

## 5. The Basic Water Quality Model

WASP6 is a dynamic compartment model that can be used to analyze a variety of water quality problems in such diverse water bodies as ponds, streams, lakes, reservoirs, rivers, estuaries, and coastal waters. This section presents an overview of the basic water quality model. Subsequent chapters detail the transport and transformation processes in WASP6 for various water quality constituents.

The equations solved by WASP6 are based on the key principle of the conservation of mass. This principle requires that the mass of each water quality constituent being investigated must be accounted for in one way or another. WASP6 traces each water quality constituent from the point of spatial and temporal input to its final point of export, conserving mass in space and time. To perform these mass balance computations, the user must supply WASP6 with input data defining seven important characteristics:

- simulation and output control
- model segmentation
- advective and dispersive transport
- boundary concentrations
- point and diffuse source waste loads
- kinetic parameters, constants, and time functions
- initial concentrations

These input data, together with the general WASP6 mass balance equations and the specific chemical kinetics equations, uniquely define a special set of water quality equations. These are numerically integrated by WASP6 as the simulation proceeds in time. At user-specified print intervals, WASP6 saves the values of all display variables for subsequent retrieval by the post-processor program. These programs allow the user to interactively produce graphs and tables of variables of all display variables.

### 5.1. General Mass Balance Equation

A mass balance equation for dissolved constituents in a body of water must account for all the material entering and leaving through direct and diffuse loading; advective and dispersive transport; and physical, chemical, and biological transformation. Consider the coordinate system shown in Equation 5-1, where the x- and y-coordinates are in the horizontal plane, and the z-coordinate is in the vertical plane.

## Water Quality Equation

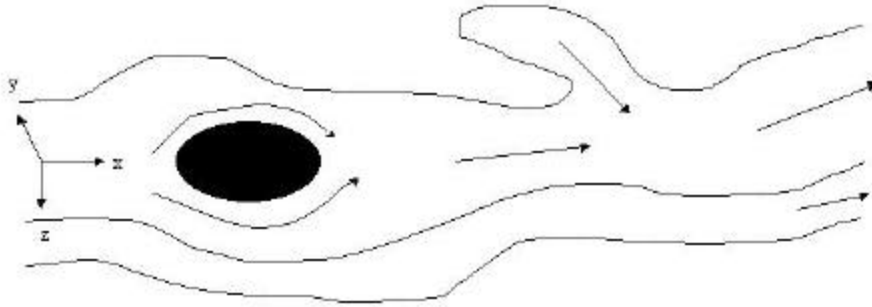


Figure 5-1 Coordinate System for Mass Balance Equation

The mass balance equation around an infinitesimally small fluid volume is:

## Equation 5-1 General Mass Balance Equation

$$\begin{aligned} \frac{\partial C}{\partial t} = & -\frac{\partial}{\partial x}(U_x C) - \frac{\partial}{\partial y}(U_y C) - \frac{\partial}{\partial z}(U_z C) \\ & + \frac{\partial}{\partial x}\left(E_x \frac{\partial C}{\partial x}\right) + \frac{\partial}{\partial y}\left(E_y \frac{\partial C}{\partial y}\right) + \frac{\partial}{\partial z}\left(E_z \frac{\partial C}{\partial z}\right) \\ & + S_L + S_B + S_K \end{aligned}$$

where:

C =	concentration of the water quality constituent, mg/L or g/m <sup>3</sup>
t =	time, days
U <sub>x</sub> , U <sub>y</sub> , U <sub>z</sub> =	longitudinal, lateral, and vertical advective velocities, m/day
E <sub>x</sub> , E <sub>y</sub> , E <sub>z</sub> =	longitudinal, lateral, and vertical diffusion coefficients, m <sup>2</sup> /day
S <sub>L</sub> =	direct and diffuse loading rate, g/m <sup>3</sup> -day
S <sub>B</sub> =	boundary loading rate (including upstream, downstream, benthic, and atmospheric), g/m <sup>3</sup> -day
S <sub>K</sub> =	total kinetic transformation rate; positive is source, negative is

sink, g/m<sup>3</sup>-day

By expanding the infinitesimally small control volumes into larger adjoining "segments," and by specifying proper transport, loading, and transformation parameters, WASP implements a finite-difference form of Equation 5-1. For brevity and clarity, however, the derivation of the finite-difference form of the mass balance equation will be for a one-dimensional reach. Assuming vertical and lateral homogeneity, we can integrate over y and z to obtain Equation 5-2

