

US EPA ARCHIVE DOCUMENT

## 8.0 Surface Water Module

### 8.1 Purpose and Scope

The Surface Water Module simulates contaminant concentrations in surface waterbodies throughout the area of interest (AOI) around each site modeled. Inputs to the Surface Water Module include contaminant loadings from direct air deposition onto surface waters, contaminant loadings from runoff and soil erosion from land areas associated with sources (LAU and waste piles only), contaminant loadings from contaminated ground water plumes that are intercepted by surface waters, contaminant loadings in runoff and eroded soil from the watersheds in the AOI, and hydrological inputs (flows, soil loads) from the watersheds. Surface Water Module outputs include water column and sediment contaminant concentrations, which are then used by the Aquatic Food Chain Module, Farm Food Chain Module, and Ecological Exposure Module. All inputs and outputs are annual average time series. Figure 8-1 shows the relationship and information flow between the Surface Water Module and the 3MRA modeling system.

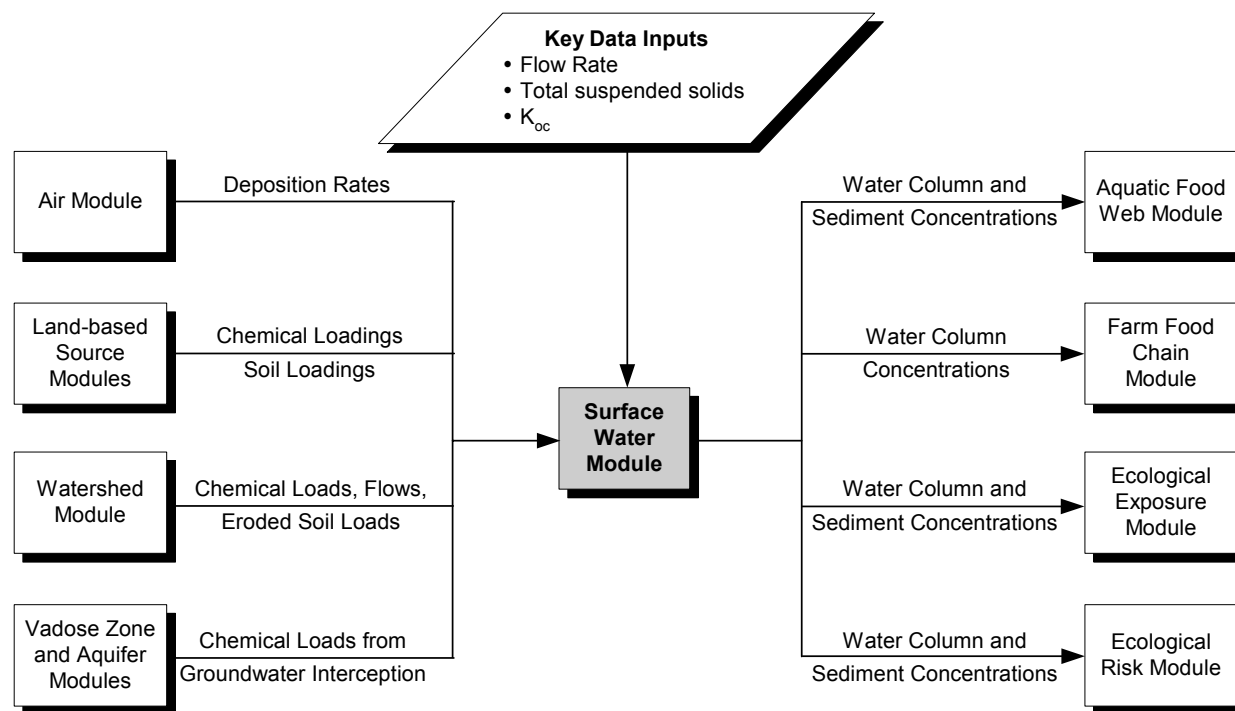


Figure 8-1. Information flow for the Surface Water Module in the 3MRA modeling system.

The major tasks performed by the Surface Water Module to simulate contaminant concentrations throughout the surface waterbody network in the AOI are as follows:

1. **Constructs waterbody network.** For each AOI, the Surface Water Module identifies the streams, wetlands, ponds, lakes, and bay reaches to be modeled, and assigns lengths, areas, depths, and volumes to them.
2. **Routes hydraulic flow and solids through the waterbody network.** The Surface Water Module conducts water and solids balances for each waterbody in each year of the simulation.
3. **Constructs and solves the mass balance equations describing contaminant fate and transport throughout the waterbody network.** The Surface Water Module calculates the contaminant concentration in each waterbody for each year. Outputs include total water column concentration and dissolved concentration.

