EXPOSURE ANALYSIS MODELING SYSTEM

User's Guide for EXAMS II Version 2.96

by

Lawrence A. Burns, Ph.D.
Research Ecologist
U.S. Environmental Protection Agency
960 College Station Road
Athens, Georgia 30605-2700

OFFICE OF RESEARCH AND DEVELOPMENT
U.S. ENVIRONMENTAL PROTECTION AGENCY
ATHENS, GEORGIA 30605-2700

DISCLAIMER

The information in this document has been funded wholly or in part by the United States Environmental Protection Agency. It has been subject to the Agency's peer and administrative review, and it has been approved for publication as an EPA document. Mention of trade names or commercial products does not constitute endorsement or recommendation for use.

FOREWORD

Environmental protection efforts are increasingly directed toward preventing adverse health and ecological effects associated with specific chemical compounds of natural or human origin. As part of this Laboratory's research on the occurrence, movement, transformation, impact, and control of environmental contaminants, the Biology Branch studies complexes of environmental processes that control the transport, transformation, degradation, fate, and impact of pollutants or other materials in soil and water and develops models for assessing the risks associated with exposures to chemical contaminants.

Concern about environmental exposure to synthetic organic chemicals has increased the need for techniques to predict the behavior of chemicals entering the environment as a result of the manufacture, use, and disposal of commercial products. The Exposure Analysis Modeling System (EXAMS), which has been undergoing continual development, test, and revision at this Laboratory since 1978, provides a convenient tool to aid in judging the environmental consequences should a specific chemical contaminant enter a natural aquatic system. Because EXAMS requires no chemical monitoring data, it can be used for new chemical not yet introduced into commerce as well as for those whose patter and volume of use are known. EXAMS and other exposure assessment models should contribute significantly to efforts to anticipate potential problems associated with environmental pollutants.

Rosemarie C. Russo
Director
Environmental Research Laboratory
Athens, Georgia

ABSTRACT

The Exposure Analysis Modeling System, first published in 1982 (EPA-600/3-82-023), provides interactive computer software for formulating aquatic ecosystem models and rapidly evaluating the fate, transport, and exposure concentrations of synthetic organic chemicals--pesticides, industrial materials, and leachates from disposal sites. EXAMS contains an integrated Database Management System (DBMS) specifically designed for storage and management of project databases required by the software. User interaction is provided by a full-featured Command Line Interface (CLI), context-sensitive help menus, an on-line data dictionary and CLI users' guide, and plotting capabilities for review of output data. EXAMS provides 20 output tables which document the input datasets and provide integrated results summaries for aid in ecological risk assessments.

EXAMS' core is a set of process modules that link fundamental chemical properties to the limnological parameters that control the kinetics of fate and transport in aquatic systems. The chemical properties are measurable by conventional laboratory methods; most are required under various regulatory authority. When run under the EPA's GEMS or pcGEMS systems, EXAMS accepts direct output from QSAR software. EXAMS limnological data are composed of elements historically of interest to aquatic scientists world-wide, so generation of suitable environmental datasets can generally be accomplished with minimal project-specific field investigations.

EXAMS provides facilities for long-term (steady-state) analysis of chronic chemical discharges, initial-value approaches for study of short-term chemical releases, and full kinetic simulations that allow for monthly variation in mean climatological parameters and alteration of chemical loadings on daily time scales. EXAMS has been written in generalized (N-dimensional) form in its implementation of algorithms for representing spatial detail and chemical degradation pathways. This DOS implementation allows for study of five simultaneous chemical compounds and 100 environmental segments; other configurations can be created through special arrangement with the author. EXAMS provides analyses of

Exposure: the expected (96-hour acute, 21-day and long-term chronic) environmental concentrations of synthetic chemicals and their transformation products,

Fate: the spatial distribution of chemicals in the aquatic ecosystem, and the relative importance of each transformation and transport process (important in establishing the acceptable uncertainty in chemical laboratory data), and

Persistence: the time required for natural purification of the ecosystem (via export and degradation processes) once chemical releases end.

EXAMS 2.96 includes file-transfer interfaces to the PRZM terrestrial model and the FGETS bio-accumulation model.

This report covers a period from October 1, 1995 to January 30, 1996 and work was completed as of January 30, 1996.

TABLE OF CONTENTS

User's Guide for EXAMS II Version 2.96

Introduction to the Exposure Analysis Modeling System (EXAMS)[1]

Industrial production of agricultural chemicals, plastics, and pharmaceuticals has increased steadily over the past four decades. More recently, growth of the chemical industry has been accompanied by increasing concern over the effects of synthetic chemicals on the environment. The suspicion has arisen that, in some cases, the benefits gained by using a chemical may not offset the cost of incidental damage to man's natural life-support systems--the biosphere. The toxicity of a chemical does not of itself indicate that the environmental risks associated with its use are unacceptable, however, as it is the dose that makes the poison. A rational evaluation of the risk posed by the use and disposal of synthetic chemicals must begin from a knowledge of the persistence and mobility of chemicals in the environment, which in turn establish the conditions of exposure leading to absorption of toxicological dose.

The Exposure Analysis Modeling System (EXAMS), developed at the Athens Environmental Research Laboratory, is an interactive computer program intended to give decision-makers in industry and government access to a responsive, general, and controllable tool for readily deriving and evaluating the behavior of synthetic chemicals in the environment. The development effort has focused on the development of the interactive command language and user aids that are the core of EXAMS, and on the genesis of reliable EXAMS mathematical models. EXAMS was designed primarily for the rapid screening and identification of synthetic organic chemicals likely to adversely impact aquatic systems. This report is intended to acquaint potential users with the underlying theory, capabilities, and use of the system.

Exposure Analysis in Aquatic Systems EXAMS was conceived as an aid to those who must execute hazard evaluations solely from laboratory descriptions of the chemistry of a newly synthesized toxic compound. EXAMS estimates exposure, fate, and persistence following release of an organic chemical into an aquatic ecosystem. Each of these terms was given a formal operational definition during the initial design of the system.

Exposure When a pollutant is released into an aquatic ecosystem, it is entrained in the transport field of the system and begins to spread to locations beyond the original point of release. During the course of these movements, chemical and biological processes transform the parent compound into daughter products. In the face of continuing emissions, the receiving system evolves toward a "steady-state" condition. At steady state, the pollutant concentrations are in a dynamic equilibrium in which the loadings are balanced by the transport and transformation processes. Residuals can be compared to the concentrations posing a danger to living organisms. The comparison is one indication of the risk entailed by the presence of a chemical in natural systems or in drinking-water

[1] Additional technical documentation for EXAMS is contained in Burns et al. 1982.

supplies. These "expected environmental concentrations" (EECs), or exposure levels, in receiving water bodies are one component of a hazard evaluation.

Persistence Toxicological and ecological "effects" studies are of two kinds: investigations of short-term "acute" exposures, as opposed to longer-term "chronic" experiments. Acute studies are often used to determine the concentration of a chemical resulting in 50% mortality of a test population over a period of hours. Chronic studies examine sub-lethal effects on populations exposed to lower concentrations over extended periods. Thus, for example, an EEC that is 10 times less than the acute level does not affirm that aquatic ecosystems will not be affected, because the probability of a "chronic" impact increases with exposure duration. A computed EEC thus must be supplemented with an estimate of "persistence" in the environment. (A compound immune to all transformation processes is by definition "persistent" in a global sense, but even in this case transport processes will eventually reduce the pollutant to negligible levels should the input loadings cease.) The notion of "persistence" can be given an explicit definition in the context of a particular contaminated ecosystem: should the pollutant loadings cease, what time span would be required for dissipation of most of the residual contamination? (For example, given the half-life of a chemical in a "first-order" system, the time required to reduce the chemical concentration to any specified fraction of its initial value can be easily computed.) With this information in hand, the appropriate duration and pollutant levels for chronic studies can be more readily decided. More detailed dynamic simulation studies can elicit the probable magnitude and duration of acute events as well.

Fate The toxicologist also needs to know which populations in the system are "at risk." In addition to the Biogeographic Endangerment Analysis conducted under PIRANHA, populations at risk can be deduced to some extent from the distribution or "fate" of the compound, that is, by an estimate of EECs in different habitats of single ecosystems. EXAMS reports a separate EEC for each compartment, and thus each local population, used to define the system.

The concept of the "fate" of a chemical in an aquatic system has an additional, equally significant meaning. Each transport or transformation process accounts for only part of the total behavior of the pollutant. The relative importance of each process can be determined from the percentage of the total system loadings consumed by the process. The relative importances of the transformations indicate which process is dominant in the system, and thus in greatest need of accuracy and precision in its kinetic parameters. Overall dominance by transport processes may imply a contamination of downstream systems, loss of significant amounts of the pollutant to the atmosphere, or pollution of ground-water aquifers.

The EXAMS program The need to predict chemical exposures from limited data has stimulated a variety of recent advances in environmental modeling. These advances fall into three general categories:

- Process models giving a quantitative, often theoretical, basis for predicting the rate of transport and transformation processes as a function of environmental variables.

- Procedures for estimating the chemical parameters required by process models. Examples include linear free energy relationships, and correlations summarizing large bodies of experimental chemical data.

- Systems models that combine unit process models with descriptions of the environmental forces determining the strength and speed of these processes in real ecosystems.

The vocabulary used to describe environmental models includes many terms, most of which reflect the underlying intentions of the modelers. Models may be predictive, stochastic, empirical, mechanistic, theoretical, deterministic, explanatory, conceptual, causal, descriptive, etc. The EXAMS program is a deterministic, predictive systems model, based on a core of mechanistic process equations derived from fundamental theoretical concepts. The EXAMS computer code also includes descriptive empirical correlations that ease the user's burden of parameter calculations, and an interactive command language that facilitates the application of the system to specific problems.

EXAMS "predicts" in a somewhat limited sense of the term. Many of the predictive water-quality models currently in use include site-specific parameters that can only be found via field calibrations. After "validation" of the model by comparison of its calibrated outputs with additional field measurements, these models are often used to explore the merits of alternative management plans. EXAMS, however, deals with an entirely different class of problem. Because newly synthesized chemicals must be evaluated, little or no field data may exist. Furthermore, EECs at any particular site are of little direct interest. In this case, the goal, at least in principle, is to predict EECs for a wide range of ecosystems under a variety of geographic, morphometric, and ecological conditions. EXAMS includes no direct calibration parameters, and its input environmental data can be developed from a variety of sources. For example, input data can be synthesized from an analysis of the outputs of hydrodynamic models, from prior field investigations conducted without reference to toxic chemicals, or from the appropriate limnological literature. The EECs generated by EXAMS are thus "evaluative" (Lassiter et al. 1978) predictions designed to reflect typical or average conditions. EXAMS' environmental database can be used to describe specific locales, or as a generalized description of the properties of aquatic systems in broad geographic regions.

EXAMS relies on mechanistic, rather than empirical, constructs for its core process equations. Mechanistic (physically determinate) models are more robust predictors than are purely empirical models, which cannot safely be extended beyond the range of prior observations. EXAMS contains a few empirical correlations among chemical parameters, but these are not invoked unless the user approves. For example, the partition coefficient of the compound on the sediment phases of the system, as a function of the organic carbon content of its sediments, can be estimated from the compound's octanol-water partition coefficient. A direct load of the partition coefficient (KOC, see the EXAMS Data Dictionary) overrides the empirical default estimate, however. (Because EXAMS is an interactive program in which the user has direct access to the input database, much of this documentation has been written using the computer variables (e.g., KOC above) as identifiers and as quantities in the process equations. Although this approach poses some difficulties for the casual reader, it allows the potential user of the program to see the connections between program variables

and the underlying process theory. The EXAMS data dictionary in this document includes an alphabetical listing and definitions of EXAMS' input variables.)

EXAMS is a deterministic, rather than a stochastic, model in the sense that a given set of inputs will always produce the same output. Uncontrolled variation is present both in ecosystems and in chemical laboratories, and experimental results from either milieu are often reported as mean values and their associated variances. Probabilistic modeling techniques (e.g., Monte Carlo simulations) can account, in principle, for this variation and attach an error bound or confidence interval to each important output variable. Monte Carlo simulation is, however, very time-consuming (i.e., expensive), and the statistical distributions of chemical and environmental parameters are not often known in the requisite detail. The objective of this kind of modeling, in the case of hazard evaluations, would in any case be to estimate the effect of parameter errors on the overall conclusions to be drawn from the model. This goal can be met less expensively and more efficiently by some form of sensitivity analysis.

Sensitivity Analysis and Error Evaluation EXAMS does not provide a formal sensitivity analysis among its options: the number of sub-simulations needed to fully account for interactions among chemical and environmental variables is prohibitively large (Behrens 1979). When, for example, the second-order rate constant for alkaline hydrolysis of a compound is described to EXAMS via an Arrhenius function, the rate constant computed for each compartment in the ecosystem depends on at least six parameters. These include the frequency factor and activation energy of the reaction, the partition coefficient of the compound (KOC), the organic carbon content of the sediment phase, the temperature, and the concentration of hydroxide ion. The overall rate estimate is thus as dependent upon the accuracy of the system definition as it is upon the skill of the laboratory chemist; in this example, the rate could vary six orders of magnitude as a function of differences among ecosystems. In order to fully map the parameter interactions affecting a process, all combinations of parameter changes would have to be simulated. Even this (simplified) example would require 63 simulations (2^n-1, where n is the number (6) of parameters) merely to determine sensitivities of a single component process in a single ecosystem compartment.

Sensitivity analysis remains an attractive technique for answering a crucial question that arises during hazard evaluation. This question can be simply stated: "Are the chemical data accurate enough, and precise enough, to support an analysis of the risk entailed by releases of the chemical into the environment?" Like many simple questions, this question does not have a simple, definitive answer. It can be broken down, however, into a series of explicit, more tractable questions whose answers sum to a reasonably complete evaluation of the significance that should be attached to a reported error bound or confidence interval on any input datum. Using the output tables and command language utilities provided by EXAMS, these questions can be posed, and answered, in the following order.

- Which geographic areas, and which ecosystems, develop the largest chemical residuals? EXAMS allows a user to load the data for any environment contained in his files, specify a loading, and run a simulation, through a simple series of one-line English commands.

- Which process is dominant in the most sensitive ecosystem(s)? The dominant process, i.e., the process most responsible for the decomposition of the compound in the system, is the process requiring the greatest accuracy and precision in its chemical parameters. EXAMS produces two output tables that indicate the relative importance of each process. The first is a "kinetic profile" (or frequency scaling), which gives a compartment-by-compartment listing with all processes reduced to equivalent ($hour^{-1}$) terms. The second is a tabulation of the overall steady-state fate of the compound, giving a listing of the percentage of the load consumed by each of the transport and transformation processes at steady state.

Given the dominant process, the input data affecting this process can be varied over the reported error bounds, and a simulation can be executed for each value of the parameters. The effect of parameter errors on the EECs and persistence of the compound can then be documented by compiling the results of these simulations.

This sequence of operations is, in effect, a sensitivity analysis, but the extent of the analysis is controlled and directed by the user. In some cases, for example, one process will always account for most of the decomposition of the compound. When the database for this dominant process is inadequate, the obvious answer to the original question is that the data do not yet support a risk analysis. Conversely, if the dominant process is well defined, and the error limits do not substantially affect the estimates of exposure and persistence, the data may be judged to be adequate for the exposure analysis portion of a hazard evaluation.

EXAMS Process Models In EXAMS, the loadings, transport, and transformations of a compound are combined into differential equations by using the mass conservation law as an accounting principle. This law accounts for all the compound entering and leaving a system as the algebraic sum of (1) external loadings, (2) transport processes exporting the compound out of the system, and (3) transformation processes within the system that degrade the compound to its daughter products. The fundamental equations of the model describe the rate of change in chemical concentrations as a balance between increases due to loadings, and decreases due to the transport and transformation processes removing the chemical from the system.

The set of unit process models used to compute the kinetics of a compound is the central core of EXAMS. These unit models are all "second-order" or "system-independent"models: each process equation includes a direct statement of the interactions between the chemistry of a compound and the environmental forces that shape its behavior in aquatic systems. Most of the process equations are based on standard theoretical constructs or accepted empirical relationships. For example, light intensity in the water column of the system is computed using the Beer-Lambert law, and temperature corrections for rate constants are computed using Arrhenius functions.

Ionization and Sorption Ionization of organic acids and bases, complexation with dissolved organic carbon (DOC), and sorption of the compound with sediments and biota, are treated as thermodynamic properties or (local) equilibria that alter the operation of kinetic processes. For example, an organic base in the water column may occur in a number of molecular species (as dissolved ions, sorbed

with sediments, etc.), but only the uncharged, dissolved species can be volatilized across the air-water interface. EXAMS allows for the simultaneous treatment of up to 28 molecular species of a chemical. These include the parent uncharged molecule, and singly, doubly, or triply charged cations and anions, each of which can occur in a dissolved, sediment-sorbed, DOC-complexed, or biosorbed form. The program computes the fraction of the total concentration of compound that is present in each of the 28 molecular structures (the "distribution coefficients," *alpha*).

These (*alpha*) values enter the kinetic equations as multipliers on the rate constants. In this way, the program accounts for differences in reactivity that depend on the molecular form of the chemical, as a function of the spatial distribution of environmental parameters controlling molecular speciation. For example, the lability of a particular molecule to hydrolytic decomposition may depend on whether it is dissolved or is sorbed with the sediment phase of the system. EXAMS makes no intrinsic assumptions about the relative transformation reactivities of the 28 molecular species. These assumptions are controlled through the structure of the input data describing the species-specific chemistry of the compound.

Transformation Processes EXAMS computes the kinetics of transformations attributable to direct photolysis, hydrolysis, biolysis, and oxidation reactions. The input chemical data for hydrolytic, biolytic, and oxidative reactions can be entered either as single-valued second-order rate constants, or as a pair of values defining the rate constant as a function of environmental temperatures. For example, the input data for alkaline hydrolysis of the compound consists of two computer variables: KBH, and EBH. When EBH is zero, the program interprets KBH as the second-order rate constant. When EBH is non-zero, EBH is interpreted as the activation energy of the reaction, and KBH is re-interpreted as the pre-exponential (frequency) factor in an Arrhenius equation giving the second-order rate constant as a function of the environmental temperature (TCEL) in each system compartment. (KBH and EBH are both actually matrices with 21 elements; each element of the matrix corresponds to one of the 21 possible molecular species of the compound.)

EXAMS includes two algorithms for computing the rate of photolytic transformation of a synthetic organic chemical. These algorithms accommodate the two more common kinds of laboratory data and chemical parameters used to describe photolysis reactions. The simpler algorithm requires only an average pseudo-first-order rate constant (KDP) applicable to near-surface waters under cloudless conditions at a specified reference latitude (RFLAT). To control reactivity assumptions, KDP is coupled to nominal (normally unit-valued) reaction quantum yields (QUANT) for each molecular species of the compound. This approach makes possible a first approximation of photochemical reactivity, but neglects the very important effects of changes in the spectral quality of sunlight with increasing depth in a body of water. The more complex photochemical algorithm computes photolysis rates directly from the absorption spectra (molar extinction coefficients) of the compound and its ions, measured values of the reaction quantum yields, and the environmental concentrations of competing light absorbers (chlorophylls, suspended sediments, DOC, and water itself). When using a KDP, please be aware that data from laboratory photoreactors usually are obtained at intensities as much as one thousand times larger than that of normal sunlight.

The total rate of hydrolytic transformation of a chemical is computed by EXAMS as the sum of three contributing processes. Each of these processes can be entered via simple rate constants, or as Arrhenius functions of temperature. The rate of specific-acid-catalyzed reactions is computed from the pH of each sector of the ecosystem, and specific-base catalysis is computed from the environmental pOH data. The rate data for neutral hydrolysis of the compound are entered as a set of pseudo-first-order rate coefficients (or Arrhenius functions) for reaction of the 28 (potential) molecular species with the water molecule.

EXAMS computes biotransformation of the chemical in the water column, and in the bottom sediments, of the system as entirely separate functions. Both functions are second-order equations that relate the rate of biotransformation to the size of the bacterial population actively degrading the compound. The second-order rate constants (KBACW for the water column, KBACS for benthic sediments) can be entered either as single-valued constants or as functions of temperature. When a non-zero value is entered for the Q_{10} of a biotransformation (parameters QTBAW and QTBAS, respectively), KBAC is interpreted as the rate constant at 20 degrees Celsius, and the biolysis rate in each sector of the ecosystem is adjusted for the local temperature (TCEL).

Oxidation reactions are computed from the chemical input data and the total environmental concentrations of reactive oxidizing species (alkylperoxy and alkoxyl radicals, etc.), corrected for ultra-violet light extinction in the water column. The chemical data can again be entered either as simple second-order rate constants or as Arrhenius functions. Oxidations due to singlet oxygen are computed from chemical reactivity data and singlet oxygen concentrations; singlet oxygen is estimated as a function of the concentration of DOC, oxygen tension, and light intensity. Reduction is included in the program as a simple second-order reaction process driven by the user entries for concentrations of reductants in the system.

Transport Processes Internal transport and export of a chemical occur in EXAMS via advective and dispersive movement of dissolved, sediment-sorbed, and biosorbed materials and by volatilization losses at the air-water interface. EXAMS provides a set of vectors (JFRAD, etc.) that specify the location and strength of both advective and dispersive transport pathways. Advection of water through the system is then computed from the water balance, using hydrologic data (rainfall, evaporation rates, streamflows, groundwater seepages, etc.) supplied to EXAMS as part of the definition of each environment.

Dispersive interchanges within the system, and across system boundaries, are computed from the usual geochemical specification of the characteristic length (CHARL), cross-sectional area (XSTUR), and dispersion coefficient (DSP) specified for each active exchange pathway. EXAMS can compute transport of synthetic chemicals via whole-sediment bedloads, suspended sediment wash-loads, exchanges with fixed-volume sediment beds, ground-water infiltration, transport through the thermocline of a lake, losses in effluent streams, etc. Volatilization losses are computed using a two-resistance model. This computation treats the total resistance to transport across the air-water interface as the sum of resistances in the liquid and vapor phases immediately adjacent to the interface.

Chemical Loadings External loadings of a toxicant can enter the ecosystem via point sources (STRLD), non-point sources (NPSLD), dry fallout or aerial drift (DRFLD), atmospheric wash-out (PCPLD), and ground-water seepage (SEELD) entering the system. Any type of load can be entered for any system compartment, but the program will not implement a loading that is inconsistent with the system definition. For example, the program will automatically cancel a rainfall loading (PCPLD) entered for the hypolimnion or benthic sediments of a lake ecosystem. When this type of corrective action is executed, the change is reported to the user via an error message.

