3510 '
3515       RN = N*17+I+1
3520       GET #1, RN
3530 '
3535       PRINT : PRINT : PRINT : PRINT
3540       FOR J = 1 TO 8
3550           PRINT "The rate constant from "; CNS(J); " to "; CNS(I); "= ";
3560           PRINT R1S(J)
3570       NEXT J
3580 '
3585       PRINT : PRINT
3590       PRINT "Do you wish to modify any of these rate constants? ";
3600       INPUT QS : QS = LEFT$(QS,1)
3610       IF QS = "Y" OR QS = "y" THEN P1 = 1 ELSE P1 = 0
3620 '
3630       IF P1 = 0 THEN GOTO 3700
3635       PRINT : PRINT : PRINT
3640       FOR J = 1 TO 8
3645           PRINT : PRINT : PRINT
3650           PRINT "The rate constant from "; CNS(J); " to "; CNS(I); "= ";
3660           PRINT R1S(J)
3665           K = J
3670           GOSUB 9000
3680       NEXT J
3700 '       endif
3710 '
3720       PRINT : PRINT : PRINT : PRINT : PRINT
3730       NEXT I
3740 '
4000       PRINT "Enter 'A' for another chemical, 'E' to exit: ";
4010       INPUT QS : QS = LEFT$(QS,1)
4020       IF QS="A" OR QS="a" THEN GOTO 2200
4030 '
4031       IF P2 = 0 THEN GOTO 4035
4032       FIELD #1, 128 AS Z$: L$ = Z$
4033       P2 = INSTR(L$,"") : IF P2 < 1 THEN P2 = 1
4034       L$ = MIDS(L$,1,P2) + DAT$ + " " + TIM$ + " by " + INI$
4035       CLOSE
4040       END
4050 '
4060 '-----
9000 '
9010 '       Modify parameter subroutine--
9020 '
9030       PRINT , "Modify (Y or <cr>)? ";
9040       INPUT QS : QS = LEFT$(QS,1)
9050       IF QS = "Y" OR QS = "y" THEN P1 = 1 ELSE P1 = 0
9060 '
9070       IF P1 = 0 THEN GOTO 9300
9080 '
9100       PRINT , "Enter new value: ";
```

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```
9200      INPUT XS
9210      LX = LEN (XS)
9220      IF LX > F(K,2) THEN GOTO 9100
9230      FIELD #1, F(K,1)-1 AS DUMBS, F(K,2) AS XFS
9240      LSET XFS = XS
9250      PUT #1, RN
9255      P2 = 1
9260 '
9300 '      endif
9310 '
9330      RETURN
9340 '
9350 '-----
```

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