## 8.2 Conceptual Approach

The Surface Water Module is based on the EPA legacy model Exposure Analysis Modeling System (EXAMS II), which has been thoroughly verified and validated in numerous applications (see Volume III of this report). EXAMS II was extended for use in the Surface Water Module primarily through development of the pre- and postprocessor, EXAMS IO. EXAMS IO is the interface between EXAMS II and the rest of the 3MRA modeling system. It reads data from other 3MRA modules and databases, builds the EXAMS input files describing the waterbody environment and chemical properties, builds a command file that specifies the contaminant loading history, and controls the EXAMS simulation. EXAMS IO passes control to EXAMS II, which conducts the simulation and produces intermediate results files. EXAMS IO then processes the intermediate files and passes the output data back to the proper 3MRA modeling system database. The complete system consisting of EXAMS II and EXAMS IO is denoted in this discussion as the Surface Water Module. A summary of EXAMS II—the science and computational core of the Surface Water Module—is presented in the accompanying text box. The full capabilities of EXAMS II are explained in Burns et al. (1982) and Burns (1997).

### 8.2.1 Construct Waterbody Network

Each Monte Carlo iteration of the 3MRA system represents a unique site covering the AOI around a waste management unit (WMU). This AOI is defined by a radius of 2 km in the sample 3MRA data set. One or more contiguous waterbody networks may be located within each AOI. For each of the 201 sites currently contained in the 3MRA modeling system database, waterbody networks were defined using the EPA Reach File system supplemented with digital elevation modeling. Each waterbody network is divided into reaches, which are characterized and stored in the site database.

### Summary of EXAMS II

EXAMS II combines contaminant loadings, transport, and transformations into a set of differential equations using the law of conservation of mass as an accounting principle. It accounts for all the contaminant mass entering and leaving a system as the algebraic sum of external loadings, transport processes that export the compound from the system, and transformation processes within the system that convert the contaminant to daughter products. (Transformation from parent to daughter products is implemented only for mercury in the Surface Water Module.)

EXAMS II represents each waterbody by a set of segments or distinct zones in the system. The program is based on a series of mass balances for the segments that give rise to a single differential equation for each segment. Working from the individual transport and transformation process equations, EXAMS II compiles an overall equation for the net rate of change of contaminant concentration in each segment. The resulting system of differential equations describes the mass balance for the entire system, which is then solved by the method of lines.

EXAMS II includes process models of the physical, chemical, and biological phenomena governing the transport and fate of compounds. Each of the unit process equations used to compute the transformation kinetics of contaminants accounts for the interactions between the chemistry of a compound and the environmental forces that shape its behavior in aquatic systems. This “second-order” or “system-independent” approach allows one to study the fundamental chemistry of compounds in the laboratory and then, based on independent studies of the levels of driving forces in aquatic systems, evaluate the probable behavior of the compound in systems that have never been exposed to it. Most of the process equations are based on standard theoretical constructs or accepted empirical relationships. The user can specify reaction pathways for the production of transformation products of concern, whose further fate and transport can then be simultaneously simulated by EXAMS II.

EXAMS II contains process modules for several chemical reactions. Equilibrium reactions are used for sorption and ionization. Kinetic reactions are used for volatilization, hydrolysis (acid, base, and neutral), biodegradation (water column and sediments), photolysis, oxidation, and reduction. (The Surface Water Module does not consider photolysis or oxidation/reduction.) EXAMS II uses these modules as determined by the input chemical properties. EXAMS II has been designed to accept standard water quality parameters and system characteristics that are commonly measured by limnologists throughout the world and contaminant data sets conventionally measured or required by EPA regulatory procedures.

The contaminant fate algorithms in EXAMS II model sorption to suspended solids, biotic solids, and sediment solids, but EXAMS II does not simulate a solids balance. Solids concentrations are specified as input data. The effects of settling and resuspension on contaminant fate are accounted for in a bulk sediment-water exchange term.

