factors that can potentially limit algal growth. Each constant is actually the level at which that particular factor limits algal growth to half the maximal or "saturated" rate (Bowie et al., 1985). Table III-3 at the end of this chapter lists typical values of the half-saturation constants for nitrogen and phosphorus. If algal concentrations are simulated and either nitrogen, phorphorus, or both are not simulated, the program assumes that the parameter not simulated is not limiting.

3.2.5 Temperature Dependence in Algae Simulation

The algal growth rate and death rates are temperature dependent. They are corrected within the model, as are all other temperature dependent systems variables, according to the procedure explained in Section 3.10.

3.3 NITROGEN CYCLE

In natural aerobic waters, there is a stepwise transformation from organic nitrogen to ammonia, to nitrite, and finally to nitrate. The nitrogen cycle in QUAL2E contains all four of these components, as shown in Figure III-1. The incorporation of organic nitrogen as a state variable, an organic nitrogen settling term, and an algal nitrogen uptake preference factor are the primary enhancements to the nitrogen cycle in QUAL2E compared to the SEMCOG version of QUAL-II. The differential equations governing transformations of nitrogen from one form to another are shown below.

3.3.1 Organic Nitrogen

$$\frac{dN_4}{dt} = \alpha_1 \rho A - \beta_3 N_4 - \sigma_4 N_4 \qquad \text{III-16}$$

where

N_4 = concentration of organic nitrogen, mg-N/L

β_3 = rate constant for hydrolysis of organic nitrogen to ammonia nitrogen, temperature dependent, day^{-1}

α_1 = fraction of algal biomass that is nitrogen, mg-N/mg-A

ρ = Algal respiration rate, day^{-1}

A = algal biomass concentration, mg-A/L

σ_4 = rate coefficient for organic nitrogen settling, temperature dependent, day^{-1}

3.3.2 Ammonia Nitrogen

$$\frac{dN_1}{dt} = \beta_3 N_4 - \beta_1 N_1 + \sigma_3/d - F_1 \alpha_1 \mu A \qquad \text{III-17}$$

where

$$F_1 = P_N N_1/(P_N N_1 + (1 - P_N)N_3) \qquad \text{III-18}$$

N_1 = the concentration of ammonia nitrogen, mg-N/L

N_3 = the concentration of nitrate nitrogen, mg-N/L

N_4 = the concentration of organic nitrogen, mg-N/L

β_1 = rate constant for the biological oxidation of ammonia nitrogen, temperature dependent, day^{-1}

β_3 = organic nitrogen hydrolysis rate, day^{-1}

α_1 = fraction of algal biomass which is nitrogen, mg-N/mg-A

σ_3 = the benthos source rate for ammonia nitrogen, mg-N/ft^2-day

d = mean depth of flow, ft

F_1 = fraction of algal nitrogen uptake from ammonia pool

μ = the local specific growth rate of algae, day^{-1}

A = algal biomass concentration, mg-A/L

P_N = preference factor for ammonia nitrogen (0 to 1.0)

The QUAL2E model includes an algal preference factor for ammonia, P_N (Bowie et al., 1985; JRB Associates, 1983). The ammonia preference factor is equivalent to the fraction of algal nitrogen uptake from the ammonia pool when the concentrations of ammonia and nitrate nitrogen are equal.

3.3.3 Nitrite Nitrogen

$$\frac{dN_2}{dt} = \beta_1 N_1 - \beta_2 N_2 \qquad \text{III-19}$$

where

N_1 = the concentration of ammonia nitrogen, mg-N/L

N_2 = the concentration of nitrite nitrogen, mg-N/L

β_1 = rate constant for the oxidation of ammonia nitrogen, temperature dependent, day^{-1}

β_2 = rate constant for the oxidation of nitrite nitrogen, temperature dependent, day^{-1}

3.3.4 Nitrate Nitrogen

$$\frac{dN_3}{dt} = \beta_2 N_2 - (1 - F)\alpha_1 \mu A \qquad \text{III-20}$$

where

F = fraction of algal nitrogen taken from ammonia pool, as defined in Section 3.3.2

α_1 = fraction of algal biomass that is nitrogen, mg-N/mg-A

μ = local specific growth rate of algae, day^{-1}

3.3.5 Inhibition of Nitrification at Low Dissolved Oxygen

QUAL2E has the capability of inhibiting (retarding) the rate of nitrification at low values of dissolved oxygen. This inhibition effect has been reported by others (Department of Scientific and Industrial Research, 1964; Texas Water Development Board, 1984).

Nitrification rates are modified in QUAL2E by computing an inhibition correction factor (having a value between zero and one) and then applying this factor to the values of the nitrification rate coefficients, β_1, and β_2. The nitrification rate correction factor is computed according to a first order equation:

$$\text{CORDO} = 1.0 - \exp(-\text{KNITRF} * \text{DO}) \qquad \text{III-21}$$

where

CORDO = nitrification rate correction factor

exp = exponential function

KNITRF = first order nitrification inhibition coefficient, mg/L^{-1}

DO = dissolved oxygen concentration, mg/L

The correction factor is applied to the ammonia and nitrite oxidation rates by:

$$\text{Ammonia:} \quad (\beta_1)_{inhib.} = CORDO * (\beta_1)_{input} \qquad \text{III-22}$$

$$\text{Nitrite:} \quad (\beta_2)_{inhib.} = CORDO * (\beta_2)_{input} \qquad \text{III-23}$$

A value of 0.6 for KNITRF closely matches the inhibition formulation in QUAL-TX, the Texas Water Development Board version of QUAL-II, whereas, a value of 0.7 closely simulates the data for the Thames Estuary (DSIR, 1964).

3.4 PHOSPHORUS CYCLE

The phosphorus cycle operates like the nitrogen cycle in many respects. Organic forms of phosphorus are generated by the death of algae, which then convert to the dissolved inorganic state, where it is available to algae for primary production. Phosphorus discharged from sewage treatment plants is generally in the dissolved inorganic form and is readily taken up by algae (Bowie et al., 1985). QUAL2E revises the SEMCOG version of QUAL-II, which included only dissolved phosphorus, to simulate the interactions between organic and dissolved phosphorus. Below are the differential equations governing transformations of phosphorus from one form to another.