**Equation 5-2 WASP Implementation of the Finite Difference Form of Mass Balance Equation**

$$\frac{\partial}{\partial t}(A C) = \frac{\partial}{\partial x} \left( -U_x A C + E_x A \frac{\partial C}{\partial x} \right) + A (S_L + S_B) + A S_K$$

where:

A = cross-sectional area, m<sup>2</sup>

This equation represents the three major classes of water quality processes -- transport (term 1), loading (term 2), and transformation (term 3). The finite-difference form is derived in Appendix E. The model network and the major processes are discussed in the following sections.

## 5.2. *The Model Network*

The model network is a set of expanded control volumes, or "segments," that together represents the physical configuration of the water body. As Figure 5-2 illustrates, the network may subdivide the water body laterally and vertically as well as longitudinally. Benthic segments can be included along with water column segments. If the water quality model is being linked to the hydrodynamic model, then water column segments must correspond to the hydrodynamic junctions. Concentrations of water quality constituents are calculated within each segment. Transport rates of water quality constituents are calculated across the interface of adjoining segments.

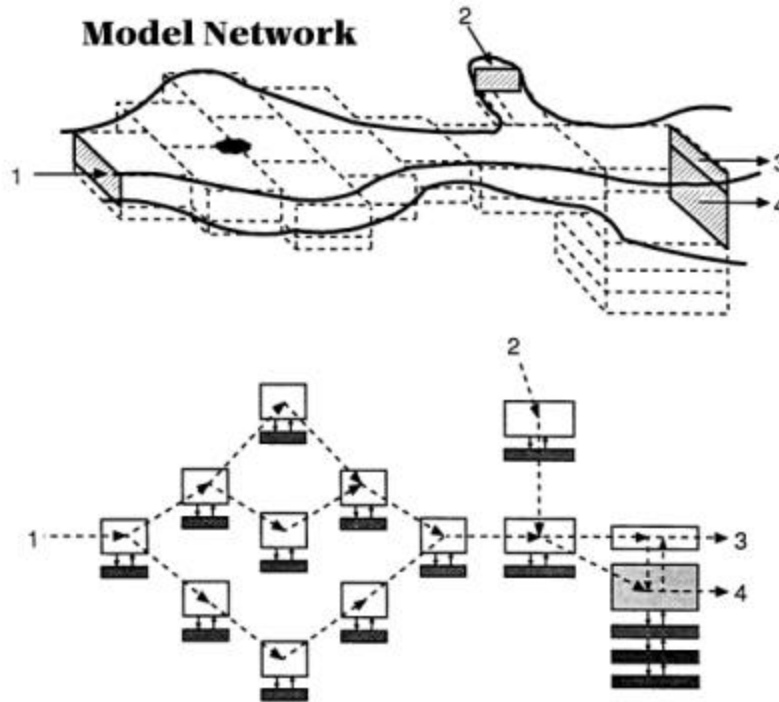
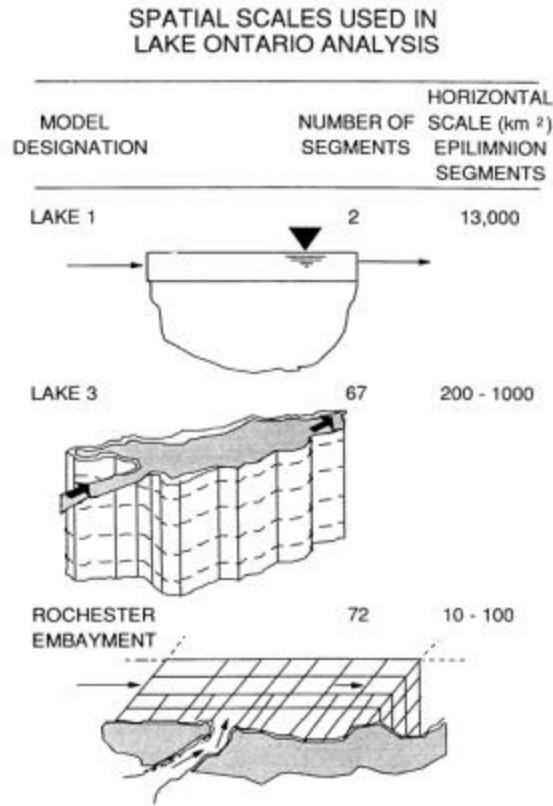


