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RMA

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HEC-5

Users Manual

SIMULATION OF FLOOD CONTROL AND CONSERVATION SYSTEMS

APPENDIX ON WATER QUALITY ANALYSIS

Prepared under the sponsorship of the

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Hydrologic Engineering Center of the Sacramento District,
Mobile District and the Kansas City District

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FOREWORD

The model described in this appendix was originally developed and has since been modified to expand the capability of the model HEC-5, "Simulation of Flood Control and Conservation Systems", to include water quality analysis. This appendix is a supplement to the HEC-5 User's Manual [HEC, 1997], and any references to HEC-5 within this document refer to the program for quantity regulation

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1 INTRODUCTION

1.1 ORIGIN OF PROGRAM

The flow simulation component of the HEC-5 model was developed at the Hydrologic Engineering Center (HEC) by Mr. Bill S. Eichert. The initial version was written for flood control operation of a single flood event and was released as HEC-5, "Reservoir System Operation for Flood Control," in May 1973. The flow simulation module was then expanded to include operation for conservation purposes and for period-of-record routings. This revised program was referred to as HEC-5C up to the February 1978 version. Further revisions to the flow simulation module were made and the revised program was referred to as the June 1979 version of HEC-5 [HEC, 1979].

In March 1979, the HEC contracted with Resource Management Associates, Inc. (RMA) to add to the HEC-5 program the capability of simulating temperature in a single reservoir (i.e., temperature simulation module or HEC-5Q).

In November 1979, the HEC contracted with Dr. James H. Duke, Jr. to add the capability to simulate conservative and non-conservative constituents, including dissolved oxygen, in a two-reservoir system and its associated downstream river reaches. These modifications were added to the temperature simulation module and the module was structured to interact with the HEC-5 program to change flow releases if such a change would improve water quality in the downstream reaches.

In February 1982, the HEC contracted with RMA and Dr. James H. Duke, Jr., to extend the November 1979 version of the model to ten reservoirs of an arbitrary tandem and parallel configuration and to perform additional options.

In October 1988, the HEC contracted with RMA and Mr. Carl Franke to jointly work on making the water quality version of HEC-5 compatible on personal computers.

The 1997 version of HEC-5Q, modified by RMA under contract to the Kansas City District, provides flexibility for application to systems consisting of multiple branches of streams flowing into or out of reservoirs which may be placed in tandem or in parallel configurations. The number of streams and reservoirs that can be modeled is subject to user-specified program dimensions and can be increased to meet project needs. The water quality simulation module, HEC-5Q, can be used to simulate concentrations of various combinations of the following water quality constituents:

- Temperature
- Dissolved oxygen
- Nitrate (NO_3) - Nitrogen
- Phosphate (PO_4) - Phosphorus
- Ammonia (NH_3) - Nitrogen
- Phytoplankton

- C-BOD
- Benthic oxygen demand
- Benthic source for nitrogen
- Benthic source for phosphorus
- Chloride
- Alkalinity
- pH
- Coliform bacteria
- 3 user-specified conservative constituents
- 3 user-specified non-conservative constituents
- Water column and sediment dissolved organic chemicals
- Water column and sediment heavy metals
- Water column and sediment dioxins and furans
- Organic and inorganic particulate matter
- Sulfur
- Iron and Manganese

This document describes the modifications made in the 1997 version of HEC-5Q, updated from the version described in HEC (1986a).

1.2 PURPOSE OF PROGRAM

The flow simulation module was developed to assist in planning studies for evaluating proposed reservoirs in a system and to assist in sizing the flood control and conservation storage requirements for each project recommended for the system. The program can also be useful for selecting proper reservoir operational releases for hydropower, water supply, and flood control.

The water quality simulation module, HEC-5Q, was developed so that temperature and selected conservative and non-conservative constituents, including dissolved oxygen, could be readily included as a consideration in system planning and management. Using estimates of system flows generated by the flow simulation module, the water quality simulation module computes the distribution of temperature and other constituents in the reservoirs and in the associated downstream reaches. For those constituents modeled, the water quality module can be used in conjunction with the flow simulation module to determine concentrations resulting from operation of the reservoir system for flow and storage considerations, or alternately, flow rates necessary to meet water quality objectives.

HEC-5Q can be used to evaluate options for coordinating reservoir releases among projects to examine the effects on flow and water quality at a specified location in the system. Examples of applications of the flow simulation model include examination of reservoir capacities for flood control and hydropower and reservoir release requirements to meet water supply and irrigation diversions. The model may be used in applications including evaluation of instream temperatures and constituent concentrations at critical locations in the system or examination of the potential effects of changing reservoir operations on temperature or water quality constituent concentrations.

Reservoirs equipped with selective withdrawal structures may be simulated to determine operations necessary to meet water quality objectives downstream. With these capabilities, the planner may evaluate the effects on water quality of proposed reservoir-stream system modifications and determine how a reservoir intake structure should be operated to achieve desired water quality objectives within the system.

1.3 HARDWARE AND SOFTWARE REQUIREMENTS

Pentium-based (or higher) personal computer recommended

32 MB RAM or higher recommended

The amount of hard disk space required for all program files, together with input and output files will vary depending on the length of the simulation and size of the system.

2 WATER QUALITY SIMULATION MODULE

2.1 GENERAL CAPABILITIES AND LIMITATIONS

The simulation model HEC-5, is currently limited to a system of up to forty reservoirs which may be in either tandem or parallel configuration, and eighty control points, although the model dimensions may be increased to meet user needs. The following guidelines must be followed when specifying a system:

1. The most upstream point, or points, of any system must be defined by reservoirs.
2. The most downstream point in the system must be defined by a stream control point.

The water quality simulation module, HEC-5Q, may use a subset of the HEC-5 simulation, a capability particularly useful for evaluating water quality in a small section of a large system without modifying the HEC-5 simulation, thus saving computation time. The following restrictions apply in addition to the two specified above:

1. All inflows into the subsystem must be included.
2. In a branched system, the sub-system boundary may be defined such that the tributary arm is represented only by its downstream-most reach, which flows into the main arm. The stream flow to the tributary arm is treated as the local flow to the main stem and the inflow quality is defined by the inflow quality data.

2.1.1 COMPUTATIONAL TIME STEPS

Typically, system hydraulics may be modeled on a daily time step, particularly if simulations of more than one year are required. If flows are available in increments of less than one day, simulations may be performed for smaller time steps, and then averaged to obtain an estimate of the daily flow rate. Water quality may also be modeled on a daily time step, but use of smaller time steps, e.g., four time steps of 6 hours each, are generally preferable for capturing diurnal variations in temperature and other heat- or light-dependent constituents such as phytoplankton. Previously, the length of simulations may have been limited due to limitations in computing capabilities, but advances in computing time and storage capacity make it possible to perform longer simulations while using shorter time steps.

The length of computational time steps used in the water quality simulation does not need to be equal to the time steps used in the flow simulation, but must be compatible with time steps used in the flow simulation, i.e., some whole number multiple or divisor. Additionally, the water quality computational time steps do not need to be the same throughout the day. For example, over a 24-hour simulation period, if 6-hour time steps are used in flow computation, the water quality simulation may use four increments of 6 hours each, two increments of 12 hours each, or a combination of the two, such as 6, 12, and 6-hour time steps. However, use of 8 hour time steps for the water quality simulation would not be acceptable, as it would not be a whole number multiple of the 6-hour increments used for flow computation. The model has typically been applied to systems using daily time steps for flow computation and 6-hour time steps for water quality to capture and quantify effects of diurnal variations in temperature and other constituents.

2.1.2 CURRENT MODEL DIMENSIONS

Current model dimension limitations and restrictions on reservoirs are shown in Table 1, but depending on system requirements, may be increased for the parameters listed. The dimensions are written to and may be checked in the output file, H5Q.LOG, created when running HEC-5Q.

Table 1 Current model limitations

Description	Dimension	Variable
Maximum number of reservoirs	20	MRS
Maximum number of reservoir elements[1]	660	MRE
Maximum number of segments in a branched longitudinally segmented reservoir	80	MBRE
Maximum number of layers in a layered longitudinally segmented reservoir	10	MXLAY
Maximum number of stream elements	300	MSE
Maximum number of meteorological data zones	10	MTZ
Maximum number of tributary quality types[2]	50	MNT
Maximum number of inflow locations (tributaries) per river reach	13	MST
Maximum number of channel cross-sections per reach	51	MSX
Maximum number of control points	80	

[1] The number of vertically segmented reservoir elements or longitudinally segmented reservoir segments times the number of layers

[2] Includes diversion returns and inflows from upstream reaches

2.1.3 OPERATION MODES

There are two 'modes of operation' which determine the computation sequence to be used by the models. They are described as follows:

Specified operation mode: Reservoirs are operated based on pre-specified outlet operation. The computation sequence is as follows:

Step 1. Simulate reservoir water quality using pre-specified outlet operation or operate withdrawals to meet tailwater temperatures and / or water quality objectives.

Step 2. Simulate stream water quality using reservoir outlet quality calculated in Step 1.

Systemwide operation mode: Reservoirs are operated to meet system-wide water quality constraints. This mode requires that reservoirs be equipped with selective withdrawal capability. The user must specify water quality constraints at control points. The computation sequence is as follows:

Step 1. Compute reservoir release targets (using the stream algorithm) such that violations of control point water quality constraints are minimized.
Step 2. Operate reservoir selective withdrawal in an attempt to supply water quality computed in Step 1.
Step 3. Simulate reservoir quality using outlet operation computed in Step 2.
Step 4. Simulate stream quality using reservoir outlet quality computed in Step 3.

In systems which have no reservoirs equipped with selective withdrawal structures, releases are constrained by instream flow and water quality requirements and the ‘specified operation’ mode must be used. To use the specified operation mode, initial conditions and either steady state or time-varying flows are specified and resulting temperatures and water quality constituent concentrations are calculated.

Reservoirs not equipped with selective withdrawal capabilities have less flexibility in operation, but there may be possible alternatives for the sequence in which reservoirs are operated to achieve water quantity and quality objectives. Each alternative must be tested separately, and flow and water quality results compared among the different alternatives.

2.1.4 WATER QUALITY SIMULATION OPTIONS

Six options are available for water quality simulation using HEC-5Q and are specified using the QC Record in the HEC-5Q input file. (The QC Record is only required if constituents other than temperature are to be simulated). Parameters that may be simulated under each option are presented in Table 2. The options are described as follows:

Option 1: No simulation of nutrients or phytoplankton
Option 2: Nutrients and phytoplankton simulation - Reservoirs only
  Option 2 ignores phytoplankton kinetics in the stream sections. This capability was typically used when computation time was a consideration. Use of this option is not recommended.
Option 3: Nutrients and phytoplankton simulation - Reservoirs and streams
Option 4: Enhanced water quality model with phytoplankton simulation
Option 5: Enhanced water quality model without phytoplankton simulation
  Option 5 is designed for simulation of contaminants when organic and / or inorganic particulates provide the predominant adsorption potential.

Option 6: Enhanced water quality model with simulation of iron, manganese, and sulfur instead of organic chemicals and dioxin. CBOD is replaced with labile and refractory dissolved organic matter.

Table 2 Variables simulated using different HEC-5Q water quality simulation options
(The numbers listed represent the water quality parameter number)

	Water Quality Simulation Option					
	Option 1	Option 2	Option 3	Option 4	Option 5	Option 6
IPHYTO	1	2	3	4	5	6
Temperature	✓	✓	✓	✓	✓	✓
Total Dissolved Solids		✓**	✓**	✓	✓	✓
NO_3 - Nitrogen		✓	✓	✓		✓
PO_4 - Phosphorus		✓	✓	✓		✓
Phytoplankton		✓	✓	✓		✓
Dissolved Organic Matter		✓	✓	✓		✓
NH_4 - Nitrogen		✓	✓	✓		✓
Dissolved Oxygen	✓	✓	✓	✓		✓
First conservative parameter	✓					
Second conservative parameter	✓					
Third conservative parameter	✓					
First non-conservative parameter	✓					
Second non-conservative parameter	✓[1]					
Third non-conservative parameter	✓[2]					
Chlorides				✓*	✓*	✓
Alkalinity - $CaCO_3$				✓*	✓*	✓
- pH & Total inorg. carbon				✓*	✓*	✓
Organic chemicals				✓*	✓*	
Heavy metals and/or radionuclides				✓*	✓*	
Dioxins and/or furans				✓*	✓*	
Organic and/or inorganic particulates				✓*	✓*	
Coliform bacteria				✓*	✓*	✓*
Iron, manganese and sulfur						✓*

* Optional variables that can be simulated in options 4, 5, and 6

**Optional TDS for options 2 and 3

[1] Carbonaceous BOD if dissolved oxygen is simulated (Option 1)

[2] Nitrogenous BOD or other oxygen consuming material if dissolved oxygen is simulated (Option 1)

2.2 RESERVOIR WATER QUALITY SIMULATION

For water quality simulations, each reservoir can be geometrically discretized and represented as a vertically segmented, longitudinally segmented, or a vertically layered and longitudinally segmented water body. Each stream is represented conceptually as a linear network of segments or volume elements.

2.2.1 VERTICALLY SEGMENTED RESERVOIRS

Vertically stratified reservoirs are represented conceptually by a series of one-dimensional horizontal slices or layered volume elements, each characterized by an area, thickness and volume, as shown in **Error! Reference source not found.**. In the aggregate the assemblage of layered volume elements is a geometrically discretized representation of the prototype reservoir.

This one-dimensional representation of reservoirs with depth has been shown to adequately represent water quality conditions in many deep, strongly stratified reservoirs [Baca, 1977; HEC, 1986b, 1987, 1994, 1996; US Army, 1977; Willey, 1987; WRE, 1968, 1969a, 1969b].

Within each horizontal layer (or 'element') in a vertically segmented reservoir, the water is assumed to be fully mixed with all isopleths parallel to the water surface both laterally and longitudinally. External inflows and withdrawals occur as sources or sinks within each element and are instantaneously dispersed and homogeneously mixed throughout the layer from the headwaters of the impoundment to the dam. Consequently, simulation results are most representative of conditions in the main reservoir body and may not accurately describe flow or quality characteristics in shallow regions or near reservoir banks. It is not possible to model longitudinal variations in water quality constituents using the vertically segmented configuration.

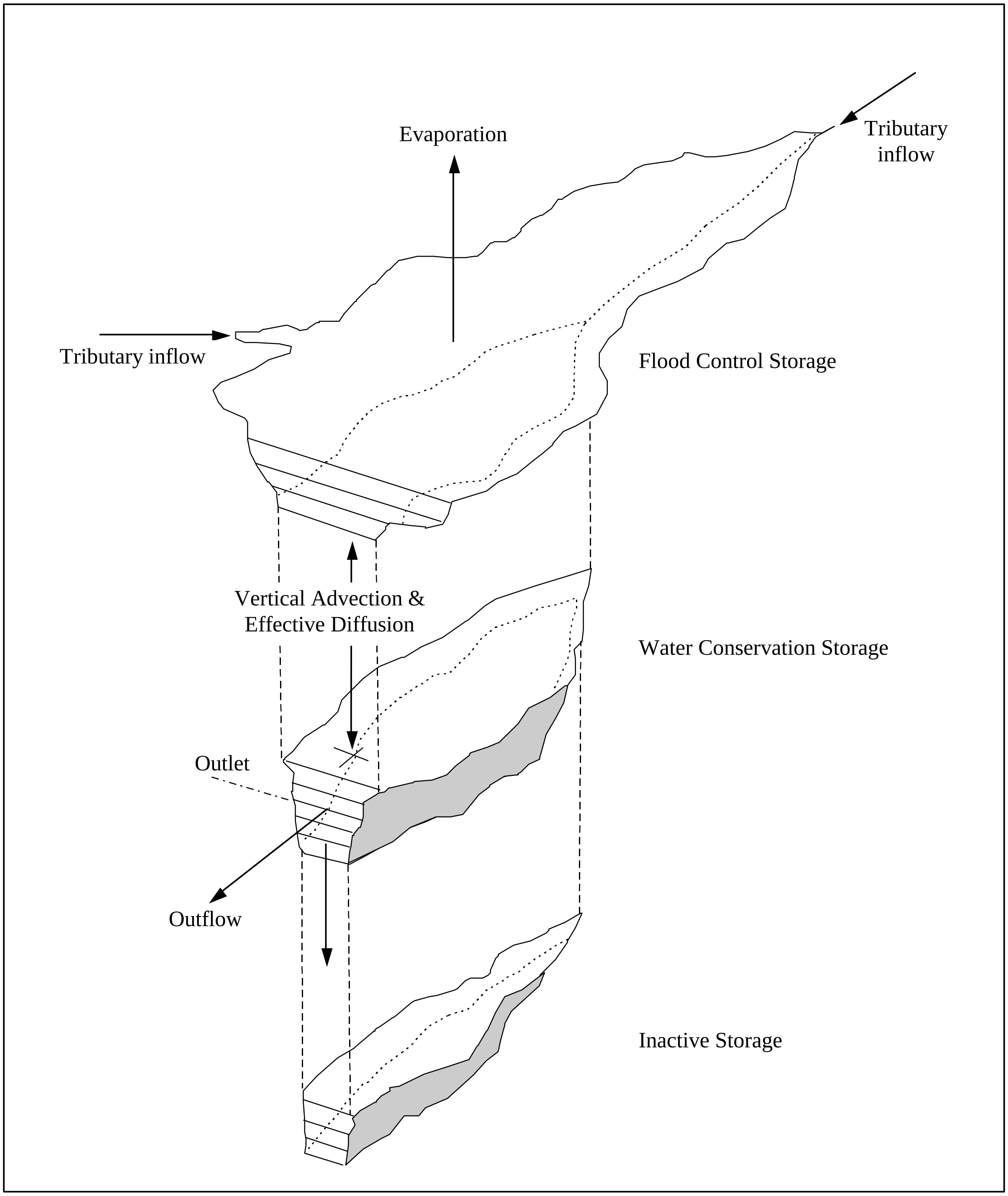

Figure 1. Schematic representation of a vertically segmented reservoir

2.2.2 VERTICAL ADVECTION

Vertical advection is one of two transport mechanisms used in the module to transport water quality constituents between elements in a vertically segmented reservoir. It is defined as the interelement flow that results in flow continuity and is calculated as the algebraic sum of inflows to and outflows from each layer beginning with the lowest layer in the reservoir. Any flow imbalance is accounted for by vertical advection into or out of the layer above, a process that is repeated for all layers in the reservoir. At the surface layer, any resulting flow imbalance is accounted for by an increase or decrease in reservoir volume.