Ecosystems Analysis and Mathematical Systems Models The EXAMS program was constructed from a systems analysis perspective. Systems analysis begins by defining a system's goals, inputs, environment, resources, and the nature of the system's components and their interconnections. The system goals describe the outputs produced by the system as a result of operating on its input stream. The system environment comprises those factors affecting system outputs over which the system has little or no control. These factors are often called "forcing functions" or "external driving variables." Examples for an aquatic ecosystem include runoff and sediment erosion from its watershed, insolation, and rainfall. System resources are defined as those factors affecting performance over which the system exercises some control. The resources of an aquatic ecosystem include, for example, the pH throughout the system, light intensity in the water column, and dissolved oxygen concentrations. The levels of these internal driving variables are determined, at least in part, by the state of the system itself. In other words, these factors are not necessarily single-valued functions of the system environment. Each of the components or "state variables" of a system can be described in terms of its local input/output behaviors and its causal connections with other elements of the system. The systems approach lends itself to the formulation of mathematical systems models, which are simply tools for encoding knowledge of transport and transformation processes and deriving the implications of this knowledge in a logical and repeatable way.

A systems model, when built around relevant state variables (measurable properties of system components) and causal process models, provides a method for extrapolating future states of systems from knowledge gained in the past. In order for such a model to be generally useful, however, most of its parameters must possess an intrinsic interest transcending their role in any particular computer program. For this reason, EXAMS was designed to use chemical descriptors (Arrhenius functions, pKa, vapor pressure, etc.) and water quality variables (pH, chlorophyll, biomass, etc.) that have been independently measured for many chemicals and ecosystems.

EXAMS *Design Strategy* The conceptual view adopted for EXAMS begins by defining aquatic ecosystems as a series of distinct subsystems, interconnected by physical transport processes that move synthetic chemicals into, through, and out of the system. These subsystems include the epilimnion and hypolimnion of lakes, littoral zones, benthic sediments, etc. The basic architecture of a computer model also depends, however, on its intended uses. EXAMS was designed for use by toxicologists and decision-makers who must evaluate the risk posed by use of a new chemical, based on a forecast from the model. The EXAMS program is itself part of a "hazard evaluation system," and

the structure of the program was necessarily strongly influenced by the niche perceived for it in this system.

Many intermediate technical issues arise during the development of a systems model. Usually these issues can be resolved in several ways; the modeling "style" or design strategy used to build the model guides the choices taken among the available alternatives. The strategy used to formulate EXAMS begins from a primary focus on the needs of the intended user and, other things being equal, resolves most technical issues in favor of the more efficient computation. For example: all transport and transformation processes are driven by internal resource factors (pH, temperature, water movements, sediment deposition and scour, etc.) in the system, and each deserves separate treatment in the model as an individual state variable or function of several state variables. The strategy of model development used for EXAMS suggests, however, that the only state variable of any transcendent interest to the user is the concentration of the chemical itself in the system compartments. EXAMS thus treats all environmental state variables as coefficients describing the state of the ecosystem, and only computes the implications of that state, as residual concentrations of chemicals in the system.

Although this approach vastly simplifies the mathematical model, with corresponding gains in efficiency and speed, the system definition is now somewhat improper. System resources (factors affecting performance that are subject to feedback control) have been redefined as part of the system environment. In fact, the "system" represented by the model is no longer an aquatic ecosystem, but merely a chemical pollutant. Possible failure modes of the model are immediately apparent. For example, introduction of a chemical subject to alkaline hydrolysis and toxic to plant life into a productive lake would retard primary productivity. The decrease in primary productivity would lead to a decrease in the pH of the system and, consequently, a decrease in the rate of hydrolysis and an increase in the residual concentration of the toxicant. This sequence of events would repeat itself indefinitely, and constitutes a positive feedback loop that could in reality badly damage an ecosystem. Given the chemical buffering and functional redundancy present in most real ecosystems, this example is inherently improbable, or at least self-limiting. More importantly, given the initial EEC, the environmental toxicologist could anticipate the potential hazard.

There is a more telling advantage, moreover, to the use of environmental descriptors in preference to dynamic environmental state variables. Predictive ecosystem models that include all the factors of potential importance to the kinetics of toxic pollutants are only now being developed, and will require validation before any extensive use. Furthermore, although extremely fine--resolution (temporal and spatial) models are often considered an ultimate ideal, their utility as components of a fate model for synthetic chemicals remains suspect. Ecosystems are driven by meteorological events, and are themselves subject to internal stochastic processes. Detailed weather forecasts are limited to about nine days, because at the end of this period all possible states of the system are equally probable. Detailed ecosystem forecasts are subject to similar constraints (Platt et al. 1977). For these reasons, EXAMS was designed primarily to forecast the prevailing climate of chemical exposures, rather than to give detailed local forecasts of EECs in specific locations.

Temporal and Spatial Resolution When a synthetic organic chemical is released into an aquatic ecosystem, the entire array of transport and transformation processes begins at once to act on the chemical. The most efficient way to accommodate this parallel action of the processes is to combine them into a mathematical description of their total effect on the rate of change of chemical concentration in the system. Systems that include transport processes lead to partial differential equations, which usually must be solved by numerical integration. The numerical techniques in one way or another break up the system, which is continuously varying in space and time, into a set of discrete elements. Spatial discrete elements are often referred to as "grid points" or "nodes", or, as in EXAMS, as "compartments." Continuous time is often represented by fixing the system driving functions for a short interval, integrating over the interval, and then "updating" the forcing functions before evaluating the next time-step. At any given moment, the behavior of the chemical is a complicated function of both present and past inputs of the compound and states of the system.

EXAMS is oriented toward efficient screening of a multitude of newly invented industrial chemicals and pesticides. Ideally, a full evaluation of the possible risks posed by manufacture and use of a new chemical would begin from a detailed time-series describing the expected releases of the compound into aquatic systems over the entire projected history of its manufacture. Given an equivalently detailed time-series for environmental variables, machine integration would yield a detailed picture of EECs in the receiving water body over the entire period of concern. The great cost of this approach, however, militates against its use as a screening tool. Fine resolution evaluation of synthetic chemicals can probably be used only for compounds that are singularly deleterious and of exceptional economic significance.

The simplest situation is that in which the chemical loadings to systems are known only as single estimates pertaining over indefinite periods. This situation is the more likely for the vast majority of new chemicals, and was chosen for development of EXAMS. It has an additional advantage. The ultimate fate and exposure of chemicals often encompasses many decades, making detailed time traces of EECs feasible only for short-term evaluations. In EXAMS, the environment is represented via long-term average values of the forcing functions that control the behavior of chemicals. By combining the chemistry of the compound with average properties of the ecosystem, EXAMS reduces the screening problem to manageable proportions. These simplified "first-order" equations are solved algebraically in EXAMS's steady-state Mode 1 to give the ultimate (i.e., steady-state) EECs that will eventually result from the input loadings. In addition, EXAMS provides a capability to study initial value problems ("pulse loads" in Mode 2), and seasonal dynamics in which environmental driving forces are updated on a monthly basis (Mode 3). Mode 3 is particularly valuable for coupling to the output of the PRZM model, which can provide a lengthy time-series of contamination events due to runoff and erosion of sediments from agricultural lands.

Transport of a chemical from a loading point into the bulk of the system takes place by advected flows and by turbulent dispersion. The simultaneous transformations presently result in a continuously varying distribution of the compound over the physical space of the system. This continuous distribution of the compound can be described via partial differential equations. In solving the equations, the physical space of the system must be broken down into discrete elements. EXAMS is a compartmental or "box" model. The physical space of the system is broken down into

a series of physically homogeneous elements (compartments) connected by advective and dispersive fluxes. Each compartment is a particular volume element of the system, containing water, sediments, biota, dissolved and sorbed chemicals, etc. Loadings and exports are represented as mass fluxes across the boundaries of the volume elements; reactive properties are treated as point processes within each compartment.

In characterizing aquatic systems for use with EXAMS, particular attention must be given the grid-size of the spatial net used to represent the system. In effect, the compartments must not be so large that internal gradients have a major effect on the estimated transformation rate of the compound. In other words, the compartments are assumed to be "well-mixed," that is, the reaction processes are not slowed by delays in transporting the compound from less reactive to more reactive zones in the volume element. Physical boundaries that can be used to delimit system compartments include the air-water interface, the thermocline, the benthic interface, and perhaps the depth of bioturbation of sediments. Some processes, however, are driven by environmental factors that occur as gradients in the system, or are most active at interfaces. For example, irradiance is distributed exponentially throughout the water column, and volatilization occurs only at the air-water interface. The rate of these transformations may be overestimated in, for example, quiescent lakes in which the rate of supply of chemical to a reactive zone via vertical turbulence controls the overall rate of transformation, unless a relatively fine-scale segmentation is used to describe the system. Because compartment models of strongly advected water masses (rivers) introduce some numerical dispersion into the calculations, a relatively fine-scale segmentation is often advisable for highly resolved evaluations of fluvial systems. In many cases the error induced by highly reactive compounds will be of little moment to the probable fate of the chemical in that system, however. For example, it makes little difference whether the photolytic half-life of a chemical is 4 or 40 minutes; in either case it will not long survive exposure to sunlight.

Assumptions EXAMS has been designed to evaluate the consequences of longer-term, primarily time-averaged chemical loadings that ultimately result in trace-level contamination of aquatic systems. EXAMS generates a steady-state, average flow field (long-term or monthly) for the ecosystem. The program thus cannot fully evaluate the transient, concentrated EECs that arise, for example, from chemical spills. This limitation derives from two factors. First, a steady flow field is not always appropriate for evaluating the spread and decay of a major pulse (spill) input. Second, an assumption of trace-level EECs, which can be violated by spills, has been used to design the process equations used in EXAMS. The following assumptions were used to build the program.

- A useful evaluation can be executed independently of the chemical's actual effects on the system. In other words, the chemical is assumed not to itself radically change the environmental variables that drive its transformations. Thus, for example, an organic acid or base is assumed not to change the pH of the system; the compound is assumed not to itself absorb a significant fraction of the light entering the system; bacterial populations do not significantly increase (or decline) in response to the presence of the chemical.

- EXAMS uses linear sorption isotherms, and second-order (rather than Michaelis-Menten--Monod) expressions for biotransformation kinetics. This approach is known to be valid for low concentrations of pollutants; its validity at high concentrations is less certain. EXAMS controls its computational range to ensure that the assumption of trace-level concentrations is not grossly violated. This control is keyed to aqueous-phase (dissolved) residual concentrations of the compound: EXAMS aborts any analysis generating EECs that exceed (the lesser of) 50% of the compound's aqueous solubility or 10 micromolar (10^{-5}M) concentrations of a dissolved unionized molecular species. This restraint incidentally allows the program to ignore precipitation of the compound from solution and precludes inputs of solid particles of the chemical.

- Sorption is treated as a thermodynamic or constitutive property of each segment of the system, that is, sorption/desorption kinetics are assumed to be rapid compared to other processes. The adequacy of this assumption is partially controlled by properties of the chemical and system being evaluated. Extensively sorbed chemicals tend to be sorbed and desorbed more slowly than weakly sorbed compounds; desorption half-lives may approach 40 days for the most extensively bound compounds. Experience with the program has indicated, however, that strongly sorbed chemicals tend to be captured by benthic sediments, where their release to the water column is controlled by their availability to benthic exchange processes. This phenomenon overwhelms any accentuation of the speed of processes in the water column that may be caused by the assumption of local equilibrium.

Further Reading

Baughman, G.L., and L.A. Burns. 1980. Transport and transformation of chemicals: a perspective. pp. 1-17 In: O. Hutzinger (Ed.). The Handbook of Environmental Chemistry, vol.2, part A. Springer-Verlag, Berlin, Federal Republic of Germany.

Burns, L.A. 1989. Method 209--Exposure Analysis Modeling System (EXAMS--Version 2.92). pp. 108-115 In: OECD Environment Monographs No. 27: Compendium of Environmental Exposure Assessment Methods for Chemicals. Environment Directorate, Organization for Economic Co-Operation and Development, Paris, France.

Burns, L.A. 1986. Validation methods for chemical exposure and hazard assessment models. pp. 148-172 In: Gesellschaft für Strahlen- und Umwelt forschung mbH München, Projektgruppe "Umwelt gefahrdungspotentiale von Chemikalien" (Eds.) Environmental Modelling for Priority Setting among Existing Chemicals. Ecomed, München-Landsberg/Lech, Federal Republic of Germany.

Burns, L.A. 1985. Models for predicting the fate of synthetic chemicals in aquatic systems. pp. 176-190 In: T.P. Boyle (Ed.) Validation and Predictability of Laboratory Methods for Assessing the Fate and Effects of Contaminants in Aquatic Ecosystems. ASTM STP 865, American Society for Testing and Materials, Philadelphia, Pennsylvania.

Burns, L.A. 1983a. Fate of chemicals in aquatic systems: process models and computer codes. pp. 25-40 In: R.L. Swann and A. Eschenroeder (Eds.) Fate of Chemicals in the Environment: Compartmental and Multimedia Models for Predictions. Symposium Series 225, American Chemical Society, Washington, D.C.

Burns, L.A. 1983b. Validation of exposure models: the role of conceptual verification, sensitivity analysis, and alternative hypotheses. pp. 255-281 In: W.E. Bishop, R.D. Cardwell, and B.B. Heidolph (Eds.) Aquatic Toxicology and Hazard Assessment. ASTM STP 802, American Society for Testing and Materials, Philadelphia,, Pennsylvania.

Burns, L.A. 1982. Identification and evaluation of fundamental transport and transformation process models. pp. 101-126 In: K.L. Dickson, A.W. Maki, and J. Cairns, Jr. (Eds.). Modeling the Fate of Chemicals in the Aquatic Environment. Ann Arbor Science Publ., Ann Arbor, Michigan.

Burns, L.A., and G.L. Baughman. 1985. Fate modeling. pp. 558-584 In: G.M. Rand and S.R. Petrocelli (Eds.) Fundamentals of Aquatic Toxicology: Methods and Applications. Hemisphere Publ. Co., New York, New York.

Burns, L.A., and D.M. Cline. 1985. Exposure Analysis Modeling System: Reference Manual for EXAMS II. EPA/600/3-85/038, U.S. Environmental Protection Agency, Athens, Georgia. 83 pp.

Burns, L.A., D.M. Cline, and R.R. Lassiter. 1982. Exposure Analysis Modeling System (EXAMS): User Manual and System Documentation. EPA-600/3-82-023, U.S. Environmental Protection Agency, Athens, Georgia. 443 pp.

Games, L.M. 1982. Field validation of Exposure Analysis Modeling System (EXAMS) in a flowing stream. pp. 325-346 In: K.L. Dickson, A.W. Maki, and J. Cairns, Jr. (Eds.) Modeling the Fate of Chemicals in the Aquatic Environment. Ann Arbor Science Publ., Ann Arbor, Michigan.

Games, L.M. 1983. Practical applications and comparisons of environmental exposure assessment models. pp. 282-299 In: W.E. Bishop, R.D. Cardwell, and B.B. Heidolph (Eds.) Aquatic Toxicology and Hazard Assessment, ASTM STP 802. American Society for Testing and Materials, Philadelphia, Pennsylvania.

Lassiter, R.R. 1982. Testing models of the fate of chemicals in aquatic environments. pp. 287-301 In: K.L. Dickson, A.W. Maki, and J. Cairns, Jr. (Eds.) Modeling the Fate of Chemicals in the Aquatic Environment. Ann Arbor Science Publ., Ann Arbor, Michigan.

Lassiter, R.R., R.S. Parrish, and L.A. Burns. 1986. Decomposition by planktonic and attached microorganisms improves chemical fate models. Environmental Toxicology and Chemistry 5:29-39.

Paris, D.F., W.C. Steen, and L.A. Burns. 1982. Microbial transformation kinetics of organic compounds. pp. 73-81 In: O. Hutzinger (Ed.). The Handbook of Environmental Chemistry, v.2, pt.B. Springer-Verlag, Berlin, Germany.

Plane, J.M.C., R.G. Zika, R.G. Zepp, and L.A. Burns. 1987. Photochemical modeling applied to natural waters. pp. 250-267 In: R.G. Zika and W.J. Cooper (Eds.) Photochemistry of Environmental Aquatic Systems. ACS Symposium Series 327, American Chemical Society, Washington, D.C.

Pollard, J.E., and S.C. Hern. 1985. A field test of the EXAMS model in the Monongahela River. Environmental Toxicology and Chemistry 4:362-369.

Reinert, K.H., P.M. Rocchio, and J.H. Rodgers, Jr. 1987. Parameterization of predictive fate models: a case study. Environmental Toxicology and Chemistry 6:99-104.

Reinert, K.H., and J.H. Rodgers, Jr. 1986. Validation trial of predictive fate models using an aquatic herbicide (Endothall). Environmental Toxicology and Chemistry 5:449-461.

Sanders, P.F., and J.N. Seiber. 1984. Organophosphorus pesticide volatilization: Model soil pits and evaporation ponds. pp. 279-295 In: R.F. Kreuger and J.N. Seiber (Eds.) Treatment and Disposal of Pesticide Wastes. ACS Symposium Series 259, American Chemical Society, Washington, D.C.

Sato, C., and J.L. Schnoor. 1991. Applications of three completely mixed compartment models to the long-term fate of dieldrin in a reservoir. Water Research 25:621-631.

Schramm, K.-W., M. Hirsch, R. Twele, and O. Hutzinger. 1988. Measured and modeled fate of Disperse Yellow 42 in an outdoor pond. Chemosphere 17:587-595.

Slimak, M.W., and C. Delos. 1982. Predictive fate models: their role in the U.S. Environmental Protection Agency's water program. pp. 59-71 In: K.L. Dickson, A.W. Maki, and J. Cairns, Jr. (Eds.) Modeling the Fate of Chemicals in the Aquatic Environment. Ann Arbor Science Publ., Ann Arbor, Michigan.

Staples, C.A., K.L. Dickson, F.Y. Saleh, and J.H. Rodgers, Jr. 1983. A microcosm study of Lindane and Naphthalene for model validation. pp. 26-41 In: W.E. Bishop, R.D. Cardwell, and B.B. Heidolph (Eds.) Aquatic Toxicology and Hazard Assessment: Sixth Symposium, ASTM STP 802, American Society for Testing and Materials, Philadelphia, Pennsylvania.

Wolfe, N.L., L.A. Burns, and W.C. Steen. 1980. Use of linear free energy relationships and an evaluative model to assess the fate and transport of phthalate esters in the aquatic environment. Chemosphere 9:393-402.

Wolfe, N.L., R.G. Zepp, P. Schlotzhauer, and M. Sink. 1982. Transformation pathways of hexachlorocylcopentadiene in the aquatic environment. Chemosphere 11:91-101.

Introduction This section describes the EXAMS command language, including usage and reference information. The first part provides an overview of the command language and its grammar. The second part contains detailed descriptions of each command. The commands are listed in alphabetical order.

Conventions used in this Section

Convention	Meaning
CTRL/X	The phrase CTRL/X indicates that you must press the key labeled CTRL while simultaneously pressing another key, for example, CTRL/Q.
EXAMS-> LIST 7 . . .	Vertical series of periods, or ellipsis, mean that not all the data EXAMS would display in response to the particular command is shown, or that not all the data a user would enter is shown.
keyword,...	Horizontal ellipsis indicates that additional key-words, command parameters, or data can be entered in a command sequence, or that EXAMS displays additional data as part of the sample output line.
[keyword]	Square brackets indicate that the item enclosed is optional, that is, the entity can be omitted from the command line altogether.
<option>	Angle brackets indicate that a command requires a choice among two or more options.

Overview The EXAMS command language provides a set of commands for

- Entering, storing, and manipulating data describing the reaction chemistry of synthetic compounds, the environmental parameters governing their transport and transformation in aquatic systems, patterns of allochthonous loadings, and product chemistry.

- Studying the results of an analysis by listing tabular output on a terminal, plotting the concentration data ("Expected Environmental Concentrations" or EECs) computed during simulations, and printing paper copy.

- Choosing among analytical frameworks for investigating exposure to chemicals in a particular case study. EXAMS includes three operational modalities or "MODEs"

MODE	Analytical Methodology
1	Long-term consequences of continued releases of chemicals; steady-state analysis.
2	Detailed examination of immediate consequences of chemical releases; initial-value problems.
3	Intermediate-scale resolution of events over several years, including effects of seasonal environmental variability; analysis of time-series data.

Entering Commands EXAMS commands are composed of English-language words (mostly verbs) that describe what you want EXAMS to do. Some commands require qualifiers and parameters. These give EXAMS more information on how to execute the command. Command parameters describe the object to be acted upon by the command. In some cases, the object is a keyword (as in the HELP command); in others, it is an EXAMS data element (SET command) or a section of a file of input data or analysis results to manipulate (STORE and LIST commands).

Throughout this section, EXAMS commands are printed in uppercase letters for the sake of clarity. However, EXAMS will accept commands entered in uppercase, lowercase, or a mixture of uppercase and lowercase letters. Most EXAMS commands and keywords can be abbreviated to the least number of characters needed to uniquely distinguish them from other options available. For example, to end EXAMS you can enter "QUIT", "QUI", "QU", or "Q". The least number of required characters depends on the context, however, but is never more than three. For example, the SHOW command includes among its options both <QUALITY> and <QUIT>; in this case you must enter three characters for EXAMS to distinguish between them. In EXAMS' "help fields" and prompts, capitalization is used to show you how many characters are required for uniqueness.

The following example shows an AUDIT command and EXAMS' response, as they would appear on a terminal.

```
EXAMS-> AUDIT ON

All input will now be copied into the file
named "AUDOUT" on Fortran Unit Number  4

EXAMS-> ! This Command File should be renamed file.EXA

EXAMS->
```

EXAMS analyzes the parts of the above example as follows.

EXAMS-> The EXAMS system prompt for command input; a greater-than (->) means that EXAMS' command interpreter is ready for a command to be entered.

AUDIT The command name, requesting that EXAMS enable/disable the User Notepad/-Command File Creation facility.

ON An option of the AUDIT command, requesting that the Notepad/Create facility be enabled.

All input will now be copied into the file named "AUDOUT" on Fortran Unit Number 4

A message from the AUDIT command, indicating that the command completed successfully. The command interpreter used the value of AUDOUT (4) to establish communication with an external file.

EXAMS-> The next system command prompt, confirming that the command has completed its operations (AUDIT has opened communications with an external file and started recording terminal inputs), and EXAMS is ready for additional input.