3.4.1 Organic Phosphorus

$$\frac{dP_1}{dt} = \alpha_2 \rho A - \beta_4 P_1 - \sigma_5 P_1 \qquad \text{III-24}$$

where

P_1 = the concentration of organic phosphorus, mg-P/L

α_2 = phosphorus content of algae, mg P/mg-A

ρ = algal respiration rate, day^{-1}

A = algal biomass concentration, mg-A/L

β_4 = organic phosphorus decay rate, temperature dependent, day^{-1}

σ_5 = organic phorphorus settling rate, temperature dependent, day^{-1}

3.4.2 Dissolved Phosphorus

$$\frac{dP_2}{dt} = \beta_4 P_1 + \sigma_2/d - \alpha_2 \mu A \qquad \text{III-25}$$

where

P_2 = concentration of inorganic or dissolved phosphorus, mg-P/L

σ_2 = benthos source rate for dissolved phosphorus, temperature dependent, mg-P/ft^2-day

d = mean stream depth, ft

μ = algal growth rate, day^{-1}

A = algal biomass concentration, mg-A/L

3.5 CARBONACEOUS BOD

The QUAL2E model assumes a first order reaction to describe deoxygenation of ultimate carbonaceous BOD in the stream. The BOD function as expressed in the model also takes into account additional BOD removal due to sedimentation, scour and flocculation, which do not exert an oxygen demand (Thomas, 1948):

$$\frac{dL}{dt} = - K_1 L - K_3 L \qquad \text{III-26}$$

where

L = the concentration of ultimate carbonaceous BOD, mg/L

K_1 = deoxygenation rate coefficient, temperature dependent, day^{-1}

K_3 = the rate of loss of carbonaceous BOD due to settling, temperature dependent, day^{-1}

QUAL2E simulates ultimate BOD in the general case; however, the user may choose to use 5-day BOD values for input and output. In this case, the model will make the necessary coversions from 5-day to ultimate BOD. The conversion equation is:

$$BOD_5 = BOD_u \, (1.0 - \exp(5 * KBOD)) \qquad \text{III-27}$$

where

BOD_5 = 5-day BOD, mg/L

BOD_u = ultimate BOD, mg/L

KBOD = BOD conversion rate coefficient, day^{-1}

The SEMCOG version of QUAL-II uses a value of 0.23 day^{-1} for KBOD. With QUAL2E, the user may specify the appropriate value for this conversion. Note: when modeling 5-day BOD, the same conversion coefficient is applied to all input BOD_5 forcing functions (headwaters, incremental flows, point loads, and the downstream boundary condition).

3.6 DISSOLVED OXYGEN

The oxygen balance in a stream system depends on the capacity of the stream to reaerate itself. This capacity is a function of the advection and diffusion processes occurring within the system and the internal sources and sinks of oxygen. The major sources of oxygen, in addition to atmospheric reaeration, are the oxygen produced by photosynthesis and the oxygen contained in the incoming flow. The sinks of dissolved oxygen include biochemical oxidation of carbonaceous and nitrogenous organic matter, benthic oxygen demand and the oxygen utilized by algae respiration (Bowie et al., 1985).

The differential equation used in QUAL2E to describe the rate of change of oxygen is shown below. Each term represents a major source or sink of oxygen.

$$\frac{dO}{dt} = K_2(O^*-O) + (\alpha_3 \mu - \alpha_4 \rho) A - K_1 L - K_4/d - \alpha_5 \beta_1 N_1 - \alpha_6 \beta_2 N_2 \quad \text{III-28}$$

where

O = the concentration of dissolved oxygen, mg/L

O^* = the saturation concentration of dissolved oxygen at the local temperature and pressure, mg/L

α_3 = the rate of oxygen production per unit of algal photosynthesis, mg-O/mg-A

α_4 = the rate of oxygen uptake per unit of algae respired, mg-O/mg-A

α_5 = the rate of oxygen uptake per unit of ammonia nitrogen oxidation, mg-O/mg-N

α_6 = the rate of oxygen uptake per unit of nitrite nitrogen oxidation, mg-O/mg-N

μ = algal growth rate, temperature dependent, day^{-1}

ρ = algal respiration rate, temperature dependent, day^{-1}

A = algal biomass concentration, mg-A/L

L = concentration of ultimate carbonaceous BOD, mg/L

d = mean stream depth, ft

K_1 = carbonaceous BOD deoxygenation rate, temperature dependent, day^{-1}

K_2 = the reaeration rate in accordance with the Fickian diffusion analogy, temperature dependent, day^{-1}

K_4 = sediment oxygen demand rate, temperature dependent, g/ft^2-day

β_1 = ammonia oxidation rate coefficient, temperature dependent, day^{-1}

β_2 = nitrite oxidation rate coefficient, temperature dependent, day^{-1}

N_1 = ammonia nitrogen concentration, mg-N/L

N_2 = nitrite nitrogen concentration, mg-N/L

3.6.1 Dissolved Oxygen Saturation Concentration

The solubility of dissolved oxygen in water decreases with increasing temperature, increasing dissolved solids concentration, and decreasing atmospheric pressure (Bowie et al., 1985). QUAL2E uses a predictive equation for the saturation (equilibrium) concentration of dissolved oxygen (APHA, 1985).

$$\ln O^* = -139.34410 + (1.575701 \times 10^5/T) - (6.642308 \times 10^7/T^2) + (1.243800 \times 10^{10}/T^3) - (8.621949 \times 10^{11}/T^4) \qquad \text{III-29}$$

where:

O^* = equilibrium oxygen concentration at 1.000 atm, mg/L

T = temperature (°K) = (°C+273.150) and °C is within the range 0.0 to 40.0°C

For non-standard conditions of pressure, the equilibrium concentration of dissolved oxygen is corrected by the equation III-30:

$$Op = O^*P \left[\frac{(1-P_{wv}/P)\ (1-\phi P)}{(1-P_{wv})\ (1-\phi)}\right] \qquad \text{III-30}$$

where

Op = equilibrium oxygen concentration at non-standard pressure, mg/L

O* = equilibrium oxygen concentration at 1.000 atm, mg/L

P = pressure (atm) and is within 0.000 to 2.000 atm

P_{wv} = partial pressure of water vapor (atm), which may be computed from:

$$\ln P_{wv} = 11.8571 - (3840.70/T) - 216961/T^2) \qquad \text{III-31}$$

and

$$\phi = 0.000975 - (1.426 \times 10^{-5}t) + (6.436 \times 10^{-8}t^2) \qquad \text{III-32}$$

where

t = temperature, °C

The equations in Standard Methods (1985) for computing dissolved oxygen saturation concentrations also include corrections for salinity and chloride. Because neither salinity nor chloride is explicitly modeled, QUAL2E does not correct O* for chloride or salinity. Furthermore, the pressure correction to O* (Equation III-30) is made only when temperature is modeled, because barometric pressure data are a primary requirement of the heat balance equations.