Vertical advection is governed by the location of inflow to, and outflow from, the reservoir. Thus the computation of the zones of distribution and withdrawal for inflows and outflows are important in operation of the model. To determine the vertical regions affected by the distribution of inflows and withdrawals, the WES withdrawal allocation method [Bohan, 1973] is used for determining the allocation of outflow and the Debler inflow allocation method [Debler, 1959] is used for the placement of inflows. These methods are described in the following sections.

2.2.3 WES WITHDRAWAL ALLOCATION METHOD

The outflow component of the model incorporates the selective withdrawal techniques developed by Bohan [1973]. Laboratory investigations were conducted to determine the withdrawal zone characteristics created in a randomly density-stratified impoundment by releasing flow through a submerged orifice. From these investigations generalized relationships were developed for describing the vertical limits of the withdrawal zone and the vertical velocity distribution within the zone.

A definition sketch of variables for orifice flow is shown in **Error! Reference source not found.**. The following transcendental equation defines the zero velocity limits of the withdrawal zone.

$$V_o = \frac{Z^2}{A_o} \sqrt{\left(\frac{\Delta\rho'}{\rho_o}\right) g\, Z} \tag{1}$$

where: V_o = average velocity through the orifice in m/sec

Z = vertical distance from the elevation of the orifice center line to the upper or lower limit of the zone of withdrawal in meters

A_o = area of the orifice opening in m^2

$\Delta\rho'$ = density of fluid[1] between the elevations of the orifice center line and the upper or lower limit of the zone of withdrawal in kg/m^3

ρ_0 = fluid density of the elevation of the orifice center line in kg/m^3

g = acceleration due to gravity in m/sec^2

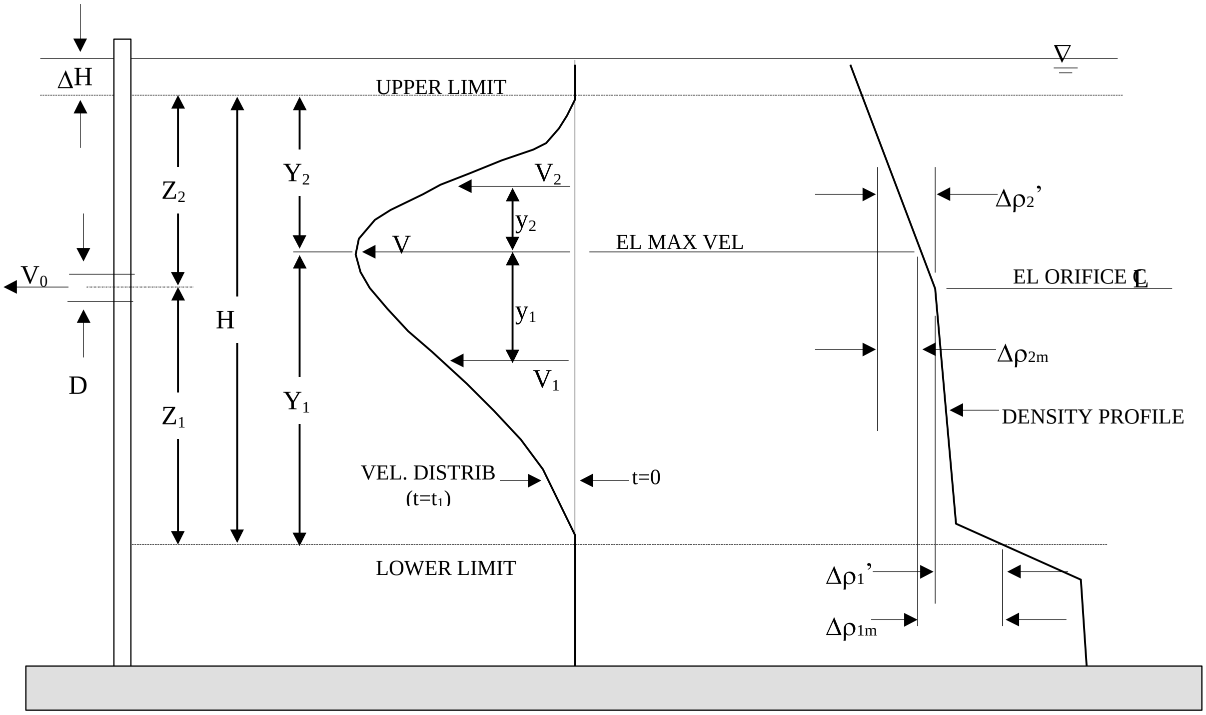

Figure 2. Definition sketch of variables for the WES Withdrawal Allocation Method

With knowledge of the withdrawal limits, the velocity profile due to outflow can be determined. First, the location of the maximum velocity is determined by:

$$\frac{Y_1}{H} = \left[\sin\left(1.57\frac{Z_1}{H}\right)\right]^2 \tag{2}$$

where: Y_1 = vertical distance from the elevation of the maximum velocity, V, to the lower limit of the zone of withdrawal in meters

H = thickness of the withdrawal zone in meters

Z_1 = vertical distance from the elevation of the orifice center line to the lower limit of the zone of withdrawal in meters

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[1] All water densities in the water quality simulation module are computed solely as a function of water temperature.

The distribution of velocities within the withdrawal zone is then determined by:

$$\frac{v}{V} = \left(1 - \frac{y\Delta\rho}{Y\Delta\,\rho_m}\right)^2 \tag{3}$$

where: v = local normalized velocity in the zone of withdrawal at a distance y from the elevation of the maximum velocity V
V = maximum velocity in the zone of withdrawal in m/sec
y = vertical distance from the elevation of the maximum velocity V to that of the corresponding local velocity v in meters
Y = vertical distance from the elevation of the maximum velocity V to the limit of the zone of withdrawal in meters
$\Delta\rho$ = density difference of fluid between the elevation of the maximum velocity V and the corresponding local velocity V in kg/m^3
$\Delta\rho_m$ = density difference of fluid between the elevation of the maximum velocity V and the limit of the zone of withdrawal in kg/m^3

This equation can be used to describe both the upper and lower sections of a velocity distribution using the elevation of the maximum velocity V as the reference elevation, except for conditions in which the withdrawal zone is limited by either the free surface or the bottom boundary. For conditions where the free surface and bottom boundary limit the withdrawal zone, the velocity distribution is computed by:

$$\frac{v}{V} = 1 - \left(\frac{y\Delta\rho}{Y\Delta\,\rho_m}\right)^2 \tag{4}$$

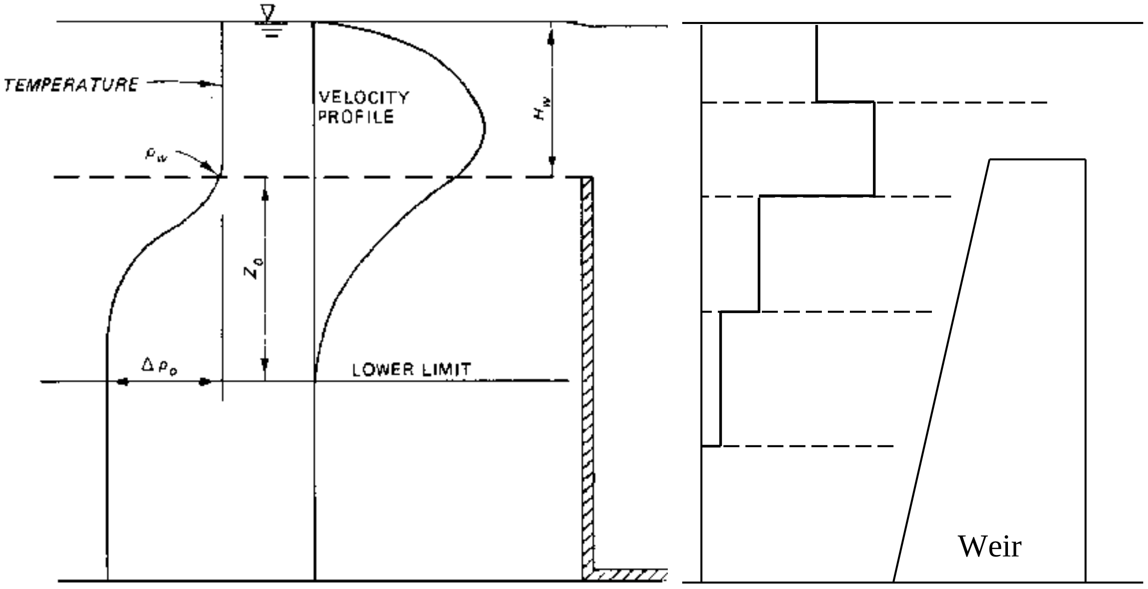
For a situation in which only one limit (upper or lower) is affected by a boundary (free surface or bottom boundary), Equation 3 can be used to determine the velocity distribution from the elevation of maximum velocity V to the limit unaffected by a boundary, and Equation 4 can be used to determine the velocity distribution from the elevation of maximum velocity V to the limit affected by a boundary. The flow from each layer is then the product of the velocity in the layer, the width of the layer and the thickness of the layer. A flow-weighted average is applied to water quality profiles to determine the value of the release content of each constituent for each time step.

<u>Submerged weir</u>: For flow over a submerged weir located upstream of a dam, the velocity profile is calculated using a procedure to that described above, namely using a modification of Equation 4:

$$\frac{v}{V} = \left[1 - \left(\frac{y\Delta\rho}{Y\Delta\,\rho_m}\right)^p\right]^q \tag{5}$$

Below the point of maximum velocity: p=1, q=3
Above the point of maximum velocity: p=2, q=1

The velocity profile calculated with the weir withdrawal method is shown schematically in Figure 3a. In HEC-5Q, the approach velocity profile is approximated as the elemental average for each layer in the reservoir, as shown in Figure 3b.



a. WES

b. HEC-5Q for 5 reservoir

Figure 3. Sketch of approach velocity profile calculated using WES weir withdrawal method and HEC-5Q

2.2.4 DEBLER INFLOW ALLOCATION METHOD

The allocation of inflows is based on the assumption that the inflow water will seek a level of neutral buoyancy within the lake, where the surrounding water is of like density. If the inflow water density is outside the range of densities found within the lake, the inflow is deposited at either the surface or the bottom depending on whether the inflow water density is less than the minimum or greater than the maximum water density found within the lake.

Once the entry level is established, the inflow water is allocated to the individual elements by one of two methods. If the inflow enters a zone of convective mixing, the inflow is distributed uniformly throughout the mixed zone. If the inflow enters a stratified region of the lake, the inflow is distributed uniformly within a flow field, the thickness of which is determined by Debler's criteria [1959].

a. WES

The thickness of the flow field is determined by:

$$D = 2.88 \left(\frac{Q}{W} \text{ x } \frac{\rho}{g\beta} \right)^{1/2} \qquad (6)$$

where: D = thickness of the flow field in meters
Q = inflow rate in m^3/sec
W = effective width[2] of reservoir at the inflow level in meters
β = density gradient at the withdrawal location in kg/m^4
g = acceleration due to gravity in m/sec^2
ρ = water density at the outlet location in kg/m^3

Once the thickness of the flow field is established, the water is deposited to the elements about the entry level assuming a uniform velocity distribution.

2.2.5 EFFECTIVE DIFFUSION

An additional mechanism used to distribute water quality constituents between elements is effective diffusion, representing the combined effects of molecular and turbulent diffusion, and convective mixing or the physical movement of water due to density instability. Wind and flow-induced turbulent diffusion and convective mixing are the dominant components of effective diffusion in the epilimnion of most reservoirs. In quiescent, well-stratified reservoirs, molecular diffusion may be an important transport mechanism in the metalimnion and hypolimnion.

For weakly stratified reservoirs where wind-induced, or wind and flow-induced turbulent diffusion are the dominant diffusion mechanisms, use of the wind method is more appropriate. For deep, strongly-stratified reservoirs with significant inflows to or withdrawals from the hypolimnion, flow-induced turbulence is the dominant diffusion mechanism in the hypolimnion. The stability method is more appropriate for this type of reservoir. The stability method may also be appropriate for shallower reservoirs where factors other than wind, such as inflows, drive turbulent mixing. The two methods for calculating effective diffusion are described as follows:

1. **Stability Method** - The stability method of computing the effective diffusion coefficients is appropriate for most deep, well-stratified reservoirs and shallower reservoirs where wind mixing is not the dominant turbulent mixing force. This method is based on the assumption that mixing will be at a minimum when the density gradient or water column stability is at a maximum.

The relationship between stability and the effective diffusion is shown graphically in Figure 4. The range of effective diffusion coefficients reported by WRE [1969b] from

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[2] The effective width of the flow field is defined as the reservoir area at the entry level divided by the effective reservoir length at the inflow location.

data collected in reservoirs of the Pacific Northwest are represented in the figure. Effective diffusion coefficients for reservoirs in other regions may fall below the lower envelope of values shown. The relationship between effective diffusion and stability is shown below.

$$D_c = A_1 \qquad \text{when } E \le E_{crit} \tag{7}$$

$$D_c = A_2 E^{A_3} \qquad \text{when } E > E_{crit} \tag{8}$$

where: D_c = effective diffusion coefficient in m^2/sec
A_1 = maximum effective diffusion coefficient in m^2/sec
$E = \frac{1}{\rho} \; \frac{\partial \rho}{\partial Z} 0$ = water column stability or normalized density gradient in m^{-1}
E_{crit} = water column critical stability in m^{-1}
A_2,A_3 = empirical constants

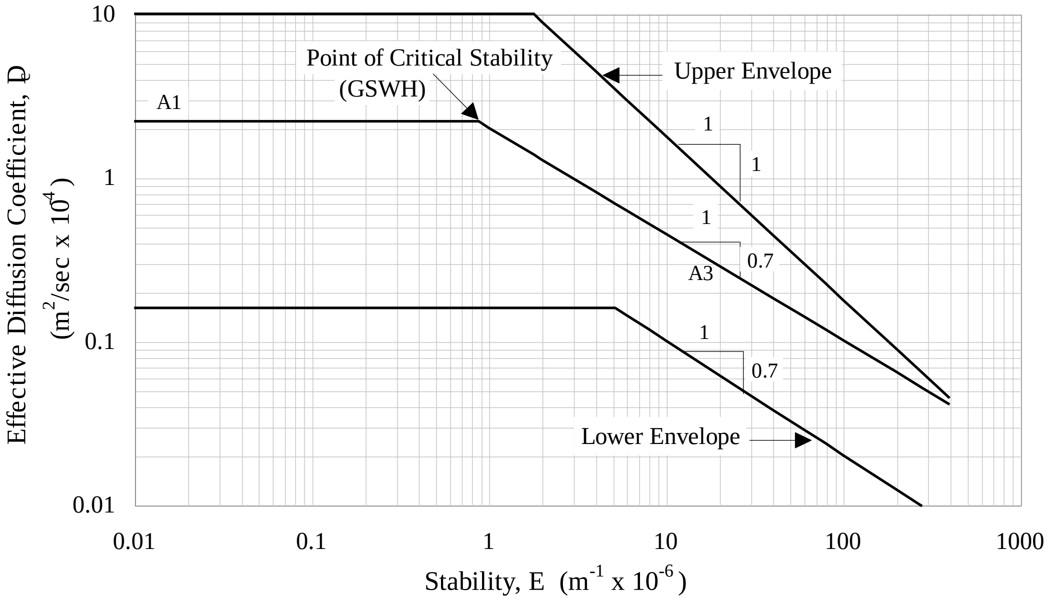

Figure 4. Log of effective diffusion vs. Log of density gradient

A typical density profile for a stratified reservoir and the resulting effective diffusion coefficient distribution are shown in Figure 5.

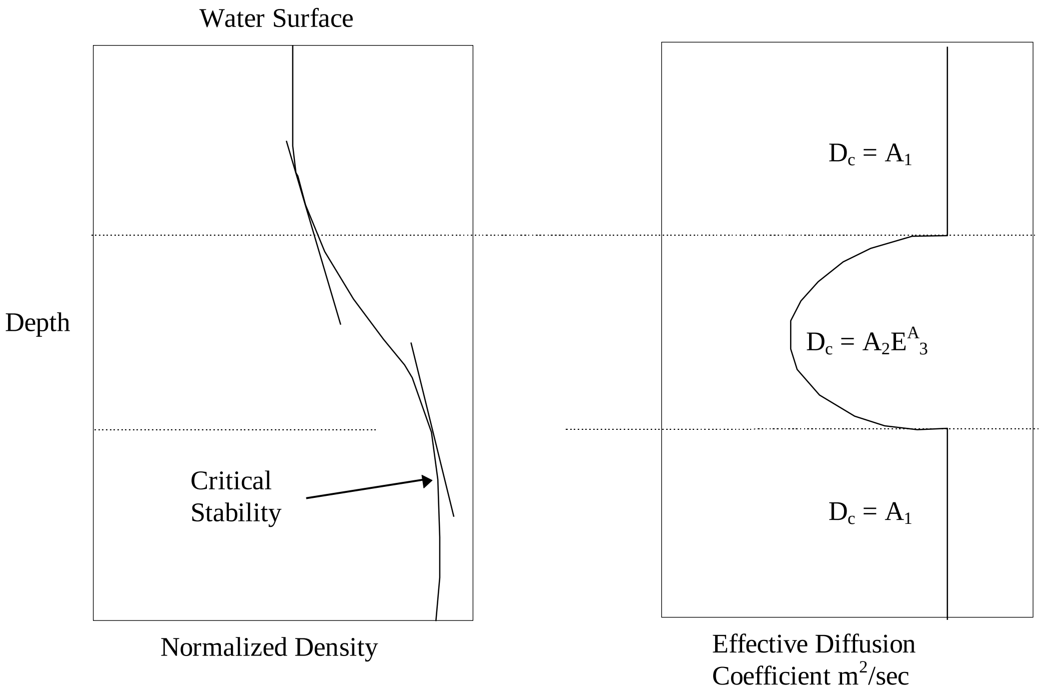

Figure 5. Stability Method - Effective diffusion coefficients vs. depth

2. **Wind Method** - The wind method for computing effective diffusion coefficients is appropriate for reservoirs in which wind mixing appears to be the dominant component of turbulent diffusion. This method assumes that wind-induced mixing is greater at the surface and diminishes exponentially with depth. The empirical expression used to calculate the effective diffusion coefficient is a combination of wind-induced diffusion and a minimum diffusion term representing the combined effects of all other mixing phenomena:

$$D_c = D_{min} + A_1 V_w e^{-kd} \tag{9}$$

where: D_{min} = minimum effective diffusion coefficient in m^2/sec
A_1 = empirical coefficient in meters
V_w = wind speed in m/sec
k = A_2/d_t
A_2 = empirical coefficient
d_t = depth of the thermocline in meters (d_t = 6m during unstratified conditions)
d = depth of specific layer in meters

Typical values reported by Baca [1977] for the minimum effective diffusion coefficient and the empirical coefficients required by Equation 10 are presented in Table 3. Within the model the actual diffusion coefficient, D_c, is constrained by a maximum D_{max}, usually approximately 5 x 10^{-4}. The variation in the diffusion coefficient calculated using the Wind method is shown in Figure 6 as a function of depth for two different cases.