! This Command File should be renamed file.EXA

A comment entered by the user. Comment lines must begin with an exclamation point (!) or an asterisk (*). You can use comments, as needed, to document EXAMS analysis sessions or command procedures.

EXAMS-> The next EXAMS system command prompt, confirming that the comment has been recorded in the Notepad/Command file and EXAMS is ready to accept another command.

Command Prompting When you enter a command at the terminal, you need not enter the entire command on a single line. If you enter a command that requires that you specify its range or the object of the requested action, and you do not include the needed information, EXAMS' command interpreter prompts you for all missing information. For example:

```
EXAMS-> AUDIT
```

The following AUDIT options are available

ON -- begins a new Audit file,
OFf -- ends Audit recording of input commands,
Help -- this message,
Quit -- return to the EXAMS prompt.

AUDIT-> ON

All input will now be copied into the
file named "AUDOUT" on Fortran unit number 4

In this example, no AUDIT option was entered, so EXAMS prompts for a more complete specification of the intended action. The line ending with a -> indicates that EXAMS is waiting for the additional input.

In many cases, EXAMS' prompts do not include an automatic description of the full range of possible response options. Often, however, entering HELP in response to the prompt will display a list of available choices, as in the following example.

EXAMS-> LIST

At the prompt, enter a Table number, "Quit,"
or "Help" to see a catalog of the output tables.

Enter Table Number -> HELP

1 Chemical inputs: FATE Data
2 Chemical inputs: PRODUCT Chemistry
3 PULSE Chemical Loadings
.
.
.
20 Exposure Analysis SUMMARY
ALL Entire Report

At the prompt, enter a Table number, "Quit,"
or "Help" to see a catalog of the output tables.

Enter Table Number -> 18

```
Ecosystem: Name of Waterbody
Chemical:  Name of chemical
-------------------------------------------------------
Table 18.01. Analysis of steady-state fate ...
-------------------------------------------------------
     .
     .    (body of table)
     .
-------------------------------------------------------
```

In the example above, LIST is entered without the number of the output table to be displayed. EXAMS prompts for the missing information; typing HELP in response to the LIST prompt displays a catalog of EXAMS output tables.

EXAMS Messages

When a command is entered incorrectly, EXAMS displays a descriptive error message indicating what is wrong. For example, if a data subscript larger that the maximum available is entered, EXAMS will respond

Subscript out-of-range.

You can then retype the command correctly.

Other error messages may be produced during the execution of a command, or during a simulation or data display sequence. These messages indicate such things as incomplete environmental data, character data entered where numeric data are required, or typographic errors during entry of commands. EXAMS will respond to typographic errors in command entries by displaying:

Command not recognized. Type HELP for command information.

Because the messages are descriptive, it is usually possible to determine what corrective action is required in order to proceed. When this is not the case, EXAMS' HELP facility contains a large body of additional and supplementary information available through the HELP, DESCRIBE, and SHOW commands.

The HELP Command Consulting a printed guide is not the most convenient way to get a summary of the syntax of a command or a definition of an input datum. EXAMS' HELP command provides this information in EXAMS' interactive environment. For example, you can type the command:

```
EXAMS-> HELP LIST
```

EXAMS responds by displaying a description of the LIST command, its syntax, and the options needed to specify the range of the command.

The HELP facility also provides on-line assistance for EXAMS' input data, e.g.,

```
EXAMS-> HELP QUANT
```

will display the subscript ranges, their meanings, the physical dimensions, and the English definition of EXAMS chemical input datum "QUANT". This information is available online for all EXAMS' input data and control parameters. The names of all of EXAMS' input variables were selected as mnemonics for their English-language names. (For example, QUANT is the photochemical quantum yield.) These mnemonics are used in EXAMS' output tables; definitions are given in the Data Dictionary of this User Manual as well as in the on-line HELP.

EXAMS' HELP facility supplies lists of individual topics and subtopics. The HELP command is described in more detail later in this Section, and a tutorial explanation of the command is available online by entering

```
EXAMS-> HELP TUTOR
```

Command Procedures A command procedure is a file that contains a sequence of EXAMS commands, optionally interspersed with descriptive comments (lines with "!" or "*" in column one). By placing sets of frequently-used commands and/or response options in a command procedure, all the commands in it can be executed as a group using a single command. For example, suppose a file called START.EXA were to contain these command lines and comments:

```
SET MODE TO 3
SET KCHEM TO 4
SET NYEAR TO 5
RECALL LOAD 7
! Loadings UDB Sector 7 is the spray drift study
```

The four commands in this file can be executed by entering the command

```
EXAMS-> DO START
```

or `EXAMS-> @START`

You do not have to specify the file type of a command procedure when you use the @ command, so long as the file type is ".EXA"--the default file type for EXAMS' @ command. You can use another file suffix, if you so inform EXAMS when you enter the command request. For example, to execute commands in a file named START.UP

```
EXAMS-> @START.UP
```

Wild Card Characters Some EXAMS commands accept a "wild card" character in the input command specifications. The asterisk (*) is the only symbol having this function in EXAMS. Wild card characters

are used to refer to a range of data subscripts, or other entities, by a general name, rather than having to enter a specific name for each member of the group. Particular uses of wild cards in EXAMS vary with the individual commands. The command descriptions later in this Section indicate where wild cards are allowed and their effects.

Truncating Command Names and Keywords All keywords and names of input data that are entered as command input can be abbreviated. Only enough characters to uniquely distinguish a keyword or datum from others with similar names need be entered (often only one).

Summary Description of EXAMS' System Commands

EXAMS Command	Summary Description
AUDIT	Start/Stop user notepad for recording procedures
CATALOG	List the contents of User Databases (UDBs)
CHANGE/SET	Enter/reset input data and program controls
CONTINUE	Resume integration (Modes 2 and 3 only)
DESCRIBE	Report dimensions and data type of parameter
DO or @	Execute file of EXAMS commands (file.EXA)
ERASE	Clear section of stored database (UDB)
HELP	Describes access to EXAMS on-line HELP facility
LIST	Show tabular results on the screen
NAME	Specify the name of a UDB, e.g., CHEM NAME IS ...
PLOT	Plot results on the screen
PRINT	Queue tabular results for hardcopy printing
QUIT	Abort command, or End interactive session
READ	Upload data from non-EXAMS ASCII disk file
RECALL	Activate data from stored database (UDB)
RUN	Begin simulation run
SHOW	Display current data values or control settings
STORE	Download current data into stored database (UDB)
WRITE	Download data to ASCII disk file
ZERO	Clear chemical loadings, pulses, or residuals

System Command Descriptions

A U D I T

Creates a copy of user input commands and responses in an external file.

Related: Control variables: AUDOUT
Commands: DO

Syntax: AUDIT <option>

Options

ON
OFf

Prompt: The following AUDIT options are available

ON -- begins a new Audit file,
OFf -- ends Audit recording of input commands,
Help -- this message,
Quit -- return to the EXAMS prompt.

AUDIT->

Options: OFf

Ends copying of EXAMS commands to the external file.

ON

Begins copying of EXAMS commands to an external file.

Description: The AUDIT command starts copying inputs typed at the terminal, into an external file. These inputs include EXAMS commands, and user responses to EXAMS prompts and option selections. The output terminus for the copy is a file named "AUDOUT," connected to Fortran logical unit number AUDOUT. The resulting output file can be used to record an analysis procedure, or as a general notepad. The output file can be renamed "file.EXA" and used as an EXAMS command (DO) file.

Examples:

1. EXAMS-> AUDIT

   The following AUDIT options are available:

ON -- begins a new Audit file,
OFf -- ends Audit recording of input commands,
Help -- this message,
Quit -- return to the EXAMS prompt.

AUDIT-> ON

All input will now be copied into the
file named AUDOUT on Fortran Unit Number 4

This command begins recording of input from the terminal into an external file. The output will go to a disk file named "AUDOUT." After leaving EXAMS, this file can be printed to give a permanent record of the analysis.

2. EXAMS-> AUDIT OFF

The AUDIT option has been terminated.

This command ends copying of EXAMS commands and responses to the external medium (usually a disk file).

3. EXAMS-> AUDIT ON

All input will now be copied into the
file named "AUDOUT" on Fortran Unit Number 4

EXAMS-> RECALL ENV 2

Selected environment is: Phantom Inlet

EXAMS-> RECALL CHEM 2

Selected compound is: Dichloroexample

EXAMS-> RECALL CHEM 4 AS 2

Selected compound is: Tetrabromoexample

EXAMS-> AUDIT OFF

These commands build a file (AUDOUT) that can later be used as a command file upon entering the EXAMS system. In this instance, the file would be renamed (e.g., MYCOMAND.EXA) and used to execute the above series of commands as a unit--

EXAMS-> DO MYCOMAND

C A T A L O G

Lists, by accession number, the title of all current entries in the specified User Database (UDB).

Related: Control variables: none
Commands: ERASE, NAME, RECALL, STORE

Syntax: CATALOG <option>

Options: CHEMICAL, ENVIRONMENT, LOAD, PRODUCT

Prompt: Enter Environment, Chemical, Load, Product, Help, or Quit->

Options:

CHEMICAL
Lists the titles, by access number, of chemical databases currently in the User Database. Each entry corresponds to a single chemical, and contains the laboratory data describing ionization and (species-specific) partitioning and reaction kinetics.

ENVIRONMENT
List the titles, by access number, of environmental databases currently in the User Database. Each entry contains a "canonical" physical and chemical model of an aquatic system, including the environmental data needed to compute reactivity and transport of synthetic chemicals in the system.

LOAD
Lists the titles, by access number, of allochthonous chemical loading patterns stored in the User Database. These data include monthly values (kg/hour) for stream-loads, non-point-source loads, groundwater seepage loads, precipitation loads, and drift loads of chemicals entering the aquatic environment, plus specification of pulse loadings. The pulse load data include the magnitude (kg), target environmental segment, and scheduling (month and day) of pulses of synthetic chemicals entering the system.

PRODUCT
Lists the titles, by access number, of reaction or transformation product chemistries stored in the User Database. These data include the Activity Database numbers of chemical parent and product compounds, the number of the process responsible for the transformation, and the yield efficiency (mole/mole) as an (optional) function of temperature.

Description: The CATALOG command inventories the contents of the specified User Database (UDB) and lists the titles of active entries on the terminal screen. Four types of UDBs are available, corresponding to the four options available to the CATALOG command. The titles are listed by accession number; this number is used to STORE, RECALL, or ERASE database entries.

Examples:

1. EXAMS-> CATALOG HELP

The CATALOG command requires that you specify either:

1. Environment,
2. Chemical,
3. Load,
4. Product,
5. Help (this option), or
6. Quit.

Enter Environment, Chemical, Load, Product, Help, or Quit-> CHEMICAL

Catalog of CHEMICAL parameter sets

UDB No.	Name of Entry Volume
1	Chemical Data Entry Template
2	p-Cresol
3	Benz[a]anthracene
.	
.	
.	

EXAMS->

This example use of the CATALOG command lists the contents of the current User Database for chemical data. Any of these datasets can be loaded into the Activity Database (ADB) for study, using the RECALL command and the appropriate access number. The first entry ("Chemical Data Entry Template") is a blank data area reserved for entering new chemical data.

2. EXAMS-> CATALOG ENVIRON

Catalog of ENVIRONMENTal models

UDB No.	Name of Entry Volume
1	Environmental Data Entry Template
2	Pond -- AERL code test data
3	Connecticut River estuary
.	
.	
.	

This example CATALOG command generates a listing of the environmental datasets present in the User Database. Any of these can be retrieved for study using a RECALL command and the accession number. The first entry ("Environmental Data Entry Template") is a template for entering a new environmental model.

C H A N G E

Use to enter data into the activity database (synonymous with SET).

Related: Commands: DESCRIBE, HELP, SET

Syntax: CHANGE <name of variable> TO <new value>
or SET <name of variable> = <new value>

Prompt: Enter name=value command->

Variable: The data entry or variable to be entered can be specified either as a single datum or, using wild cards (*), as an entire vector, row/column of a matrix, etc.

Description: Use the CHANGE command to specify the values of data in the activity database. "Value" can be any numerical quantity or literal characters, as appropriate. "Variable" specifies an individual element of input data or a program control parameter. Entire vectors, rows/columns of matrices, etc. can be set to a single uniform value using wild cards (*).

Examples:

1. EXAMS-> CHANGE VOL(153) TO 7E5

   Subscript out-of-range.

   EXAMS-> DESCRIBE VOL

   VOL is a Real Vector with 100 elements.

   EXAMS> CHANGE VOL(2) TO E

   Invalid numeric quantity after TO or =.

   EXAMS-> CHANGE VOL(2) TO 7E5

This command sets the environmental volume of segment 2 to 7.0E+05 cubic meters. The initial attempt to set the volume of segment 153 was rejected by EXAMS because the version in use was set up for environmental models of 100 segments at most. The DESCRIBE command was used to check the number of subscripts and the dimensional size of the variable "VOL". The accidental entry of an alphabetic character ("E") for the volume was trapped by the CHANGE command; VOL(2) was not altered.

2. EXAMS-> HELP TCEL

TCEL is a Real Matrix with 100 rows and 13 columns.
Temperature-CELsius (segment,month) Units: degrees C.
Average temperature of ecosystem segments. Used (as enabled by input data) to compute effects of temperature on transformation rates and other properties of chemicals.

EXAMS-> CHANGE TCEL(2,7) TO 24

This command changes the July temperature in segment 2 to 24° C. The HELP command was used to check subscript dimensions, maximum values, the meaning of the subscripts (subscript #1 denotes the segment, subscript #2, the month), and the proper units for the input datum (degrees Celsius).

3. EXAMS-> HELP POH

POH is a Real Matrix with 100 rows and 13 columns.
pOH (segment,month) Units: pOH units
The negative value of the power to which 10 is raised in order to obtain the temporally averaged concentration of hydroxide [OH^-] ions in gram-equivalents per liter.

EXAMS-> CHANGE POH(*,13) TO 6.2

This command sets the average pOH (sector 13) of every segment to 6.2. Note use of wild card "*" to specify that all segments are to be changed. As in the previous example, HELP was used to check subscript dimensions, units, etc. This step, of course, is optional.

C O N T I N U E

The CONTINUE command resumes EXAMS' simulation analysis of chemical dynamics beginning from the current state of the system.

Related: Control variables: CINT, TINIT, TEND, TCODE, NYEAR
Commands: RUN, SHOW_TIME_FRAME

Syntax: CONTINUE

Prompt: (In Mode 2 only:)
Initial time for integration will be (nn.n) units
Enter ending time of integration, Help, or Quit->

Options: None. Reply to prompt with a value greater than (nn.n).

Description: The CONTINUE command resumes EXAMS' simulation analysis of chemical dynamics, beginning from the current state of the system. Chemical loadings and other input data can be altered (CHANGEd or SET) between simulation time segments; EXAMS will re-evaluate equation parameters as needed to incorporate the changed conditions into the analysis. CONTINUE cannot be invoked from Mode 1, where it is not appropriate. The SHOW TIME FRAME (abbreviate to SH T F) command can be used to examine the current state of the integrator timer controls. In Mode 2, the Communications INTerval CINT can be used to vary the temporal resolution in different segments of the analysis (see Example 1). In Mode 3, NYEAR, the number of years in a simulation time segment, can similarly be altered.

Examples:

1.
```
EXAMS-> SET MODE=2

EXAMS-> SHOW TIME FRAME

A RUN will integrate from      0. to     24. Hours
with output at intervals of    2.00 Hours

EXAMS-> SET TCODE=2

EXAMS-> SET TEND=10

EXAMS-> SET CINT=0.25

EXAMS-> SH TI F

A RUN will integrate from      0. to     10. Days
with output at intervals of    0.25 Days
```

EXAMS-> RUN

Simulation beginning for:
Environment: Pond -- AERL code test data
Chemical 1: Dichloroexample

Run complete

EXAMS-> PLOT KIN PL (3,0,0 -- see PLOT command)

```
System:  Pond -- AERL code test data
Chemical:  Dichloroexample

  2.00          IBB BBB
                I      B BBBB BBBB
                I                    BBBB BBBB BBB
                I                                 B BBBB BBBB BB
                I                                                BB BBB
  1.33          I
                I
                I
                I
                I
  0.667         I
                I
                I
                I
                I
  0.000         I
                 +----+----+----+----+----+----+----+----+----+----+
                0.000     2.00      4.00      6.00      8.00      10.0
                     1.00      3.00      5.00      7.00      9.00
                                    Time, Days
```

EXAMS-> SET CINT=1
EXAMS-> CONTINUE

Initial time for integration will be 10.0 Days
Enter ending time of integration, Help, or Quit-> 30

Simulation beginning for:
Environment: Pond -- AERL code test data
Chemical 1: Dichloroexample

Run complete.

EXAMS-> SET CINT=10
EXAMS-> ZERO PULSE LOAD

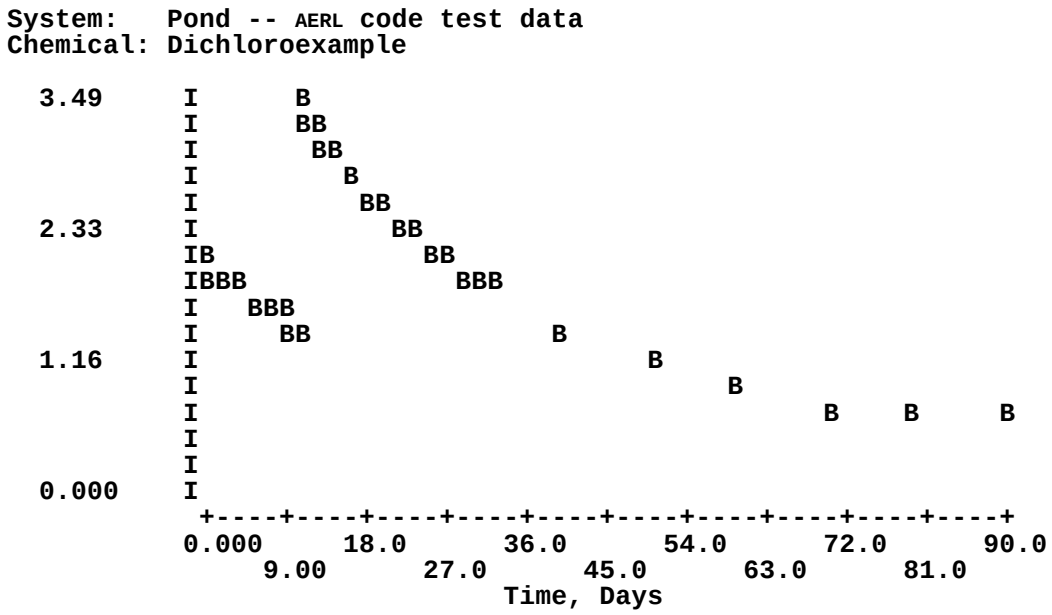
EXAMS-> CONTINUE

Initial time for integration will be 30.0 Days
Enter ending time of integration, Help, or Quit-> 90

Simulation beginning for:
Environment: Pond -- AERL code test data
Chemical 1: Dichloroexample

Run complete.

EXAMS-> PLOT KINETIC PLOT (3,0,0)



These commands show the use of the CONTINUE command in Mode 2. The objective of the analysis was to introduce two pulses of chemical separated by 10 days and to follow exposure over 90 days. Note the phased increase in the Communications INTerval CINT from 0.25 to 1 and then 10 days. Note the use of the ZERO command to clear the pulse load ADB before the simulation of dissimilation from day 30 through day 90. If this were not done, EXAMS would introduce an additional pulse on day 30.

2. EXAMS-> SET MODE=3

EXAMS-> SHO TI FR

A RUN will integrate from 1 January 1989
through 31 December 1989.
(YEAR1 = 1989, and NYEAR = 1.)

EXAMS-> RUN

Simulation beginning for:
Environment: Pond -- AERL code test data
Chemical 1: Dichloroexample

Run complete.

EXAMS-> SHO TI FR

A RUN will integrate from 1 January 1989
through 31 December 1989.
(YEAR1 = 1989, and NYEAR = 1.)

CONTinuation will proceed through 31 December 1990
(NYEAR = 1.)

EXAMS-> SET NYEAR=3

EXAMS-> SH TI F

A RUN will integrate from 1 January 1989
through 31 December 1991.
(YEAR1 = 1989, and NYEAR = 3.)

CONTinuation will proceed through 31 December 1992
(NYEAR = 3.)

EXAMS-> CONTINUE

CONTinuing integration through 31 December 1992.

Simulation beginning for:
Environment: Pond -- AERL code test data
Chemical 1: Dichloroexample

Run complete.

EXAMS->

These commands illustrate the use of the CONTINUE command in Mode 3. "SHOW TIME FRAME" is used to check the state of the integrator timer controls.

D E S C R I B E

Reports the data type, dimensionality, and implemented size of parameters.

Related: Control variables:
Commands: HELP

Syntax: DESCRIBE <parameter>

Parameters:

Any "system parameter"--any chemical or environmental input datum, control parameter (e.g., MODE, CINT), etc.

Prompt: Enter name of input parameter->

Options: Any parameter accessible to the CHANGE and SET commands can be inspected using the DESCRIBE command.

Description: The DESCRIBE command returns information about EXAMS' input data and control parameters. All variables whose values can be altered using the CHANGE and SET commands can be inspected by the DESCRIBE command. The information returned by DESCRIBE includes the data type (real, integer, character), dimensionality (scalar, vector, matrix (2-dimensional), table (3-dimensional matrix)) and implemented size in the version of EXAMS in use. The DESCRIBE command is the first recourse when a CHANGE or SET command fails.

Examples:

1. EXAMS-> DESR MODE

   Command not recognized. Type HELP for command information.

   EXAMS-> DESCR

   Enter name of input parameter-> MODE

   MODE is an Integer Scalar.

   These commands establish that "MODE" is an integer scalar. Note that the initial typing error (DESR) resulted in a "not recognized" error message followed by return to the EXAMS prompt.

2. EXAMS-> CHANGE VOL(133) TO 7E5

Subscript out-of-range.

EXAMS-> DESCRIBE VOL

VOL is a Real Vector with 100 elements.

This command reports that VOL is a real variable, with 100 elements. In this example, the number of segments (NPX) in the version of EXAMS currently in use is set for 100 at most. Any (intentional or accidental) attempt to set "KOUNT" to a value > 100, or to enter a value for the VOLume of a segment > 100 (e.g., VOL(133)) will fail, as illustrated above. DESCRIBE can be used to check the reason for a failure of the CHANGE or SET command when a problem with dimension sizes is suspected.