The dissolved oxygen saturation concentrations computed from the Texas and SEMCOG versions of QUAL-II are compared to those from the Standard Methods formulations of QUAL2E in Table III-1.

3.6.2 Atmospheric Reaeration Coefficient Estimation

The reaeration coefficient (K_2) is most often expressed as a function of stream depth and velocity. QUAL2E provides eight options for estimating or reading in K_2 values, which are discussed in the sections below. A comparative study of reaeration prediction equation performance has been reported by St. John et al. (1984).

TABLE III-1
COMPARISON OF DISSOLVED OXYGEN SATURATION CONCENTRATIONS
(Barometric Pressure = 1 atm, Chloride = 0.0mg/L,
Equilibrium with Air Saturated with Water Vapor)

Temperature, °C	QUAL-II SEMCOG	QUAL-TX Texas	QUAL2E Std. Meth.
0.	14.631	14.584	14.621
1.	14.227	14.187	14.217
2.	13.837	13.806	13.830
3.	13.461	13.441	13.461
4.	13.100	13.091	13.108
5.	12.752	12.755	12.771
6.	12.418	12.433	12.448
7.	12.096	12.124	12.139
8.	11.787	11.828	11.843
9.	11.489	11.544	11.560
10.	11.203	11.271	11.288
11.	10.927	11.009	11.027
12.	10.661	10.758	10.777
13.	10.406	10.517	10.537
14.	10.159	10.285	10.306
15.	9.922	10.062	10.084
16.	9.692	9.848	9.870
17.	9.471	9.642	9.665
18.	9.257	9.444	9.467
19.	9.050	9.253	9.276
20.	8.849	9.069	9.093
21.	8.655	8.891	8.915
22.	8.465	8.720	8.744
23.	8.281	8.555	8.578
24.	8.101	8.396	8.418
25.	7.925	8.241	8.264
26.	7.753	8.092	8.114
27.	7.584	7.948	7.969
28.	7.417	7.807	7.828
29.	7.252	7.672	7.691
30.	7.089	7.540	7.559
31.	6.927	7.412	7.430
32.	6.765	7.288	7.305
33.	6.604	7.167	7.183
34.	6.442	7.049	7.065
35.	6.280	6.935	6.949
36.	6.116	6.823	6.837
37.	5.950	6.715	6.727
38.	5.782	6.609	6.620
39.	5.612	6.506	6.515
40.	5.438	6.406	6.413

K_2 Option 1

Option 1 allows the user to read in K_2 values that have been previously selected by the modeler. This option is useful in modeling unusual situations such as ice cover (see Section 3.6.3).

K_2 Option 2

Using data collected in field measurements of stream reaeration, Churchill, Elmore, and Buckingham (1962) developed the following expression for K_2 at 20°C.

$$K_2^{20} = 5.026\ \bar{u}^{0.969}\ d^{-1.673} \times 2.31 \qquad \text{III-33}$$

where

$\bar{u}$ = average velocity in the stream, ft/sec.

d = average depth of the stream, ft

K_2 = reaeration coefficient, day^{-1}

K_2 Option 3

O'Connor and Dobbins (1958) proposed equations based on the turbulence characteristics of a stream. For streams displaying low velocities and isotropic conditions, Equation III-34 was developed:

$$K_2^{20} = \frac{(D_m\ \bar{u})^{0.5}}{d^{1.50}} \qquad \text{III-34}$$

For streams with high velocities and nonisotropic conditions, the relationship is:

$$K_2^{20} = \frac{480 D_m^{0.5}\ S_o^{0.25}}{d^{1.25}} \times 2.31 \qquad \text{III-35}$$

where

S_o = slope of the streambed, ft/ft

d = mean stream depth, ft

$\bar{u}$ = mean velocity, ft/day

K_2 = reaeration coefficient, day^{-1}

and D_m is the molecular diffusion coefficient (ft^2/day), which is given by:

$$D_m = 1.91 \times 10^3 \ (1.037)^{T-20} \qquad \text{III-36}$$

Equation III-34 has been found to be generally applicable for most cases and is the equation used in QUAL2E for Option 3. Equation III-35 can be used to calculate K_2 outside the model and input it directly under Option 1.

K_2 Option 4

Based on the monitoring of six streams in England, Owens et al. (1964) obtained reaeration estimates for shallow, fast moving streams. Combining their data with that of Churchill et al., they developed an euation for streams exhibiting depths of 0.4 to 11.0 feet and velocities of 0.1 to 5.0 ft/sec:

$$K_2^{20} = 9.4 \ \bar{u}^{0.67}/d^{1.85} \times 2.31 \qquad \text{III-37}$$

where

$\bar{u}$ = mean velocity, ft/sec

d = mean depth, ft

K_2 Option 5

Thackston and Krenkel (1966) proposed the following equation based on their investigation of several rivers in the Tennessee Valley Authority system.