Table 3 Wind Mixing Method: Effective diffusion and empirical coefficients

Coefficient	Well Mixed Reservoirs	Stratified Reservoirs
Minimum Effective Diffusion (D_{min})	$1x10^{-5}$ to $5x10^{-5}$	$1x10^{-6}$ to $1x10^{-7}$
Empirical (A_1)	$1x10^{-4}$ to $2x10^{-4}$	$1x10^{-5}$ to $5x10^{-5}$
Empirical (A_2)	4.6	4.6

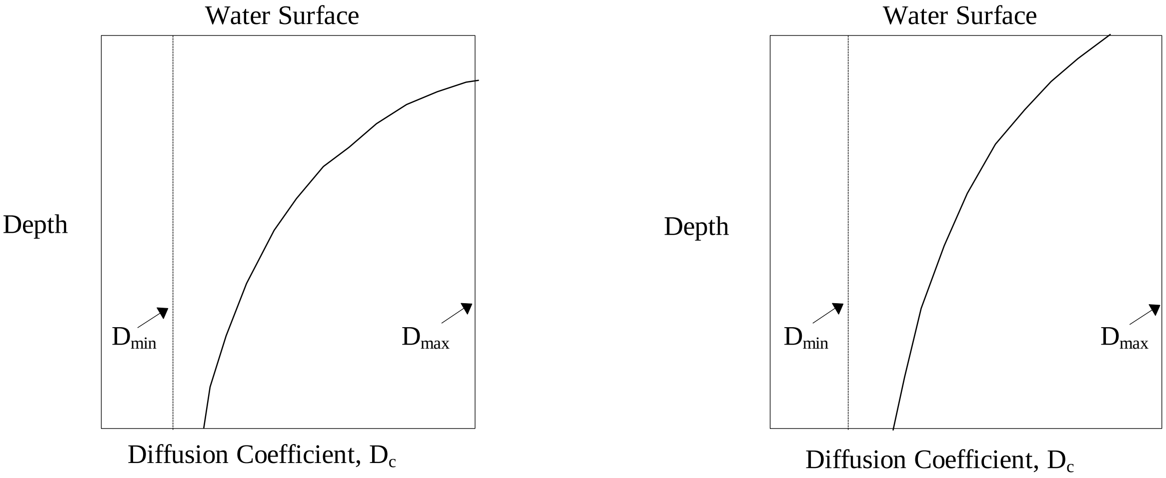

Figure 6. Wind method - Diffusion coefficient vs. depth

2.2.6 LONGITUDINALLY SEGMENTED RESERVOIRS

Longitudinal segmentation is appropriate for shallower, weakly stratified reservoirs where the flow velocity is relatively constant over depth and the major thermal or concentration gradients occur over the reservoir length.

Longitudinally segmented reservoirs are represented conceptually as a linear network of a specified number of segments or volume elements, shown schematically in Figure 7. Each reservoir segment is characterized by its length, area and volume or by its length and a relationship between width and elevation. Each longitudinally segmented reservoir is subdivided into elements in the direction of flow with each element assumed to be fully mixed in the vertical and lateral directions.

When reservoir geometry is defined using detailed cross-section information, the model performs a backwater computation to define the water surface profile as a function of the hydraulic gradient based on flow and Manning's equation. A backwater calculation is also performed with less detailed cross-sections if the bottom width is defined.

External flows such as withdrawals and tributary inflows occur as sinks or sources distributed uniformly over the depth of an element. This method of representing inflows is a limitation of the one-dimensional approximation. The uniform distribution approximation is appropriate for use with smaller tributaries, which do not significantly affect flow dynamics in the main stem but contribute flows that may be sufficiently large to affect water quantity and quality in the main channel. Because the flows are distributed uniformly, there is no mechanism for examining local temperature variations or mixing behavior. External flows may be allocated along the length of the reservoir to represent dispersed, or non-point, source inflows including agricultural drainage or groundwater accretions.

2.2.7 LAYERED AND LONGITUDINALLY SEGMENTED RESERVOIRS

A reservoir may be represented with layers and longitudinal segmentation when horizontal gradients exist in flow or quality in addition to vertical gradients in temperature or water quality constituent concentrations. For reservoirs represented as layered and longitudinally segmented, all cross-sections must contain the same number of layers and each layer must be assigned the same fraction of the reservoir cross-sectional area, as shown in Figure 8. For example, if three layers are specified for each segment and the top two layers are assigned one quarter of the cross-sectional area each and the bottom layer is assigned one-half, then every element within the reservoir will have 3 layers, with the top two layers comprising one quarter of the segment cross-sectional area each and the bottom comprising a half. Typically, the smaller fractions of the cross-sectional area, and therefore a greater level of detail, are assigned to layers where the largest vertical gradients are expected. Tributary inflows to layered and longitudinally segmented reservoirs are allocated in proportion to the fraction of the cross-section assigned to each layer.

Vertical variations in constituent concentrations can be computed for the layered and longitudinally segmented reservoir model. Mass transport between vertical layers is represented by diffusion. Spatially varying initial conditions may only be specified in the longitudinal direction; variations in the vertical direction are not allowed.

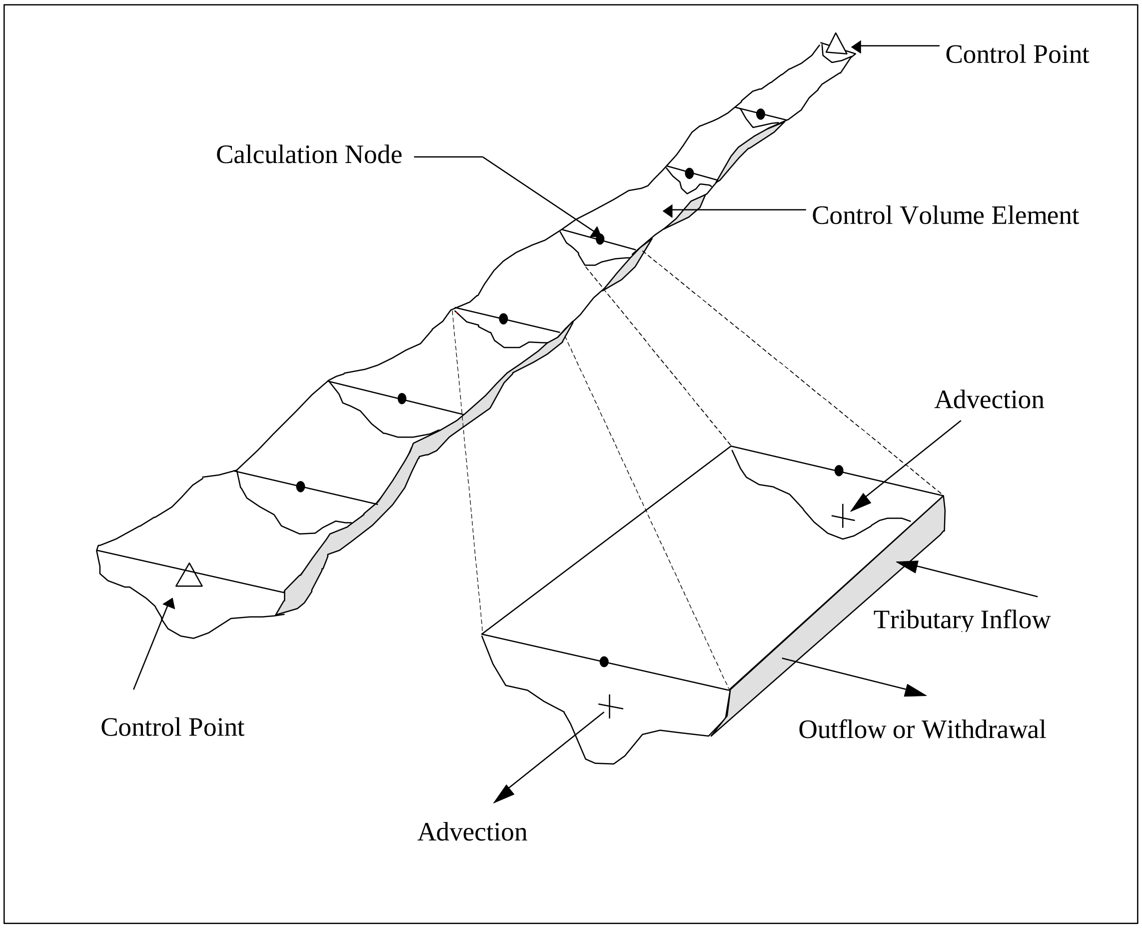

Figure 7. Schematic representation of a longitudinally segmented reservoir

Unless otherwise specified, the velocity within each layer of a layered and longitudinally segmented reservoir is assumed to be uniform over depth and parallel to the direction of flow. The uniform velocity assumption may not be appropriate for the following flow fields, potentially causing differences from observed values:

1. Shallow regions of a reservoir or near the reservoir bottom where effects of bottom roughness may be important.
2. Reservoirs with density currents resulting in vertical or cross-stream velocity components.
3. Reservoirs with outflow through a submerged orifice in the dam or a submerged weir upstream of the dam.

A non-uniform vertical velocity distribution may be specified at any location within the reservoir to incorporate the effects listed above. If a weir exists upstream of the dam or outflow is considered through a submerged orifice in the dam, the velocity distribution throughout the water column is calculated as a function of thermal stratification using the WES weir withdrawal or withdrawal allocation method, described in Section 2.2.3. HEC-5Q uses an elemental average of the approach velocity for each layer in the reservoir. Weirs may be specified within the reservoir to reflect natural constrictions or to attenuate the effects of dam withdrawals upstream. The specification of weirs and vertical velocity distribution may not achieve the desired effect under all hydraulic conditions and the user is cautioned to use these options with care. The HEC-5Q model is not intended for simulating complex two-dimensional effects on flow and water quality.

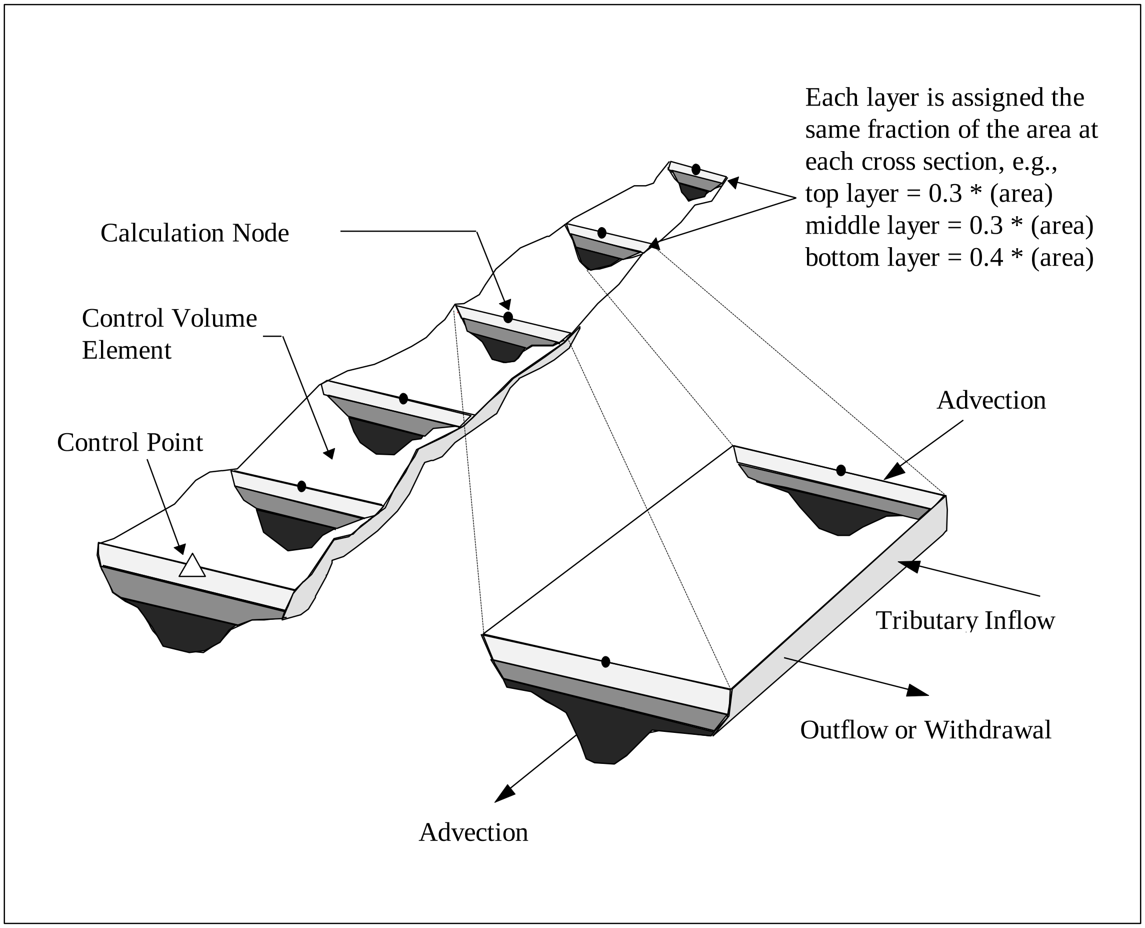

Figure 8. Schematic representation of a layered and longitudinally segmented reservoir

2.3 STREAM HYDRAULICS

A reach of a river or stream is represented conceptually as a linear network of volume elements. Within a stream, each element is characterized by its length, width, cross-sectional area, 2/3 power of the hydraulic radius, bottom roughness given in terms of Manning's n and an optional flow-depth relationship.

Flow rates at stream control points are calculated within the flow simulation module by using one of the hydrologic routing methods. Within the flow simulation module, incremental local flows (i.e., inflow between adjacent control points) are assumed to be deposited at the control point. Within the water quality simulation module, the incremental local flow may be divided into components and placed at different locations within the stream reach (i.e., that portion of the stream bounded by the two control points). A flow balance is used to determine the flow rate at element boundaries.

Net pipe diversions are specified to represent inflows or withdrawals that would not normally be a part of the channel flow. They may include any flows that result in variation from unimpaired flows, e.g., agricultural or wastewater return flows and withdrawals for drinking water supply. For simulation of water quality, the tributary locations and associated quality must be specified. To allocate components of the diversion flow balance, HEC-5Q performs a calculation using any specified withdrawals, inflows, or return flows and distributes the balance uniformly along the stream reach. Once interelement flows are established, the depth, surface width and cross-section area are computed at each element boundary (assuming normal flow).

2.4 WATER QUALITY ANALYSIS

2.4.1 THERMAL ANALYSIS

Streams and reservoirs are represented by an assemblage of fluid elements linked together by interelement flow and diffusion (stream diffusion is assumed near zero). The principle of conservation of heat (thermal energy) can be represented by the following differential equation model for the dynamics of temperature within each fluid element.

$$V \frac{\partial T}{\partial t} = \Delta z Q_z \frac{\partial T}{\partial z} + \Delta z A_z D_z \frac{\partial^2 T}{\partial z^2} + Q_i T_i - Q_o T \pm \frac{A_h H}{\rho c} - T \frac{\partial V}{\partial t} \qquad (10)$$

where: T = temperature in degrees Celsius
V = fluid element volume in m^3
t = time in seconds
z = space coordinate in meters (vertical for vertically segmented reservoirs, horizontal for streams and longitudinally segmented reservoirs)
Q_z = interelement flow in m^3/sec
A_z = element surface area normal to the direction of flow in m^2
D_z = effective diffusion coefficient in m^2/sec
Q_i = lateral inflow in m^3/sec
T_i = inflow water temperature in degrees Celsius
Q_o = lateral outflow in m^3/sec
A_h = element surface area in m^2
H = external heat sources and sinks in J/m^2/sec
ρ = water density in kg/m^3
c = specific heat of water in J/kg/°C

Equation 10 represents the dynamics of heat within a fluid element. By forming a set of equations for all elements within the system, the dynamics of heat within that system can be represented. Terms on the right side of Equation 10 represent physical heat transfers including external heat sources and sinks. The external heat sources and sinks that are considered in HEC-5Q are assumed to occur at the air-water interface. The rate of heat transfer per unit of surface area can be expressed as the sum of the following heat exchange components:

$$H_n = H_s - H_{sr} + H_a - H_{ar} \pm H_c - H_{br} - H_e \tag{11}$$

where: H_n = the net heat transfer
H_s = the short-wave solar radiation arriving at the water surface
H_{sr} = the reflected short-wave radiation
H_a = the long-wave atmospheric radiation
H_{ar} = the reflected long-wave radiation
H_c = the heat transfer due to conduction
H_{br} = the back radiation from the water surface
H_e = the heat loss due to evaporation

All units are in $J/m^2/sec$

Complete discussions of the individual terms have been presented by Anderson [1954] and by the Tennessee Valley Authority [1972].