Figure 5-2 Model Segmentation Schematic

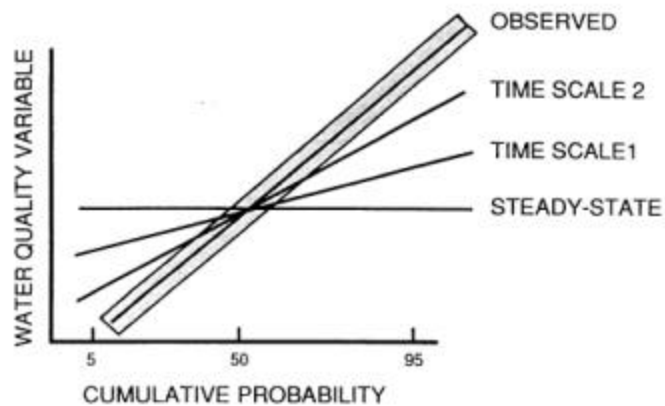
Segments in WASP may be one of four types, as specified by the input variable ITYPE. A value of 1 indicates the epilimnion (surface water), 2 indicate hypolimnion layers (subsurface), 3 indicate an upper benthic layer, and 4 indicate lower benthic layers. The segment type plays an important role in bed sedimentation and in certain transformation processes. The user should be careful to align segments properly. The segment immediately below each segment is specified by the input variable IBOTSG. This alignment is important when light needs to be passed from one segment to the next in the water column, or when material is buried or eroded in the bed.

Segment volumes and the simulation time step are directly related. As one increase or decreases, the other must do the same to insure stability and numerical accuracy. Segment size can vary dramatically, as illustrated in Figure 5-3. Characteristic sizes are dictated more by the spatial and temporal scale of the problem being analyzed than by the characteristics of the water body or the pollutant per se. For example, analyzing a problem involving the upstream tidal migration of a pollutant into a water supply might require a time step of minutes to an hour. By contrast, analyzing a problem involving the total residence time of that pollutant in the same water body could allow a time step of hours to a day. The first network was used to study the general eutrophic status of Lake Ontario. The second network was used to investigate the lake-wide spatial and seasonal variations in eutrophication. The third network was used to predict changes in near-shore eutrophication of Rochester Embayment resulting from specific pollution control plans.



**Figure 5-3 Spatial Scales used in Lake Ontario Analysis**

As part of the problem definition, the user must determine how much of the water quality frequency distribution must be predicted. For example, a daily-average dissolved oxygen concentration of 5 mg/L would not sufficiently protect fish if fluctuations result in concentrations less than 2 mg/L for 10% of the time. Predicting extreme concentration values is generally more difficult than predicting average values. Figure 5-4 illustrates typical frequency distributions predicted by three model time scales and a typical distribution observed by rather thorough sampling, as they would be plotted on probability paper. The straight lines imply normal distributions. Reducing the model time step (and consequently segment size) allows better simulation of the frequency distribution. This increase in predictive ability, however, also entails an increase in the resolution of the input data.