$$K_2^{20} = 10.8 \ (1 + F^{0.5}) \ \frac{u^*}{d} \times 2.31 \qquad \text{III-38}$$

where F is the Froude number, which is given by:

$$F = \frac{u^*}{\sqrt{g\ d}} \qquad \text{III-39}$$

and u* is the shear velocity, ft/sec.:

$$u^* = \sqrt{d\ S_e g} = \frac{\bar{u}\ n\ \sqrt{g}}{1.49\ d^{1.167}} \qquad \text{III-40}$$

where

d = mean depth, ft

g = acceleration of gravity, ft/sec^2

S_e = slope of the energy gradient

$\bar{u}$ = mean velocity, ft/sec

n = Manning's coefficient

K_2 Option 6

Langbien and Durum (1967) developed a formula for K_2 at 20°C:

$$K_2^{20} = 3.3\ \bar{u}/d^{1.33} \times 2.31 \qquad \text{III-41}$$

where

$\bar{u}$ = mean velocity, ft/sec

d = mean depth, ft

K_2 Option 7

This option computes the reaeration coefficient from a power function of flow. This empirical relationship is similar to the velocity and depth correlations with flow used in the hydraulics section of QUAL2E, i.e.,

$$K_2 = aQ^b \qquad \text{III-42}$$

where

a = coefficient of flow for K_2

Q = flow, ft^3/sec

b = exponent on flow for K_2

K_2 Option 8

The method of Tsivoglou and Wallace (1972) assumes that the reaeration coefficient for a reach is proportional to the change in elevation of the water surface in the reach and inversely proportional to the flow time through the reach. The equation is:

$$K_2^{20} = c \frac{\Delta h}{t_f} \qquad \text{III-43}$$

where

c = escape coefficient, ft^{-1}

Δh = change in water surface elevation in reach, ft

t_f = flow time within reach, days

Assuming uniform flow, the change in water surface elevation is

$$\Delta h = S_e \Delta x \qquad \text{III-44}$$

where

S_e = slope of the energy gradient, ft/ft

Δx = reach length, ft

and the time of passage through a reach is

$$t_f = \frac{\Delta x}{\bar{u}} \qquad \text{III-45}$$

where

$\bar{u}$ = mean velocity in reach, ft/sec

Substituting the above in equation III-43 gives

$$K_2^{20} = (3600 \times 24)\, c S_e \bar{u} \qquad \text{III-46}$$

Equation III-46 is the form of Option 8 used in QUAL2E. The constants 3600 and 24 convert velocity to units of feet per day. The slope may be input directly for computing K_2 with this option, or it can be calculated from Manning's equation as follows

$$S_e = \frac{\bar{u}^2 n^2}{(1.49)^2 d^{4/3}} \qquad \text{III-47}$$

where

d = mean depth, ft

n = Manning's coefficient

The escape coefficient is usually treated as a variable and determined empirically. TenEch (1978) recommends the following guideline in determining c values, analogous to that recommended for uncalibrated stream segments by Tsivoglou and Neal (1976):

$c = 0.054\ ft^{-1}$ (at 20°C) for $15 <= Q <= 3000\ ft^3/sec$

$c = 0.110\ ft^{-1}$ (at 20°C) for $1 <= Q <= 15\ ft^3/sec$

3.6.3 Ice Cover

Ice cover on streams during winter low flow conditions may significantly affect reaeration. Reaeration rates are decreased because ice cover reduces the surface area of the air-water interface through which reaeration occurs (TenEch, 1978). Approaches recommended by TenEch (1978) for estimating the extent of ice cover include:

- Statistical analyses of past records
- Steady state heat budget analysis (including the U.S. Army Corps of Engineers differential equations)
- Extensive field observations

To adjust the reaeration rate for winter ice cover conditions in the QUAL2E model, the calculated reaeration rate must be multiplied by an "ice cover factor" and input under Option 1. TenEch recommends factors ranging from 0.05 for complete ice cover to 1.0 for no ice cover. Depending on the extent of cover, reaeration values can be greatly reduced.

3.6.4 K_2 Default Values

There are no default K_2 values in QUAL2E. In some versions of QUAL-II, a default value of K_2 is computed, accounting for the influences of wind-induced turbulence and diffusion under low-velocity conditions. In those models, when the calculated values of K_2 are less than two divided by the depth of the reach (2/d), K_2 is set equal to 2/d. This feature has not always proved useful, particularly when simulating the very low reaeration rates; thus it is not included in QUAL2E.

3.6.5 Dam Reaeration

QUAL2E has the capability of modeling oxygen input to the system from reaeration over dams. The following equation described by Butts and Evans (1983) and attributable to Gameson is used to estimate oxygen input from dam reaeration.

$$D_a - D_b = \left[1 - \frac{1}{1 + 0.116abH(1 - 0.034H)(1 + 046T)}\right] D_a \quad \text{III-48}$$

where

D_a = oxygen deficit above dam, mg/L

D_b = oxygen deficit below dam, mg/L

T = temperature, °C

H = height through which water falls, ft

a = empirical water quality factor

= 1.80 in clean water

= 1.60 in slightly polluted water

= 1.0 in moderately polluted water

= 0.65 in grossly polluted water

b = empirical dam aeration coefficients

= 0.70 to 0.90 for flat broad crested weir

= 1.05 for sharp crested weir with straight slope face

= 0.80 for sharp crested weir with vertical face

= 0.05 for sluice gates with submerged discharge

The factors H, a and b are input for each dam. The model includes a provision for bypassing some or all of the flow around the dams (e.g., through generators). The fraction of the total flow that spills over the dam is supplied as an input variable.

3.7 COLIFORMS

Coliforms are used as an indicator of pathogen contamination in surface waters. Expressions for estimating coliform concentrations are

usually first order decay functions, which only take into account coliform die-off (Bowie et al., 1985). The QUAL2E model uses such an expression:

$$\frac{dE}{dt} = - K_5 E \qquad \text{III-49}$$

where

E = concentration of coliforms, colonies/100 ml

K_5 = coliform die-off rate, temperature dependent, day^{-1}

3.8 ARBITRARY NONCONSERVATIVE CONSTITUENT

QUAL2E has the provision for modeling an arbitrary nonconservative constituent (ANC). In addition to a first order decay mechanism, there are source and sink terms in the mass balance. The differential equation describing the interactions for an arbitrary nonconservative constituent is:

$$\frac{dR}{dt} = -K_6 R - \sigma_6 R + \sigma_7/d \qquad \text{III-50}$$

where

R = concentration of the nonconservative constituent, mg-ANC/L

K_6 = decay rate for the constituent, temperature dependent, day^{-1}

σ_6 = rate coefficient for constituent settling, temperature dependent, day^{-1}

σ_7 = benthal source for constituent, temperature dependent, mg-ANC/ft^2-day

d = mean stream depth, ft

3.9 TEMPERATURE

Temperature is modeled by performing a heat balance on each computational element in the system. The heat balance accounts for temperature inputs and losses from the forcing functions as well as the heat exchanged between the water surface and the atmosphere. The air-water heat balance terms include long and short wave radiation, convection, and evaporation using:

$$H_n = H_{sn} + H_{an} - H_b - H_c - H_e \qquad \text{III-51}$$

where

H_n = net heat flux passing the air water surface, Btu/ft^2-day

H_{sn} = net short wave solar radiation after losses from absorption and scattering in the atmosphere and by reflection at the interface, Btu/ft^2-day

H_{an} = net long wave atmosphere radiation after reflection, Btu/ft^2-day

H_b = outgoing long wave back radiation, Btu/ft^2-day

H_c = convective heat flux, Btu/ft^2-day

H_e = heat loss by evaporation, excluding sensible heat loss, Btu/ft^2-day

In order for QUAL2E to perform the heat balance computations, the user must supply a variety of data, including the longitude and latitude of the basin, the time of year, evaporation coefficients, and a dust attenuation coefficient. Local climatological information in the form of time of day, wet and dry bulb air temperatures, atmospheric pressure, cloud cover and wind velocity also must be provided.