The method used in the module to evaluate the net rate of heat transfer at the air-water interface has been developed by Edinger and Geyer [1965]. Their method utilizes the concepts of equilibrium temperature and coefficient of surface heat exchange, described by the equation:

$$H_n = K_e (T_e - T_s) \tag{12}$$

where: H_n = net rate of heat transfer in $J/m^2/sec$
K_e = coefficient of surface heat exchange in $J/m^2/sec/^\circ C$
T_e = equilibrium temperature in degrees Celsius
T_s = surface temperature in degrees Celsius

The equilibrium temperature is defined as the water temperature at which the net rate of heat exchange between the water surface and the overlying atmosphere is zero. The coefficient of surface heat exchange is the rate at which the heat transfer process proceeds. The Heat Exchange Programs that compute these terms are described in Exhibit 5 and reside in directory EQ_TEMP of the CD.

All heat transfer mechanisms, except short-wave solar radiation, are applied at the water surface. Short-wave radiation penetrates the water surface and may affect water temperatures several meters below the surface. The depth of penetration is a function of adsorption and scattering properties of the water [Hutchinson, 1957]. This phenomenon is unimportant in the calculation of heat in longitudinally segmented reservoirs and in streams since elements are assumed vertically mixed.

In the vertically segmented reservoirs, however, the short-wave solar radiation may penetrate several elements. The amount of heat that reaches each element is determined by:

$$I = (1 - \beta)\, I_o e^{-kz} \tag{13}$$

where: I = light energy at any depth in $J/m^2/sec$
β = fraction of the radiation absorbed in the top foot of depth
I_o = light energy at the water surface in $J/m^2/sec$
k = light extinction coefficient in l/meter
z = depth in meters

Combining Equations 12 and 13 for the reservoir surface element, the external heat source and sink term becomes:

$$H = K_e(T_e - T_s) - (1 - \beta)\, I_o e^{-k\Delta z} \tag{14}$$

and the external heat source for all remaining reservoir elements becomes:

$$I = I_z(1 - e^{-k\Delta z}) \tag{15}$$

where: I_z = the light intensity at the top of the element in $J/m^2/sec$

2.4.2 PHYSICAL AND CHEMICAL CONSTITUENTS

Water quality constituents other than temperature are represented by Equation 10 with minor modifications:

a. The definition of the variable T is generalized to represent the concentration of any water quality constituent.

b. The distributed heat gain/loss term $\frac{A_h H}{\rho c}$, which represents external sources and sinks, is:

1. Eliminated for conservative constituents

2. Replaced by a first order kinetic formulations representing decay, reaeration, growth, respiration, settling, volatilization, oxidation and reduction.

Constituents simulated under each water quality simulation option are listed in Table 2. For each constituent, the distributed heat gain/loss term in the advection -

dispersion equation is replaced by terms given in the following sections. The constituent relations are written in complete format to include all source and sink terms which may be simulated, but the terms that are not chosen for simulation will be omitted by the model during runs.

2.4.2.1 NUTRIENTS

Nutrients, including nitrogen, phosphorus and carbon dioxide can enter a system via inflow, decomposition of dissolved organic material (DOM) and detritus, phytoplankton dark respiration, and wind driven resuspension (reservoirs only). Aerobic and anaerobic exchange with sediments, and surface exchange such as denitrification and reaeration can act as either sources or sinks for nutrients. Outflow, transformation (for example NH_3 to NO_3), and phytoplankton photosynthesis can be nutrient sinks. Nutrient flux relationships are illustrated in Figure 9

2.4.2.1.1 AMMONIA NITROGEN

$$\ldots + V \cdot (\, KB \cdot PN \; \cdot P \cdot (PR \cdot FR1 + PM \cdot FM1 - PG \cdot FN) + SN \tag{16}$$

$$+\, OMN \cdot KOM \cdot DOM \; + SSN \cdot KSS \cdot OSS \,)$$

where: V = fluid element volume
KB = phytoplankton activity rate at ambient temperature
PN = nitrogen fraction of phytoplankton (PN=0.08)
P = phytoplankton concentration
PR = phytoplankton respiration rate
FR1 = fraction of respired phytoplankton converted directly to nutrients
PM = phytoplankton mortality rate
FM1 = fraction of expired phytoplankton converted directly to nutrients
PG = phytoplankton growth rate
FN = ammonia fraction of available nitrogen
SN = benthic source rate for ammonia nitrogen
DOM = labile and refractory dissolved organic material
OMN = nitrogen fraction of DOM
KOM = first order decay rate for DOM at ambient temperature
OSS = organic suspended solids
SSN = nitrogen fraction of organic OSS
KSS = first order decay rate for OSS at ambient temperature

Figure 9. Nutrient Fluxes.

NITRATE NITROGEN

$$\ldots + V \cdot (KNH_3 \cdot NH_3 - KB \cdot PN \cdot P \cdot PG \cdot (1\text{-}FN) - KNO_3 \cdot NO_3) \qquad (17)$$

where: V = fluid element volume
KNH_3 = ammonia decay rate adjusted to ambient temperature
NH_3 = ammonia concentration
KB = phytoplankton activity rate at ambient temperature
PN = nitrogen fraction of phytoplankton (PN=0.08)
P = phytoplankton concentration
PG = phytoplankton growth rate
FN = ammonia fraction of available nitrogen
KNO_3 = nitrate decay rate
NO_3 = nitrate concentration

2.4.2.1.1 PHOSPHATE PHOSPHOROUS

$$\ldots + V \cdot (KB \cdot PP \cdot P \cdot (PR \cdot FR1 + PM \cdot FM1 - PG) + SP + FP \cdot PO4 \cdot [SS]_i \qquad (18)$$

$$+ OMP \cdot KOM \cdot DOM + SSP \cdot KSS \cdot OSS)$$

where: V = fluid element volume
KB = phytoplankton activity rate at ambient temperature
PP = phosphorus fraction of phytoplankton (PP=0.012)
P = phytoplankton concentration
PR = phytoplankton respiration rate
$FR1$ = fraction of respired phytoplankton converted directly to nutrients
PM = phytoplankton mortality rate
$FM1$ = fraction of expired phytoplankton converted directly to nutrients
PG = phytoplankton growth rate
SP = benthic source rate for phosphorus
FP = fraction of phosphorus partitioned into suspended solids
$PO4$ = phosphorus concentration
$[SS]_i$ = concentration of i^{th} organic or inorganic particulate
DOM = labile and refractory dissolved organic material
OMP = phosphorus fraction of DOM
KOM = first order decay rate for DOM at ambient temperature
OSS = organic suspended solids
SSP = phosphorus fraction of organic OSS
KSS = first order decay rate for OSS at ambient temperature

2.4.2.2 PHYTOPLANKTON

Phytoplankton can enter a system via inflow or diffusion from other layers. It can leave a system via outflow, diffusion to other layers, settling, or mortality. Photosynthesis acts as a phytoplankton source that is dependent on inorganic carbon, phosphate, ammonia, and nitrate. Photosynthesis is therefore a sink for these nutrients. Conversely, phytoplankton respiration produces inorganic carbon, phosphate, and ammonia. Phytoplankton is an oxygen source during photosynthesis and an oxygen sink during respiration. Mortality contributes to detritus and photorespiration contributes to DOM. The phytoplankton fluxes are illustrated in Figure 10.

$$\ldots + V \cdot KB \cdot P \cdot (PG - PR - PM) - \frac{\partial}{\partial z}(P\, A_s) \cdot PS - V \cdot PF \cdot P \tag{19}$$

where: V = fluid element volume
KB = phytoplankton activity rate at ambient temperature
P = phytoplankton concentration
PG = phytoplankton growth rate

$$= P_{max} \left| \frac{C}{C_2 + C} \right|_{min} \tag{20}$$

P_{max} = maximum phytoplankton growth rate
C = nutrient concentration or light intensity
C_2 = half saturation constant for phytoplankton utilizing nutrients or light
PR = phytoplankton respiration rate
PM = phytoplankton mortality rate
A_s = element surface area (top or bottom of element) through which phytoplankton settles
PS = phytoplankton settling rate
PF = fraction of phytoplankton which increments the labile DOM compartment
(as a result of mortality, decay)

Figure 10. Phytoplankton Fluxes

In addition, the following are included in simulation of phytoplankton:

1. The light intensity is associated with the three types of organic or inorganic particulate matter and phytoplankton self-shading. The light extinction coefficient for each type of particulate matter is supplied by the user.
2. The total nitrogen, total phosphorous and carbon dioxide concentrations are computed. The limiting factor (nutrient or light) is used to adjust the growth rate using a Michaelis-Menten formulation as given by Equation 19.
3. Respiration and mortality rates are supplied by the user, and are adjusted to the ambient temperature.

2.4.2.3 DISSOLVED OXYGEN

Oxygen sources can be inflow, diffusion from adjacent elements, surface exchange, or phytoplankton photosynthesis. Possible sinks for oxygen are outflow, diffusion to adjacent elements, surface exchange, phytoplankton respiration, decomposition of detritus, labile DOM (or BOD), refractory DOM and sediment, and oxidation of sulfide, reduced iron, reduced manganese and ammonia nitrogen. Dissolved oxygen flux relationships are illustrated in Figure 11.

$$
\begin{aligned}
&...+ A_s \cdot K_2 \cdot (DO^* - DO) - V \cdot KL \cdot L \qquad (21)\\
&- V \cdot KB \cdot P \cdot (PR \cdot O2R + PM \cdot O2R - PG \cdot O2G) - K_1 \cdot\cdot K_3 \cdot V \cdot SS \cdot T_c^{(T-20)}\\
&- K_{C1} \cdot K_{C3} \cdot V \cdot CBOD \cdot T_c^{(T-20)} - K_{N1} \cdot K_{N3} \cdot V \cdot NH_3 \cdot T_c^{(T-20)}\\
&- V \cdot KNH_3 \cdot NH_3 \cdot O2N - SO - V \cdot KS_2 \cdot S_2 \cdot O2S - V \cdot KFE \cdot FE \cdot O2FE\\
&- V \cdot KMN \cdot MN \cdot O2MN - V \cdot KDOM \cdot DOM \cdot O2DOM\\
&- V \cdot KRFR \cdot RFR \cdot O2RFR
\end{aligned}
$$

where: A_s = element surface area
K_2 = reaeration rate (calculated using Equations 22 and 23)
DO^* = dissolved oxygen saturation concentration at the ambient temperature
DO = existing dissolved oxygen concentration
V = fluid element volume
KL = BOD decay rate at ambient temperature
L = BOD concentration
KB = phytoplankton activity rate at ambient temperature
P = phytoplankton concentration
PR = phytoplankton respiration rate

O2R = ratio between oxygen consumed and phytoplankton respiration and decay (O2R = 1.6)

PM = phytoplankton mortality rate

PG = phytoplankton growth rate

O2G = ratio between oxygen produced and phytoplankton growth (O2G = 1.6)

K_1 = decay coefficient for organic particulates

K_3 = coefficient to convert from mass of decayed organic particulate to ultimate oxygen demand

SS = organic particulate concentration (A term of this form is included for each organic particulate simulated)

T_c = thermal correction factor for decay of organic particulate

T = temperature in degrees Celsius

K_{C1} = first order decay coefficient for carbonaceous oxygen demand

K_{C3} = coefficient to convert from mass of decayed [5-day CBOD] to ultimate oxygen demand

CBOD = carbonaceous oxygen demand concentration

K_{N1} = first order decay coefficient for [NH_3-N]

K_{N3} = coefficient to convert from decayed [NH_3-N] to ultimate oxygen demand

NH_3 = ammonia concentration

KNH_3 = ammonia decay rate adjusted to ambient temperature

O2N = ratio between oxygen consumed and ammonia decay (O2N = 4.6)

SO = benthic uptake rate

KS_2 = sulfur decay rate

S_2 = sulfur concentration

O2S = amount of oxygen required to form oxidized sulfur species

KFE,KMN = iron, manganese decay rate

FE, MN = iron, manganese concentration

O2FE, O2MN = amount of oxygen required to form oxidized iron, manganese species

KDOM,KRFR = labile, refractory dissolved organic matter decay rate

DOM, RFR = labile, refractory dissolved organic matter concentration

O2DOM, O2RFR = amount of oxygen required for decomposition of labile and refractory DOM

Figure 11. Dissolved oxygen fluxes

(Note: Option 1 provides a simplified method for simulating DO concentration, based only on terms representing reaeration, carbonaceous and nitrogenous BOD decay, and benthic uptake. The user is cautioned that this simplistic method may not be applicable to many systems and that use of the other simulation options (2 through 6) may be more appropriate. Cases where Option 1 may apply include simple systems with discharge to a stream or a reservoir system where different operation scenarios are investigated. It does not apply to a system receiving inflows of different quality or where nutrient effects on DO concentrations become important. In such cases, use of other simulation Options (2-6) is recommended.)

Reaeration

The reservoir reaeration rate is computed as follows:

$$K_2 = \frac{(a + bW^2)}{\Delta z} \tag{22}$$

where: K_2 = reaeration rate in 1/day at 20°C
a,b = empirical coefficients derived by curve fit from Kanwisher [1963] to be 0.64 and 0.032, respectively.
W = wind speed in meters per second
Δz = surface element thickness in meters

The stream reaeration rate is computed using the O'Conner-Dobbins [1958] method:

$$K_2 = \frac{\left(D_m U\right)^{0.5}}{D^{1.5}} \tag{23}$$

where: K_2 = reaeration rate in 1/day at 20°C
D_m = molecular diffusion coefficient in m^2/day
U = flow velocity in m/s
D = average stream depth in meters

The rates at which chemical and biological processes take place are normally a function of temperature. To account for this temperature dependence, all first order kinetic rates are adjusted for local ambient temperatures using a multiplicative correction factor:

$$\theta = T_c^{(T-20)} \tag{24}$$

where: θ = reaeration rate multiplicative correction factor
T_c = empirically determined temperature correction factor
T = local ambient water temperature in °C

Computation of the reaeration rate for dissolved oxygen and the first order rate adjustment for the ambient temperature is the same when phytoplankton is not simulated, except for the term representing an adjustment for phytoplankton growth and respiration. The ambient temperature adjustment factor for phytoplankton growth utilizes the temperature limit approach, which assumes that the rate at which a reaction takes place is a function of two exponential expressions similar to those depicted in Figure 12. The temperature tolerances define the functions used to modify the growth and respiration rates. The temperatures T1 and T4 are the lower and upper tolerance limits for growth, respectively. T2 and T3 define the optimum range at which the growth is a maximum. The upper range of the optimum temperature T3 and the upper tolerance limit T4 for phytoplankton respiration and mortality processes are assumed outside the range of normal prototype temperatures.

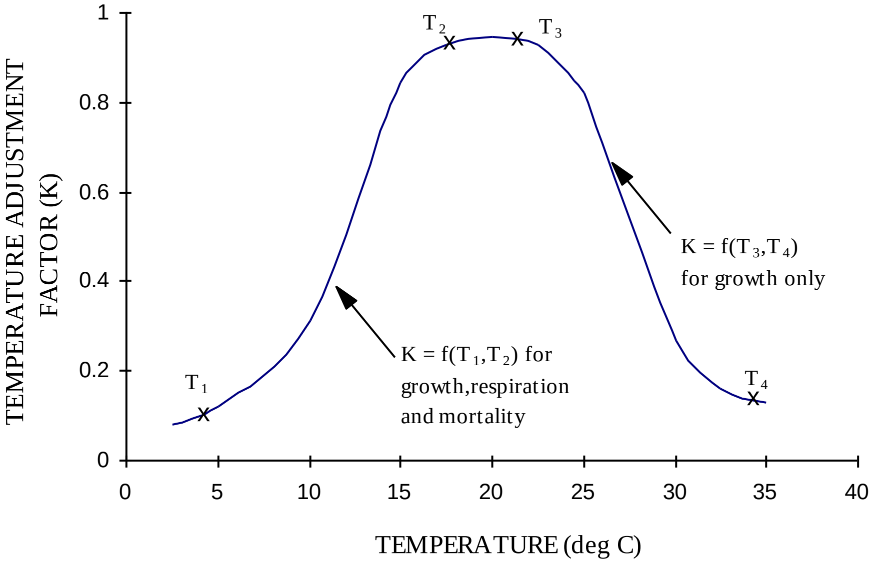

Figure 12. Rate coefficient temperature adjustment function

2.4.2.4 pH AND CO_2...

These constituents are computed according to equilibrium theory considering $CaCO_3$, CO_2, OH^- and H^+, where TIC = $[CO_2\text{-}C] + [CO_3\text{-}C]$

2.4.2.5 TOTAL INORGANIC CARBON (TIC)

$$\ldots + A_s \cdot K_2 \cdot ([CO_2\text{-}C]^* - [CO_2\text{-}C]) + V \cdot (\, OMC \cdot KOM \cdot DOM \tag{25}$$

$$+ SSC \cdot KSS \cdot OSS + PC \cdot (PR \cdot FR1 + PM \cdot FM1 - PG)\,)$$

where: A_s = element surface area
K_2 = reaeration rate (calculated using Equations 22 and 23)
$[CO_2\text{-}C]^*$ = $[CO_2\text{-}C]$ saturation concentration at the ambient temperature
$[CO_2\text{-}C]$ = $[CO_2\text{-}C]$ concentration
DOM = labile and refractory dissolved organic material
OMC = carbon fraction of DOM
KOM = first order decay rate for DOM at ambient temperature
OSS = organic suspended solids
SSC = carbon fraction of organic TSS
KSS = first order decay rate for TSS at ambient temperature
PC = carbon fraction of phytoplankton
PR = phytoplankton respiration rate
FR1 = fraction of respired phytoplankton converted directly to nutrients
PM = phytoplankton mortality rate
FM1 = fraction of expired phytoplankton converted directly to nutrients
PG = phytoplankton growth rate

2.4.2.6 CONTAMINANTS

Under aerobic conditions, contaminants, including dissolved organic chemicals, heavy metals, dioxins and furans can enter the system via inflow, diffusion from adjacent layers, or wind driven resuspension (reservoirs only). Sinks for contaminants can be outflow, volatilization, decay, settling, or diffusion to adjacent layers. Contaminant fluxes are shown in Figure 13.