EXAMS II incorporates a few major assumptions. The model was designed to evaluate the consequences of longer-term, primarily time-averaged contaminant loadings that ultimately result in trace-level contamination of aquatic systems. EXAMS II generates a steady-state, average flow field (long-term or monthly) for the ecosystem. The program cannot therefore fully evaluate the transient, high concentrations that arise from chemical spills, although spills under average hydrological conditions can be studied. An assumption of trace-level contaminant concentrations was used to design the process equations. The contaminant is assumed not to radically change the environmental variables that drive its transformations. EXAMS II uses linear sorption isotherms and second-order (rather than Michaelis-Menten-Monod) expressions for biotransformation kinetics, which are known to be valid for low concentrations of pollutants. Sorption is treated as a thermodynamic or constitutive property of each compartment in the system; that is, sorption-desorption kinetics are assumed to be rapid compared with other processes. Although this assumption may be violated by extensively sorbed contaminants, these contaminants tend to be captured by benthic sediments, where their release to the water column is controlled by benthic exchange processes.

From the 3MRA modeling system site database, stream reaches are assigned lengths, and wetland, pond, lake, and bay reaches are assigned surface areas. Site-specific reach depths and volumes were not available. Instead, depths were assigned to water column and sediment compartments for wetlands, ponds, lakes, and bays based on national distributions. The Surface Water Module calculates volumes from the site-specific surface areas and the estimated depths. For stream reaches, the Surface Water Module calculates widths and depths using discharge coefficients based on empirical observations of stream hydrogeometric relationships (Leopold and Maddox, 1953) and then calculates volumes using site-specific reach lengths.

## 8.2.2 Route Hydraulic Flow Through the Waterbody Network

**Water Balance.** The Surface Water Module conducts a water balance for each simulated year, routing incoming flows from the headwater reaches down through the network and out of the exiting reach. For a given reach in a given year, the outflow is the sum of all the inflows minus evaporation, as shown in the water balance equation:

$$Q_{r,t} = \sum_{i=1}^{NumTrib_r} QTrib_{i,r,t} + \sum_{i=1}^{NumWS_r} QRunoff_{i,r,t} \times WSFrac_{i,r} + QBase_r + \frac{(R_t - E_t) \times AS_r}{100 \times 365} \quad (8-1)$$

where

$Q_{r,t}$	=	average outflow from reach $r$ during year $t$ ( $m^3/d$ )
$NumTrib_r$	=	number of upstream reaches flowing into reach $r$
$QTrib_{i,r,t}$	=	average upstream outflow from reach $i$ , tributary to reach $r$ during year $t$ ( $m^3/d$ )
$NumWS_r$	=	number of adjacent watersheds flowing into reach $r$
$QRunoff_{i,r,t}$	=	annual average surface runoff inflow from watershed $i$ immediately adjacent to reach $r$ during year $t$ ( $m^3/d$ )
$WSFrac_{i,r}$	=	area fraction of adjacent watershed $i$ contributing to reach $r$
$QBase_r$	=	average constant baseflow flow to reach $r$ ( $m^3/d$ )
$R_t$	=	precipitation for year $t$ (cm/yr)
$E_t$	=	evaporation for year $t$ (cm/yr)
$AS_r$	=	surface area for reach $r$ under baseflow conditions ( $m^2$ ).

The Surface Water Module also checks and ensures positive flow in every reach for every year. If evaporation exceeds the total inflow to a reach for a year, the evaporation in that reach is reduced to a level supporting an outflow equivalent to precipitation of 0.5 mm/yr over the entire contributing watershed.

Long-term average baseflow from each adjacent watershed is calculated in the Watershed Module using empirical correlations based on watershed surface area and regional location (see Section 7). The input data map these watersheds to the appropriate reaches and also specify the fraction of each contributing watershed's baseflow that should be associated with each reach. Total reach baseflow is then calculated by the fraction-weighted sum over all contributing watersheds. This baseflow estimate is derived from observed stream flow data and accounts for both seepage inflow and evaporation loss during dry periods.

This water balance is conducted for each simulated year on a reach-specific basis by EXAMS IO. The resulting internal flows are used to calculate stream hydrogeometry and the waterbody solids balance. Information on stream widths and depths and all hydrologic inflows is used to recalculate the water balance on a compartment-specific basis for use in the chemical advection calculations.