3. EXAMS-> DESCRIBE QUANT

QUANT is a Real Table with dimensions (3,7,4)

EXAMS-> HELP QUANT

QUANT is a Real Table with dimensions (3,7,4)
QUANTum yield (form,ion,chemical) Units: dimensionless
Reaction quantum yield for direct photolysis of chemicals--fraction of the total light quanta absorbed by a chemical that results in transformations. Separate values (21) for each potential molecular type of each chemical allow the effects of speciation and sorption on reactivity to be specified in detail. The matrix of 21 values specifies quantum yields for the (3) physical forms: (1) dissolved, (2) sediment-sorbed, and (3) DOC--complexed; of each of (7) possible chemical species: neutral molecules (1), cations (2-4), and anions (5-7). (QUANT is an efficiency.)

These commands report the data type and dimensionality of EXAMS' input "QUANT" (result of "DESCRIBE QUANT") and then report the meaning of the dimensions and the physical units of the variable (result of "HELP QUANT"). The local implementation of EXAMS used in this example has the capacity to simulate the behavior of no more than four chemicals simultaneously. Thus, QUANT was DESCRIBEd as consisting of a set of four matrices, each of (fixed) size (3,7).

D O

Executes a command procedure; requests that EXAMS read subsequent input from a specific file.

Related: Control variables:
Commands: AUDIT

Syntax: DO <name of command file>

Prompt: Enter name of file (no more than nn characters), Help, or Quit->

Parameters: name of file

Specifies the file from which to read a series of EXAMS commands. If you do not specify a file type suffix, EXAMS uses a default file type of EXA (e.g., "filename.EXA"). Wild cards are not allowed in the file specification.

Description: Use command procedures to catalog frequently used sequences of commands. An EXAMS command procedure can contain

- Any valid EXAMS command. The command line can include all the necessary options and data to build a complete command (exception: kinetic plots).
- Parameters or response options for a specific command. When the currently executing command requires additional parameters, the next line of the command file is searched for appropriate input.
- Data. When the currently executing command requires numerical or character data entry, the next line of the command file is searched for input.
- Comment lines. Any line that contains an exclamation point (!) or asterisk (*) in column one is ignored by EXAMS' command interpreter. These lines can be used as needed to document the command procedure.

Command procedures must not contain a request to execute another command procedure. (In other words, a DO file must not contain a DO (@) command; EXAMS' DO commands cannot be nested.) Command procedures can be constructed as external files using your favorite editor, or they can be constructed interactively through the EXAMS system command processor, as illustrated below. The default file type is "EXA", but files of any type (suffix) can be used if the entire file name is specified when entering the DO command.

Examples: 1. EXAMS-> AUDIT ON

All input will now be copied into the
file named "AUDOUT" on Fortran Unit Number 4

EXAMS-> RECALL

Enter Environment, Chemical, Load, Product, Help or Quit-> ENV
Enter environment UDB catalog number, Help, or Quit-> 2
Selected environment is: Phantom Inlet

EXAMS-> RECALL CHEM 2

Selected compound is: Dichloroexample

EXAMS-> RECALL LOAD 2

Selected load is: Aedes control spray drift

EXAMS-> ! Load 2 is the Phantom Inlet salt marsh study

EXAMS-> SET KCHEM TO 2

EXAMS-> RECALL CHEM 4 AS 2

Selected compound is: Tetrabromoexample

EXAMS-> AUDIT OFF

These commands build a file (AUDOUT.DAT) that can later be used as a command file upon entering the EXAMS system. In this instance, the file could be renamed (e.g., SETUP.EXA) and used to execute the above series of commands as a unit:

EXAMS-> DO SETUP
or, EXAMS-> @SETUP

The completed command file appears as follows

```
RECALL
ENV
2
RECALL CHEM 2
RECALL LOAD 2
! Load 2 is the Phantom Inlet salt marsh study
SET KCHEM TO 2
RECALL CHEM 4 AS 2
AUDIT OFF
```

Note that command files that are constructed interactively will include "AUDIT OFF" as the final instruction. This can, of course, be removed by editing the file if it is undesirable.

2. EXAMS-> DO

Enter name of file (no more than nn characters), Help, or Quit-> HELP

The "DO" or "@" command provides a means of executing stored EXAMS commands. In response to the prompt, enter the name of the file that contains the stored commands. A three-character filename extension of "EXA" is added to the name if no period is present in the name as entered. The maximum length for file names is nn characters; this limit includes the .EXA suffix.

Enter name of file (no more than nn characters), Help, or Quit-> AUDOUT

EXAMS/DO-> ! Audit trail of input sequence from EXAMS.
EXAMS/DO-> RECALL

Enter Environment, Chemical, Load, Product, Help, or Quit->
EXAMS/DO-> ENV

Enter environment UDB catalog number, Help, or Quit->
EXAMS/DO-> 2

Selected environment is: Phantom Inlet
EXAMS/DO-> RECALL CHEM 2

Selected compound is: Dichloroexample
EXAMS/DO-> RECALL LOAD 2

Selected load is: Aedes control spray drift
EXAMS/DO-> ! Load 2 is the Phantom Inlet salt marsh study
EXAMS/DO-> SET KCHEM TO 2
EXAMS/DO-> RECALL CHEM 4 AS 2

Selected compound is: Tetrabromoexample
EXAMS/DO-> AUDIT OFF

The AUDIT option has been terminated.

This command requests execution of the command procedure constructed in Example 1 above. The default name (AUDOUT) was not altered, so the complete file specification was given to the DO command as the entry parameter. The DO file transfers a set of two chemicals, an environmental model, and a load pattern from the stored UDB to the ADB for study and analysis.

E R A S E

Deletes, by accession number, the data stored at a single sector of a User Database (UDB) library (chemical, environmental, loadings, product chemistry).

Related: Control variables:
Commands: CATALOG, RECALL, STORE

Syntax: ERASE <option> <accession number>

Options

CHEMICAL
ENVIRONMENT
LOAD
PRODUCT

Prompt: Enter Environment, Chemical, Load, Product, Help, or Quit->

Options: CHEMICAL
Deletes the contents, by entry access number, of chemical databases currently in the User Database. Each entry corresponds to a single chemical, and contains the laboratory data describing ionization and (species-specific) partitioning and reaction kinetics.

ENVIRONMENT
Deletes the contents, by entry access number, of environmental databases currently in the User Database. Each entry contains a canonical physical and chemical model of an aquatic system, including the environmental data needed to compute the reactivity and transport of synthetic chemicals in the system.

LOAD
Deletes the contents, by entry access number, of chemical loading patterns stored in the User Database. These data include monthly values (kg/hour) for streamloads, non--point-source loads, groundwater seepage loadings, precipitation loads, and drift loads of chemicals entering the aquatic environment, plus the magnitude (kg), target environmental sector, and scheduling (month and day) of chemical pulse loads.

PRODUCT
Deletes the contents, by entry access number, of chemical product data stored in the User Database (UDB). These data include the Activity Database numbers of reactants and

products, the number code of the chemical process, and yield efficiencies (mole/mole) as an (optional) function of temperature.

Description: ERASE deletes the contents of a single sector of the specified User Database (UDB) library (chemical, environmental, loads, or product chemistry). The data to be deleted are selected by choosing the appropriate accession number. (If you work in a multi-user environment, be sure to avoid erasing others' data.)

Examples:

1. EXAMS-> ERASE ENV 20

   Environment 20 erased.

   This command erases the data stored at Environmental UDB sector number twenty. The space is now available for storing another dataset.

2. EXAMS-> ERASE

   Enter Environment, Chemical, Load, Product, Help, or Quit-> HELP

   The ERASE command requires that you specify either:
   1. Environment,
   2. Chemical,
   3. Load,
   4. Product,
   5. Help (this option), or
   6. Quit.

   Enter Environment, Chemical, Load, Product, Help, or Quit-> LOAD

   Enter allochthonous loading UDB catalog number, Help, or Quit-> 10

   Load 10 erased.

   This command erases the data stored at Loadings UDB sector number ten. The space is now available for another dataset.

E X I T

EXIT can be used as a synonym for QUIT to end an interactive session.

Related: Control variables:
Commands: QUIT is used to abort commands in progress.

Syntax: EXIT

Prompt: None

Options: None

Description: If EXIT is entered from the EXAMS prompt command level, EXAMS stops and returns control to the computer operating system.

Examples:

1. EXAMS-> EXIT

   This command terminates an interactive EXAMS session.

H E L P

Displays, on the terminal, information available in EXAMS' help files. EXAMS provides descriptions of its commands, input data, control parameters, and general concepts and analysis procedures.

Related: Control variables:
Commands: DESCRIBE

Syntax: HELP [keyword]

Prompt: None

Keyword: Specifies a keyword (a topic or an element of EXAMS input data) that tells EXAMS what information to display.

- None--if HELP is typed with no keyword, EXAMS lists the keywords that can be specified to obtain information about other topics.
- Topic-name--describes either a basic EXAMS command, an information page, or a "system parameter." System parameters include chemical and environmental input data, system control parameters (e.g., CINT), and parameters that control the current analysis (e.g., IMASS).

Ambiguous abbreviations result in a failure to achieve a match on the keyword, and an error message is displayed.

Description: The HELP command provides access to EXAMS' collection of on-line user aids and information texts. This material includes

- Brief discussions of the syntax and function of each of EXAMS' command words (RECALL, RUN, etc.)
- Definitions, physical dimensions, and meanings of subscripts for EXAMS' chemical and environmental input data and control parameters.
- A series of information pages providing orientation to the concepts implemented in the EXAMS program, the range of capabilities and analyses that can be executed with the program, and brief expositions on data structures and program control options.

Examples:

1. EXAMS-> HELP

EXAMS includes these system commands:

.
. HELP message text and list of command and
. information topics

Issuing the HELP command without any keywords produces a list of the HELP topics in EXAMS main command library. When responding to one of the topics on the list, EXAMS displays a HELP message on that topic, and a list of subtopics (if any).

2. EXAMS-> HELP QUOIT

No information available for this request.

EXAMS->

When you request information for a topic not on file, EXAMS displays a message to that effect and returns you to the EXAMS-> prompt.

3. EXAMS-> HELP QUANT

QUANT is a Real Table with dimensions(3,7,4)
QUANTum yield (form,ion,chemical) Units: dimensionless
Reaction quantum yield for direct photolysis of chemicals--fraction of the total light quanta absorbed by a chemical that results in transformations. Separate values (21) for each potential molecular type of each chemical allow the effects of speciation and sorption on reactivity to be specified in detail. The matrix of 21 values specifies quantum yields for the (3) physical forms: (1) dissolved, (2) sediment-sorbed, and (3) DOC--complexed; of each of (7) possible chemical species: neutral molecules (1), cations (2-4), and anions (5-7). (QUANT is an efficiency.)

You can request information about any input datum (chemical, environmental, control parameters, analysis parameters) accessible to the CHANGE and SET commands. EXAMS then displays on the screen the characteristics of the variable (equivalent to the results of DESCRIBE), followed by a discussion of the variable that echoes the entry in the Data Dictionary section of the EXAMS User Manual.

L I S T

Displays an EXAMS output table on the terminal screen.

Related: Control variables: FIXFIL
Commands: PLOT, PRINT

Syntax: LIST <option>

Options

table-#
ALL
HELP

Prompt: Enter Table Number -> option

Options:

table-#	specifies the number of an EXAMS output table to be displayed.
ALL	Sequential display of all current output tables.
HELP	Displays a list of titles of EXAMS output tables.

Description: The LIST command displays EXAMS' output tables at the terminal. To temporarily halt the output and resume it at the line where it was interrupted, use CTRL/S followed by CTRL/Q.

When you request a primary table number (that is, an integer from 1 to 20) EXAMS displays the first table of that number present in the analysis file. If additional tables of that type are present in the file, EXAMS will display the first, and then search for more tables of that type and, if any are found, ask if you want to see them.

Examples:

1. EXAMS-> LIST

   A PRINT, LIST, or PLOT command was issued before executing a RUN. If results exist from a previous simulation, these can be accessed after issuing the command: SET FIXFIL TO 1

   EXAMS-> SET FIXFIL TO 1

EXAMS-> LIST

Enter Table Number -> HELP

1 Chemical inputs: FATE Data
2 Chemical inputs: PRODUCT Chemistry
3 PULSE Chemical Loadings
.
.
.
18 Sensitivity Analysis of Chemical FATE
19 Summary TIME-TRACE of Chemical Concentrations
20 Exposure Analysis SUMMARY
ALL Entire Report

Table-> 18

```
Ecosystem: Name of Waterbody
Chemical:  Name of chemical
-----------------------------------------------------
TABLE 18.01.  Analysis of steady-state fate ...
-----------------------------------------------------
      .
      .  (body of table)
      .
-----------------------------------------------------
```

The LIST command requests that output Table 18 from an EXAMS results file be displayed on the terminal. For illustrative purposes, it was assumed that the user had left EXAMS and then returned to inspect Table 18 generated in the previous session.

2. EXAMS-> LIST 20

```
Ecosystem: Name of Waterbody
Chemical:  Name of FIRST chemical
-----------------------------------------------------
TABLE 20.01.  Exposure analysis summary: 1983--1985.
-----------------------------------------------------
      .
      .  (body of table)
      .
```

More? (Yes/No/Quit)-> Y

```
Ecosystem: Name of Waterbody
Chemical:  Name of SECOND chemical
-----------------------------------------------------------
TABLE 20.02.  Exposure analysis summary: 1983--1985.
-----------------------------------------------------------
      .
      .  (body of table)
      .
```

In this example, EXAMS was used to investigate the behavior of two chemicals over a period of several years, using Mode 3 simulations. The analysis began with year 1983, and NYEAR was set to 3 to produce an analysis of the period 1983 through 1985. The LIST command requests that all versions of Table 20 in the analysis file be displayed, with a pause between each for inspection of the results. In the example, the analyst chose to examine the output for both chemicals. If the analysis is now CONTINUEd, the current set of tables will be replaced with new results. The PRINT command should be used to make copies of all intermediate results you want to save.

The sub-table numbers of EXAMS' output tables identify the ADB number of the chemical, the indexes of any ions (see SPFLG in the EXAMS Data Dictionary), and the month of the year, as follows.

Table	Sub-tables	Examples	Sub-table Meaning
1	1.cc.i	1.01.1	Table.chemical.ion
4-6, 8, 10,11,13	NN.mm	4.01 10.13	Table.month (13 = annual mean)
12	12.cc.mm	12.01.12	Table.chemical.month
14 (Mode 1/2)	14.cc	14.01	Table.chemical
14 (Mode 3)	14.cc.mm	14.01.12	Table.chemical.month
15-18,20	NN.cc	18.01 20.01	Table.chemical

N A M E

Use the NAME command to attach unique names to datasets.

Related: Control Variables: MCHEM
Commands: CATALOG, ERASE, STORE, RECALL

Syntax: <datatype> NAME IS a[aa...] (up to 50 characters), where <datatype> can be CHEmical, ENvironment, LOad, or PROduct

Prompt: Options available are:

Help - this message.
Quit - return to EXAMS command mode.
<carriage return> = Help
<any other response> - accepted as the new name.

Enter new name->

<datatype>: EXAMS uses these four kinds of datasets:

1. CHEMICAL reactivity and partitioning,

2. ENVIRONMENTal physico/chemical parameters,

3. allochthonous chemical LOADings, and

4. PRODUCT chemistry for generating interconversions among multiple chemicals in an analysis

Description: The NAME command is used to associate unique names with datasets in the UDB. These names can be STOREd in the CATALOGs; they are printed in the headers of EXAMS' output tables. When naming CHEMICAL datasets, the ADB number of the chemical to be named is given by MCHEM; use "SET MCHEM TO n" before naming dataset "n".

Examples:

1. EXAMS-> CHEM NAME IS Tetrachloroexample

The NAME command associates the name "Tetrachloro..." with the chemical data in the sector of the activity database (ADB) given by the current value of MCHEM. This name will be printed on all subsequent appropriate output tables, and it will be used as a title for the database if the STORE command is used to download the data into the User Database (UDB).

2. EXAMS-> SET MCHEM = 2

   EXAMS-> CHEM NAME IS Dichloroexample

   The chemical name command always addresses the MCHEM sector of the chemical ADB, thus, this example names chemical number 2 to "Dichloro...".

3. EXAMS-> ENVIR NAME IS Pogue Sound

   This command names the current environmental dataset "Pogue Sound". The name will now appear on output tables, and remain with the dataset if it is downloaded to the UDB permanent files.

P L O T

Used to plot character graphics for the chemical state of the ecosystem.

Related: Control Variables: MCHEM
Commands: LIST, PRINT

Syntax: PLOT <Option1, Option2, Option3>

Options 1:

POINT
PROFILE
KINETIC

Prompt: The following options are available:

POint - Vertical concentration profile
PRofile - Longitudinal concentration profile
Kinetic - List or plot kinetic outputs
Help - This message
Quit - Return to the EXAMS program prompt

Option->

Plot options: POINT

"POINT" plots are generalized profiles of chemical concentrations. These also require selection of a variable to be displayed (total concentration, dissolved concentration, etc.) and a "statistical" class (average values, minima, or maxima).

PROFILE

"PROFILE" plots are longitudinal profiles of chemical concentrations. These require selection of a concentration variable (total concentration, dissolved concentration, etc.) and an environmental sector (water column or benthic sediments). The abscissa of the resulting plot is set up by increasing segment number, which in most cases should represent an upstream-downstream progression. When the aquatic model includes both longitudinal and vertical segmentation, each section of the plot begins at the air-water or water/benthic interface and proceeds vertically downward (the bars are presented along the abscissa).

KINETIC

"KINETIC" plots display the results of integration of the governing equations over the time spans selected for simulation. These plots also require selection of concentration variables and either particular segments, or summary "statistics," for display. Time is used as the abscissa for the plot.

Description: Use the PLOT command to display results of the current analysis. Three kinds of character graphic PLOTs are available on-line from EXAMS: POINT, PROFILE, and KINETIC. Each PLOT requires the specification of several options; these can either be entered on the system command line or entered in response to EXAMS prompts. The available second- and third-level options are illustrated in the examples below. The results available to POINT and PROFILE plots depend on the Mode used in the simulation. In Mode 1, the outputs are steady-state concentrations. In Mode 2, the results are a snap-shot of concentrations as of the end of the current temporal simulation segment. In Mode 3, the results are time-averaged concentrations over the most recent temporal simulation segment of length NYEAR.

Examples:

1. EXAMS-> PLOT POINT

The following concentration options are available:

Total	-	mg/L in Water Column, mg/kg in Benthic Sediments
Dissolved	-	"Dissolved" (mg/L) (aqueous + complexes with "dissolved" organics)
Particulate	-	Sediment-sorbed (mg/kg dry weight)
Biota	-	Biosorbed (ug/g dry weight)
Mass	-	Chemical mass as grams/square meter AREA
Help	-	This message
Quit	-	Return to the EXAMS prompt

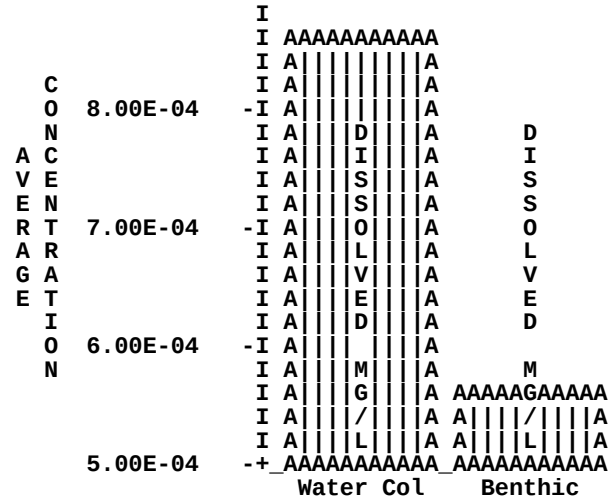
Option-> DISSOLVED

The following statistical options are available:

MAX - Maximum concentration
MIN - Minimum concentration
AVE - Average concentration
Help - This message
Quit - Return to the EXAMS prompt

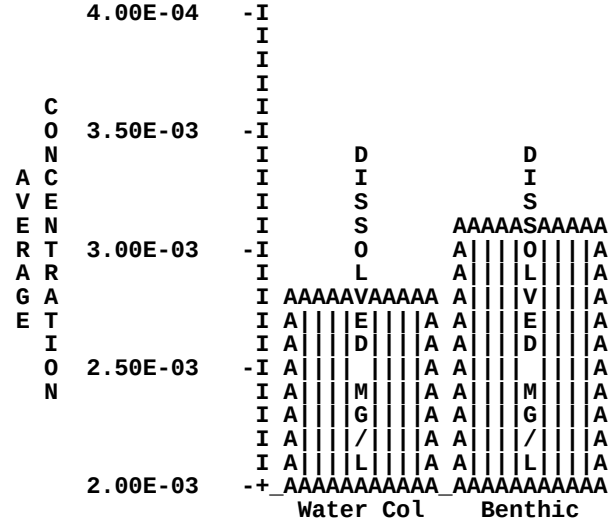
Option-> AVERAGE

9.00E-04 -I



EXAMS-> SET MCHEM=2

EXAMS-> PL PO DI AV



This example illustrates EXAMS' internal prompting for POINT plots. Note that the analysis included two chemicals; the plot for chemical number two was obtained by first SETting MCHEM=2. The second plot was requested via a single command line, thus bypassing the PLOT prompts.