2.4.2.6.1 DISSOLVED ORGANIC CHEMICALS

$$...- K_1 \cdot [ORG]_d - K_2 \cdot [ORG]_d - K_3 \cdot [ORG]_d - \Sigma_{i=1,4}[(w_s)_i \cdot ([ORG]_s)_i / DEP] \quad (26)$$

$$- K_4 \cdot ([ORG]_d - [ORG]_p) / DEP$$

where: K_1 = first order decay coefficient for the dissolved organic chemical

K_2 = first order volatilization coefficient for the dissolved organic chemical (i.e., volatilization rate in m/sec divided by depth)

K_3 = first order complexation/precipitation coefficient for the dissolved organic chemical

$[ORG]_d$ = dissolved organic chemical concentration

$([ORG]_s)_i$ = for i = 1..3, sorbed organic chemical concentration associated with ith organic or inorganic particulate

= for i = 4, sorbed organic chemical concentration associated with phytoplankton

DEP = water column depth

$(w_s)_i$ = for i = 1..3, settling velocity of ith organic or inorganic particulate

= for i = 4, settling velocity of phytoplankton

K_4 = diffusion rate between the sediment pore water and the overlying water

$[ORG]_p$ = dissolved organic chemical in the sediment pore water

The formulation given above is used in water quality simulation options 4 and 5. The dissolved and sorbed fractions of the dissolved organic chemical are determined according to the solution of the following simultaneous equations:

$$[ORG] = [ORG]_d \cdot (1 + \Sigma_{i=1,4}[(K_5)_i \cdot [SS]^a])$$

and $$[ORG] = [ORG]_d + [ORG]_s$$

where: $(K_5)_i$ = partitioning coefficient for the organic chemical with the ith organic or inorganic particulate (L/kg)

$[SS]_i$ = concentration of ith organic or inorganic particulate (mg/L)

a = exponent

Figure 13. Contaminant Fluxes

An iterative process is used to solve for $[ORG]_s$ and $[ORG]_d$.

Associated with the water column model is a sediment bed model. The bed model represents that portion of the reservoirs and stream bottom that interacts with the overlying water through diffusion of the dissolved organic chemicals in the pore water. A partitioning coefficient similar to that described above is used to compute the pore water concentration as a function of total mass of the pollutant contained in the bed. Fluxes to and from the bed model mirror the last two terms of the equation describing dissolved organic chemical kinetics, but with a sediment concentration exponent equal to 1. The bed thickness is assumed constant and the burial rate is equal to the suspended sediment settling flux.

2.4.2.6.2 HEAVY METALS OR RADIONUCLIDES

<u>Note:</u> The formulation shown below for simulating heavy metals is used when water quality simulation options 4 or 5 are specified (as specified in Table 2). For more detailed descriptions of iron and manganese species, Option 6 must be used.

$$...- K_1 \cdot [HMT]_d - K_3 \cdot [HMT]_d - \Sigma_{i=1,4}[(w_s)_i \cdot ([HMT]_s)_i \;/\; DEP] \qquad (27)$$

$$- K_4 \cdot ([HMT]_d - [ORG]_p) \;/\; DEP$$

where: K_1 = first order decay coefficient for radionuclide (= 0 if heavy metal)

K_3 = first order complexation/precipitation coefficient for heavy metal or radionuclide

$[HMT]_d$ = dissolved heavy metal or radionuclide concentration

$([HMT]_s)_i$ = for i = 1..3, sorbed heavy metal or radionuclide concentration associated with ith organic or inorganic particulate

= for i = 4, sorbed heavy metal or radionuclide concentration associated with phytoplankton

DEP = depth of the water column

$(w_s)_i$ = for i = 1..3, settling velocity of ith organic or inorganic particulate

= for i = 4, settling velocity of phytoplankton

K_4 = diffusion rate between the sediment pore water and the overlying water

$[HMT]_p$ = heavy metals in the sediment pore water

The dissolved and sorbed fractions of the heavy metal or radionuclide is determined according to the solution of the following simultaneous equations:

$$[HMT] = [HMT]_d \cdot (1 + \Sigma_{i=1,4}[(K_5)_i \cdot [SS]_i{}^a])$$

and $$[HMT] = [HMT]_d + [HMT]_s$$

where: $(K_5)_i$ = partitioning coefficient for the heavy metal or radionuclide with the i^{th} organic or inorganic particulate (L/kg)
$[SS]_i$ = concentration of i^{th} organic or inorganic particulate (mg/L)
a = exponent

An iterative process is used to solve for $[HMT]_s + [HMT]_d$. A bed model is used to compute the concentration of heavy metals in the sediment pore water and is similar to the bed model described for dissolved organic chemicals.

2.4.2.6.3 DIOXINS OR FURANS

$$\ldots \quad - K_1 \cdot [DIO]_d - K_3 \cdot [DIO]_d - \Sigma_{i=1,4}[(w_s)_i \cdot ([DIO]_s)_i / DEP] \qquad (28)$$

$$- K_4 \cdot ([DIO]_d - [DIO]_p) / DEP$$

where: K_1 = first order decay coefficient for dioxin or furan
K_3 = first order complexation/precipitation coefficient for dioxin or furan,
$[DIO]_d$ = dissolved dioxin or furan concentration
$([DIO]_s)_i$ = for i = 1..3, sorbed dioxin or furan concentration associated with i^{th} organic or inorganic particulate
= for i = 4, sorbed dioxin or furan concentration associated with phytoplankton
DEP = depth of the water column
$(w_s)_i$ = for i = 1..3, settling velocity of i^{th} organic or inorganic particulate
= for i = 4, settling velocity of phytoplankton
K_4 = diffusion rate between the sediment pore water and the overlying water
$[DIO]_p$ = dioxin or furan in the sediment pore water

The dissolved and sorbed fractions of the dioxin or furan are determined according to the solution of the following simultaneous equations:

$$[DIO]_s = [DIO]_d(1 + \Sigma_{i=1,4}[(K_5)_i \cdot [SS]^{a}])$$

and $$[DIO] = [DIO]_d + [DIO]_s$$

where: $(K_5)_i$ = partitioning coefficient for the dioxin or furan with the ith organic or inorganic particulate (L/kg)

$[SS]_i$ = concentration of ith organic or inorganic particulate (mg/L)

a = exponent

An iterative process is used to solve for $[DIO]_s + [DIO]_d$. A bed model is used to compute the concentration of dioxin and furans in the sediment pore water and is similar to the bed model described for dissolved organic chemicals.

2.4.2.7 ORGANIC OR INORGANIC PARTICULATES

Possible sources of organic and inorganic particulates (detritus) are inflow (TSS from treatment plants), phytoplankton mortality, diffusion of detritus from other layers, and wind driven resuspension (reservoirs only). Sinks for detritus can include outflow, settling, diffusion to other layers, and decomposition to inorganic carbon, phosphate, and ammonia. Detritus is an oxygen sink. Inorganic suspended solids are simulated by setting the decay rate to zero. Organic and inorganic particulate (detritus) fluxes are shown in Figure 14.

Figure 14. Detritus fluxes.

$$\ldots - w_s \cdot K_5 \cdot A_s \cdot SS - V \cdot (K_1 \cdot SS + PF \cdot ALG) \qquad (29)$$

where: w_s = settling velocity for organic or inorganic particulate, according to the relation:

$$w_s = a_0 + a_1 \cdot T + a_2 \cdot T^2$$

a_0,a_1,a_2 = quadratic coefficients for function defined by three pairs of (T, w_s) data
T = temperature in degrees Celsius

K_5 = loss coefficient computed according to Rouse velocity distribution [ASCE, 1977]
A_s = element surface area
SS = organic or inorganic particulate concentration
K_1 = first order decay coefficient for organic particulate at ambient temperature (= 0 for inorganic particulate)
T_c = thermal correction factor for organic or inorganic particulate
PF = fraction of phytoplankton which increments the organic particulate (as a result of mortality and respiration)
ALG = phytoplankton concentration

2.4.2.8 COLIFORM BACTERIA

$$\ldots - K_1 \cdot CB \cdot T_c^{(T-20)} \qquad (30)$$

where: K_1 = first order mortality rate for coliform bacteria
CB = coliform bacteria concentration
T_c = thermal correction factor for coliform mortality

2.4.2.9 DISSOLVED ORGANIC MATTER

Dissolved organic matter represents BOD in the model. Five-day BOD is transformed to ultimate BOD based on decay rate as shown in the following equation:

where k is the decay rate and t is time. Ultimate BOD is converted to DOM as follows:

where O_2 Org is oxygen consumed by 1 unit of DOM.

Two BOD classes with different decay rates are simulated, one for labile DOM and the other for refractory DOM. The labile DOM represents the more rapidly decaying oxygen consuming material typically found in wastewater discharge. The refractory DOM represents the more stable oxygen consuming material which are present in natural streams. At the user's option, total carbonaceous BOD may be represented by labile DOM and the total DOM represented by refractory DOM. With this option, oxygen consumption is associated with BOD and nutrient sources are associated with DOM (refractory) and organic particulates.

Sources of DOM can be inflow, phytoplankton photorespiration, and diffusion from other layers. DOM sinks can be outflow, diffusion to other layers, decomposition to inorganic carbon, phosphate and ammonia, and wind driven resuspension (reservoirs only). DOM components may act as oxygen sinks. The transformation rate from labile to refractory DOM is set to zero when labile DOM represents BOD and refractory DOM represents total dissolved organic material. DOM flux relationships are illustrated in Figure 15.

<u>Labile DOM</u>

$$...- V \cdot (K_d \cdot DOM \ - K_t \cdot DOM \ + PF \cdot ALG) \qquad (31)$$

where: V = element volume
K_d = first order rate for decomposition to elemental constituents
K_t = first order rate for decomposition to refractory DOM
DOM = labile dissolved organic matter concentration
PF = fraction of phytoplankton which increments the labile DOM compartment
(as a result of mortality and respiration)
ALG = phytoplankton concentration

<u>Refractory DOM</u>

$$...- V \cdot K_d \cdot RFR \ + \ V \cdot K_t \cdot DOM \qquad (32)$$

where: V = fluid element volume
K_d = first order rate for decomposition of refractory DOM to elemental constituents
RFR = refractory dissolved organic matter concentration
K_t = first order rate for decomposition to refractory DOM
DOM = labile dissolved organic matter concentration

Figure 15. DOM fluxes.

2.4.2.10 MANGANESE, IRON, AND SULFUR

Heavy metal relations were developed to allow for simulation of oxidized and reduced species' concentrations under aerobic and anaerobic conditions in the water column and sediments. The species and processes used to calculate sources and sinks for manganese, iron and sulfur are summarized in Table 4. The relations were developed based upon methods presented in WES [1986] and DiToro, et al. [1994]. In the water column component of HEC-5Q, the advection-dispersion equation is used to calculate the concentrations of the different constituents. For the sediments, however, advection is not applicable, so the dominant processes including diffusion, redox, sorption, and settling are incorporated into a simplified two-layered (aerobic and anaerobic) sediment model to calculate species' concentrations. The relations used in the model are shown schematically in Figure 16 and Figure 17.

Many of the components implemented in the sediment model were common to iron, manganese, and sulfur calculations and are given as follows:

Constituent	Partitioning	Oxidation / Reduction	Diffusive exchange with bed	Settling	Sorption	Burial (sediments)
Mn^{2+}	✓	✓	✓		✓	✓
MnO_2		✓		✓		✓
$MnCO_3$	✓			✓		✓
Fe^{2+}	✓	✓	✓		✓	✓
FeOOH		✓		✓		✓
FeS	✓			✓		✓
S^{2-}	✓	✓	✓			✓
SO_4^{2-}		✓	✓			✓

Table 4 Processes included for generation and removal of manganese, iron and sulfur in the water column and sediments✓

Figure 16. Schematic diagram of iron, manganese, and sulfur speciation in the water column and sediments: Aerobic and anaerobic sediments, aerobic water column

Figure 17. Schematic diagram of iron, manganese, and sulfur speciation in the water column and sediments: Anaerobic sediments, aerobic and anaerobic water column

1. Aerobic vs. anaerobic conditions. In the modified model, processes including oxidation and reduction are represented which are dependent on the oxygen concentration within the sediment layer or in the water column. Additionally, sorption, settling, and diffusion across the sediment - water interface and at the boundary between the anaerobic and aerobic water column or sediment layers are included. If the water column overlying the sediments is oxygenated, the top section of the sediments will also be aerobic down to a certain depth, shown schematically in Figure 18. It is assumed that the dissolved oxygen (D.O.) concentration decreases linearly within the aerobic sediment layer, with a D.O. concentration of zero at the interface with the anaerobic layer. Accordingly, as the D.O. concentration in the overlying water column decreases, the thickness of the aerobic layer will also decrease. For conditions where the overlying water column is anoxic, a minimum surface sediment layer thickness is specified in the model at which point the layer is considered to be anaerobic.

   Raising and lowering of the interface between the aerobic and anaerobic sediments only depends on the overlying water column D.O. concentration. The rate at which the interface between the two layers moves affects the concentration of constituents associated with each layer: as the interface moves upwards, constituents previously associated with the upper sediment layer become a part of the volume comprising the newly-expanded lower layer. Similarly, as the D.O. concentration in the water column increases, the aerobic-anaerobic sediment interface moves downward and constituents previously in the top portion of the anaerobic layer become associated with the upper aerobic layer. The thickness of the aerobic and anaerobic sediment layers will affect the flux of constituents at the sediment-water interface and is estimated as a function of the overlying water column dissolved oxygen concentration.

2. Solid and dissolved species in the sediments and water column. Concentrations of reduced dissolved and particulate species are recorded for each time step in the water column and sediments. Total concentrations of the reduced species within the sediments, i.e., Mn^{2+}, Fe^{2+}, and S^{2-}, are calculated and used to compute dissolved and particulate fractions using a sediment partition coefficient [Thomann, 1987]. The appropriate physical (e.g., settling) or chemical (e.g., oxidation, reduction) processes may then be applied to each species to predict resulting concentrations.

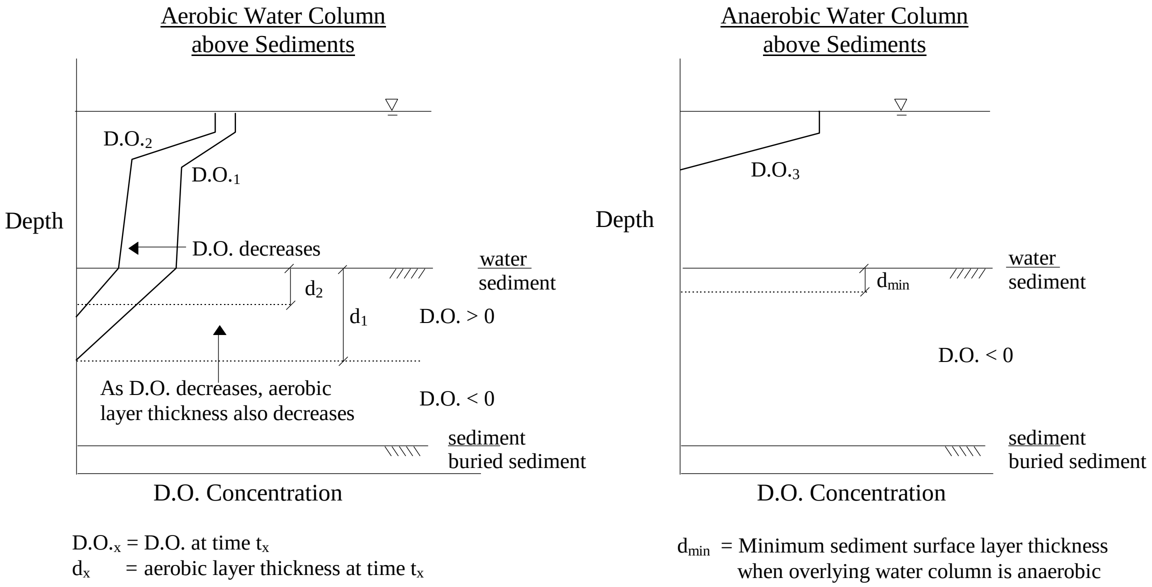

Figure 18. Dependence of sediment layer thickness on water column D.O. concentration

Production of $MnCO_3$, the dominant particulate form of manganese in a reducing environment, is calculated as a function of the inorganic carbon concentration so that the model will still be valid even under conditions of low alkalinity. Iron and sulfur have a common particulate phase, FeS. Therefore, in calculating the concentration of FeS, it becomes necessary to compare concentrations of the dissolved forms of each constituent, i.e., Fe^{2+} and S^{2-}, to determine which limits formation of FeS.

3. Sorption. The concentration of free metal ions in solution can be strongly affected by the presence of organic material as the positively-charged ions bind to negatively charged sites on the organic particulate matter in the water column and sediments [Stumm, 1992]. Once sorbed, the bound metals in the water column can settle to the sediments. Sorption to organic matter has been included in the model for the dissolved reduced species of manganese (Mn^{2+}) and iron (Fe^{2+}), but not for sulfur (S^{2-}). For the purposes of this study, sorption has been assumed to be an irreversible process, i.e., once reduced dissolved species are sorbed to suspended material they cannot be desorbed. Concentrations of suspended solids are computed in HEC-5Q for labile dissolved organic matter (DOM), refractory DOM, detritus and phytoplankton and are used in the metals component of the program for computation of removal by sorption and subsequent settling.