**Solids Balance.** EXAMS IO conducts a solids balance for each simulated year, routing incoming solids from the headwater reaches down through the network and out of the exiting reach. The total suspended solids (TSS) in a reach may originate in erosion from adjacent watershed subbasins, from internal bank erosion, or from internal production of biotic solids. Solids deposition and burial are not simulated in this version of the Surface Water Module; consequently, TSS is modeled as a conservative substance. Therefore, for a given reach in a given year, the average solids flux per year through the reach is the sum of all the solids mass inflows, including upstream loads, loads delivered from adjacent surface erosion, and loads generated internally to the reach:

$$TSS_{r,t} = \sum_{i=1}^{NumTrib_r} QTrib_{i,r,t} \times TSS_{Trib_{i,r,t}} + \sum_{i=1}^{NumWS_r} TSS_{Runoff_{i,r,t}} \times WS_{Frac_{i,r}} + Q_{r,t} \times \left[ SolBnk_r + \frac{Phyt(TI_r)}{FocBio} \right] \quad (8-2)$$

where

$TSS_{r,t}$	=	average solids load exiting reach $r$ in year $t$ (g/day)
$QTrib_{i,r,t}$	=	average upstream outflow from reach $i$ , tributary to reach $r$ during year $t$ (m <sup>3</sup> /d)
$TSS_{Trib_{i,r,t}}$	=	TSS concentration exiting upstream reach $i$ , tributary to reach $r$ , in year $t$ (g/m <sup>3</sup> )
$TSS_{Runoff_{i,r,t}}$	=	solids load delivered from erosion of watershed $r$ , immediately adjacent to reach $r$ , in year $t$ (g/day)
$SolBnk_r$	=	TSS concentration from incremental bank erosion in reach $r$ (g/m <sup>3</sup> )
$Phyt(TI_r)$	=	biotic carbon concentration for trophic index for reach $r$ (g-C/m <sup>3</sup> )
$TI_r$	=	trophic index for reach $r$ (unitless)
$FocBio$	=	organic carbon fraction of biotic solids (g-C/g-solids)

The first right-hand term in this equation accounts for upstream tributary solids loads. The second term accounts for adjacent watershed erosion loads. This erosion load is generated by the Watershed Module and already incorporates an area-dependent sediment delivery ratio. The third term accounts for bank erosion loading, where the TSS concentration from incremental bank erosion is the resulting incremental concentration in reach  $r$ . This is set to 5 g/m<sup>3</sup> for stream reaches and 1 g/m<sup>3</sup> otherwise. The final term accounts for internal biotic production of solids. The trophic index is related to the net biotic production.

### 8.2.3 Construct and Solve the Mass Balance Equations Describing Contaminant Fate and Transport throughout the Waterbody Network

The primary function of the Surface Water Module is to simulate the spatial and temporal contaminant concentrations for both fate within the individual waterbody segments (or compartments) and transport among these compartments that make up the overall waterbody network.

Contaminant fate and transport are calculated on a compartment-specific basis, by accounting for a set of transport and transformation processes applied within a mass balance framework. The Surface Water Module is based on a series of mass balances, which give rise to a single differential equation for each compartment. Working from the transport and transformation process equations, the Surface Water Module generates an equation for the net rate of change of contaminant concentration in each compartment. The resulting system of differential equations describes a mass balance for the entire waterbody network. These equations have the following general form:

$$V \frac{dC}{dt} = L_e + L_i - V \times K \times C \quad (8-3)$$

where

- V = volume of water in the compartment (m<sup>3</sup>)
- C = total contaminant concentration (mg/L)
- L<sub>e</sub> = total external loading to the compartment (g/h)
- L<sub>i</sub> = total internal loading to the compartment resulting from contaminated flows among system compartments and the formation of chemical reaction products (g/h)
- K = overall pseudo-first-order loss constant that expresses the combined effect of transport and transformation processes (i.e., advection, dispersion, volatilization, biodegradation) that decrease contaminant concentration (h<sup>-1</sup>)

The Surface Water Module provides for a total of five kinds of compartment loadings:

- Point source or stream-borne loadings,
- Nonpoint source loadings,
- Contaminated ground water seepage,
- Precipitation washout from the atmosphere, and
- Spray drift (or miscellaneous) loading.

The inputs include monthly and annual average loadings to all appropriate compartments.