FREQUENCY DISTRIBUTION OF OBSERVED AND  
CALCULATED VALUES OF A QUALITY VARIABLE

**Figure 5-4 Frequency Distribution of Observed and Calculated Values of a Quality Variable**

Once the nature of the problem has been determined, then the temporal variability of the water body and input loadings must be considered. Generally, the model time step must be somewhat less than the period of variation of the important driving variables. In some cases, this restriction can be relaxed by averaging the input over its period of variation. For example, phytoplankton growth is driven by sunlight, which varies diurnally. Most eutrophication models, however, average the light input over a day, allowing time steps on the order of a day.

Care must be taken so that important non-linear interactions do not get averaged out. When two or more important driving variables have a similar period of variation, then averaging may not be possible. One example is the seasonal variability of light, temperature, nutrient input, and transport in lakes subject to eutrophication. Another example involves discontinuous batch discharges. Such an input into a large lake might safely be averaged over a day or week, because large-scale transport variations are relatively infrequent. The same batch input into a tidal estuary cannot safely be averaged, however, because of the semi-diurnal or diurnal tidal variations. A third example is salinity intrusion in estuaries. Tidal variations in flow, volume, and dispersion can interact so that accurate long-term predictions require explicit simulation at time steps on the order of hours.

Once the temporal variability has been determined, then the spatial variability of the water body must be considered. Generally, the important spatial characteristics must be homogeneous within a segment. In some cases, this restriction can be relaxed by judicious averaging over width, depth, and/or length. For example, depth governs the impact of reaeration and sediment oxygen demand in a column of water. Nevertheless, averaging the depth across a river would generally be acceptable in a conventional waste

load allocation, whereas averaging the depth across a lake would not generally be acceptable. Other important spatial characteristics to consider (depending upon the problem being analyzed) include temperature, light penetration, velocity, pH, benthic characteristics or fluxes, and sediment concentrations.

The expected spatial variability of the water quality concentrations also affects the segment sizes. The user must determine how much averaging of the concentration gradients is acceptable. Because water quality conditions change rapidly near a loading point and stabilize downstream, studying the effects on a beach a quarter-mile downstream of a discharge requires smaller segments than studying the effects on a beach several miles away.

A final, general guideline may be helpful in obtaining accurate simulations: water column volumes should be roughly the same. If flows vary significantly downstream, then segment volumes should increase proportionately. The user should first choose the proper segment volume and time step in the critical reaches of the water body ( $V_c$ ,  $\Delta t_c$ ), and then scale upstream and downstream segments accordingly:

$$V_i = V_c Q_i / Q_c$$

Of course, actual volumes specified must be adjusted to best represent the actual spatial variability, as discussed above. This guideline will allow larger time steps and result in greater numerical accuracy over the entire model network, as explained in the section on "Simulation Parameters" in Chapter 2.

### 5.3. *The Model Transport Scheme*

Transport includes advection and dispersion of water quality constituents. Advection and dispersion in WASP are each divided into six distinct types, or "fields." The first transport field involves advective flow and dispersive mixing in the water column. Advective flow carries water quality constituents "downstream" with the water and accounts for instream dilution. Dispersion causes further mixing and dilution between regions of high concentrations and regions of low concentrations.

The second transport field specifies the movement of pore water in the sediment bed. Dissolved water quality constituents are carried through the bed by pore water flow and are exchanged between the bed and the water column by pore water diffusion.

The third, fourth, and fifth transport fields specify the transport of particulate pollutants by the settling, resuspension, and sedimentation of solids. Water quality constituents sorbed onto solid particles are transported between the water column and the sediment bed. The user can define the three solids fields as size fractions, such as sand, silt, and clay, or as inorganic, phytoplankton, and organic solids.

The sixth transport field represents evaporation or precipitation from or to surface water segments.

Most transport data, such as flows or settling velocities, must be specified by the user in a WASP input dataset. For water column flow, however, the user may "link" WASP with a hydrodynamics model. If this option is specified, during the simulation WASP will read the contents of a hydrodynamic file for unsteady flows, volumes, depths, and velocities.