4. Diffusion at the aerobic-anaerobic and sediment-water interfaces. Exchange of the dissolved reduced species, Mn^{2+}, Fe^{2+}, and S^{2-}, at the sediment-water interface and at the aerobic-anaerobic sediment layer interface are modeled as diffusive processes, shown in Figure 19. The dissolved reduced species are released predominantly under anaerobic conditions. However, for modeling purposes, diffusion at the sediment

interfaces is also allowed to occur under aerobic conditions, although the contribution to metals in the water column will typically be small due to oxidation and partitioning within the surface sediment layer and the overlying water column element.

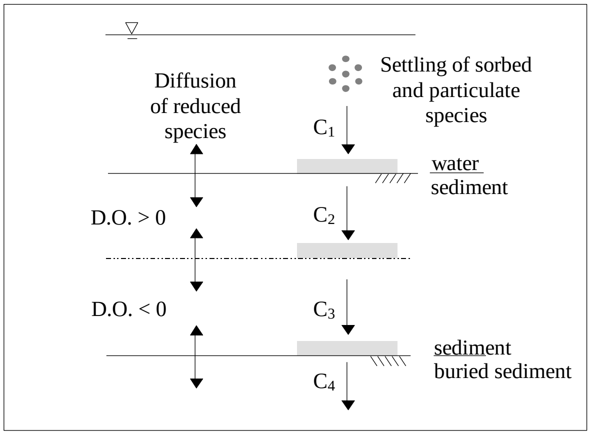

Figure 19. Diffusion and settling in the water column and sediments

5. Oxidation and reduction. Under aerobic conditions, the dissolved reduced species (Fe^{2+}, Mn^{2+}, S^{2-}) are oxidized at user-specified rates. Since oxidation is not an instantaneous process, reduced species may exist under aerobic conditions until they are oxidized. This condition applies to both particulate and dissolved species. Particulate species are first partitioned to the dissolved form as an intermediate species prior to oxidation. Reduction is modeled in a manner similar to oxidation. Under anaerobic conditions, oxidized species are reduced according to user-specified reduction rates. Oxidized species are allowed to exist under anaerobic conditions, gradually reducing according to the specified rates.

6. Settling. The model is capable of simulating settling of heavy metals in two ways: oxidized or reduced particulate species (e.g., MnO_2, $MnCO_3$, FeOOH, FeS) may settle at a user-specified settling rate. If suspended solids (labile DOM, refractory DOM, detritus or phytoplankton) are simulated, settling may be represented by settling of the dissolved reduced species that are sorbed to organic material. Since reduced sulfur is negatively charged, it is assumed not to sorb to suspended material and can only settle in the particulate form, FeS.

7. Burial. It is assumed that as metals and sulfur (either sorbed or in particulate form) settle to the bed from the water column, a fraction settles between the sediment layers and finally, from the anaerobic sediments into the buried sediments, shown in Figure 19. Since concentrations in the buried sediments are assumed to be much larger than concentrations in other system components, the concentration of a constituent added to or removed from buried sediments is not explicitly retained. It is assumed that buried sediments contain very high concentrations of dissolved reduced species and are a non-depleting source of reduced species to the anaerobic sediments via

diffusion. This assumption was made to avoid complete depletion of reduced species in the sediments.

8. Bottom Exchange. For each reservoir segment modeled in HEC-5Q, the surface area representing the reservoir sides or bottom can be calculated. Exchange of material with the reservoir sides or bottom includes diffusion and settling of material to the bed.

2.4.2.10.1 PARTITIONING

Partitioning is used as the mechanism for transforming the reduced species between dissolved and particulate forms. Under anaerobic conditions, a portion of dissolved manganese, Mn^{2+}, is used to form the particulate species, $MnCO_3$. Similarly, under aerobic conditions, $MnCO_3$ is partitioned back to the dissolved species as an intermediate prior to oxidation. Reduced solid and dissolved phase species for each constituent, i.e., Mn^{2+}, $MnCO_3$, Fe^{2+}, FeS, S^{2-}, may exist under aerobic conditions in the water column and sediments, until oxidized. Reduced species concentrations of Fe(II) and S(II) are calculated and the values are compared to determine which limits formation of FeS. At the start of each time step, the total reduced species' concentration in each water column element and sediment layer is calculated for iron, manganese, and sulfur as the sum of the dissolved and particulate species:

$$C_T = C_{diss}^{red} + C_{part}^{red} \tag{33}$$

where C_T = Total reduced species' concentration in the water column or sediment element

C_{diss}^{red} = Dissolved reduced species' (Mn^{2+}, Fe^{2+}, S^{2-}) concentration

C_{part}^{red} = Particulate reduced species' ($MnCO_3$, FeS) concentration

The reduced species concentration for the time step is calculated using the relations:

$$C_{diss}^{red} = f_d \cdot C_T$$ (Dissolved species: Mn^{2+}, Fe^{2+}, S^{2-})

$$C_{part}^{red} = f_p \cdot C_T$$ (Particulate species: $MnCO_3$, FeS)

where: C_T = Total reduced species' concentration in the element, i.e., (Mn^{2+} + $MnCO_3$), (Fe^{2+} + FeS), (S^{2-} + FeS)

f_d = Dissolved fraction coefficient calculated by: $f_d = \frac{1}{1 + Pm}$

f_p = Particulate fraction coefficient calculated by: $f_p = 1 - f_d$

P = Partition coefficient in water column or sediments [L/mg]

m = Mass of solids in water column or sediments [mg/L]

Under anaerobic conditions, a portion of dissolved reduced species will partition to the particulate form. Similarly, under aerobic conditions, the particulate form is partitioned back to the dissolved form as an intermediate species prior to oxidation. Because the partitioning term is given as a fraction of the reduced particulate and dissolved species concentrations, it is not included as a 'source/sink' term.

At each time step and within each element, the concentration of the reduced particulate iron species, FeS, is dependent upon both the reduced dissolved iron and sulfur species' concentrations. Therefore, at the start of each time step Fe^{2+} and S^{2-} concentrations are compared to determine which will limit formation of iron sulfide. If the reduced iron species' concentration (Fe^{2+}) in the sediment layer is less than the reduced sulfur (S^{2-}) concentration, the particulate species' (FeS) concentration is calculated as a function of the iron concentration. Similarly, the concentrations of Mn^{2+} and inorganic carbon (representing CO_3^{2-}) are compared to determine which component limits formation of $MnCO_3$.

Using the example provided by iron, if FeS formation is limited by S^{2-} concentration, for each mole of FeS which is partitioned into Fe^{2+} and S^{2-} under aerobic conditions, the amount of Fe^{2+} released must be determined by scaling the concentrations by a ratio of the molecular weights of iron and sulfur:

$$\text{Change in } Fe^{2+} \text{ concentration} = \text{Change in } S^{2-} \text{ concentration} \cdot \frac{\text{Mol. wt. Fe}(55.8)}{\text{Mol. wt. S}(32)}$$

Similarly, for each mole of FeS formed, the reduction in Fe^{2+} concentration would be determined by the relation given above. The FeS relations are calculated only once at each time step, in the iron or sulfur subroutines, depending on which component is the limiting substance.

2.4.2.10.2 SEDIMENT RELATIONS

Reduced Dissolved Species - Aerobic sediment layer

$$\ldots - K_{ox} \cdot \left(C_{diss}^{red}\right)_a \cdot t + \sum_{i=1,4} r_{setl,SS} \cdot f(SS_e)_i \cdot \left(C_{diss}^{red}\right)_e \cdot t \pm r_{interface} \cdot \left(C_{diss}^{red}\right)_{a,b} \cdot t \quad (34)$$

$$\pm K_{interface} \cdot \Delta\left(C_{diss}^{red}\right)_{a,b} \cdot t \pm K_{wc} \cdot \Delta\left(C_{diss}^{red}\right)_{e,a} \cdot t - r_{burial} \cdot \left(C_{diss}^{red}\right)_a \cdot t$$

where K_{ox} = Oxidation rate of reduced species, sediments [1/s]

$\left(C_{diss}^{red}\right)_a$ = Reduced dissolved species' concentration in top sediment layer [mg/L]

t = Time step [s]

$r_{setl,SS}$ = Water column suspended solids settling rate [1/s]

$f(SS_e)_i$ = Function dependent on suspended solids concentration [dimensionless]

i represents the suspended solid type calculated by HEC-5Q: labile DOM, refractory DOM, detritus or phytoplankton

$\left(C^{red}_{diss}\right)_e$ = Reduced dissolved species' concentration in overlying water column element [mg/L]

$r_{interface}$ = Rate of movement of aerobic - anaerobic sediment interface [1/s]

$\left(C^{red}_{diss}\right)_{a,\,b}$ = Reduced dissolved species' concentration in aerobic or anaerobic sediment layer [mg/L]. If water column is aerobic, the sediment interface moves downward, therefore the concentration in the aerobic layer increases (+) as a function of the anaerobic layer concentration $\left(C^{red}_{diss}\right)_b$. If water column is anaerobic, the sediment interface moves upward, and the concentration in the aerobic layer decreases (-) as a function on the aerobic layer concentration.

$K_{interface}$ = Coefficient of mass transfer at aerobic-anaerobic sediment interface [1/s]

$\Delta\left(C^{red}_{diss}\right)_{a,\,b}$ = Concentration difference between aerobic and anaerobic sediment layers [mg/L]

K_{wc} = Coefficient of mass transfer at sediment-water interface [1/s]

$\Delta\left(C^{red}_{diss}\right)_{e,\,a}$ = Concentration difference between water column element and top sediment layer [mg/L]

r_{burial} = Rate of burial to deep sediments; calculated as a function of the accumulation rate. This term represents a component of the constituent eventually transferred to buried sediments [1/s]

The above terms represent the following:

Oxidation of reduced species, settling of sorbed dissolved species from the water column, gain/loss due to movement of the aerobic-anaerobic sediment interface, mass transfer (diffusion) between the sediment layers, diffusion at sediment-water interface (small under aerobic conditions), and fraction of the accumulated sediment transferred to layer below (for burial).

Note: The sorption term is not used for modeling of reduced sulfur.

Reduced dissolved species - Anaerobic sediment layer

$$\ldots + K_{red} \cdot \left(C^{ox}\right)_b \cdot t \;\underline{+}\; r_{interface} \cdot \left(C^{red}_{diss}\right)_{a,b} \cdot t \;\underline{+}\; K_{interface} \cdot \Delta\left(C^{red}_{diss}\right)_{a,b} \cdot t \qquad (35)$$

$$\underline{+}\; r_{burial} \cdot \Delta\left(C^{red}_{diss}\right)_{a,b} \cdot t + K_{buried\ sed} \cdot \left(C^{red}_{diss}\right)_{buried} \cdot t$$

where K_{red} = Reduction rate of oxidized species, first order reaction rate constant [1/s]

$\left(C^{ox}\right)_b$ = Concentration of oxidized species in the anaerobic sediment layer (MnO_2, FeOOH, SO_4^{2-}) [mg/L]

$K_{buried\ sed}$= Coefficient of mass transfer between buried sediment and anaerobic layer [1/s]

The above terms represent the following:

Reduction, gain/loss due to movement of the aerobic-anaerobic sediment interface, mass transfer (diffusion) between the sediment layers, gain/loss due to accumulation from aerobic layer and transfer to buried sediments, and diffusion from buried sediments.

Oxidized Species - Aerobic sediment layer

$$\ldots + K_{ox} \cdot \left(C^{red}_{diss}\right)_a \cdot t + r_{setl,part} \cdot \left(C^{ox}\right)_e \cdot t \;\underline{+}\; r_{interface} \cdot \left(C^{ox}\right)_{a,b} \cdot t \qquad (36)$$

$$- \; r_{burial} \cdot \left(C^{ox}\right)_a \cdot t$$

where $r_{setl,part}$ = Water column particulate species settling rate [1/s]

$\left(C^{ox}\right)_e$ = Oxidized species’ concentration in overlying water column element [mg/L]

$\left(C^{ox}\right)_{a,b}$ = Oxidized species’ concentration in aerobic or anaerobic sediment layer [mg/L]

The above terms represent the following:

Oxidation of reduced species, settling of oxidized species from overlying water column, gain/loss due to movement of the aerobic-anaerobic sediment interface, and fraction of the accumulated sediment transferred to layer below (for burial).

Oxidized Species - Anaerobic sediment layer

$$\ldots\ -\ K_{red} \cdot \left(C^{ox}\right)_b \cdot t\ \ \underline{+}\ \ r_{interface} \cdot \left(C^{ox}\right)_{a,\,b} \cdot t\ \ \underline{+}\ \ r_{burial} \cdot \Delta\left(C^{ox}\right)_{a,\,b} \cdot t \qquad (37)$$

where $\Delta\left(C^{ox}\right)_{a,\,b}$ = Concentration difference between aerobic and anaerobic sediment layers [mg/L]

The above terms represent the following:

Reduction of oxidized species, gain / loss due to movement of the aerobic-anaerobic sediment interface, fraction of accumulated sediment transferred from aerobic layer, and gain/loss due to accumulation from aerobic layer and transfer to buried sediments.

Reduced Particulate Species - Aerobic sediment layer

$$\ldots\ +\ r_{setl,part} \cdot \left(C^{red}_{part}\right)_e \cdot t\ \ \underline{+}\ \ r_{interface} \cdot \left(C^{red}_{part}\right)_{a,\,b} \cdot t\ \ -\ \ r_{burial} \cdot \left(C^{red}_{part}\right)_a \cdot t \qquad (38)$$

where $\left(C^{red}_{part}\right)_e$ = Reduced particulate species' concentration in overlying water column element [mg/L]

$\left(C^{red}_{part}\right)_{a,\,b}$ = Reduced particulate species' concentration in aerobic or anaerobic sediment layer [mg/L]

$\left(C^{red}_{part}\right)_a$ = Reduced particulate species' concentration in aerobic sediment layer [mg/L]

The above terms represent the following:

Settling of reduced particulate from the overlying water column element, gain / loss due to movement of the aerobic-anaerobic sediment interface, and fraction of the accumulated sediment transferred to layer below (for burial).

Reduced Particulate Species - Anaerobic sediment layer

$$\ldots\ \underline{+}\ \ r_{interface} \cdot \left(C^{red}_{part}\right)_{a,\,b} \cdot t\ \ -\ \ r_{burial} \cdot \Delta\left(C^{red}_{part}\right)_{a,b} \cdot t \qquad (39)$$

$\left(C_{part}^{red}\right)_b$ = Reduced particulate species' concentration in anaerobic sediment layer [mg/L]

$\Delta\left(C_{part}^{red}\right)_{a,b}$ = Concentration difference between aerobic and anaerobic sediment layers [mg/L]

The above terms represent the following:

Gain / loss due to movement of the aerobic-anaerobic sediment interface, and gain/loss due to accumulation from aerobic layer and transfer to buried sediments.

2.4.2.10.3 WATER COLUMN RELATIONS

The relations developed for transformation of reduced and oxidized species of manganese, iron, and sulfur in the water column under aerobic and anaerobic conditions are similar to those used to describe source and sink terms for the sediments. The source/sink terms developed for the water column are added to the advection - dispersion equation, used by HEC-5Q to predict the transport and fate of water quality constituents. In the following equations, the subscript 'e' refers to the water column element.

<u>Reduced Dissolved Species - Aerobic water column element</u>

$$\ldots - K_{ox} \cdot \left(C_{diss}^{red}\right)_e \cdot t \pm \sum_{i=1,4} r_{setl,SS} \cdot f(SS_e)_i \cdot \left(C_{diss}^{red}\right)_e \cdot t \qquad (40)$$

$$\pm K_{wc} \cdot \Delta\left(C_{diss}^{red}\right)_{e,a} \cdot t$$

where K_{ox} = Oxidation rate of reduced species, water column [1/s]

$\left(C_{diss}^{red}\right)_e$ = Reduced dissolved species' concentration in water column element (Mn^{2+}, Fe^{2+}, S^{2-}) [mg/L]

t = Time step [s]

$r_{setl,SS}$ = Settling velocity of suspended solids [1/s]

$f(SS_e)_i$ = Function dependent on suspended solids concentration [dimensionless]

i represents the suspended solid type calculated by HEC-5Q: labile DOM, refractory DOM, detritus or phytoplankton

K_{wc} = Coefficient of mass transfer at sediment-water interface[1/s]

$\Delta\left(C_{diss}^{red}\right)_{e,a}$ = Concentration difference between water column element and top sediment layer [mg/L]

The above terms represent the following:

Oxidation, settling of sorbed dissolved species from the water column (from element above, to element below), and mass transfer (diffusion) between the water column and sediment (small under aerobic conditions).

Note: The sorption term is not used for modeling of reduced sulfur.

Reduced Dissolved Species - Anaerobic water column element

$$\ldots - K_{red} \cdot \left(C^{ox}\right)_e \cdot t \pm \sum_{i=1,4} r_{setl,SS} \cdot f(SS_e)_i \cdot \left(C_{diss}^{red}\right)_e \cdot t \tag{41}$$

$$\pm K_{wc} \cdot \Delta\left(C_{diss}^{red}\right)_{e,a} \cdot t$$

where K_{red} = Reduction rate of oxidized species, water column [1/s]

$\left(C^{ox}\right)_e$ = Oxidized species' concentration in water column element (MnO_2, $FeOOH$, SO_4^{2-}) [mg/L]

The above terms represent the following:

Reduction of oxidized species, settling of sorbed dissolved species from the water column (from element above, to element below), and mass transfer (diffusion) between the water column and sediment.

Note: The sorption term is not used for modeling of reduced sulfur.

Oxidized Species - Aerobic water column element

$$\ldots + K_{ox} \cdot \left(C_{diss}^{red}\right)_e \cdot t \pm r_{setl,part} \cdot ((C^{ox})_{e,t} - (C^{ox})_e) \cdot t \tag{42}$$

where $r_{setl,part}$ = Water column particulate species settling rate [1/s]

$(C^{ox})_{e,t}$ = Oxidized species' concentration in overlying water column element [mg/L]

The above terms represent the following:

Oxidation of reduced species, and settling (from the water column element above to the element below).