2. EXAMS-> PLOT PROF

The following concentration options are available:

Total	-	mg/L in Water Column, mg/kg in Benthic Sediments
Dissolved	-	"Dissolved" (mg/L)

(aqueous + complexes with "dissolved" organics)

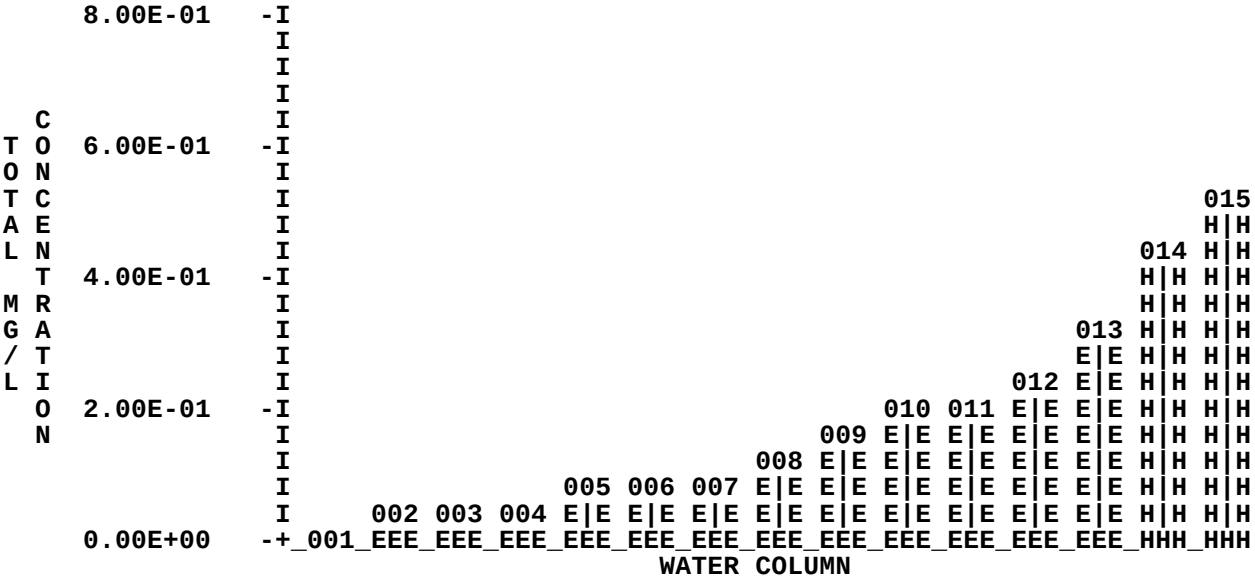
Particulate	-	Sediment-sorbed (mg/kg dry weight)
Biota	-	Biosorbed (ug/g dry weight)
Mass	-	Chemical mass as grams/square meter AREA
Help	-	This message
Quit	-	Return to the EXAMS prompt

Option-> TOTAL

The following options are available:

WATER	-	Water Column concentrations
SEDIMENTS	-	Benthic Sediment concentrations
Help	-	This message
Quit	-	Return to the EXAMS prompt

Option-> WATER



The above example illustrates EXAMS' internal prompts for a PROFILE plot. As with the POINT option, this entire command could be entered on a single line:

EXAMS-> PLOT PROF TOT WAT

3. EXAMS-> PLOT KIN

The following KINETIC options are available:

List - lists selected KINETIC output parameters

Plot - plots selected KINETIC output parameters
Help - this message
Quit - return to the EXAMS prompt

Option-> PLOT

Chemical: Methyl Parathion
Environment: Pond -- AERL code test data

Simulation units: Days
Number of segments: 2

	1	2
Type of segment (TYPE):	L	B

The following parameters are available for time-trace plotting
of values averaged over the ecosystem space:
("Dissolved" = aqueous + complexes with "dissolved" organics.)

1	-	Water Column: average "dissolved" (mg/L)	
2	-	average sorbed (mg/kg)	
3	-	total mass (kg)	
4	-	Benthic:	average "dissolved" (mg/L)
5		average sorbed (mg/kg)	
6		total mass (kg)	

Enter parameters, one per line;
enter 0 to end data entry and proceed.

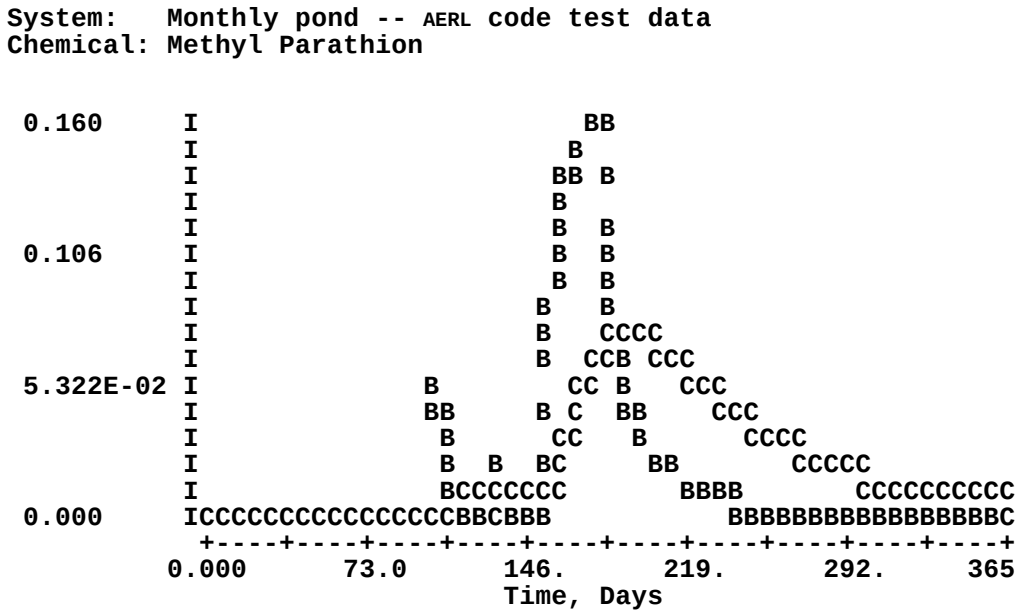
Parameter-> 3
Parameter-> 6
Parameter-> 0

The following parameters are available for each segment:

1	-	Total concentration	(Water Column, mg/L; benthic, mg/kg)
2	-	"Dissolved"	(mg/liter of fluid volume)
3	-	Sorbed	(mg/kg of sediment)
4	-	Biosorbed	(ug/g)
5	-	Mass	(grams/square meter of AREA)

Enter segment-parameter number pair, one number per line;
enter 0 when data entry is complete; Quit to abort.

Enter segment number---> 0



This example illustrates EXAMS' prompting in KINETIC plots. The numerical options cannot be entered on the command line, but must be entered in response to the prompts.

P R I N T

Use the PRINT command to queue an output table for hardcopy printing.

Related: Control variables: FIXFIL
Commands: LIST

Syntax: PRINT <option>

Options:

table-#
ALL
Help
Quit

Prompt: Enter Table Number->

Options:

table-#	specifies the number of an EXAMS output table to be displayed.
ALL	Sequential printing of all current output tables.
HELP	Displays a list of titles of EXAMS output tables.

Description: The PRINT command transfers EXAMS results tables to an output queue for printing. The command functions identically with the LIST command, except that output is saved for hardcopy printing rather than being routed to your interactive terminal. If the PRINT command results in output at your terminal, you may need to consult with site ADP personnel to properly direct the print stream to a lineprinter.

Examples: See the documentation for the LIST command.

Q U I T

Use QUIT to abort a command in progress or to end an interactive EXAMS session.

Related: Control variables:
Commands: EXIT

Syntax: QUIT

Prompt: None

Options: None

Description: Entering QUIT at the EXAMS prompt command level will terminate an interactive session, returning control to the computer's operating system. QUIT is included as an option of many EXAMS commands to allow the command to be aborted.

Examples:

1. EXAMS-> AUDIT

   The following AUDIT options are available
   ON -- begins a new audit file,
   OFf -- ends Audit recording of input commands,
   Help -- this message,
   Quit -- return to the Exams prompt.

   AUDIT-> QUIT

   EXAMS->

   This command terminates processing of the AUDIT command and returns control to the EXAMS prompt command level. The current status of AUDIT is not altered.

2. EXAMS-> QUIT

   This command terminates an interactive EXAMS session.

R E A D

Use the READ command to transfer data from a properly organized non-EXAMS file into the Activity Data Base (ADB).

Related: Control variables: MODE, MCHEM, PRBEN
Commands: WRITE

Syntax: READ <datatype> <name of file>

Prompt: Enter Environment, Chemical, PRZM, Help, or Quit->

Description: The READ command provides a facility for up-loading EXAMS datasets from external ASCII sequential files. These non-EXAMS files can be stored entirely separately from the main EXAMS User Data Base (UDB), which is contained in a direct access file named "EXAMS.DAF". Data are transferred directly to the Activity Data Base (foreground memory ADB) rather than to the User Data Base (UDB) file area, so the STORE command must be used to transfer data to the UDB from the ADB after invoking READ or they will be discarded when you exit from EXAMS.

Under the ENVIRONMENT option of READ, the setting of MODE controls how many data are read from the external file. When MODE is 1 or 2, only the dataset sector indicated by the current value of MONTH is transferred. For example, if MODE=1 and MONTH=13, explicit mean values (only) will be uploaded. When MODE=3, the entire ADB dataset ("months" 1 through 13) will be uploaded from the external file called <name of file>.

Under the CHEMICAL option of READ, the chemical dataset to be uploaded from <name of file> is put into the MCHEM sector of the Activity Data Base (ADB).

In the PRZM option of the READ command, a set of external loadings generated by the Pesticide Root Zone Model (PRZM). This facility transfers chemicals exported from the land surface into an adjacent aquatic system. The PRZM transfer file is a mode 3 construct, in which the first set of loadings contain the application rate of the pesticide, and the succeeding loadings contain water-borne and sediment-borne chemical transfers to the aquatic system. The parameter PRBEN (c.f.) controls EXAMS' treatment of sediment-borne materials. When PRBEN is zero, all sediment-borne materials are equilibrated with the water column upon entry into the system. When PRBEN is 1.0, all sediment-borne materials are routed to the benthic zone. PRBEN has a default value of 0.5, based on the observation that, in general, about 50% of sorbed chemical is usually labile, and about 50% recalcitrant, to rapid re-equilibration in water.

Examples:

1. Transfer of a single set of values of an environmental dataset takes place in Mode 1 and 2. In this example, MODE and MONTH are set to upload average data (only) from a file called "INLET.DAT" on the default directory; the dataset is then STORED in EXAMS' direct access UDB file.

EXAMS-> SET MONTH=13

EXAMS-> SET MODE=1

EXAMS-> READ

Enter Environment, Chemical, Load, Help, or Quit-> EN

Enter name of file, Help, or Quit-> INLET.DAT

2. To continue the above example, an entire monthly dataset can be read from another file by changing the mode to 3. Note that a directory other than the default can be specified as part of the READ command <name of file> option.

EXAMS-> SET MODE=3

EXAMS-> READ EN C:\EXAMS\PROJECTX\INLET.DAT

3. To read a PRZM transfer file, first set MODE to 3, and then read the dataset. Note the convention for naming of PRZM transfer files--the base name is always "PRZM2EXA" and the suffix indicates the year--in this case data from 1989 ("D89"). Because EXAMS will accept any file name for acquisition by the READ command, these files can be renamed to any convenient file name for archiving or to prevent subsequent PRZM runs from over-writing them.

EXAMS-> READ PRZM PRZM2EXA.D89

R E C A L L

Use RECALL to upload data from the permanent database (UDB) into current foreground memory (ADB).

Related: Control Variables: MCHEM

Commands: CATALOG, ERASE, NAME, STORE

Syntax: RECALL <datatype> <UDB#> [AS ADB#]

Prompt: Enter Environment, Chemical, Load, Product, Help, or Quit->

Command parameters:

<datatype> can be Chemical, Environment, Load, or Product
(EXAMS uses these four kinds of datasets.)

AS ADB# is an optional explicit specification of MCHEM (see Example 1).

UDB# specifies the accession number or location in the User Database for the source data for transfer to the ADB (Example 2).

Description: RECALL transfers data from permanent storage (UDB) to activity databases (ADBs). The data in active use by EXAMS are held in a foreground memory bank (Activity DataBase or ADB) with four sectors, one for each datatype required by EXAMS--

<C>hemical reactivity and partitioning,

<E>nvironmental physical and chemical parameters,

allochthonous chemical <L>oadings, and

<P>roduct chemistry for generating interconversions among multiple chemicals in an analysis.

When EXAMS is started, the ADB is empty. Use the RECALL command to transfer data from the permanent User Databases (UDBs) to foreground memory (ADB). When an analysis session is ended (QUIT or EXIT), ADBs are discarded. Use the STORE command to transfer new data from the ADB to the UDB sector of the same datatype for permanent retention of the data.

Examples:

1. Because EXAMS can process several chemicals in a single analysis, the target sector of the chemical activity database should be specified when using the RECALL command to activate CHEMICAL data. (This section of the command should be omitted for other data types.) When the ADB# (an integer between 1 and KCHEM) is omitted, the chemical data are transferred to the sector of the activity database given by the current value of MCHEM. For example, to activate data from the chemical UDB, putting UDB dataset number 9 into ADB sector 1, and UDB #14 into sector 2:

Either:

```
EXAMS-> SET MCHEM TO 1

EXAMS-> RECALL CHEMICAL 9

EXAMS-> SET MCHEM TO 2

EXAMS-> RECALL CHEMICAL 14
```

or, equivalently:

```
EXAMS-> RECALL CHEMICAL 9 AS 1

EXAMS-> RECALL CHEMICAL 14 AS 2
```

2. Long-term retention of data required by EXAMS is provided by storage in the "User Database" (UDB, generally resident on a physical device--e.g., a hard disk) for Chemicals, Environments, Loads, or Products. Within each UDB sector, each dataset is catalogued via a unique accession number (UDB#). When transferring data to foreground memory (the activity database or ADB) from a UDB, the source location must be specified by the name of the UDB sector and the accession number within the sector. For example, to RECALL an environmental dataset:

```
EXAMS-> RECALL ENVIR 2

Selected environment is:  Phantom Inlet, Bogue Sound

EXAMS->
```

R U N

The RUN command begins a simulation analysis.

Related: Control Variables: MODE
Commands: CONTINUE

Syntax: RUN

Prompt: None

Description: The RUN command executes an analysis and creates the output files accessed by the LIST and PLOT commands. The activity database (ADB) must be loaded, either via entry of new data or by RECALL from the UDB, before a RUN can be started.

Examples:

1. EXAMS-> RECALL CHEMICAL 22

   Selected compound is: Dibromoexample

   EXAMS-> RECALL ENVIRON 17

   Selected environment is: Albemarle Sound--Bogue Bank

   EXAMS-> SET STRL(1,1,13)=.01

   EXAMS-> RUN

   Simulation beginning for:
   Environment: Albemarle Sound--Bogue Bank
   Chemical 1: Dibromoexample

   Run complete.

   EXAMS->

   In this example, a steady-state (MODE=1) analysis is conducted by selecting a chemical and an environment, imposing a loading of chemical 1 on segment 1 under average conditions (i.e., data sector 13, EXAMS initial default value) and invoking EXAMS' simulation algorithms with the RUN command.

S E T

Use SET to specify the values of data in the activity database.

Related: Commands: CHANGE (synonym), DESCRIBE, HELP

Syntax: SET <name of variable> TO <new value>
or
SET <name of variable> = <new value>

Prompt: Enter name=value command->

Variable: The data entry or variable to be SET can be specified either as a single datum or, using wild cards (*), as an entire vector, row/column of a matrix, etc.

Description: Use the SET command to specify the values of data in the activity database. "Value" can be any numerical quantity or literal, as appropriate. "Variable" specifies an individual element of input data or a program control parameter. Entire vectors, rows/columns of matrices, etc. can be set to single values using wild cards (*).

Examples:

1. EXAMS-> SET VOL(167) TO 7E5

   Subscript out-of-range.

   EXAMS-> DESCRIBE VOL

   VOL is a Real Vector with 100 elements.

   EXAMS> SET VOL(2) TO E

   Invalid numeric quantity after TO.

   EXAMS-> SET VOL(2) TO 7E5

   This command sets the environmental volume of segment 2 to 7.0E+05 cubic meters. The initial attempt to set the volume of segment 67 was rejected by EXAMS because the version in use was set up for environmental models of 100 segments at most. The DESCRIBE command was used to check the number of subscripts and the dimensional size of the variable "VOL". The erroneous

entry of an alphabetic for the volume was trapped by the SET command; the initial value of VOL(2) was not altered.

2. EXAMS-> HELP TCEL

TCEL is a Real Matrix with 100 rows and 13 columns.
Temperature-CELsius (segment,month) Units: degrees C.
Average temperature of ecosystem segments. Used (as enabled by input data) to compute effects of temperature on transformation rates and other properties of chemicals.

EXAMS-> SET TCEL(2,7)=24

This command changes the July temperature in segment 2 to 24° C. The HELP command was used to check subscript dimensions, maximum values, the meaning of the subscripts (subscript #1 denotes the segment; subscript #2, the month), and the proper units for the input datum (degrees Celsius).

3. EXAMS-> HELP POH

POH is a Real Matrix with 100 rows and 13 columns.
pOH (segment, month) Units: pOH units
The negative value of the power to which 10 is raised in order to obtain the temporally averaged concentration of hydroxide [OH^-] ions in gram-molecules per liter.

EXAMS-> SET POH(*,13) TO 6.2

This command sets the average pOH (sector 13) of every segment to 6.2. Note use of wild card "*" to specify that all segments are to be changed. As in the previous example, HELP was used to check subscript dimensions, units, etc. This step, of course, is optional.

S H O W

Use SHOW to display current data values or control settings.

Related: Control Variables: MCHEM, MONTH

Commands: CHANGE, SET

Syntax: SHOW <option> [range]

Prompt: The following options are available:

Advection,	Chemistry,	Dispersion,	GEometry,
GLobals,	Loads,	PLot,	PUlse Loads,
PRoducts,	QUAlity,	Time Frame,	Variables,
Help, or	QUIt->		

Command parameters:

Range: Some options of the SHOW command accept the specification of a range of values to define the scope of the data to be displayed (see Example 1). Use MCHEM to delimit the range of SHOW Chemistry, and MONTH for GEometry, QUAlity, etc.

Options:

ADVECTION

SHOW ADVECTION gives the advective hydrologic flow structure of the current aquatic system. A single element in a dataset might typically look like the following example.

J FR AD	1	J FRom ADvection: Source Segment
I TO AD	3	I TO ADvection: Terminus
ADV PR	1.00	ADVection Proportion: Percent of total JFRAD flow on path
Path No.:	1	Vector index for SETting data

No more than NCON hydrologic pathways can be specified. If more are needed, special versions of EXAMS can be produced. Specify export pathways by entering a zero (0) for the number of the segment to receive the flow (ITOAD). Do not specify a hydrologic source term by entering zero in the JFRAD vector; instead use streamflows, non-point-source flows, etc.

DISPERSION

SHOW DISPERSION displays the input data describing transport in the active (loaded in the ADB) Environmental dataset. The index vectors (JTURB, ITURB) define the existence of inter-segment dispersive transport paths. A zero in either vector, when paired with a non- zero value at the corresponding position in the other index vector, is taken as a boundary condition with an uncontaminated body of water. A single element in a dataset might typically be displayed like the following example.

J TURB	1	Segment number for dispersion
I TURB	2	Segment number for dispersion
XS TUR m^2	5.000E+04	Cross-sectional area of path
CHARL m	2.53	CHARacteristic_Length of path
DSP m^2/hr	4.676E-05	Eddy DiSPersion coefficient
Path No.:	1	Vector index for data entry

No more than NCON hydrologic pathways can be specified. If more are needed, this number can be increased and EXAMS recompiled.

CHEMISTRY

SHOW CHEMISTRY displays the chemical output data currently in the ADB (foreground memory bank). The sector of the ADB denoted by the current value of MCHEM is displayed. Within each sector of the ADB (that is, for each chemical under active review), the data for each ionic species are presented separately, and photochemical data are presented on separate screens.

GEOMETRY

SHOW GEOMETRY returns a segment-by-segment description of the geometry (volumes, areas, etc.) of the current ecosystem. The segment number reported with each block of data is the first subscript for modifying the datum using CHANGE or SET. The month to be displayed is set by the current value of MONTH (explicit mean values are denoted by MONTH number 13): the month is the second subscript of such data as WIND, STFLO, etc.

GLOBALS

SHOW GLOBALS displays the input data that are "global" in extent, that is, "global" data apply to all segments of the current ecosystem.

LOADS

SHOW LOADS displays the current state of allochthonous chemical loadings. The form of the display depends on the current operational MODE: initial values are ignored in Mode 1 as they have no effect on the analysis results. The value of PRSW also affects the display: when PRSW is 0, SHOW LOADS returns a summary of annual loadings; when PRSW=1, a month-by-month tabulation is displayed as well. This display may not represent the final values used in the

analysis, because EXAMS will modify loads that result in violation of the linearizing assumptions used to construct the program. After a RUN has been executed, however, SHOW LOADS will display the corrected values.

PRODUCTS

SHOW PRODUCTS displays the specifications for product chemistry currently in the ADB. Each entry is identified and loaded according to a unique "pathway number." A single element of a dataset might look like this:

CH PAR	1	ADB number of CHemical PARent
T PROD	2	ADB number of Transformation PRODuct
N PROC	7	Number of transforming PROCess
R FORM	29	Reactive FORM (dissolved, etc.)
YIELD M/M	0.100	Mole/Mole YIELD of product
EAYLD Kcal	0.000	Enthalpy of yield (if appropriate)
Pathway:	1	Number of the pathway

More detail as to the numbering of NPROC and RFORM is given in the EXAMS Data Dictionary, which can also be accessed on-line using the HELP command. No more than NTRAN transformation pathways can be specified. If more are needed, a special version of EXAMS can be created.

PLOT

SHOW PLOT examines the contents of the concentration time-series and steady-state files, and reports the names of the chemicals and ecosystem used in the analysis.

PULSE LOADS

SHOW PULSE LOADS displays the specifications for allochthonous pulses of chemicals entering the system. This display may not represent the final values used in the analysis, because EXAMS will modify loads that result in violation of the linearizing assumptions used to construct the program. Although faulty pulse loads are discarded, EXAMS does not correct the input pulse load data, because the occurrence of load constraint violations depends on the context (i.e., the size of current stream loadings, etc.). Thus, unlike SHOW LOADS, the SHOW PULSE display following execution of a RUN does not display corrected data. The pulses actually used during an analysis are instead entered into EXAMS' output tables, where they can be examined using the LIST and PRINT commands.

QUALITY

SHOW QUALITY returns a segment-by-segment display of the canonical water-quality data included in the current Environmental ADB dataset. The month to be displayed is set by the current value of MONTH (explicit mean values are denoted by MONTH number 13). The month is the second

subscript of such data as pH, pOH, etc. The first subscript is the segment number; thus these data are entered (CHANGE/SET) as "datum(segment,month)".

TIME FRAME

SHOW TIME FRAME displays the current status of the parameters needed to control the temporal aspects of a Mode 2 or Mode 3 simulation.

VARIABLES

SHOW VARIABLES displays a list of the names of EXAMS input data and control parameters. These names must be used to SET/CHANGE, SHOW values, HELP/DESCRIBE, etc.