In the dynamic mode, local climatological data must be supplied at regular (typically 3 hour) intervals. In this manner the source/sink term for the heat balance is updated in time to simulate the diurnal response of the steady hydraulic system to changing temperature conditions.

In the steady state mode, average local climatological data must be supplied by the user. The program uses linear approximations for the long-wave back radiation and evaporation terms for solution of the steady state heat balance. The reader is referred to Chapter 4 of this report for a detailed treatment of the temperature simulation.

In the dynamic mode, local climatology data are applied uniformly over the entire river basin (i.e., there is no spatial variation). In the steady state mode, local climatology data may vary spatially by reach.

3.10 TEMPERATURE DEPENDENCE OF RATE COEFFICIENTS

The temperature values computed in QUAL2E are used to correct the rate coefficients in the source/sink terms for the other water quality variables. These coefficients are input at 20°C and are then corrected to temperature using a Streeter-Phelps type formulation:

$$X_T = X_{20}\ \theta^{(T-20°)} \qquad \text{III-52}$$

where

X_T = the value of the coefficient at the local temperature (T)

X_{20} = the value of the coefficient at the standard temperature (20°C)

θ = an empirical constant for each reaction coefficient

The values of the temperature correction factors, θ, may be specified by the user. In the absence of user specified values, the default values shown in Table III-2 are employed. For comparison purposes, the θ values used in the SEMCOG version of QUAL-II are also listed in Table III-2.

If temperature is not simulated, the temperature value specified for the initial condition is assumed to be the temperature for the simulation.

3.11 REACTION RATES AND PHYSICAL CONSTANTS

The chemical and biological reations that are simulated by QUAL2E are represented by a complex set of equations that contain many system parameters; some are constant, some are spatially variable, and some are temperature dependent. Table III-3 lists these system parameters and gives the usual range of values, units, and types of variation. Kramer (1970), Chen and Orlob (1972), and Bowie et al. (1985) give detailed discussions of the basic sources of data, ranges and reliabilities of each of these parameters. Final selection of the values for many of these system parameters or measurement of sensitive ones should be made during model calibration and verification.

TABLE III-2
DEFAULT TEMPERATURE CORRECTION, θ, VALUES FOR QUAL2E

Rate Coefficient	Symbol	Default Values SEMCOG	Default Values QUAL2E
BOD Decay	K_1	1.047	1.047
BOD Settling	K_3	-	1.024
Reaeration	K_2	1.0159	1.024
SOD Uptake	K_4	-	1.060
Organic N Decay	β_3	-	1.047
Organic N Settling	σ_4	-	1.024
Ammonia Decay	β_1	1.047	1.083
Ammonia Source	σ_3	-	1.074
Nitrite Decay	β_2	1.047	1.047
Organic P Decay	β_4	-	1.047
Organic P Settling	σ_5	-	1.024
Dissolved P Source	σ_2	-	1.074
Algal Growth	μ	1.047	1.047
Algal Respiration	ρ	1.047	1.047
Algal Settling	σ_1	-	1.024
Coliform Decay	K_5	1.047	1.047
ANC	K_6	1.047	1.000
ANC	σ_6	-	1.024
ANC	σ_7	-	1.000

Note: - = not temperature dependent in QUAL-II SEMCOG.

ANC = Arbitrary Nonconservative Constituent

TABLE III-3
TYPICAL RANGES FOR QUAL2E REACTION COEFFICIENTS

Variable	Description	Units	Range of Values	Variable by Reach	Temperature Dependent
α_0	Ratio of chlorophyll-a to algal biomass	$\frac{\text{ug-Chla}}{\text{mg A}}$	10-100	No	No
α_1	Fraction of algal biomass that is Nitrogen	$\frac{\text{mg-N}}{\text{mg A}}$	0.07-0.09	No	No
α_2	Fraction of algal biomass that is Phosphorus	$\frac{\text{mg-P}}{\text{mg A}}$	0.01-0.02	No	No
α_3	O_2 production per unit of algal growth	$\frac{\text{mg-O}}{\text{mg A}}$	1.4-1.8	No	No
α_4	O_2 uptake per unit of algae respired	$\frac{\text{mg-O}}{\text{mg A}}$	1.6-2.3	No	No
α_5	O_2 uptake per unit of NH_3 oxidation	$\frac{\text{mg-O}}{\text{mg N}}$	3.0-4.0	No	No
α_6	O_2 uptake per unit of NO_2 oxidation	$\frac{\text{mg-O}}{\text{mg N}}$	1.0-1.14	No	No
μ_{max}	Maximum algal growth rate	day^{-1}	1.0-3.0	No	No
ρ	Algal respiration rate	day^{-1}	0.05-0.5	No	No
K_L	Michaelis-Menton half-saturation constant for light (Option 1)	Btu/ft^2-min	0.02-0.10	No	No
K_N	Michaelis-Mention half-saturation constant for nitrogen	mg-N/L	0.01-0.30	No	No
K_P	Michaelis-Menton half-saturation constant for phosphorus	mg-P/L	.001-0.05	No	No
λ_0	Non-algal light extinction coefficient	ft^{-1}	Variable	No	No
λ_1	Linear algal self-shading coefficient	$\frac{\text{1/ft}}{\text{ug Chla/L}}$	0.002-0.02	No	No