Oxidized Species - Anaerobic water column element

$$\ldots\ -\ K_{red} \cdot \left(C^{ox}\right)_{e} \cdot t \ \ \underline{+}\ \ r_{setl,part} \cdot ((C^{ox})_{e,t} - (C^{ox})_{e}) \cdot t \qquad (43)$$

The above terms represent the following:

Reduction of oxidized species, and settling (from the water column element above to the element below).

Reduced Particulate Species - Aerobic or anaerobic water column element

$$\ldots\ \underline{+}\ \ r_{setl,part} \cdot (\left(C^{red}_{part}\right)_{e,\,t} - \left(C^{red}_{part}\right)_{e}) \cdot t \qquad (44)$$

where $r_{setl,part}$ = Water column particulate species settling rate [1/s]

$\left(C^{red}_{part}\right)_{e}$ = Reduced particulate species' concentration in water column element [mg/L]

The above term represents the following:

Settling of reduced particulate species from the water column element above and to the element below.

3 SOLUTION TECHNIQUES

3.1.1 RESERVOIRS

A Gaussian reduction scheme is used for solving the differential equations, which represent the response of the water quality constituents within the reservoirs. Equation 10 is rewritten in a form where a "forward time and central difference in space" scheme is used to describe all the derivative processes. For element i adjacent to elements i-1 and i+1, as shown in Figure 20, the general mass balance equation can be written:

$$\begin{aligned} V_i\left[\frac{\partial T}{\partial t}\right]_i = {} & T_{i-1}\left\{\left[\frac{A_z D_z}{\Delta z}\right]_i + Q_{u_i}\right\} - T_i\left\{\left[\frac{A_z D_z}{\Delta z}\right]_i + \left[\frac{A_z D_z}{\Delta z}\right]_{i+1}\right. \\ & \left. + Q_{d_i} + Q_{u_{i+1}} + Q_w + \frac{\partial V}{\partial t}\right\} + T_{i+1}\left\{\left[\frac{A_z D_z}{\Delta z}\right]_{i+1} + Q_{d_{i+1}}\right\} + \sum Q_x T_x + \frac{A_h H}{\rho c} 0 \end{aligned} \tag{45}$$

where: V = volume of the fluid element in m^3
T = temperature in degrees Celsius or water quality constituent concentration in mg/L
t = computation time step in seconds
A_z = element area at the fluid element boundary in m^2
D_z = effective diffusion coefficient in m^2/sec
Δz = element thickness (length is stream) in meters
Q_u = upward advective flow (stream flow) between elements in m^3/sec
Q_d = downward advective flow between elements in m^3/sec
Q_w = rate of flow removal from the element in m^3/sec
Q_x = rate of inflow to the element in m^3/sec
T_x = inflow water temperature in °C or constituent concentration in mg/l
A_h = element surface area in m^2
H = external sources and sinks of heat in J/m^2/sec
ρ = water density in kg/m^3
c = specific heat of water in J/kg/°C

Subscripts i, i-1, i+1 denote element numbers.

Equation 45 represents the general mass balance for water quality constituents in reservoirs. It is modified for specific application to the different reservoir types simulated, i.e., vertically, longitudinally or layered and longitudinally segmented.

Recall that the term $\frac{H}{\rho c}$ is replaced by $-K_1T$ or $K_2(DO^* - DO)$ for non-conservative water quality constituents and dissolved oxygen, respectively. A finite difference equation of this type is formed for each element and integrated with respect to time. The system of finite difference mass balance equations represents the response of water quality within the entire reservoir. With the aid of a numerical integration technique, the equations are solved with respect to time.

The heat or mass balance at any element, i, can take the form:

$$v_i \dot{c}_i = c_{i-1} s_{i-1} - c_i s_i + c_{i+1} s_{i+1} + p_i \tag{46}$$

where: v_i = volume of element i
$\dot{c}_i$ = time rate of temperature or water quality constituent concentration in element i
c_i = temperature or constituent concentration in element i
s_i = the bracketed terms of the mass balance equations (i.e., advection, diffusion and change of volume)
p_i = the constant term for each element i (i.e., sources and sinks)

The complete system of mass balance equations for the n elements can be written in the matrix form:

$$[v]\{\dot{c}\} = [s]\{c\} + \{p\} \tag{47}$$

where: [v] = an n x n matrix with the element volumes on the diagonal and zeroes elsewhere
$\{\dot{c}\}$ = a column matrix of the rates of change for temperature or constituent concentrations in each of the n elements
[s] = an n x n matrix of the coefficients which multiply the temperature or constituent concentrations
{c} = a column matrix of the temperature or constituent concentrations in each segment
{p} = a column matrix of the constant terms for each segment

To integrate the basic equation over time, the following numerical approximation for each element is made.

$$c_{t+\Delta t} = c_t + \frac{\Delta t}{2}(\dot{c}_t + \dot{c}_{t+\Delta t}) \tag{48}$$

where: $c_t, c_{t+\Delta t}$ = temperature or constituent concentration at the beginning and end of an integration interval, respectively
$\dot{c}_t, \dot{c}_{t+\Delta t}$ = rate of change of temperature or constituent concentration at the beginning and end of an integration interval, respectively
Δt = the length of an integration interval

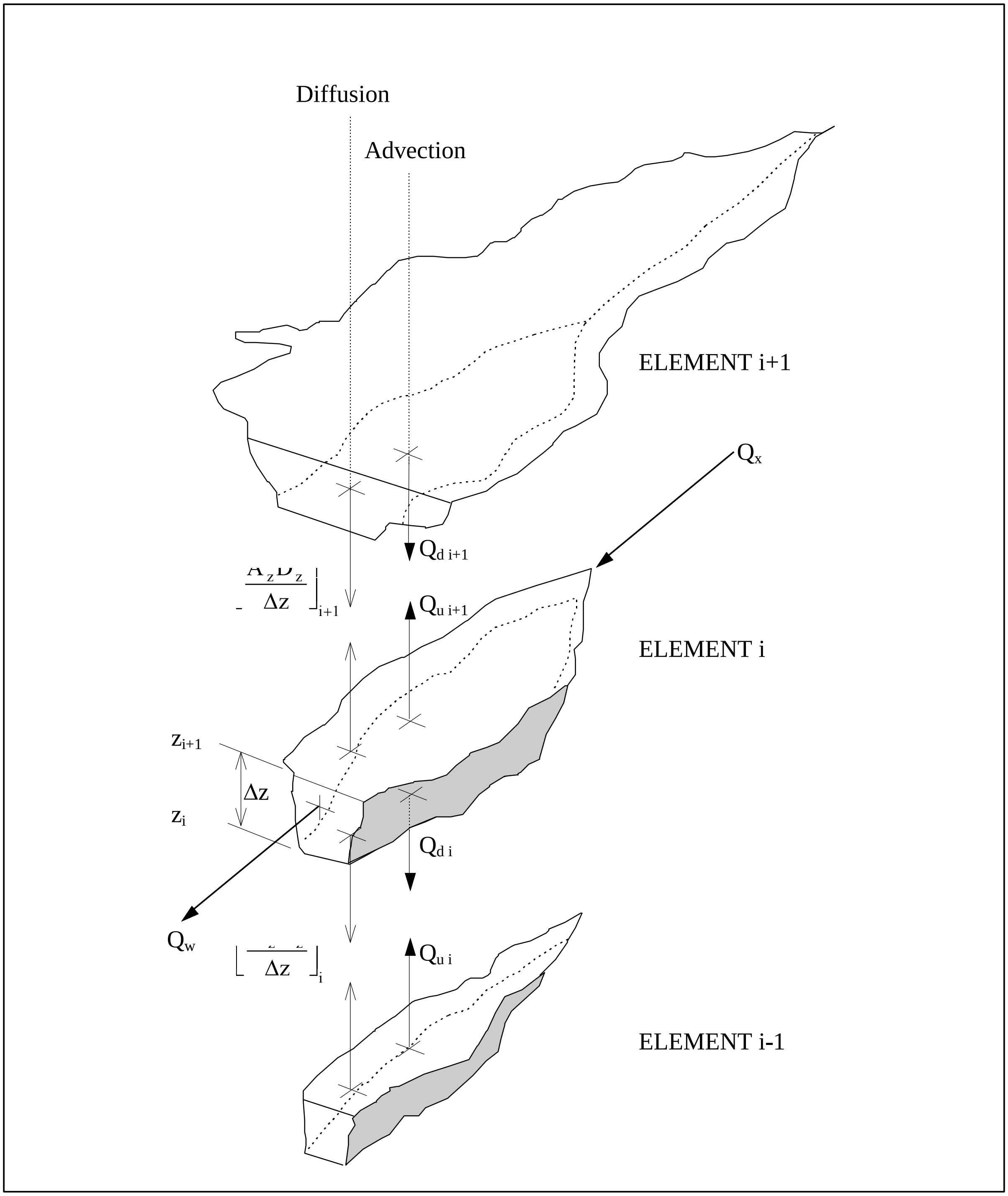

Figure 20. Physical mass transfers between elements

At any point in time c_t and $\dot{c}_t$ are known, thus the expression becomes:

$$c_{t+\Delta t} = B + \frac{\Delta t}{2} \dot{c}_{t+\Delta t} \tag{49}$$

where: $B = c_t + \frac{\Delta t}{2} \dot{c}_t 0$

Equation 49 rewritten in matrix form is:

$$\{c\} = \{B\} + \frac{\Delta t}{2} \{\dot{c}\} \tag{50}$$

where: $\{c\}$ = a column matrix of temperatures or constituent concentrations at the end of the time interval
$\{B\}$ = a column matrix of the terms defined in Equation 49
$\{\dot{c}\}$ = a column matrix of the time rate of change in temperature or constituent concentrations

Substituting Equation 50 into Equation 47:

$$[v]\{c\} = [s]\{B\} + \frac{\Delta t}{2} [s]\{\dot{c}\} + \{p\} \tag{51}$$

or:

$$[s^*]\{\dot{c}\} = \{p^*\} \tag{52}$$

where: $[s*] = [v] - \frac{\Delta t}{2}[s] 0$

$\{p^*\} = [s]\{B\} + \{p\}$

Equation 52 forms the basis for a solution, as there is only one unknown in the equation (i.e., $\{\dot{c}\}$). The following recursive scheme can be used for the numerical solution of Equation 52.

1. Form the vector {B} from the initial condition or the solution just completed.

2. Form the known hydraulic solution and known boundary conditions; define the conditions that will exist at the end of the interval.

3. With known values of [v], [s], and {p}, form $[s^*]$ and $\{p^*\}$.

4. Solve for $\{\dot{c}\}$ at time $(t + \Delta t)$.

5. Compute {c} by substitution in Equation 50.

The above recursive scheme is that used in many computer codes and has proven to be very stable.

3.1.2 STREAMS

A linear programming algorithm is used to solve a fully implicit backward difference in space, forward difference in time, and finite difference approximation of Equation 45. This approximation has the general form:

$$a_{i,i-1}c_{i-1}^{t+1} + a_{i,i}c_{i}^{t+1} + a_{i,i+1}c_{i+1}^{t+1} - c_{i}^{t} = b_{i} \qquad (53)$$

where the "a" terms are coefficients formed from the area, dispersion coefficients, flows, lengths of the computational elements, and time step for each volume element; the "c" terms are the unknown temperatures and constituent concentrations in each volume element; the "b" terms are constants formed from initial conditions or previously computed conditions, tributary inputs of heat or mass loads and potentially the reservoir releases.

Two matrix formats are used in the stream water quality simulation module. The first can be used to solve for temperature and constituent concentrations given all external inputs. It is represented by::

$$|\mathbf{A}|\vec{c} = \vec{b} \qquad (54)$$

where |A| is the matrix of coefficients; c is the vector of unknown temperatures or constituent concentrations; and b is the vector of constants. In this format, the **|A|** matrix is a tri-diagonal matrix consisting of m x m elements, where m is the number of stream elements. The vectors $\vec{c}$ and $\vec{b}$ both consist of m elements. This solution method is used in the water quality simulation module to compute the final results after all reservoir operations have been completed. In effect, the linear programming algorithm is used as a matrix solver for a simulation model.

The second, and more complex, matrix format used in the water quality simulation module is used for determining the temperature and constituent concentrations that are required for the reservoir releases to satisfy all water quality targets in the stream system. In effect, the second format is used to determine which control point controls the release for each constituent and to determine the reservoir release water quality that most closely satisfies the targets at the controlling points. This decision making capability is achieved by transforming the constituent concentrations at each control point into a specification of the target and the deviation of the concentration above or below the target and by making the concentrations in the reservoir releases unknown so that they can be computed. An additional set of equations is used to define the range of constituent concentrations that may be released from the reservoirs.

The linear programming approached is used to select the results that best satisfy the objectives for downstream water quality. An objective function is used to quantitatively describe the desirability of any given solution to a formulated problem. In the water quality simulation module, a minimization routine is used, expressed as:

$$\text{minimize } z = \vec{p}\,\vec{c} \tag{55}$$

The actual value of z is immaterial to the water quality simulation module; it is just an index by which the desirability of the solution is determined. The vector $\vec{c}$ represents the vector of constituent concentrations, but it also includes the variables representing the following:

1. The deviations from the control point targets for those volume elements that represent control points
2. The constituent concentrations in all other volume elements
3. The constituent concentrations in the reservoir releases.

The vector $\vec{p}$ represents the penalty associated with the appearance of a given variable in the final solution. The penalties are nonzero only at control points and are applied only for the variables that represent deviations from the target. Different penalties can be assigned for each control point, for each constituent and for each deviation, above and below the target. When trying to minimize z, the linear programming algorithm tries to ensure that the variable representing the negative deviation appears in the final solution since a lower value of the index z would result. Similar logic is used for setting penalties for constituents that must always exceed a target value, such as dissolved oxygen. The nonzero penalties are applied to the variables representing negative deviations, and the variables that represent positive deviations are given penalties equal to zero. For a more detailed discussion of the stream solution algorithm, the reader is referred to HEC [1986a].

3.1.3 GATE SELECTION

The port selection algorithm serves to determine the configuration of ports and flow rates to maximize a function of the downstream water quality concentrations. Solution of this problem is accomplished by using mathematical optimization techniques. The objective function is related to meeting downstream target qualities subject to various hydraulic constraints on the individual ports.

Kaplan [1974] solved a similar, although more difficult, problem by including in the constraint set upper and lower bounds on the release concentration of each water quality constituent. Kaplan also considered as part of his objective function the reservoir water quality that resulted from any particular operation strategy. A penalty function approach was used to incorporate the many constraints into the objective function, which could then be solved as an unconstrained nonlinear problem. For the problem of interest with respect to HEC-5Q, with appropriate transformations it is possible to formulate a quadratic objective function with linear constraints. Mathematical optimization techniques are available to exploit the special structure of this problem and to solve it efficiently.

The hydraulic structure under consideration is composed of two wet wells, containing up to eight ports each, and a flood control outlet. It is assumed that releases through any of these ports (including the flood control outlet) leave the reservoir through a common pipe. At any given time, only one port in either wet well and the flood control outlet may be operated. Hence, the algorithm provides flows through three ports at most.

The HEC-5 model also provides for releases through an uncontrolled spillway. These releases are not a part of the gate selection algorithm, but the water quality of the spillway releases are considered by the gate selection algorithm.

The algorithm proceeds by considering a sequence of problems, each representing a different combination of open ports. For each combination, the optimal allocation of total flow to ports is determined. The combination of open ports with the highest water quality index defines the optimal operation strategy for the time period under consideration.

There are four different types of combinations of open ports. For one-port problems all of the flow is taken from a single port, and the water quality index is computed. For two-port problems, combinations of one port in each wet well and combinations of each port with the floodgate are considered. For three-port problems, combinations of one port in each wet well and the floodgate are considered. The total flow to be released downstream is specified external to the port selection module, but if the flow alteration option is selected, then the flow can be treated as an additional decision variable; and the flow for which the water quality index is maximized is also determined.

For each combination of open ports, a sequence of flow allocation strategies is generated using a gradient method, a gradient projection method, or a Newton projection method as appropriate. The value of any flow allocation strategy is determined by evaluation of a water quality index subject to the hydraulic constraints of the system. The sequence converges to the optimal allocation strategy for the particular combination of open ports.

To evaluate the water quality index for a feasible flow allocation strategy, first the release concentration for every water quality constituent is computed.

$$R_c = \frac{\sum_{p=1}^{N_p}(\phi_{cp} Q_p)}{\sum_{p=1}^{N_p}(Q_p)}; \quad c = 1, N_c \tag{56}$$

where: R_c = release concentration for constituent c
c = index for constituents
p = index for open ports
N_p = number of open ports
Φ_{cp} = concentration of constituent c at port p
Q_p = flow rate through port p
N_c = number of constituents under consideration

The deviation of release qualities from downstream target qualities can be computed.

$$D_c = R_c - T_c ; \qquad c = 1, N_c \tag{57}$$

where: D_c = deviation of constituent C
T_c = downstream target quality for constituent C

The subindex S_c for each constituent can be determined by:

$$S_c = f(D_c) ; \qquad c = 1, N_c \tag{58}$$

Where the function f takes the form of the sixth order polynomial:

$$f(D_c) = a + bD_c + c\, D_c^2 + dD_c^3 + eD_c^4 + fD_c^5 \tag{59}$$

In selecting these coefficients, the magnitude and importance of the water quality parameter should be considered. To aid in the coefficient selection process, Table 5, Figure 21 and the following discussion are provided.

Table 5 Typical coefficients in constituent suboptimization function

Curve	Coefficient					
Number	a*	b	c	d	e	f
1	100	0.0	-0.1	0.0	0.000	0
2	100	0.0	-2.0	0.0	0.000	0
3	100	0.0	-10.0	0.0	0.000	0
4	100	-3.2	-0.7	-0.1	-0.005	0
5	100	3.2	-0.7	0.1	-0.005	0

* a must equal 100.