#### 5.4. *Application of the Model*

The first step in applying the model is analyzing the problem to be solved. What questions are being asked? How can a simulation model be used to address these questions? A water quality model can do three basic tasks-- describe present water quality conditions, provide generic predictions, and provide site-specific predictions. The first, descriptive task is to extend in some way a limited site-specific database. Because monitoring is expensive, data seldom give the spatial and temporal resolution needed to fully characterize a water body. A simulation model can be used to interpolate between observed data, locating, for example, the dissolved oxygen sag point in a river or the maximum salinity intrusion in an estuary. Of course such a model can be used to guide future monitoring efforts. Descriptive models also can be used to infer the important processes controlling present water quality. This information can be used to guide not only monitoring efforts, but also model development efforts.

Providing generic predictions is a second type of modeling task. Site-specific data may not be needed if the goal is to predict the types of water bodies at risk from a new chemical. A crude set of data may be adequate to screen a list of chemicals for potential risk to a particular water body. Generic predictions may sufficiently address the management problem to be solved, or they may be a preliminary step in detailed site-specific analyses.

Providing site-specific predictions is the most stringent modeling task. Calibration to a good set of monitoring data is definitely needed to provide credible predictions. Because predictions often attempt to extrapolate beyond the present database, however, the model also must have sufficient process integrity. Examples of this type of application include waste load allocation to protect water quality standards and feasibility analysis for remedial actions, such as tertiary treatment, phosphate bans, or agricultural best-management practices.

Analysis of the problem should dictate the spatial and temporal scales for the modeling analysis. Division of the water body into appropriately sized segments was discussed in Section "Model Network." The user must try to extend the network upstream and downstream beyond the influence of the waste loads being studied. If this is not possible, the user should extend the network far enough so that errors in specifying future boundary concentrations do not propagate into the reaches being studied.

The user also should consider aligning the network so that sampling stations and points of interest (such as water withdrawals) fall near the center of a segment. Point source waste loads in streams and rivers with unidirectional flow should be located near the upper end of a segment. In estuaries and other water bodies with oscillating flow, waste loads are best centered within segments. If flows are to be input from DYNHYD, then a WASP

segment must coincide with each hydrodynamic junction. Benthic segments, which are not present in the hydrodynamic network, may nevertheless be included in the WASP network. WASP segment numbering does not have to be the same as DYNHYD junction numbering. Segments stacked vertically do not have to be numbered consecutively from surface water segments down.

Once the network is set up, the model study will proceed through four general steps involving, in some manner, hydrodynamics, mass transport, water quality transformations, and environmental toxicology. The first step addresses the question of where the water goes. This can be answered by a combination of gaging, special studies, and hydrodynamic modeling. Flow data can be interpolated or extrapolated using the principle of continuity. Very simple flow routing models can be used; very complicated multi-dimensional hydrodynamic models can also be used with proper averaging over time and space. At present, the most compatible hydrodynamic model is DYNHYD.

The second step answers the question of where the material in the water is transported. This can be answered by a combination of tracer studies and model calibration. Dye and salinity are often used as tracers.

The third step answers the question of how the material in the water and sediment is transformed and what its fate is. This is the main focus of many studies. Answers depend on a combination of laboratory studies, field monitoring, parameter estimation, calibration, and testing. The net result is sometimes called model validation or verification, which are elusive concepts. The success of this step depends on the skill of the user, who must combine specialized knowledge with common sense and skepticism into a methodical process.

The final step answers the question of how this material is likely to affect anything of interest, such as people, fish, or the ecological balance. Often, predicted concentrations are simply compared with water quality criteria adopted to protect the general aquatic community. Care must be taken to insure that the temporal and spatial scales assumed in developing the criteria are compatible with those predicted by the model. Sometimes principles of physical chemistry or pharmacokinetics are used to predict chemical body burdens and resulting biological effects. The bioaccumulation model FGETS (Barber, et al., 1991) and the WASTOX food chain model (Connolly and Thomann, 1985) are good examples of this.