TABLE III-3 (cont'd)
TYPICAL RANGES FOR QUAL2E REACTION COEFFICIENTS

Variable	Description	Units	Range of Values	Variable by Reach	Temperature Dependent
λ_2	Nonlinear algal self-shading coefficient	$\frac{1/ft}{(\lambda g\ Chla/L)^{2/3}}$	0.0165 (Riley)	No	No
P_N	Algal preference factor for ammonia	-	0.0-1.0	No	No
σ_1	Algal settling rate	ft/day	0.5-6.0	Yes	Yes
σ_2	Benthos source rate for dissolved phosphorus	$\frac{mg\text{-}P}{ft^2\text{-}day}$	Variable	Yes	Yes
σ_3	Benthos source rate for ammonia nitrogen	$\frac{mg\text{-}O}{ft^2\text{-}day}$	Variable	Yes	Yes
σ_4	Organic nitrogen settling rate	day^{-1}	0.001-0.1	Yes	Yes
σ_5	Organic phosphorus settling rate	day^{-1}	0.001-0.1	Yes	Yes
σ_6	Arbitrary non-conservative settling rate	day^{-1}	Variable	Yes	Yes
σ_7	Benthal source rate for arbitrary non-conservative settling rate	$\frac{mg\text{-}ANC}{ft^2\text{-}day}$	Variable	Yes	Yes
K_1	Carbonaceous deoxygenation rate constant	day^{-1}	0.02-3.4	Yes	Yes
K_2	Reaeration rate constant	day^{-1}	0.0-100	Yes	Yes
K_3	Rate of loss of BOD due to settling	day^{-1}	-0.36-0.36	Yes	Yes
K_4	Benthic oxygen uptake	$\frac{mg\text{-}O}{ft^2\text{-}day}$	Variable	Yes	Yes
K_5	Coliform die-off rate	day^{-1}	0.05-4.0	Yes	Yes
K_6	Arbitrary non-conservative decay coefficient	day^{-1}	Variable	Yes	Yes

TABLE III-3 (cont'd)
TYPICAL RANGES FOR QUAL2E REACTION COEFFICIENTS

Variable	Description	Units	Range of Values	Variable by Reach	Temperature Dependent
β_1	Rate constant for the biological oxidation of NH_3 to NO_2	day^{-1}	0.10-1.00	Yes	Yes
β_2	Rate constant for the biological oxidation of NO_2 to NO_3	day^{-1}	0.20-2.0	Yes	Yes
β_3	Rate constant for the hydrolysis of organic-N to ammonia	day^{-1}	0.02-0.4	Yes	Yes
β_4	Rate constant for the decay of organic-P to dissolved-P	day^{-1}	0.01-0.7	Yes	Yes

4. FUNCTIONAL REPRESENTATION OF TEMPERATURE

4.1 BASIC TEMPERATURE EQUATION

The basic mass transport equation for QUAL2E was given in Section II as (see equation II-3):

$$\frac{\partial C}{\partial t} = \frac{\partial(A_x D_L \frac{\partial C}{\partial x})}{A_x \partial x} - \frac{\partial(A_x \bar{u} C)}{A_x \partial x} + \frac{dC}{dt} + \frac{s}{V} \qquad \text{IV-1}$$

In temperature modeling, C is taken as the concentration of heat (HL^{-3}) and can be equated to temperature through the relationship

$$C = \rho c (T - T_o) \qquad \text{IV-2}$$

where

ρ = the density of water ($M L^{-3}$)

c = the heat capacity of water ($HM^{-1} D^{-1}$)

T = the water temperature

T_o = an arbitrary base temperature

M = mass

H = heat energy flux

D = degrees

The parameters ρ and c can be considered constant for practical purposes. Also, the internal heat generation $\frac{dC}{dt}$, which results from viscous dissipation of energy and boundary friction, is generally small enough to be

considered negligible. Thus setting $\frac{dC}{dt} = 0$ in equation IV-1 and substituting equation IV-2 for C gives us (after some simplification):

$$\frac{\partial T}{\partial t} = \frac{\partial(A_x D_L \frac{\partial T}{\partial x})}{A_x \partial x} - \frac{\partial(A_x \bar{u} T)}{A_x \partial x} + \frac{1}{\rho c} \frac{s}{V} \qquad \text{IV-3}$$

The source term s/V (with units of $HL^{-3}T^{-1}$) accounts for all heat transferred across the system boundaries, i.e., heat transferred across the air-water interface and heat conducted across mud-water interface. Heat transfer across the mud-water interface is generally insignificant; hence, s/V takes on the identity of the net rate of heat input per unit volume of stream through the air-water interface.

It is most convenient to represent the interfacial heat transfer rate as a flux (H_N) having units of $HL^{-2}T^{-1}$. For a stream element of length dx and mean surface width W, H_N is related to s/V as follows.

The total rate of heat input across the air-water interface is $H_N \frac{dx}{} W$. This heat is distributed uniformly throughout the underlying volume of $\bar{A}_x$ dx, where $\bar{A}_x$ is the mean cross-sectional area of the element. Thus the rate of heat gain per unit volume of water, s/V, is computed as:

$$\frac{s}{V} = \frac{s}{A_x \, dx} = \frac{H_N \, (W dx)}{\bar{A}_x \, dx} = \frac{H_N}{d} \qquad \text{IV-4}$$

where $d = \bar{A}_x/W$ is the hydraulic depth of the stream. Substituting equation IV-4 into equation IV-3 gives the generalized form of the temperature equation:

$$\frac{\partial T}{\partial t} = \frac{\partial(A_x D_L \frac{\partial T}{\partial x})}{A_x \partial x} - \frac{\partial(A_x \bar{u} T)}{A_x \partial x} + \frac{H_N}{\rho c d} \qquad \text{IV-5}$$

4.2 DEFINITION OF H_N

Heat is transferred across the air-water interface of a surface water body by three difference processes: radiation exchange, evaporation, and conduction. The individual heat terms associated with these processes are shown in Figure IV-1 and are defined in Table IV-1 with the typical ranges of their magnitudes in northern latitudes also listed.