The Surface Water Module evaluates the status of individual loadings entering the compartments to prevent conditions outside of its numerical operating range. For example, the Surface Water Module makes no provision for crystallization of the compound from solution, nor for dissolution of a compound from a solid or liquid phase. In addition, reaction nonlinearities potentially present at high contaminant concentrations are not incorporated into

the model. The Surface Water Module calculates the dissolved contaminant concentration within each input flow, using receiving compartment pH and temperature to account for ionization and using entrained sediment loads to account for sorption. If the dissolved concentration for any of the species is greater than half its solubility, then the simulation is not used by the 3MRA modeling system.

The system of mass balance differential equations is solved numerically, using the method of lines algorithm. The solution to the system of mass balance equations yields the distribution of contaminant concentration throughout the surface waterbody network (water column and sediments) over time. Three temporal options are available for EXAMS II:

- Steady-state (no change over time),
- Quasi-dynamic with time-constant environmental data, and
- Quasi-dynamic with monthly-varying environmental data.

The Surface Water Module implements the quasi-dynamic mode with time-constant environmental data. In this mode, the dynamic simulations consider annually-varying flows and loadings but assume other environmental conditions are at their long-term average values.

## 8.3 Module Discussion

### 8.3.1 Strengths and Advantages

The Surface Water Module has the following strengths and advantages:

- **Use of a proven chemical fate model.** The Surface Water Module uses EXAMS to simulate chemical fate for the scenarios presented by the 3MRA framework. EXAMS is an EPA legacy model that has been used for two decades to assess the fate of organic chemicals in aquatic systems. It has been used routinely to evaluate pesticide exposure scenarios for the Office of Pesticide Programs. During its extensive application history, EXAMS has been tested in a wide variety of waterbodies for a wide range of organic chemicals. The code has been verified, and its predictions have been confirmed in several site-specific evaluations published in the technical literature.
- **Applicable to a variety of conditions.** EXAMS is a robust model that solves the governing differential equations effectively under a variety of conditions.

### 8.3.2 Uncertainty and Limitations

The following uncertainties and limitations are inherent in the Surface Water Module:

- **Limited temporal resolution of numerical solution.** The current 3MRA modeling system methodology calls for repeated, relatively long simulations (e.g., 200 or more years). Accordingly, run time must be relatively fast, which precludes small time steps that might otherwise give insight into contaminant behavior on a finer temporal scale.



- **Limited resolution of loadings and flows.** Use of annual-average loadings and flows rather than daily loadings and flows leads to calculated annual-average concentrations that are biased high, depending on the correlation between flow and loading at a particular site. This bias is somewhat mitigated for reactive and volatile contaminants where the loss rate is proportional to the concentration.
- **Limited site-specific data.** Use of national distributions rather than site-specific environmental data could cause calculated concentrations to be low or high at a given location, with no known general bias.
- **Simplistic solids balance.** The simple solids balance overestimates suspended solids concentrations slightly in streams and more significantly in ponds, wetlands, and lakes. Calculated total water column contaminant concentrations will be high, whereas the dissolved contaminant fraction will be low. The net result for dissolved water column contaminant concentrations, which are used for fish exposure, is not expected to be biased significantly high or low.
- **Procedure for preventing drying of surface water reaches.** For sites that experience periodic drying (due to limited inflows), a small default positive flow equivalent to 0.5 mm per year of direct precipitation onto the waterbody surface is maintained to keep the model functioning. This procedure conducts contaminant loads downstream within a remnant waterbody reach rather than within runoff over a dry bed or subsurface flow within the bed. Although the mass balance is maintained, the contaminant and solids concentrations will tend to be elevated within the remnant reach. These elevated concentrations are probably realistic for years in which evaporation exceeds all hydrologic inflows.

## 8.4 References

- Burns, L.A., D.M. Cline, and R.R. Lassiter. 1982. *Exposure Analysis Modeling System (EXAMS): User Manual and System Documentation*. U.S. Environmental Protection Agency, Athens, GA. EPA-600/3-83-023.
- Burns, L.A. 1997. *Exposure Analysis Modeling System (EXAMS II): User's Guide for Version 2.97.5*. U.S. Environmental Protection Agency, Athens, GA. EPA-600/R-97/047.
- Leopold, L.B. and T. Maddox. 1953. *The Hydraulic Geometry of Stream Channels and Some Physiographic Implications*. Professional Paper 252, U.S. Geological Survey, Washington, DC.