Description: Use the SHOW command to examine the current contents of the ADB, that is, the foreground datasets used for the current analysis. The SHOW command can be used to examine clusters of similar data, the values of individual parameters, or the data contained in entire vectors. Typing SHOW without an option will display a list of the available options.

Examples: 1. The SHOW command can be used to examine the value of single parameters. For example, the pH of segment 7 of the current ecosystem during September could be inspected by entering:

```
EXAMS-> SHOW PH(7,9)
```

Using wild cards (*), the SHOW command can also be used to display the data in an entire vector or row/column of a data matrix. For example, the pH in every segment of the current ecosystem during September could be displayed by entering:

```
EXAMS-> SHOW PH(*,9)
```

and the pH of segment 7 through the year could be displayed by:

```
EXAMS-> SHOW PH(7,*)
```

S T O R E

Use STORE to download current (ADB) data into the permanent database (UDB).

Related: Control Variables: MCHEM

Commands: CATALOG, ERASE, NAME, RECALL

Syntax: STORE <datatype> [ADB# IN] <UDB#>

Prompt: Enter Environment, Chemical, Load, Product, Help, or Quit->

Command parameters:

<datatype> can be Chemical, Environment, Load, or Product
(EXAMS uses these four kinds of datasets.)

ADB# IN is an optional explicit specification of MCHEM (see Example 1).

UDB# specifies the accession number or location in the User Database for storage of the current ADB sector (Example 2).

Description: STORE downloads data from activity databases (ADBs) into the permanent User DataBases (UDBs). The data in active use by EXAMS are held in a foreground memory bank (Activity DataBase or ADB) with four sectors, one for each datatype required by EXAMS:

CHEMICAL reactivity and partitioning,

ENVIRONMENTal physical and chemical parameters,

allochthonous chemical LOADings, and

PRODUCT chemistry for generating interconversions among multiple chemicals in an analysis.

When an analysis session is ended (QUIT or EXIT), these data are discarded. Use the STORE command to transfer data from the ADB to the UDB sector of the same datatype for permanent retention of the data.

Examples: 1. Because EXAMS can process several chemicals in a single analysis, the source sector of the chemical activity database should be specified when using the STORE command to download CHEMICAL data. (This section of the command should be omitted for other data types.) When the ADB# (an integer from 1 to KCHEM) is omitted, the chemical data are taken from the sector of the activity database given by the current value of MCHEM. For example, to STORE data in the UDB, putting ADB sector 1 into the chemical UDB under catalog/accession 9 and ADB sector 2 into UDB sector 14:

Either:

```
EXAMS-> SET MCHEM TO 1

EXAMS-> STORE CHEMICAL 9

EXAMS-> SET MCHEM TO 2

EXAMS-> STORE CHEMICAL 14
```

or, equivalently:

```
EXAMS-> STORE CHEMICAL 1 IN 9

EXAMS-> STORE CHEMICAL 2 IN 14
```

2. Long-term retention of data required by EXAMS is provided by storage in the "User Database" (UDB, generally resident on a physical device--e.g., a hard disk) for Chemicals, Environments, Loads, or Products. Within each of these UDB sectors, each dataset is CATALOGued via a unique accession number (UDB#). When transferring data between foreground memory (the activity database or ADB) and a UDB, the target location must be specified by the name of the UDB sector and the accession number within the sector. For example, to STORE the current environmental dataset:

```
EXAMS-> STORE ENVIR 2

Environment record   2 is in use with
Pond -- AERL code test data
Replace?-> no

Nothing changed.

EXAMS-> STORE ENVIR 14

Environment stored: Phantom Inlet-Bogue Sound Study Data

EXAMS->
```

Note that EXAMS provides a measure of protection against accidental overwriting of existing datasets, an important courtesy in a multi-user environment.

W R I T E

Use the WRITE command to transfer data from the Activity Data Base (ADB) to an external (non-EXAMS) sequential file.

Related: Control variables: MODE, MCHEM
Commands: READ

Syntax: WRITE <datatype> <name of file>

Prompt: Enter Environment, Chemical, Load, Help, or Quit->

Description: The WRITE command provides a facility for off-loading EXAMS datasets into external ASCII sequential files. These non-EXAMS files can be stored separately from the main EXAMS User Data Base (UDB). Data are transferred from the Activity Data Base (foreground memory ADB) rather than directly from the User Data Base (UDB) file, so the RECALL command must be used to transfer data from the UDB to the ADB before invoking WRITE.

Under the ENVIRONMENT option of WRITE, the setting of MODE controls how many data are stored in the external file. When MODE is 1 or 2, only the dataset sector indicated by the current value of MONTH is transferred. For example, if MODE=1 and MONTH=13, explicit mean values (only) will be downloaded. When MODE=3, the entire ADB dataset ("months" 1 through 13) will be downloaded to the external file called <name of file>.

Under the CHEMICAL option of WRITE, the chemical dataset to be downloaded to <name of file> is chosen from the MCHEM sector of the Activity Data Base (ADB).

In the LOAD option of WRITE, a set of external chemical loadings are written to an ASCII file. As with environmental data, the setting of MODE controls the amount of data written to the file. In Mode 1, only long-term, average data are written from the ADB; in Mode 2, initial conditions are added, and in Mode 3 a full set of monthly loads and daily pulse loads are written from the ADB to the external file. The first item written to the external file is the Mode for which the loadings are designed. This datum serves as a check value when EXAMS reads data from a file of external loadings (see discussion under READ command.

Examples:

1. Transfer of a single set of values of an environmental dataset takes place in Mode 1 and 2. In this example, the data is RECALLed from the UDB, and MODE and MONTH are set to download the average data to a file called "INLET.DAT" on the default directory.

EXAMS-> RECALL ENVIRONMENT 12

Selected environment is: Chinquoteague Inlet

EXAMS-> SET MONTH=13

EXAMS-> SET MODE=1

EXAMS-> WRITE

Enter Environment, Chemical, Load, Help, or Quit-> EN

Enter name of file, Help, or Quit-> INLET.DAT

2. To continue the above example, the entire dataset could be stored in another file by changing mode to 3. Note that a directory other than the default can be specified as part of the WRITE command <name of file> option.

EXAMS-> SET MODE=3

EXAMS-> WRITE ENV C:\EXAMS\PROJECTX\INLET.DAT

Z E R O

Use the ZERO command to initialize (set to zero) loadings databases or the concentration of pollutant chemicals throughout the ecosystem.

Related: Control variables: MODE
Commands: CONTINUE, RUN

Syntax: ZERO <option>

Options:

PULSE LOADS
LOADS
RESIDUALS

Prompt: The following options are available:

Pulse Loads	-	zero all pulse loads,
Loads	-	zero all other loads,
Residuals	-	zero all pollutant concentrations,
Help	-	this message, or
Quit	-	return to command mode with no action.

ZERO->

Description: The ZERO command initializes (sets to zero) the entire suite of allochthonous chemical pulse loadings (IMASS), longer term loadings (stream loads, drift loads, etc.), or the current values of pollutant chemical concentrations throughout the ecosystem. The ZERO command is designed primarily for use during the course of temporally segmented simulation studies. The same effect can be achieved with multiple applications of the CHANGE/SET command; ZERO is a block-mode implementation that reduces the work needed to remove loadings datasets. (See Example 1 in the documentation of the CONTINUE command.)

Examples:

1. EXAMS-> SET MODE=2

   EXAMS-> RECALL CHEMICAL 22

   Selected compound is: Dibromoexample

```
EXAMS-> RECALL ENVIRON 17

Selected environment is:  Albemarle Sound--Bogue Bank

EXAMS-> SET STRL(1,1,13)=.01

EXAMS-> SET IMASS(1)=2.0

EXAMS-> SET ISEG(1)=14

EXAMS-> SET ICHEM(1)=1

EXAMS-> RUN

Simulation beginning for:
Environment: Albemarle Sound--Bogue Bank
Chemical  1: Dibromoexample

Run complete.

        .
        .
        .

EXAMS-> ZERO PULSE LOADS

EXAMS-> CONTINUE
```

In this example, an initial-value (MODE=2) analysis is begun by selecting a chemical and an environment, imposing an allochthonous load of chemical 1 on segment 1 under average conditions (i.e., data sector 13, EXAMS' initial default value), and specifying the initial presence (or introduction at time zero) of 2.0 kg of material in segment 14. At the end of the initial RUN segment, one might want to examine the output tables, plot the results, etc. Then, before CONTINUing, the ZERO command is used to remove the pulse load specifications. If this were not done, EXAMS would introduce a second 2.0 kg pulse into segment 14 at the beginning of the continuation segment. Alternatively, the other loadings could have been removed, and the effect of a series of pulse loads could be studied by issuing a sequence of CONTINUE commands.

ABSER

ABSolute ERror tolerance of integrators

When the characteristics of the chemical and ecosystem are such as to result in "stiff" equations, numerical errors may lead to small negative numbers in the time series. If desired, the value of ABSER and RELER can be decreased in order to achieve greater precision in the simulation outputs.

ADB

Activity DataBase

EXAMS provides for long-term storage of CHEMical, ENVironmental, transformation PRODuct chemistry, and allochthonous LOADings databases in a User DataBase or UDB. The actual analyses are conducted on particular datasets drawn from these files (or entered via SET/CHANGE). Particular cases are loaded from the UDB into the foreground transient memory of your computer in an Activity DataBase or ADB, using the RECALL command. Because EXAMS simulates the behavior of several (MCHEM) chemicals simultaneously, the ADB for chemicals has MCHEM separate sectors. These data are lost when you EXIT from EXAMS, so be sure to STORE any new or corrected datasets before leaving EXAMS.

ABSOR

ABSORption spectra (wavelength, ion, chemical) Units: $cm^{-1}(mole/L)^{-1}$

Mean decadic molar light extinction coefficients in 46 wavelength intervals over 280--825 nm. For wavelength "w" and chemical "c":

ABSOR(w,1,c) is molar absorption coefficient of	SH_3	(neutral molecule)
ABSOR(w,2,c) is molar absorption coefficient of	SH_4^+	(+1 cation)
ABSOR(w,3,c) is molar absorption coefficient of	SH_5^{2+}	(+2 cation)
ABSOR(w,4,c) is molar absorption coefficient of	SH_6^{3+}	(+3 cation)
ABSOR(w,5,c) is molar absorption coefficient of	SH_2^-	(-1 anion)
ABSOR(w,6,c) is molar absorption coefficient of	$SH^=$	(-2 anion)
ABSOR(w,7,c) is molar absorption coefficient of	S^{3-}	(-3 anion)

ADVPR

ADVection PRoportion (path) Units: n/a Range: > 0 - 1.0

PRoportion of flow ADVected from segment JFRAD that enters ITOAD. The matching (same subscript) members of JFRAD, ITOAD, and ADVPR define an advective hydrologic flow pathway. Although usually 1, ADVPR lets one enter braided channels, etc. The total of ADVPRs for each segment must sum to either 0 or 1, failing which, EXAMS aborts the RUN. The flow data can be inspected by typing SHOW ADV; path numbers are given above each active dataset. Enter data via CHANGE or SET commands.

Additional information available: JFRAD, ITOAD

AEC

Anion Exchange Capacity (segment, month) Units: meq/100 g (dry)

Anion exchange capacity of sediment phase of each segment. Useful in relating sediment sorption (partitioning) of anions to a variable characteristic of system sediments.

AIRTY

AIR mass TYpe (month) Units: letter codes

Select: Rural (default), Urban, Maritime, or Tropospheric

AREA

AREA (segment) Units: m^2

Top plan area of each model segment of the waterbody. For Epilimnion and Littoral segments, AREA is the area of the air-water interface; for Hypolimnion segments AREA is the area of the thermocline; for Benthic segments it is the surface area of the bottom. In the latter case AREA may differ from XSTUR in a dispersive exchange pair because of reduction in exchanging area due to rock outcrops, etc.

ATURB

Atmospheric TURBidity (month) Units: km

Equivalent aerosol layer thickness.

AUDOUT

While the AUDIT directive is in effect, a copy of user inputs and responses is written to the file connected to FORTRAN Logical Unit Number AUDOUT.

BACPL

BACterioPLankton population density (segment, month) Units: cfu/mL

Population density of bacteria capable of degrading xenobiotics. The abbreviation "cfu" stands for a "colony forming unit."

BNBAC

BeNthic BACteria (segment, month) Units: cfu/100g dry sediment

Population density of benthic bacteria that degrade xenobiotics. The abbreviation "cfu" stands for a "colony forming unit."

BNMAS

BeNthic bioMASs (segment, month) Units: $g(dry)/m^2$

Biomass of small benthos--infauna subject to biosorption.

BULKD

BULK Density (segment, month) Units: g/cm^3

Fresh weight per unit volume of benthic sediments.

CEC

Cation Exchange Capacity (segment, month) Units: meq/100g (dry)

Cation exchange capacity of sediment phase in each segment. Useful in relating sediment sorption (partitioning) of cations to a variable characteristic of system sediments.

CHARL

CHARacteristic Length or mixing length (path) Units: m

Average of segment dimensions normal to the exchange interface linking segment numbers JTURB(p) and ITURB(p). The matching (same "p" subscript) members of JTURB, ITURB, CHARL, DSP, and XSTUR together define a dispersive transport pathway. A given segment may have different mixing lengths at different interfaces. CHARL can also be calculated from the distance along a path that connects the centers of segments JTURB(p) and ITURB(p), passing through the interface whose area is XSTUR(p).

See also: DSP, ITURB, JTURB, XSTUR

CHEMNA

CHEMical NAme(s) of compounds (50 characters,chemical) Units: n/a

Do *not* use "CHANGE" or "SET" to enter names! The NAme for a CHEMical is entered into the database via the command sequence:

EXAMS-> CHEMICAL NAME IS nnn...

where "nnn... " can include as many as 50 characters. This name is associated with chemical library entries and is printed in the header information of the appropriate output tables.

CHL

CHLorophylls + pheophytins (segment, month) Units: mg/L

Concentration of chlorophyll plus chlorophyll-like pigments. Used to compute spectral light absorption coefficients due to pigments which absorb light from the water column and thus compete with photolysis of xenobiotics.

CHPAR

CHemical PARent compound (path) Units: n/a Range: 1--KCHEM

CHPAR(p) gives the ADB location of the parent source of TPROD(p). The matching (same transformation path number "p") members of CHPAR and TPROD give the location numbers in the active database of the parent chemical and the transformation product for pathway "p". For example, "SET CHPAR(p) TO 1", and TPROD(p) TO 4, to show that the chemical in ADB sector 4 is produced via transformation of the chemical in ADB sector 1, via process data defined by the remaining members of product chemistry sector "p".

See also: EAYLD, NPROC, RFORM, TPROD, YIELD

CINT

Communications INTerval for dynamic simulations. Units: see TCODE

CINT is the interval between output cycles from the integrators. In Mode 2, CINT can be set to produce any desired output frequency, so long as the resulting reporting interval is >1 hour. When CINT is set to 0, EXAMS (Mode 2) sets CINT to report at the 12 equal-increment periods most closely matching the duration specified by (TEND - TINIT). CINT is under full user control only in Mode 2; in Modes 1 and 3 EXAMS itself sets the value of CINT according to the needs of the analysis.

CLOUD

CLOUDiness (month) Units: dimensionless Range: 0 -- 10

Mean monthly cloudiness in tenths of full sky cover.

DEPTH

DEPTH (segment) Units: m

Average vertical depth of each segment.

DFAC

Distribution FACtor (segment, month) Units: dimensionless ratio

Ratio of optical path length to vertical depth, range 1.0--2.0. A vertical light beam has a DFAC of 1.0; a fully diffused light field has a DFAC of 2.0. For whole days, a value of 1.19 is often adequate; EXAMS defaults to this value when the entry for DFAC is outside the range 1.0-2.0.

DISO2

DISsolved O2 (segment, month) Units: mg/L

Concentration of dissolved oxygen (O_2) in each segment of ecosystem.

DOC

Dissolved Organic Carbon (segment, month) Units: mg/L

Used for computing spectral light absorption and complexation.

DRFLD

DRiFt LoaD (segment, chemical, month) Units: kg/hour

Drift loadings: aerial drift, direct applications, stack fallout (etc.) of chemical on each system element.

DSP

DiSPersion coefficient (path, month) Units: m^2/hour

Eddy diffusivity to be applied to dispersive exchange pairing "p". The matching (same "p" subscript) members of JTURB, ITURB, CHARL, and XSTUR together define a dispersive transport pathway. In the case of horizontal mixing, DSP is the longitudinal dispersion coefficient; for vertical mixing it may represent exchange across the thermocline or exchanges with bottom sediments. In the latter case DSP is a statistical kinetic composite incorporating direct sorption to the sediment surface, mixing of the sediments by benthos (bioturbation), stirring by demersal fishes, etc.

See also: CHARL, ITURB, JTURB, XSTUR

EAH

E_a for Acid Hydrolysis (form, ion, chemical) Units: kcal/mole

Arrhenius activation energy E_a of specific-acid-catalyzed hydrolysis of chemicals. Matrix indices match those of KAH, giving, for each chemical, data for 3 forms (1: dissolved, 2: solids-sorbed, 3: DOC-complexed) of 7 ionic species (1: neutral; 2, 3, 4: cations; 5, 6, 7: anions). When EAH is non-zero, the second-order rate constant is calculated from:

$$\log K = \text{KAH}(f,i,c) - \frac{1000 * \text{EAH}(\text{form,ion,chemical})}{4.58\ (\text{TCEL}(\text{segment,month}) + 273.15)}$$

$M^{-1}h^{-1}$

EAYLD

EA YieLD (path) Units: kcal

EAYLD(p) is activation energy Ea to compute transformation product yield as a function of environmental temperatures (TCEL). When EA_YieLD(p) is zero, YIELD(p) gives the dimensionless molar product yield. A non-zero EAYLD(p) invokes a re-evaluation in which YIELD(p) is interpreted as the pre-exponential factor in an Arrhenius-type function, giving product yield as a function of spatially and temporally specific temperatures (TCEL(segment, month)):

$$\log \text{Yield}(p) = \text{YIELD}(p) - \frac{1000 * \text{EAYLD}(\text{path})}{4.58\ (\text{TCEL}(\text{segment,month}) + 273.15)}$$

See also: CHPAR, NPROC, RFORM, TPROD, YIELD

EBH

Ea for Base Hydrolysis (form, ion, chemical) Units: kcal/mole

Arrhenius activation energy E_a of specific-base catalyzed hydrolysis of chemicals. Matrix indices match those of KBH, giving, for each chemical, data for 3 forms (1: dissolved, 2: solids-sorbed, 3: DOC-complexed) of 7 ionic species (1: neutral, 2, 3, 4: cations, 5, 6, 7: anions). When EBH is non-zero, the second-order rate constant is calculated from:

$$\log K = \text{KBH}(f,i,c) - \frac{1000 * \text{EBH}(\text{form,ion,chemical})}{4.58\ (\text{TCEL}(\text{segment,month}) + 273.15)}$$

$M^{-1}h^{-1}$

EHEN

Enthalpy term for HENry's law (chemical) Units: kcal/mole

Used to compute Henry's law constants as a function of TCEL (environmental temperature). When EHEN is non-zero, the Henry's law constant (H) affecting volatilization at a particular (segment, month) is computed from TCEL:

$$\log H = \text{HENRY}(\text{chemical}) - \frac{1000 * \text{EHEN}(\text{chemical})}{4.58\ (\text{TCEL}(\text{segment,month}) + 273.15)}$$

EK1O2

Ea K1O2 (singlet oxygen) (form, ion, chemical) Units: kcal/mole

Arrhenius activation energy for singlet oxygen photo-oxygenation of chemicals. Matrix indices match those of K1O2, giving, for each chemical, data for 3 forms (1: dissolved, 2: solids-sorbed, 3: DOC-complexed) of 7 ionic species (1: neutral, 2, 3, 4: cations, 5, 6, 7: anions). When EK1O2 is non-zero, the second-order rate constant is calculated as:

$$\log K = \text{K1O2}(f,i,c) - \frac{1000 * \text{EK1O2}(\text{form,ion,chemical})}{4.58\ (\text{TCEL}(\text{segment,month}) + 273.15)}$$

$M^{-1}h^{-1}$

ELEV

ELEVation Units: meters above mean sea level

Ground station elevation.

ENH

Ea for Neutral Hydrolysis (form, ion, chemical) Units: kcal/mole

Arrhenius activation energy for neutral hydrolysis of chemicals. Matrix indices match those of KNH, giving, for each chemical, data for 3 forms (1: dissolved, 2: solids-sorbed, 3: DOC--complexed) of 7 ionic species (1: neutral, 2, 3, 4: cations, 5, 6, 7: anions). When ENH is non-zero, the pseudo-first-order rate constant is calculated from:

$$\log K = \text{KNH}(f,i,c) - \frac{1000 * \text{ENH}(\text{form,ion,chemical})}{4.58\ (\text{TCEL}(\text{segment,month}) + 273.15)}$$

h^{-1}

EOX

Ea OXidation (form, ion, chemical) Units: kcal/mole

Arrhenius activation energy for oxidative transformations of chemicals. Matrix indices match those of KOX, giving, for each chemical, data for 3 forms (1: dissolved, 2: solids-sorbed, 3:DOC-complexed) of 7 ionic species (1: neutral, 2, 3, 4: cations, 5, 6, 7: anions). When EOX is non-zero, the second-order rate constant is calculated from:

$$\log K = KOX(f,i,c) - \frac{1000 * EOX(form,ion,chemical)}{4.58\ (TCEL(segment,month) + 273.15)}$$

$M^{-1}h^{-1}$

EPK

Enthalpy term for pK (ion, chemical) Units: kcal/mole

When EPK is non-zero, pK is computed as a function of temperature via:

$$\log pK = PK(i,c) - \frac{1000 * EPK(ion,chemical)}{4.58\ (TCEL(segment,month) + 273.15)}$$

The vector indices for EPK ("c" denotes the chemical) are

EPK(1,c) contains datum for generation of SH_4^+ from SH_3

EPK(2,c) contains datum for generation of SH_5^{2+} from SH_4^+

EPK(3,c) contains datum for generation of SH_6^{3+} from SH_5^{2+}

EPK(4,c) contains datum for generation of SH_2^- from SH_3

EPK(5,c) contains datum for generation of SH^{2-} from SH_2^-

EPK(6,c) contains datum for generation of S^{3-} from SH^{2-}

ERED

Ea REDuction (form, ion, chemical) Units: kcal/mole

Arrhenius activation energy for reductive transformations of chemicals. Matrix indices match those of KRED, giving, for each chemical, data for three forms (1: dissolved, 2: solids-sorbed, 3: DOC-complexed) of seven ionic species (1: neutral, 2, 3, 4: cations, 5, 6, 7: anions). When ERED is non-zero, the second-order rate constant is calculated as:

$$\log K = KRED(f,i,c) - \frac{1000 * ERED(form,ion,chemical)}{4.58\ (TCEL(segment,month) + 273.15)}$$

$M^{-1}h^{-1}$

ESOL

Enthalpy term for SOLubility (ion, chemical) Units: kcal/mole

ESOL describes chemical solubility as a function of temperature (TCEL). The matrix indices ("c" denotes the chemical) denote:

ESOL(1,c) is datum for solubility of neutral molecules SH_3

ESOL(2,c) is datum for solubility of singly charged cations SH_4^+

ESOL(3,c) is datum for solubility of doubly charged cations SH_5^{2+}

ESOL(4,c) is datum for solubility of triply charged cations SH_6^{3+}

ESOL(5,c) is datum for solubility of singly charged anions SH_2^-

ESOL(6,c) is datum for solubility of doubly charged anions SH^{2-}

ESOL(7,c) is datum for solubility of triply charged anions S^{3-}

EVAP

EVAPoration (segment, month) Units: mm/month

(Monthly) evaporative water losses from ecosystem segments.