The expression that results from the summation of these various energy fluxes is:

$$H_N = H_{sn} + H_{an} - (H_b \pm H_c + H_e) \qquad \text{IV-6}$$

where

H_N = net energy flux passing the air-water interface, Btu/ft^2-day

H_{sn} = net short-wave solar radiation flux passing through the interface after losses due to absorption and scattering in the atmosphere and by reflection at the interface, Btu/ft^2-day

H_{an} = net long-wave atmospheric radiation flux passing through the interface after reflection, Btu/ft^2-day

H_b = outgoing long-wave back radiation flux, Btu/ft^2-day

H_c = conductive energy flux passing back and forth between the interface and the atmosphere, Btu/ft^2-day

H_e = energy loss by evaporation, Btu/ft^2-day

These mechanisms by which heat is exchanged between the water surface and the atmosphere are fairly well understood and are adequately documented in the literature by Edinger and Geyer (1965). The functional representation of these terms has been defined by Water Resources Engineers, Inc. (1967).

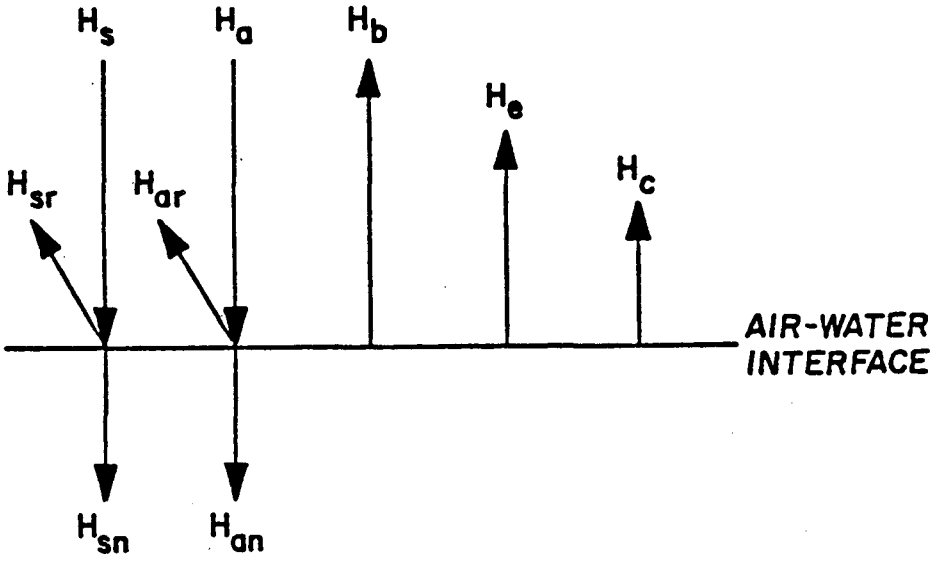

Figure IV-1. Heat Transfer Terms Associated with Interfacial Heat Transfer

TABLE IV-1
DEFINITION OF HEAT TRANSFER TERMS
ILLUSTRATED IN FIGURE 1

Heat Term			Units	Magnitude ($BTU/ft^2\text{-}day^1$)
H_s	=	total incoming solar or short-wave radiation	$HL^{-2}T^{-1}$	400-2800
H_{sr}	=	reflected short-wave radiation	$HL^{-2}T^{-1}$	40-200
H_a	=	total incoming atmospheric ratiation	$HL^{-2}T^{-1}$	2400-3200
H_{ar}	=	reflected atmospheric radiation	$HL^{-2}T^{-1}$	70-120
H_b	=	back radiation from the water surface	$HL^{-2}T^{-1}$	2400-3600
H_e	=	heat loss by evaporation	$HL^{-2}T^{-1}$	150-3000
H_c	=	heat loss by conduction to atmosphere	$HL^{-2}T^{-1}$	-320 to +400

The formulations reported here were extracted from that more detailed work by Frank D. Masch and Associates and the Texas Water Development Board (1971).

4.3 NET SHORT-WAVE SOLAR RADIATION

The net incoming solar radiation is short-wave radiation which passes directly from the sun to the earth's surface. Its magnitude depends on: the altitude of the sun, which varies daily as well as seasonally for a fixed location on the earth; the dampening effect of scattering and absorption in the atmosphere due to cloud cover, and the reflection from the water surface.

The net amount of solar radiation which reaches the surface of the earth may be represented functionally on an hourly basis by:

$$H_{sn} = \underset{(i)}{H_o} \quad \underset{(ii)}{a_t} \quad \underset{(iii)}{(1 - R_s)} \quad \underset{(iv)}{(1 - 0.65C_L^2)} \qquad \text{IV-7}$$

where

H_{sn} = net short-wave solar radiation flux, Btu/ft^2-hr

H_o = amount of radiation flux reaching the earth's atmosphere, Btu/ft^2-hr

a_t = atmospheric transmission term

R_s = Albedo or reflection coefficient

C_L = cloudiness as a fraction of sky covered

It is appropriate for purposes of this discussion to identify and treat separately the four components in equation IV-7 as (i) extraterrestrial solar radiation, (ii) radiation scattering and absorption, (iii) reflectivity, and (iv) cloudiness.

4.3.1 Extraterrestrial Radiation

The short-wave solar radiation flux that strikes the earth's outer atmosphere over a given period of time is given by Water Resources Engineers, Inc. (1967) as:

$$H_o = \frac{H_{sc}}{r^2}\left\{\sin\frac{\pi\phi}{180}\sin\delta\,(t_e - t_b) + \frac{12}{\pi}\cos\frac{\pi\phi}{180}\cos\delta\left[\sin\left(\frac{\pi t_e}{12}\right) - \sin\left(\frac{\pi t_b}{12}\right)\right]\right\}\Gamma \qquad \text{IV-8}$$

where

H_{sc} = solar constant = 438.0 Btu/ft^2-hr

r = normalized radius of the earth's orbit

ϕ = latitude of the site, degrees

δ = declination of the sun, degrees

t_b, t_e = hour angles corresponding to the beginning and end, respectively, of any time interval between sunrise and sunset

r = a correction factor for diurnal exposure to radiation flux

Listed below are several parameters in equation IV-8 requiring further definition as described by Water Resources Engineers, Inc. (1967).