Curves 1 through 3 in Figure 21 are functions where equal weight is given to deviation on either side of the target concentration. Under normal conditions, this type of function should be used.

Curve number 1 would be used for a quality parameter such as TDS since wide variations from the target are normally allowable. For a parameter such as nitrate where the concentration is low, curve number 3 would be appropriate. Curve number 2 might be used for temperature or other parameters where the concentration range is 5 to 25. Curves number 4 and 5 are functions where deviations about the target are not weighted equally. Curve number 4 could be used for a toxic parameter where the lowest discharge concentration would be desirable. Conversely, curve 5 could be used for a parameter where a higher concentration is always desirable, for example, for dissolved oxygen in some applications.

In summary, almost any shape of function can be developed (a curve fit routine will be very helpful) using the sixth order polynomial function. In developing these functions, the importance of the parameter and the anticipated magnitude of the concentration are the major considerations. Keep in mind that the weighting factor can be set to zero if the quality parameter is unimportant.

Finally, the scalar water quality index can be determined by:

$$Z = \sum_{c=1}^{N_c} W_c \; S_c \tag{60}$$

where: Z = water quality index
W_c = weighting factor for constituent c
S_c = subindex for constituent c and:

$$\sum_{c=1}^{N_c} W_c = 1 \tag{61}$$

The problem of determining the optimal allocation of flows to ports for a particular combination of open ports and for a specified total flow rate Q can be expressed as follows:

$$\underset{Q_p}{\text{MAX}} \quad \left(\sum_{c=1}^{N_c} W_c S_c \right) \tag{62}$$

Subject to:

$$\sum_{p=1}^{N_p} Q_p = Q\,0$$

$$F_{min,p} \le Q_p \le F_{max,p} \; ; \; p = 1, N_p$$

where F_{min} and F_{max} are the minimum and maximum acceptable flow rates through a port.

When an acceptable flow range Q_{lower} to Q_{upper} is specified, then the problem is written as:

$$\underset{Q_p}{\text{MAX}} \quad \left(\sum_{c=1}^{N_c} W_c S_c \right) \tag{63}$$

Subject to:

$$Q_{lower} \le \sum_{p=1}^{N_p} Q_p \le Q_{upper}\, 0$$

$$F_{min,p} \le Q_p \le F_{max,p}; \quad p = 1, N_p$$

These problems are solved very efficiently by using mathematical optimization techniques that take advantage of the problem structure, namely a quadratic objective function with linear constraints.

Figure 21. Relationship between the deviation from the release target quality and the suboptimization function for the coefficients presented in Table 5

3.1.4 FLOW AUGMENTATION ROUTINE

The flow augmentation algorithm is designed to modify reservoir release rates to better satisfy downstream water quality constraints. The data for each control point include a list of reservoirs that are operated to meet the water quality objectives. The water quality objective data consist of a target concentration and weighting factor, which reflects the relative importance of the parameter. The target concentration can be either specified in terms of minimum or maximum concentrations. The revised algorithm uses these data and the water quality solution from the previous time step in the following manner.

Step 1. Estimate the water quality for reservoir release rates from 0.2 to 3.0 times the reservoir release rate from the previous time step assuming a simple mass balance as follows:

$$C = \frac{Qs\ Cs + Qr\ Cr\ (K-1)}{Qr\ (K-1) + Qs} \tag{64}$$

where: C = estimated stream quality
Cs = computed stream quality for the previous time step
Cr = quality of the reservoir release
Qs = stream flow rate
Qr = reservoir release rate
K = scaling factor (from 0.2 to 3.0 in increments of 0.2)

Step 2. Compute the violation plus a penalty for water use for each reservoir release increment by:

$$V = W\ (C - C_t)^n + P\ Q_r \tag{65}$$

where: V = violation at flow scaling factor K
W = weighting factor
C = estimated stream quality
C_t = control point quality objective
n = exponent (currently = 1.33)
P = penalty for water use
Q_r = reservoir release rate

Step 3. Form a single relationship between reservoir release and total violations for each reservoir release increment by summing the violation from step 2 for each control point influenced by the reservoir for each water quality parameter.

Step 4. A curve fit is utilized to develop a second order relationship between violation and reservoir release increment which is then used to determine the flow increment which results in the estimated minimum violation. The change in flow is presently constrained by a factor of 0.75 or 2.0 times the previous reservoir release rate.

The equations above assume a penalty for exceeding the control point target quality, however penalties for falling below objectives are also allowed.

The magnitude of the violation can be made sensitive to increases or decreases in a certain water quality parameter. The flow augmentation routine is capable of determining reservoir releases necessary to compensate for a violation of water quality objective due to, for example, an exceedance of target concentrations caused by the local inflow. The effects of differences in penalties for use of water from different reservoirs can also be examined.

The present flow augmentation algorithm should be considered as a first step in developing a more comprehensive approach. The algorithm has one major limitation in that there is no accounting for changes in travel time when estimating the effects of modifying reservoirs releases. Also, the penalty function for water use is fairly crude and constraints on changes in flow are somewhat arbitrary. Accounting for travel time involves projecting the effects of local inflows on stream quality and incorporating the projection into the decision process. Travel time should also be considered when regulating flow for temperature and dissolved oxygen. Refinements of the water use penalty function and constraints on the rate of change in reservoir release rate involves modifying input routines to allow specification by the user and model testing to determine the optimal procedure for the solution. The penalty function could include the total amount of water available for augmentation, credits for power production (i.e., decreased penalty for higher head releases), and credits for releasing water as the reservoir volume approaches the top of the conservation pool.

4 INPUT STRUCTURE

4.1 ORGANIZATION OF INPUT

The input structure is designed to be flexible with respect to specifying characteristics of the reservoir system and other inputs to the system. Each input record is described in detail in the HEC-5Q manual on description of program input, presented in Exhibit 3. An example of input data is shown in Exhibit 1.

4.2 TYPE OF INPUT RECORDS

Two characters in columns 1 and 2 identify the various types of records used. For numerous records these characters trigger program options and cannot be omitted. Many of the records are optional depending on the simulation options selected. Types of records are as follows:

a. Title Information and Job Controls – TI through JZ Records. These records specify the title and simulation controls including the length of simulation and information about water quality output to the GUI interface and DSS files.

b. Water Surface Heat Exchange – EZ and ET Records. These records provide meteorological data for the temperature simulation. One EZ record identifies the meteorological zone and averaging time for the ET records that follow. ET Records define mean surface heat exchange characteristics for the averaging period (usually 6 to 24 hours).

c. Water Quality Constituents – QC and TQ Records. These records identify which water quality constituents will be modeled.

d. General Reservoir Data - L1 through AC Records. These records control the reservoir simulation and describe the physical characteristics of the reservoir. They define the printout interval, miscellaneous physical constants, and additional reservoir storage, area and elevation data (i.e., extension of, or modifications to, the HEC-5 RS, RA, RE Records). AC Records provide time dependent penalty functions for flow augmentation.

e. Vertically Segmented Reservoir Data - LR through PL Records. These records define additional reservoir and dam geometry, diffusion coefficients and outlet water quality suboptimization objective functions.

f. Longitudinally Segmented Reservoir Data - LS through LW Records. These records define layering and vertical flow distribution, depth versus elevation relationships for the individual reservoir elements and locations of inflows and withdrawals.

g. Initial Temperature and Water Quality Conditions - L9 and LX Records. The L9 record identifies the water quality parameter and uniform initial concentration for both types of reservoirs. LX Records define spatially varying quality. Default values are provided but their use is not recommended. If the initial quality is similar throughout the system, the initial quality need only be set for the first reservoir since water quality of all subsequent reservoirs is automatically set to the latest initial quality input values. In any event, sufficient startup time should be allowed as to minimize the impacts of the initial conditions.

h. Stream Related Data - S1 through ES Records. These records define printout controls, reach limits, local inflow and withdrawal locations, reaeration controls, channel cross section geometry data and energy grade line elevations. Uniform initial conditions may be defined (Y5 through SB Records) for all non-advected parameters such as benthic contamination. Steady state water quality is assumed for all advected parameters.

i. Chemical, Biological and Physical Coefficients - KA through EK Records. These records specify the various chemical, biological and physical coefficients required by the water quality relationships. The KA through KF records are global and apply to all reservoir and stream sections. They can only be set in association with the data for the first reservoir. Default values are assigned if the record is omitted. The remaining K1 through EK records are required for the first reservoir and first stream reach, but are optional for all other reservoirs and stream reaches. Coefficients specified for previous reservoirs or stream sections will apply if none are specified for subsequent reservoirs and stream reaches.

j. Control Point Objectives - CU through EC Records. These records specify control point water quality objectives and weighting functions for stream control points.

k. Local Inflow Temperature and Water Quality - I1 through EI Records. The I1 Record defines the time period of the inflow data. Each tributary inflow point requires an I2 Record plus sets of any of I3 through I8 Records to define water quality over the period of record. IG and IL Records are used to specify scaling factors for inflow temperature and water quality.

l. Gate Operations - G1 and G2 Records. These records define the operation schedule for the wet wells, flood control outlet and uncontrolled spillway. The values can be actual flows or relative weightings. As an option, temperature and water quality outflow objectives may be input and the outlet structure operated to meet these objectives.

5 OUTPUT

HEC-5Q model output is written to several files that are specified by input data controls. These output options include:

- ASCII HEC-5Q output file or traditional printer output
- Output file with results saved in a format required by the HEC-5Q Graphical User Interface (GUI)
- DSS water quality output file in which data are stored in the DSS file format for use by the HEC-5Q GUI or DSS utilities including DSSUTL, DSPLAY.

The GUI and DSS output options are generally preferred since the give a more comprehensive and informative display of the model results. The GUI output capabilities are described Exhibit 4 and DSS capabilities are described in the appropriate HECDSS documents.

5.1 ASCII OUTPUT FILE

The ASCII output file is designed to echo the input data for checking and documenting the simulation conditions. Results for the system components are written to the output file in the same order in which they are specified in the HEC-5Q input file. Its contents are itemized below. An example of the ASCII program output file is contained in Exhibit 2.

- General information about the reservoir, including water surface elevation, surface area, storage volume, and factors used in calculation of the heat budget,
- Inflow data including flows from tributaries, identified by tributary types, and flows specified at control points. The flow rate and water quality is shown for each inflow.
- Reservoir outflow data that include flows and water quality of releases from the flood control outlet, wet wells, diversions, and the total release downstream.
- Reservoir water quality for each element in the system. The format of this section varies depending on the reservoir representation, i.e., vertically, longitudinally, or layered and longitudinally segmented reservoir. All water quality constituents modeled are included in the output.
- Stream water quality for each element in the system. All water quality constituents modeled are included in the output.

The reservoir water quality output takes the following forms.

<u>Vertically Segmented Reservoirs:</u> For each vertically segmented reservoir, water quality data are presented for each constituent as a function of the mid-depth of the reservoir element. The depth of any flood control outlet (‘FC’) or wet well (‘W#’, with # representing the wet well number) is listed adjacent to the corresponding depth. The residence time in each element (or layer) is presented in the last column.

<u>Longitudinally Segmented Reservoirs:</u> Within the Reservoir Water Quality section, longitudinally segmented reservoirs are identified by the element river mile. The control point or tributary identification number of any local inflows and the associated flow fraction, as specified in the input file, are listed. If a tributary or control point number and flow fraction is not listed in the output file, the number following the river

mile designation represents the reservoir element number. The element water surface elevation is listed along with the flow. The ‘Reservoir Water Quality’ section also presents the time (in days) upstream of the dam, or the number of days (travel time) required for the volume of water in that element to reach the dam.

Layered and Longitudinally Segmented Reservoirs: In general, the format of the ‘Reservoir Water Quality’ section is the same as for longitudinally segmented reservoirs, with some additions necessary to present results for the different layers. At each river mile, the elevation at the mid-depth is presented for each layer in the ‘Mid-Elev’ column. Output results show water quality constituent concentrations, the water surface elevation, and the velocity within each layer at each river mile location. The travel time is based on the total flow rate and volume and does not consider variation in velocity over the depth.

Stream Related Output: Results for streams in the system are presented in the same order specified in the HEC-5Q input file (S2 Records). The section begins with a summary of the meteorological zone data, followed by reservoir release flows and water quality. Local flows, return flows and diversions and their associated water quality are also summarized. Stream results are presented for each reach in the system, designated by river mile from the upstream end to the downstream end of the reach and the control points at each end. For each reach, tributary flows and the local flow fraction are listed at the river mile location at which they have been applied. Mean flow and water surface elevation is presented at each river mile. The value in the ‘time’ column represents the travel time calculated from the dam at the upstream end of the reach.

6 REFERENCES

American Society of Civil Engineers (ASCE), 1977. Sedimentation Engineering, V. A. Vanoni, ed., New York: ASCE.

Anderson, E.R., 1954. "Water Loss Investigations: Lake Hefner Studies," Technical Report, Project Paper 269, Geological Survey, U.S. Department of Interior, Washington, D.C..

Baca, R.G., A.F. Gasperino, A. Brandstetter and M.S. Annette, 1977. "Water Quality Models for Municipal Water Supply Reservoirs," a report prepared for the Engineering and Water Supply Department, Adelaide, South Australia.

Bohan, J.P. and J.L. Grace, Jr., 1973.."Selective Withdrawal from Man-made Lakes; Hydraulic Laboratory Investigation," Technical Report H-73-4, U.S. Army Engineer Waterways Experiment Station, CE, Vicksburg, MS.

Debler, W.R., 1959. "Stratified Flow into a Line Sink," ASCE Journal of Engineering Mechanics Division, Vol. 85, EM3.

DiToro, D. M., J. F. Fitzpatrick and R. R. Islieb, 1994. “A Model of Manganese and Iron Fluxes from Sediments,” Report to the U. S. Army Corps of Engineers’ Waterways Experiment Station, Report No. W-94-1.

Edinger, J.E. and J.C. Geyer, 1965. "Heat Exchange in the Environment," Department of Sanitary Engineering and Water Resources, Research Project No. 49, The John Hopkins University, Baltimore, Maryland.

Hutchinson, G.E., 1957. "A Treatise on Limnology," Volume I, Geography, Physics and Chemistry, New York: John Wiley and Sons, Inc..

Hydrologic Engineering Center, 1979. "HEC-5, Simulation of Flood Control and Conservation Systems, User's Manual", Davis, CA.

Hydrologic Engineering Center, 1986a. "HEC-5, Simulation of Flood Control and Conservation Systems, Appendix on Water Quality Analysis", Davis, CA.

Hydrologic Engineering Center (HEC), 1986b. “Kanawha River Basin Water Quality Modeling,” Project Report to U.S. Army Corps of Engineers, Huntington District.

Hydrologic Engineering Center (HEC), 1987. “Monongahela River Basin Water Quality Modeling,” Project Report to U.S. Army Corps of Engineers, Pittsburgh District.

Hydrologic Engineering Center (HEC), 1994. “McKenzie River Water Temperature Study,” Project Report to U.S. Army Corps of Engineers, Portland District.

Hydrologic Engineering Center (HEC), 1996. “Big Sandy River Water Conservation and Water Quality Study,” Project Report to U.S. Army Corps of Engineers, Huntington District.

Hydrologic Engineering Center (HEC), 1996. “HEC-5 Simulation of Flood Control and Conservation Systems, Appendix on Water Quality Analysis,” Computer Program Manual, Description of Program Input.

Hydrologic Engineering Center (HEC), 1997. “HEC-5 Simulation of Flood Control and Conservation Systems,” Computer Program User’s Manual.

Kanwisher, J., 1963. "On the Exchange of Gases Between the Atmosphere and Sea," Deep Sea Research, Vol. 10, pp. 195-207.

Kaplan, E., 1974. "Reservoir Optimization for Water Quality Control", PH.D dissertation, University of Pennsylvania.

O'Connor, D.J. and W.E. Dobbins, 1958. "Mechanism of Reaeration in Natural Streams," Transactions, American Society of Civil Engineers, Volume 123.

Stumm, W. and J. J. Morgan, 1981. Aquatic Chemistry: An Introduction Emphasizing Chemical Equilibria in Natural Waters, 2nd ed. New York: John Wiley.

Stumm, W. and J. J. Morgan, 1996. Aquatic Chemistry: Chemical Equilibria and Rates in Natural Waters, 3rd ed. New York: John Wiley.

Stumm, W., 1992. Chemistry of the Solid-Water Interface, New York: John Wiley.

Tennessee Valley Authority, 1972. "Heat and Mass Transfer Between a Water Surface and the Atmosphere," Report No. 14.

Thomann, R. V. and J. A. Mueller, 1987. Principles of Surface Water Quality Modeling and Control, New York: Harper Collins.

U. S. Army Corps of Engineers (USACE), 1974. Baltimore District, "Thermal Simulation of Lakes, User's Manual".

U. S. Army Corps of Engineers, Baltimore District, 1977. “Thermal Simulation of Lakes,” Computer Program Description.

Water Resources Engineers (WRE), 1968. "Prediction of Thermal Energy Distribution in Streams and Reservoirs," Report to Department of Fish and Game, State of California.

Water Resources Engineers (WRE), 1969a. "The Thermal Simulation of Applegate Reservoir to Evaluate the Effect of Outlet Placement and Discharge on Downstream Temperature," report to Corps of Engineers, Portland District.

Water Resources Engineers (WRE), 1969b. "Mathematical Models for the Prediction of Thermal Energy Changes in Impoundments," report to the Environmental Protection Agency.

Waterways Experiment Station (WES), U. S. Army Corps of Engineers, 1986. “CE-QUAL-R1: A Numerical One-Dimensional Model of Reservoir Water Quality,” User’s Manual, Report no. E-82-1.

Willey, R. G., 1987. “Water Quality Modeling of Reservoir System Operations Using HEC-5,” Training Document 24, Hydrologic Engineering Center, U.S. Army Corps of Engineers, Davis, California.