EVPR

Molar hEat of VaPoRization (chemical) Units: kcal/mole

Enthalpy term for computing vapor pressure as a function of TCEL (environmental temperature (segment,month)). When EVPR is non-zero, vapor pressure Va is computed from:

$$\log Va = VAPR(\text{chemical}) - \frac{1000 * EVPR(\text{chemical})}{4.58\ (TCEL(\text{segment,month}) + 273.15)}$$

FIXFIL

FIXFIL signals the existence of output data for LISTs and PLOTs.

To access results from a prior run, "SET FIXFIL TO 1." FIXFIL is set to zero when EXAMS is invoked, so that the LIST and PLOT commands are protected from attempts to access non-existent output data files. When results exist from a previous simulation, you can reset FIXFIL to 1 in order to gain access to them.

FROC

FRaction Organic Carbon (segment, month) Units: dimensionless

Organic carbon content of solids as fraction of dry weight. FROC is coupled to KOC to generate the sediment partition coefficient for neutral chemicals (SH_3) as a function of a property (organic carbon content) of the sediment.

HENRY

HENRY's law constant (chemical) Units: atmosphere-m^3/mole

Used in computation of air/water exchange rates (volatilization). If parameter EHEN is non-zero, HENRY is used as the pre-exponential factor in computing the Henry's law constant H as a function of environmental temperatures (TCEL):

$$\log H = \text{HENRY}(\text{chemical}) - \frac{1000 * \text{EHEN}(\text{chemical})}{4.58\ (\text{TCEL}(\text{segment,month}) + 273.15)}$$

ICHEM

I CHEMical (event) Units: n/a Range: 1--KCHEM

Event "e" is a pulse of chemical number ICHEM(e) in the active database ICHEM identifies the location in the Activity Database (ADB) of the chemical entering the ecosystem via pulse load event "e". When, for example, chemical data are loaded into ADB sector 3 (whether RECALLed from the User Database Library (UDB) (via, for example, the command sequence "RECALL CHEM 7 AS 3") or entered as new data), ICHEM(e) can be SET to 3 to create a pulse load event of that chemical.

See also: IDAY, IMASS, IMON, ISEG

IDAY

I DAY (event) Units: n/a Range: 1--31

Pulse load event "e" takes place on day IDAY(e) of month IMON(e). The pulse load data are organized by vertical event columns, that is, the set of pulse load variables (IMASS(e), ICHEM(e), ISEG(e), IMON(e), and IDAY(e)) with the same vector subscript describes a single chemical pulse event. Thus a pulse of chemical ICHEM(e), of magnitude IMASS(e), is released into segment ISEG(e) on day IDAY(e) of month IMON(e). During mode 2 simulations, IDAY and IMON are inoperative.

See also: ICHEM, IMASS, IMON, ISEG

IMASS

Initial MASS (event) Units: kg

IMASS gives the magnitude of chemical pulse load event "e". In mode 2, pulses are entered at time 0 (i.e., as initial conditions), and at the outset of each CONTINUation of the simulation. In mode 3, IMON and IDAY specify the date of the load events. An event recurs in each year of the RUN or CONTINUed simulation. The pulse load data are organized by vertical event columns, that is, the series of pulse load variables (IMASS, ICHEM, ISEG, IMON, and IDAY) with the same vector subscript describes a single event.

See also: ICHEM, IDAY, IMON, ISEG

IMON

I MONth (event) Units: n/a Range: 1--12

Pulse load event "e" takes place on day IDAY(e) of month IMON(e). The pulse load data are organized by vertical event columns, that is, the set of pulse load variables (IMASS(e), ICHEM(e), ISEG(e), IMON(e), and IDAY(e)) with the same vector subscript describes a single chemical pulse event. Thus a pulse of chemical ICHEM(e), of magnitude IMASS(e), is released into segment ISEG(e) on day IDAY(e) of month IMON(e). During mode 2 simulations, IDAY and IMON are inoperative.

See also: IDAY, ICHEM, IMASS, ISEG

ISEG

I SEGment (event) Units: n/a Range: 1--KOUNT

Pulse load event "e" loads chemical ICHEM(e) on segment ISEG(e). Any segment can receive a pulse load. Should the pulse loads increase the *free* concentration of unionized chemical above 10^{-5} M (or half its aqueous solubility, whichever is less), the size of the event is reduced, to avoid violating the linearizing assumptions used to create EXAMS. The pulse load data are organized by vertical event columns, that is, the pulse load variables having the same vector subscript define a single chemical pulse event.

See also: ICHEM, IDAY, IMASS, IMON

ITOAD

I TO ADvection (path) Units: n/a Range: 0--KOUNT (0 = export)

Chemicals are advected to segment ITOAD(p) from segment JFRAD(p). The matching (same subscript) members of JFRAD, ITOAD, and ADVPR define an advective hydrologic flow pathway carrying entrained chemicals and solids through the waterbody. When ITOAD(p) is 0, the pathway advects water and entrained substances across system boundaries, i.e., ITOAD(p) = 0 specifies an export pathway. The flow data can be inspected by typing "SHOW ADV"; path numbers are given above each active dataset. Enter data with SET or CHANGE commands.

See also: JFRAD, ADVPR

ITURB

I TURBulent dispersion (path) Units: n/a Range: 0--KOUNT

Segments ITURB(p) and JTURB(p) exchange via turbulent dispersion. The matching (same "p" subscript) members of ITURB, JTURB, CHARL, DSP, and XSTUR together define a dispersive transport pathway; ITURB(p) and JTURB(p) indicate which segments are linked by dispersive transport

pathway "p". A "0" in ITURB paired with a non-zero segment number in JTURB denotes a boundary condition with a pure (zero chemical) water-body. The input data can be examined via SHOW TURBULENCE; pathway numbers are shown with each dataset.

See also: CHARL, DSP, JTURB, XSTUR

IUNIT

IUNIT controls the printing of diagnostics from the integrators.

Normally zero (off), it may be turned on when problems occur. To manually set IUNIT to generate integrator diagnostic messages, SET IUNIT TO 1. The message generator can be disabled at any time by SETting IUNIT to 0.

JFRAD

J FRom ADvection (path) Units: n/a Range: 1--KOUNT

Chemicals are advected from segment JFRAD(p) to segment ITOAD(p). The matching (same subscript) members of JFRAD, ITOAD, and ADVPR define an advective hydrologic flow pathway. EXAMS computes the total net flow available for advection from segment JFRAD(p). Of the total flow, the fraction ADVPR(p) flows from segment JFRAD(p) into segment ITOAD(p). The hydrologic flow carries an entrained mass of chemical along the pathway. The flow specifications can be inspected by typing SHOW ADV; pathway numbers are given above each active dataset. Enter data with SET or CHANGE commands.

See also: ITOAD, ADVPR

JTURB

J TURBulent dispersion (path) Units: n/a Range: 0--KOUNT

Segments JTURB(p) and ITURB(p) exchange via turbulent dispersion. The matching (same "p" subscript) members of JTURB, ITURB, CHARL, DSP, and XSTUR together define a dispersive transport pathway; JTURB(p) and ITURB(p) indicate which segments are linked by dispersive transport pathway "p". A "0" in JTURB paired with a non-zero segment number in ITURB denotes a boundary condition with a pure (zero chemical) water-body. The input data can be examined via SHOW TURBULENCE; pathway numbers are shown with each dataset.

See also: CHARL, DSP, ITURB, XSTUR

KAH

K Acid Hydrolysis (form, ion, chemical) Units: per mole $[H^+]$ per hour

Second-order rate constant for specific-acid-catalyzed hydrolysis of chemicals. When the matching (same subscripts) Arrhenius activation energy (EAH) is zero, KAH is interpreted as the

second-order rate constant. When the matching entry in EAH is non-zero, KAH is interpreted as the (Briggsian) logarithm of the frequency factor in an Arrhenius equation, and the 2nd-order rate constant is computed as a function of segment temperatures TCEL. Matrix indices refer to three forms--1: aqueous, 2: solids-sorbed, and 3: DOC-complexed; by seven ions--1: neutral, 2-4: cations, and 5-7: anions.

KBACS

K BACteria benthoS (form, ion, chemical) Units: $(cfu/mL)^{-1}$ $hour^{-1}$

Second-order rate constants--benthic sediment bacterial biolysis of chemicals normalized by "colony forming units" (cfu) per mL. When the matching (same subscripts) Q_{10} (QTBAS) is zero, KBACS is interpreted as the second-order rate constant. When the matching entry in QTBAS is non-zero, KBACS is interpreted as the numerical value of the second-order rate constant at 20° C, and local values of the rate constant are computed as a function of temperature (TCEL) in each ecosystem segment. Indices refer to four forms--1: aqueous, 2: solids-sorbed, 3: DOC-complexed, and 4: bio-sorbed; by seven ions--1: neutral, 2-4: cations, and 5-7: anions.

KBACW

K BACterioplankton Water (form, ion, chemical) Units: $(cfu/mL)^{-1}$ $hour^{-1}$

Second-order rate constants K for water column bacterial biolysis of chemicals normalized by "colony forming units" (cfu) per mL. When the matching (same subscripts) Q_{10} (QTBAW) is zero, KBACW is interpreted as the second-order rate constant. When the matching entry in QTBAW is non-zero, KBACW is interpreted as the numerical value of the second-order rate constant at 20° C, and local values of the rate constant are computed as a function of temperature (TCEL) in each ecosystem segment. Indices refer to four forms--1: aqueous, 2: solids-sorbed, 3: DOC-complexed, and 4:bio-sorbed; by seven ions--1: neutral, 2-4: cations, and 5-7: anions.

KBH

K Base Hydrolysis (form, ion, chemical) Units: per mole $[OH^-]$ per hour

Second-order rate constant for specific-base-catalyzed hydrolysis of chemicals. When the matching (same subscripts) Arrhenius activation energy (EBH) is zero, KBH is interpreted as the second-order rate constant. When the matching entry in EBH is non-zero, KBH is interpreted as the (Briggsian) logarithm of the frequency factor in an Arrhenius equation, and the 2nd-order rate constant is computed as a function of segment temperatures TCEL. Matrix indices refer to three forms--1: aqueous, 2: solids-sorbed, and 3: DOC-complexed; by seven ions--1: neutral, 2-4: cations, and 5-7: anions.

KCHEM

Number of chemicals under review in current study. Units: n/a

KDP

K Direct Photolysis (ion, chemical) Units: $hour^{-1}$

Estimated photolysis rates--use only when ABSOR, the actual light absorption spectra of the compound in pure water, are unavailable. KDP is an annual average pseudo-first-order photolysis rate constant under cloudless conditions at RFLAT, where

KDP(1,c) are pseudo-first-order photolysis rate constants of neutral molecules SH_3

KDP(2,c) are pseudo-first-order photolysis rate constants of singly charged cations SH_4^+

KDP(3,c) are pseudo-first-order photolysis rate constants of doubly charged cations SH_5^{2+}

KDP(4,c) are pseudo-first-order photolysis rate constants of triply charged cations SH_6^{3+}

KDP(5,c) are pseudo-first-order photolysis rate constants of singly charged anions SH_2^-

KDP(6,c) are pseudo-first-order photolysis rate constants of doubly charged anions SH^{2-}

KDP(7,c) are pseudo-first-order photolysis rate constants of triply charged anions S^{3-}

KIEC

Kp for Ion Exchange Capacity (ion, chemical) Units: Kp $(meq/100g\ dry)^{-1}$

Coefficient relating sediment partition coefficient Kp of ions to exchange capacity of sediments. KIEC times the cation exchange capacity CEC(seg, month) (or anion exchange capacity AEC for anionic species) gives the Kp for sorption of ions with solid phases. This computation is overridden by explicit (non-zero) values of KPS, i.e., a non-zero value of KPS takes precedence over a Kp computed by EXAMS using KIEC.

KIEC(1,c) is datum for relating CEC and sorption of singly charged cation SH_4^+

KIEC(2,c) is datum for relating CEC and sorption of doubly charged cation SH_5^{2+}

KIEC(3,c) is datum for relating CEC and sorption of triply charged cation SH_6^{3+}

KIEC(4,c) is datum for relating AEC and sorption of singly charged anion SH_2^-

KIEC(5,c) is datum for relating AEC and sorption of doubly charged anion SH^{2-}

KIEC(6,c) is datum for relating AEC and sorption of triply charged anion S^{3-}

KINOUT

Logical Unit Number for writing results of numerical integration to kinetics plotting file.

KNH

K Neutral Hydrolysis (form, ion, chemical) Units: $hour^{-1}$

Pseudo-first-order rate constants for neutral hydrolysis of chemicals. When the matching (same subscripts) Arrhenius activation energy (ENH) is zero, KNH is interpreted as the first-order rate constant. When the matching entry in ENH is non-zero, KNH is interpreted as the (Briggsian) logarithm of the frequency factor in an Arrhenius equation, and the 1st-order rate constant is computed as a function of segment temperatures TCEL. Matrix indices refer to three forms--1: aqueous, 2: solids-sorbed, and 3: DOC-complexed; by seven ions--1: neutral, 2-4: cations, and 5-7: anions.

KOC

KOC (chemical) Units: [(mg/kg)/(mg/L)] $(organic\ carbon\ fraction)^{-1}$

KOC is partition coefficient (Kp) keyed to organic carbon content FROC(s, m) of the sediment solids in each (s) segment, during each (m) month of simulation of chemical behavior in the system. Multiplication of KOC by the organic carbon fraction FROC(s) of the solids in each segment yields the partition coefficient (Kp) for sorption of unionized (SH3) species with those solids:

Kp(chemical, segment, month) = KOC(chemical) * FROC(segment, month)

KOUNT

Number of segments used to define current ecosystem. Units: n/a

KOW

Octanol-Water partition coefficient (chemical) Units: (mg/L)/(mg/L)

Kow is an experimentally determined chemical descriptor. Kow (KOW(c)) can be used to estimate Koc (c.f.), and thus relate the Kp of a chemical to the organic carbon content of sediments.

KOX

K OXidation (form, ion, chemical) Units: per mole [OXRAD] per hour

Second-order rate constants for free-radical (OXRAD) oxidation of chemicals. When the matching (same subscripts) Arrhenius activation energy (EOX) is zero, KOX is interpreted as the second-order rate constant. When the matching entry in EOX is non-zero, KOX is interpreted as the (Briggsian) logarithm of the frequency factor in an Arrhenius equation, and the 2nd-order rate constant is computed as a function of segment temperatures TCEL. Matrix indices refer to three forms--1: aqueous, 2: solids-sorbed, and 3: DOC-complexed; by seven ions--1: neutral, 2-4: cations, and 5-7: anions.

KO2

KO2 (segment, month) Units: cm/hour

Oxygen exchange constant or piston velocity at 20 degrees C in each ecosystem segment.

KPB

KP for Biomass (ion, chemical) Units: (ug/g) / (mg/L)

Partition coefficient (Kp) for computing equilibrium biosorption. The "ion" subscripts (the "c" subscript denotes the chemical) identify:

KPB(1,c) datum for biosorption of neutral molecules SH_3

KPB(2,c) datum for biosorption of singly charged cations SH_4^+

KPB(3,c) datum for biosorption of doubly charged cations SH_5^{2+}

KPB(4,c) datum for biosorption of triply charged cations SH_6^{3+}

KPB(5,c) datum for biosorption of singly charged anions SH_2^-

KPB(6,c) datum for biosorption of doubly charged anions SH^{2-}

KPB(7,c) datum for biosorption of triply charged anions S^{3-}

KPDOC

KP Dissolved Organic Carbon (ion, chemical) Units: (ug/g)/(mg/L)

Partition coefficient (Kp) for equilibrium complexation with DOC. The "ion" subscripts (the "c" subscript denotes the chemical) identify:

KPDOC(1,c) datum for complexation of neutral molecules SH_3

KPDOC(2,c) datum for complexation of singly charged cations SH_4^+

KPDOC(3,c) datum for complexation of doubly charged cations SH_5^{2+}

KPDOC(4,c) datum for complexation of triply charged cations SH_6^{3+}

KPDOC(5,c) datum for complexation of singly charged anions SH_2^-

KPDOC(6,c) datum for complexation of doubly charged anions SH^{2-}

KPDOC(7,c) datum for complexation of triply charged anions S^{3-}

KPS

KP for Sediment solids (ion, chemical) Units: (mg/kg)/(mg/L)

Partition coefficients (Kp) for computing sorption with sediments. The "ion" subscripts (the "c" subscript denotes the chemical) identify:

KPS(1,c) datum for sorption of neutral molecules SH_3

KPS(2,c) datum for sorption of singly charged cations SH_4^+

KPS(3,c) datum for sorption of doubly charged cations SH_5^{2+}

KPS(4,c) datum for sorption of triply charged cations SH_6^{3+}

KPS(5,c) datum for sorption of singly charged anions SH_2^-

KPS(6,c) datum for sorption of doubly charged anions SH^{2-}

KPS(7,c) datum for sorption of triply charged anions S^{3-}

KRED

K REDuction (form, ion, chemical) Units: per mole [REDAG] per hour

Second-order rate constants for REDucing AGent chemical reduction of compounds. When the matching (same subscripts) Arrhenius activation energy (ERED) is zero, KRED is interpreted as the second-order rate constant. When the matching entry in ERED is non-zero, KRED is interpreted as the (Briggsian) logarithm of the frequency factor in an Arrhenius equation, and the 2nd-order rate constant is computed as a function of segment temperatures TCEL. Matrix indices refer to three forms--1: aqueous, 2: solids-sorbed, and 3: DOC-complexed; by seven ions--1: neutral, 2-4: cations, and 5-7: anions.

KVO

KVOlatilization (chemical) Units: dimensionless ratio

Liquid-phase transport resistance, as ratio to reaeration rate.

K1O2

K1O2 (singlet oxygen) (form, ion, chemical) Units: per M [$^1O_2$] per hour

Second-order rate constants for singlet oxygen photo-oxygenation of chemicals. When the matching (same subscripts) Arrhenius activation energy (EK1O2) is zero, K1O2 is interpreted as the second-order rate constant. When the matching entry in EK1O2 is non-zero, K1O2 is interpreted as the (Briggsian) logarithm of the frequency factor in an Arrhenius equation, and the 2nd-order rate constant is computed as a function of segment temperatures TCEL. Matrix indices

refer to three forms--1: aqueous, 2: solids-sorbed, and 3: DOC-complexed; by seven ions--1: neutral, 2-4: cations, and 5-7: anions.

LAMAX

LAMbda MAXimum (ion, chemical) Units: nanometers

Wavelength of maximum absorption of light by each ionic species, or wavelength of maximum overlap of solar spectrum and chemical's absorption spectrum (of each ion). Indices match with KDP matrix. LAMAX selects the wavelengths used to compute light extinction factors for photochemical transformation, in those cases where the absorption spectrum of the compound is not available, but the results of simple photochemical experiments can be used as a coarse estimate of rates of photochemical transformations (i.e., KDP > 0.0). When set to zero, LAMAX defaults to 300 nm.

LAT

LATitude Units: degrees and tenths (e.g., 37.24)

Geographic latitude of the ecosystem.

LENG

LENGth (segment) Units: m

Length of a reach -- used to compute volume, area, depth.

LOADNM

LOADings database NaMe (50 characters) Units: n/a

Do *not* use "CHANGE" or "SET" to enter names! The NaMe for a LOADings database is entered via the command sequence:

EXAMS-> LOAD NAME IS nnn...

where "nnn... " can include as many as 50 characters. This name is associated with chemical loadings database library entries, so that load patterns can be found in the catalog. The Ith character can be corrected with a CHANGE or SET command. For example, to repair the 7th character, "SET LOADNM(7) TO ... ."

LONG

LONGitude Units: degrees and tenths (e.g., 154.2)

Geographic longitude of the ecosystem.

MCHEM

M CHEMical Units: n/a

Number of chemical in activity data base.

MODE

MODE sets the operating "mode" of EXAMS.

Three operating modes are available; these are selected by SETting MODE to 1, 2, or 3.

MODE	Operational characteristics of EXAMS
1	Long-term (steady-state) analysis.
2	Pulse analysis -- specifiable initial chemical mass (IMASS) and time frame, time-invariant environment.
3	Monthly environmental data, daily pulse loads IMASS and monthly chemical loadings of other types.

MONTH

MONTH Units: n/a

Set MONTH to inspect a specific block of environmental data.

MWT

Gram Molecular WeighT (chemical) Units: g/mole

Molecular weight of the neutral species of each study chemical. Changes in molecular weight due to ionization are neglected.

NPROC

Number of PROCess (path) Units: n/a Range: 1--9

Signals the type of process transforming CHPAR(p) into TPROD(p). NPROC can be set to the following:

1 --> specific acid hydrolysis
2 --> neutral hydrolysis
3 --> specific base hydrolysis
4 --> direct photolysis
5 --> singlet oxygen reactions
6 --> free radical oxidation
7 --> water column bacterial biolysis
8 --> benthic sediment bacterial biolysis
9 --> reductions, e.g., reductive dechlorination

See also: CHPAR, EAYLD, RFORM, TPROD, YIELD

NPSED

Non-Point-Source SEDiment (segment, month) Units: kg/hour

Non-point-source sediment loads entering ecosystem segments.

NPSFL

Non-Point-Source FLow (segment, month) Units: m^3/hour

Non-point-source water flow entering ecosystem segments.

NPSLD

Non-Point-Source LoaD (segment, chemical, month) Units: kg/hour

Chemical loadings entering segments via non-point sources.

NYEAR

Number of YEARs Units: n/a

NYEAR is number of years to be simulated for a mode 3 run.

OXRAD

OXidant RADicals (month) Units: moles/L

Concentration of environmental oxidants in near-surface waters (e.g., peroxy radicals). EXAMS computes segment-specific oxidant concentrations using ultra-violet light extinction in the system.

OZONE

OZONE (month) Units: centimeters NTP Typically 0.2--0.3 cm

Mean (monthly) ozone (O_3) content of atmosphere.

PCPLD

PreCiPitation LoaD (segment, chemical, month) Units: kg/hour

Chemical loadings entering each segment via rainfall.

PCTWA

PerCenT WAter (segment, month) Units: dimensionless

Percent water in bottom sediments of benthic segments. Elements of these vectors that correspond to water column segments are not used (dummy values). PCTWA should be expressed as the conventional soil science variable (the fresh weight : dry weight ratio times 100); all values must be greater than or equal to 100. An entry in PCTWA that is less than 100.0 for a benthic segment raises an error condition, and control is returned to the user for correction of the input data.

PH

pH (segment, month) Units: pH units

The negative value of the power to which 10 is raised in order to obtain the temporally averaged concentration of hydronium ions [H_3O^+] in gram-equivalents per liter.

PK

pK (ion, chemical)

Negative of base-10 logarithm of acid/base dissociation constants. When the matching value in the EPK matrix is zero, PK(i, c) is taken as the pK value. (To "match" is to have the same subscript values.) When EPK(i, c) is non-zero, PK is taken as the base-10 logarithm of the pre-exponential factor in the equation for pK as a function of environmental temperature TCEL, that is,

$$\log pK = PK(i,c) - \frac{1000\ EPK(ion,chemical)}{4.58\ (TCEL(segment,month) + 273.15)}$$

The vector indices for PK ("c" denotes the chemical) are

PK(1,c) contains datum for generation of SH_4^+ from SH_3

PK(2,c) contains datum for generation of SH_5^{2+} from SH_4^+

PK(3,c) contains datum for generation of SH_6^{3+} from SH_5^{2+}

PK(4,c) contains datum for generation of SH_2^- from SH_3

PK(5,c) contains datum for generation of SH^{2-} from SH_2^-

PK(6,c) contains datum for generation of S^{3-} from SH^{2-}

PLMAS

PLanktonic bioMASs (segment, month) Units: mg (dry weight)/L

Total plankton subject to biosorption of xenobiotic chemicals.

POH

pOH (segment, month) Units: pOH units

The negative value of the power to which 10 is raised in order to obtain the temporally averaged concentration of hydroxide [OH^-] ions in gram-equivalents per liter.

PRBEN

PROportion of sorbed chemical delivered to BENthic zone Unitless

The PRZM model generates an output file that can be read by the READ command in EXAMS. PRZM reports, for each runoff date, contaminant dissolved in the flow, and contaminant sorbed to entrained particulate matter. Use PRBEN (SET to a value between 0.0 and 1.0) to indicate how much of the sorbed material is to sink through the water column and become incorporated into the benthic sediments. Based on the generalizaiton that about 50% of sorbed contaminant is typically quite labile, and 50% is refractory, the default value of PRBEN is set to 0.50.

PRINTR

Logical Unit Number used for printing results on a line printer.

PRODNM

PRODuct chemistry database NaMe (50 characters) Units: n/a

Do *not* use "CHANGE" or "SET" to enter names! The NaMe for a PRODuct chemistry database is entered via the command sequence:

EXAMS-> PRODUCT NAME IS nnn...

where "nnn... " can include as many as 50 characters. This name is associated with product chemistry database library entries, so that databases can be found in the catalog. Use a CHANGE or SET command to repair single characters in the name. For example, to repair character seven, enter "SET PRODNM(7) TO ... ."

PRSW

PRint SWitch Units: n/a

PRSW is a switch for controlling printing options. In mode 3, when PRSW is set to 0 (the default), average values of the environmental parameters are recorded in the run log. When PRSW is 1, a separate table is produced for each (monthly) data set, except for those values which are invariant (VOL etc.).

QTBAS

Q Ten BACteria benthoS (form, ion, chemical) Units: dimensionless

Q_{10} values for benthic bacterial biolysis (see KBACS) of chemical. "Q_{10}" is the increase in the second-order rate constant due to a 10° C increase in temperature. Indices refer to 28 molecular spp: 4 forms--1:aqueous, 2:solids-sorbed, 3:DOC-complexed, and 4: bio-sorbed; by 7 ions--1:neutral, 2-4:cations, and 5-7:anions. When QTBAS is non-zero, the matching (same subscripts) rate constant is computed as:

$$KBACS(f,i,c) = QTBAS(f,i,c)^{(TCEL(seg,month)-20)/10} * KBACS(f,i,c)$$

QTBAW

Q Ten BACteria Water (form, ion, chemical) Units: dimensionless

Q_{10} values for bacterioplankton biolysis (see KBACW) of chemical. "Q_{10}" is the increase in the second-order rate constant due to a 10° C increase in temperature. Indices refer to 28 molecular spp: 4 forms--1:aqueous, 2:solids-sorbed, 3:DOC-complexed, and 4: bio-sorbed; by 7 ions--1:neutral, 2-4:cations, and 5-7:anions. When QTBAW is non-zero, the matching (same subscripts) rate constant is computed as:

$$KBACW(f,i,c) = QTBAW(f,i,c)^{(TCEL(seg,month)-20)/10} * KBACW(f,i,c)$$

QUANT

QUANTum yield (form, ion, chemical) Units: dimensionless

Reaction quantum yield for direct photolysis of chemicals--fraction of the total light quanta absorbed by a chemical that results in transformations. Separate values (21) for each potential molecular type of each chemical allow the effects of speciation and sorption on reactivity to be specified in detail. The matrix of 21 values specifies quantum yields for the (3) physical forms: (1) dissolved, (2) sediment-sorbed, and (3) DOC-complexed; of each of (7) possible chemical species: neutral molecules (1), cations (2-4), and anions (5-7). (QUANT is an efficiency.)

RAIN

RAINfall (month) Units: mm/month

Average (monthly) rainfall in geographic area of system.

RANUNT

Logical Unit Number for the UTILITY file support.

The UTILITY file is used for retrieving and storing chemical and environmental parameters, for supporting the on-line assistance facility, and to support the SYSTEM PARAMETERS operations.

REDAG

REDucing AGents (segment, month) Units: moles/L

Molar concentration of reducing agents in each system segment.

RELER

RELative ERror tolerance for integrators.

When the characteristics of the chemical and ecosystem are such as to result in "stiff" equations, numerical errors may lead to small negative numbers in the time series. If desired, the value of ABSER and RELER can be decreased in order to achieve greater precision in the simulation outputs.

RFLAT

ReFerence LATitude (ion, chemical) Units: degrees (e.g., 40.72)

(RFLAT - LAT) corrects for North or South displacement of the ecosystem LATitude from the location (RFLAT) of a photochemical study used to develop a matched (same subscript) KDP pseudo-first-order rate constant.

RFLAT(1,c) refer to photolysis of neutral molecules SH_3

RFLAT(2,c) refer to photolysis of singly charged cations SH_4^+

RFLAT(3,c) refer to photolysis of doubly charged cations SH_5^{2+}

RFLAT(4,c) refer to photolysis of triply charged cations SH_6^{3+}

RFLAT(5,c) refer to photolysis of singly charged anions SH_2^-

RFLAT(6,c) refer to photolysis of doubly charged anions SH^{2-}

RFLAT(7,c) refer to photolysis of triply charged anions S^{3-}

RFORM

Reactive FORM (path) Units: n/a Range: 1--32

RFORM gives the reactive molecular form (ionic species in each of the possible sorptive states) of CHPAR(p) resulting in product TPROD(p). The table shows the value of RFORM for each molecular entity, including values for total dissolved (29), solids-sorbed (30), etc.

	Ionic species	Neutral	Cations			Anions			Total
	Valence	0	1+	2+	3+	1-	2-	3-	(all)
Forms:	Dissolved	1	5	9	13	17	21	25	29
	Solids-sorbed	2	6	10	14	18	22	26	30
	DOC-complexed	3	7	11	15	19	23	27	31
	Biosorbed	4	8	12	16	20	24	28	32

See also: CHPAR, EAYLD, NPROC, TPROD, YIELD

RHUM

Relative HUMidity (month) Units: %, i.e., saturation = 100% R.H.

Mean (monthly) relative humidity during daylight hours. Data typical of daylight hours are needed because their primary use is to characterize light transmission in the atmosphere.

RPTOUT

Logical Unit Number for data written to tabular report file.

SEELD

SEEpage LoaD (segment, chemical, month) Units: kg/hour

Chemical loadings entering the system via "interflows" or seepage (all sub-surface water flows entering the system, (usually) via a benthic segment).

SEEPS

SEEPage flowS (segment, month) Units: m^3/hour

Interflow (subsurface water flow, seepage) entering each segment. SEEPS usually enter via a benthic segment. SEEPS are assumed to lack an entrained sediment flow, that is, they are flows of water only.

SOL

SOLubility (ion, chemical) Units: mg/L

Aqueous solubility of each species (neutral molecule + all ions). When the matching value in the ESOL matrix is zero, SOL(i, c) is taken as the aqueous solubility in mg/L. (To "match" is to have

the same subscript values.) When ESOL(i, c) is non-zero, SOL(i, c) is taken as the base-10 logarithm of the pre-exponential factor of the equation describing the *molar* solubility of the species as a function of environmental temperature (TCEL). The vector indices for SOL are given in the text describing ESOL. Solubility must be specified, because it is used as a constraint on loads.

SPFLG

SPecies FLaGs (ion, chemical)--can be "1" (exists) or "0".

This vector of "flags" or "switches" shows which ions exist. Set the flags ("SET SPFLG(i, c)=1") when entering chemical data in order to show EXAMS the ionic structure of the chemical. When EXAMS starts, only SPFLG(1,*) are set, i.e., the default chemical structure is a neutral (non-ionizing) molecule. As additional SPFLG are set, EXAMS displays the additional chemical data tables needed to display the properties of the ionic species.

set SPFLG(1,c)=1 to signal existence of a neutral molecule SH_3

set SPFLG(2,c)=1 to signal existence of a singly charged cation SH_4^+

set SPFLG(3,c)=1 to signal existence of a doubly charged cation SH_5^{2+}

set SPFLG(4,c)=1 to signal existence of a triply charged cation SH_6^{3+}

set SPFLG(5,c)=1 to signal existence of a singly charged anion SH_2^-

set SPFLG(6,c)=1 to signal existence of a doubly charged anion SH^{2-}

set SPFLG(7,c)=1 to signal existence of a triply charged anion S^{3-}

SSOUT

Logical Unit Number for data written to plotting file containing EXAMS' steady-state chemical concentrations.

STFLO

STream FLOws (segment, month) Units: m^3/hour

Flow into head reach of river or estuary; segment tributaries and creeks or other streamflows entering a lake or pond. Note that STFLO represents stream flow entering system segments from external sources *only*. EXAMS itself computes hydrologic flows among segments that are part of the waterbody being studied, via the specified advective and dispersive flow patterns (see JFRAD, JTURB, etc.). Therefore, *do not* compute net water balances for each segment and enter these into the database--enter *only* those flows entering the system across external boundaries!

STRLD

STReam LoaD (segment, chemical, month) Units: kg/hour

Chemical loadings entering ecosystem segments via stream flow.

STSED

STream-borne SEDiment (segment, month) Units: kg/hour

Stream-borne sediment load entering ecosystem segments.

SUSED

SUspended SEDiment (segment, month) Units: mg/L

Suspended particulate matter--applicable to the water column only.

SYSTYP

Name of aquatic ecoSYStem TYPe (50 characters) Units: n/a

Do *not* use "CHANGE" or "SET" to enter names! The name of a waterbody is entered into the database via the command sequence:

EXAMS-> ENVIRONMENT NAME IS nnn...

where "nnn... " can include as many as 50 characters. This name is associated with environmental library entries (the UDB catalog) and is printed in the header information of the appropriate output tables. Use SET and CHANGE to correct single characters in the name. For example, to correct the seventh character in a name,

EXAMS-> CHAN SYSTYP(7) TO ...

TCEL

Temperature in CELsius (segment, month) Units: degrees C

Average temperature of ecosystem segments. Used (as enabled by input data) to compute effects of temperature on transformation rates and other properties of chemicals.

TCODE

The value of Time CODE sets the units of TINIT, TEND, and CINT.

TCODE can be SET to 1 (hours), 2 (days), 3 (months), or 4 (years). TCODE is under full user control only in Mode 2. In mode 2, TCODE controls the time frame of the study. For example, given TINIT=0., TEND=24., and CINT=2.; CHANging TCODE from 1 to 3 converts a 0-24 hour study into

0-24 months, with bimonthly reports. In mode 1, EXAMS selects the units for reporting results, from the probable half-life of the study chemical(s). In mode 3, a RUN encompasses one year or longer, and the timing is set to produce standard outputs.

TEND

Time END for a dynamic simulation segment. Units: see TCODE

A simulation segment encompasses the period TINIT through TEND. At the end of each integration, TINIT is reset to TEND. The simulation can be extended by invoking the "CONTINUE" command; EXAMS will then request a new value of TEND. Pulse loads (IMASS) and longer-term chemical loads (STRLD, NPSLD, etc.) can be modified or deleted during the pause between simulation segments.

TINIT

Time INITial for a dynamic simulation segment. Units: see TCODE

A simulation RUN encompasses the period TINIT through TEND. At the end of each integration, TEND is transferred to TINIT. The simulation results can be evaluated, and the study continued via the "CONTINUE" command. EXAMS will note the new value of TINIT and request a new endpoint. Pulse and other chemical loadings can be modified or deleted between simulation segments.

TPROD

Transformation PRODuct (path) Units: n/a Range: 1-KCHEM

TPROD(p) -- ADB location of the transformation product of CHPAR(p). The matching (same transformation path number "p") members of CHPAR and TPROD give the location numbers in the active database of the parent chemical and the transformation product for pathway "p". For example, SET CHPAR(p) TO 1, and TPROD(p) to 4, to show that the chemical in ADB sector 4 is produced via transformation of the chemical in ADB sector 1, via process data defined by the remaining members of product chemistry sector "p".

See also: CHPAR, EAYLD, NPROC, RFORM, YIELD

TTYIN

Logical Unit Number for interactive input commands.

TTYOUT

Logical Unit Number for output error messages and warnings, and for EXAMS' interactive responses.

TYPE

Segment TYPE (segment) Units: letter codes

Letter codes designating segment types used to define ecosystems.
Available types: Littoral, Epilimnion, Hypolimnion, and Benthic.

UDB

User DataBase

Long-term retention of data required by EXAMS is provided by storage in the "User Database" (UDB, generally resident on a physical device, e.g., a hard disk) for CHEMICALs, ENVIRONMENTs, LOADs, or PRODUCTs. Within each of these UDB sectors, each dataset is CATALOGued via a unique accession number (UDB#). When transferring data between foreground memory (the activity database or ADB) and a UDB, the target location must be specified by the name of the UDB sector and the accession number within the sector. For example, to STORE the current pattern of chemical loadings: STORE LOAD 7. Similarly, to retrieve or RECALL data from a UDB into the ADB for use in an analysis, one could enter: RECALL LOAD 7.

VAPR

VAPOR pressure (chemical) Units: Torr

Used to compute Henry's law constant when HENRY datum is zero (0) but VAPR is non-zero:

HENRY = (VAPR/760) / (SOL/MWT)

If the associated molar heat of vaporization (EVPR) is non-zero, VAPR is taken as the base-10 logarithm of the pre-exponential factor in an exponential function describing vapor pressure as a function of temperature (TCEL).

VOL

VOLume (segment) Units: m^3

Total environmental volume of ecosystem segments.

WIDTH

WIDTH (segment) Units: m

Average bank-to-bank distance--for computing volume, area, depth of lotic systems described via length, width, and cross-sectional areas.

WIND

WINDspeed (segment, month) Units: m/second

Average wind velocity at a reference height of ten centimeters above the water surface. Parameter is used to compute a piston velocity for water vapor (Liss 1973, Deep-Sea Research 20:221) in the 2-resistance treatment of volatilization losses.

XSA

Cross-sectional (XS) Area (segment) Units: m^2

Area of waterbody in section along advective flowpath.

XSTUR

X Section for TURbulent dispersion (path) Units: m^2

XSTUR is cross-sectional area of a dispersive exchange interface at the boundary between segments JTURB(p) and ITURB(p). The matching (same "p" subscript) members of JTURB, ITURB, CHARL, DSP, and XSTUR collectively define a dispersive transport pathway. The exchange constant E(p) is computed as:

E(p) (m^3/hour) = DSP(p) XSTUR(p) / CHARL(p)

See also: CHARL, DSP, ITURB, JTURB

YEAR1

YEAR 1 Units: n/a

Starting year for mode 3 simulation (e.g., 1985).

YIELD

YIELD of product (path) Units: mole per mole

YIELD(p) is the product yield from the transformation pathway "p" with dimensions mole of transformation product TPROD(p) produced per mole of parent compound CHPAR(p) reacted (dimensionless).

See also: CHPAR, EAYLD, NPROC, RFORM, TPROD

EXAMS data entry template for chemical molar absorption spectra (ABSOR).

Waveband					Waveband			
No.	Center nm	Band-width nm	ABSOR cm^{-1} M^{-1}		No.	Center nm	Band-width nm	ABSOR cm^{-1} M^{-1}
1	280.0	2.5			24	380.0	10.0	
2	282.5	2.5			25	390.0	10.0	
3	285.0	2.5			26	400.0	10.0	
4	287.5	2.5			27	410.0	10.0	
5	290.0	2.5			28	420.0	10.0	
6	292.5	2.5			29	430.0	10.0	
7	295.0	2.5			30	440.0	10.0	
8	297.5	2.5			31	450.0	10.0	
9	300.0	2.5			32	460.0	10.0	
10	302.5	2.5			33	470.0	10.0	
11	305.0	2.5			34	480.0	10.0	
12	307.5	2.5			35	490.0	10.0	
13	310.0	2.5			36	503.75	17.5	
14	312.5	2.5			37	525.0	25.0	
15	315.0	2.5			38	550.0	25.0	
16	317.5	2.5			39	575.0	25.0	
17	320.0	2.5			40	600.0	25.0	
18	323.1	3.75			41	625.0	25.0	
19	330.0	10.0			42	650.0	25.0	
20	340.0	10.0			43	675.0	25.0	
21	350.0	10.0			44	706.25	37.5	
22	360.0	10.0			45	750.0	50.0	
23	370.0	10.0			46	800.0	50.0	

Implementing the microcomputer MS-DOS Runtime EXAMS 2.96

The diskette contains a total of five EXAMS program files stored in a combined archival compressed format. The files require a total of about 360 Kb of mass storage for transfer to your hard disk, plus an additional six megabytes for storage of the files as they are retrieved from the Archives, plus additional working space for the files produced while EXAMS runs.

The disk includes, besides the file README.XMS you are now reading,

- **A file for installing the EXAMS program, in file INSTXMS.EXE, which will create files EXAMS.EXE, EXAMSDAF.TPL, ...**

- **the task image in file EXAMS.EXE, which allows space for five simultaneous chemicals (or one chemical and two degradation products, etc.), and environmental models of up to one hundred segments;**

- **the unformatted direct access data- and help-file EXAMSDAF.TPL, with space for 25 chemical datasets, 10 environmental datasets, 5 external chemical load series, and 5 product chemistries. This file is a template file and should be protected via the DOS command ATTRIB +R if at all possible.**

- **an EXAMS command file for testing the installation, in TEST.EXA;**

- **a sample output for comparison with the results of your test run, in file TESTOUT.XMS**

- **a file for assisting in the interpretation of error messages, and**

- **the User's Guide for EXAMS 2.96 in file EXAMS.PS. This file can be printed by routing it to a PostScript printer.**

First, make sure that your IBM PC/AT 386/486/Pentium or "Compatible" measures up to the following minimum hardware and software specifications.

- **EXAMS makes use of the Phar Lap DOS-extender to access extended memory. EXAMS will require time to set up its virtual memory system when loaded from DOS; load time can be reduced by running as a Windows 3.1+ task.**

- **appropriate diskette drive (for installation only)**

- **5- or 10-megabyte available mass storage (hard disk)**

- **80x87 math co-processor**

- **MS-DOS version 5.0 or higher**

If your machine does not conform to these minimum specifications, the EXAMS program WILL NOT execute properly.

- more -

Then, to install the program

1. Transfer the contents of the diskette to your hard disk in some suitable subdirectory or partition.

a. Set the default drive to the mass storage device (e.g., hard disk "C"): C:

b. Create an EXAMS directory: MKDIR EXAMS
(N.B. if installing as part of PIRANHA, the PIRANHA\EXAMS directory already exists--do NOT create another EXAMS directory)

c. Request verification of copy results: VERIFY ON

d. Change default directory to EXAMS: CD\EXAMS
or to PIRANHA EXAMS subdirectory CD\PIRANHA\EXAMS

e. Transfer the files from the diskette (e.g., drive "A") to the hard disk: COPY A:*.*

f. Execute the file INSTXMS.EXE to recover files from the archives: INSTXMS

g. Protect the direct access file template from accidental corruption: ATTRIB +R EXAMSDAF.TPL

h. Create a working copy of the file:
(N.B. Skip this step if upgrading PIRANHA)
COPY EXAMSDAF.TPL EXAMS.DAF

2. Start the EXAMS program from the EXAMS directory.

a. Start the EXAMS program: EXAMS

b. When you reach the EXAMS system prompt, start the test command file: EXAMS-> DO TEST

3. When the test run finishes compare the outcome (in file REPORT) with the file TESTOUT supplied with the program:

```
FC   REPORT.XMS TESTOUT.XMS
```

Files TESTOUT.XMS and TEST.EXA are not needed for routine operation of EXAMS and can be deleted, as can file INSTXMS.EXE.

4. EXAMS uses Logical Unit Number (LUN) Seven, writing to device PRN, for its Print command. As part of starting the program under DOS, you may wish to make the DOS print routine memory-resident (i.e., set up a print spooler) before starting EXAMS.

a. Load the DOS print routine (optional) PRINT

b. Start the EXAMS program: EXAMS