a. Relative Earth-Sun Distance--

$$r = 1.0 + 0.017 \cos \left[\frac{2\pi}{365} (186-Dy)\right] \qquad \text{IV-9}$$

where Dy is the number of the day of the year (beginning January 1)

b. Declination--

$$\delta = \frac{23.45}{180} \pi \cos \left[\frac{2\pi}{365} (173-Dy)\right] \qquad \text{IV-10}$$

c, Hour Angles--

$$t_b = ST_b - \Delta t_s + ET - 12 \qquad \text{IV-11}$$

and

$$t_e = ST_e - \Delta t_s + ET - 12 \qquad \text{IV-12}$$

where ST_b, ST_e are the standard times at the beginning and end of the time interval selected

ET = an expression for time from a solar ephemeris that represents the difference in hours between "true solar time" and that computed on the basis of a yearly average. It is given for each day of the year, Dy, by

$$ET = 0.000121 - 0.12319 \sin \left[\frac{2\pi}{365} (Dy-1) - 0.0714\right]$$

$$= \quad 0.16549 \sin \left[\frac{4\pi}{365} (Dy-1) + 0.3088\right] \qquad \text{IV-13}$$

Δt_s = difference between standard and local civil time in hours as determined from:

$$\Delta t_s = \frac{\varepsilon}{15} (L_{sm} - L_{lm}) \qquad \text{IV-14}$$

where

ε = -1 for west longitude

ε = +1 for east longitude

L_{sm} = longitude of standard meridian, degrees

L_{lm} = longitude of local meridian, degrees

d. Diurnal Exposure--

$$r = 1 \text{ when } ST_r \leq ST_b \text{ or } ST_e \leq ST_s \qquad \text{IV-15}$$

$$r = 0 \text{ when } ST_s \leq ST_b \text{ or } ST_e \leq ST_r \qquad \text{IV-16}$$

where ST_r and ST_s are the standard times of sunrise and sunset, respectively as determined from:

$$ST_r = 12 - \frac{12}{\pi} \text{ arc cos } [\tan (\frac{\pi\phi}{180}) \tan \delta] + \Delta t_s \qquad \text{IV-17}$$

and

$$ST_s = 24 - ST_r + 2\Delta t_s \qquad \text{IV-18}$$

4.3.2 Radiation Scattering and Absorption

The atmospheric transmission term, a_t, is given by Water Resources Engineers, Inc. (1967) as:

$$a_t = \frac{a'' + 0.5 (1 - a' - d)}{1 - 0.5 R_s (1 - a' + d)} \qquad \text{IV-19}$$

in which a" is the mean atmospheric transmission coefficient after scattering and absorption, given by:

$$a'' = \exp \{ - [0.465 + 0.0408 P_{wc}] [0.179 + 0.421 \exp (-0.721 \theta_{am})] \theta_{am} \} \quad \text{IV-20}$$

where θ_{am} is the optical air mass given by the expression:

$$\theta_{am} = \frac{\exp (-Z/2531)}{\sin \alpha + 0.15 \left(\frac{180\alpha}{\pi} + 3.885\right)^{-1.253}} \quad \text{IV-21}$$

in which

Z = elevation of the site in feet

α = sun's altitude in radians, given by:

$$\alpha = \arcsin \left[\sin \frac{\pi\phi}{180} \sin \delta + \cos \frac{\pi\phi}{180} \cos \delta \cos \frac{\pi t}{12}\right] \quad \text{IV-22}$$

in which t is the hour angle, described by an equation similar to equation IV-11 and IV-12.

P_{wc} in equation IV-20 is the mean daily precipitable water content in the atmosphere, given by the expression:

$$P_{wc} = 0.00614 \exp (0.0489 T_d) \quad \text{IV-23}$$

where T_d is the dewpoint in °F, which can be obtained from the expression:

$$T_d = 1n [(e_a + 0.0837)/0.1001]/0.03 \quad \text{IV-24}$$

where e_a is the water vapor pressure of the air.

The mean atmospheric coefficient, a', can also be represented by an equation of the form of equation IV-20 as:

$$a' = \exp \{ - [0.465 + 0.0408 P_{wc}] [0.129 + 0.171 \exp (-0.880 \theta_{am})] \theta_{am} \} \quad \text{IV-25}$$

Dust attenuation of the solar radiation flux, which is represented in equation IV-19 by the quantity d, varies with optical air mass, season of the year, and geographic location. Water Resources Engineers, Inc. (1967) gives a range of 0-0.13 for several locations.

4.3.3 Cloudiness

The dampening effect on the solar radiation flux is given by Water Resources Engineers, Inc. (1967) as

$$C_s = 1.0 - 0.65 C_L^2 \quad \text{IV-26}$$

where C_L is the decimal fraction of the sky covered. Water Resources Engineers, Inc. (1967) reports that equation IV-26 gives satisfactory results except for heavy overcast conditions, i.e., when C_L approaches 1.0.

4.3.4 Reflectivity

The reflection coefficient, R_s, can be approximately computed as a function of the solar altitude, α, by Anderson's (1954) empirical formula:

$$R_s = A\alpha^B \quad \text{IV-27}$$

where α is in degrees, and A and B are functions of cloudiness, C_L. Values for A and B given by Anderson (1954) are shown in Table IV-2.

TABLE IV-2
EMPIRICAL COEFFICIENTS FOR DETERMINING R_s
After Anderson (1954)

Cloudiness C_L	0 Clear		0.1 - 0.5 Scattered		0.6 - 0.9 Broken		1.0 Overcast	
Coefficients	A	B	A	B	A	B	A	B
	1.18	-0.77	2.20	-0.97	0.95	-0.75	0.35	-0.45

4.4 LONG-WAVE ATMOSPHERIC RADIATION

The long-wave radiation emitted by the atmosphere varies directly with the moisture content of the atmosphere. Although it is primarily dependent on air temperature and humidity, it can also be affected by ozone, carbon dioxide, and possibly other materials in the atmosphere. Anderson (1954) indicated that the amount of atmospheric radiation is also significantly affected by cloud height. The amount of long-wave atmospheric radiation that is reflected is approximately a constant fraction of the incoming radiation, found by Anderson (1954) to be approximately 0.03.

The net atmospheric radiation flux can be expressed as:

$$H_{an} = [2.89 \times 10^{-6}]\ \sigma\ (T_a + 460)^6\ (1.0 + 0.17C_L^2)(1-R_L) \qquad \text{IV-28}$$

where

H_{an} = net long-wave atmospheric radiation flux, Btu/ft^2-hr

σ = Stefan-Boltzman constant, 1.73×10^{-9} Btu/ft^2/hr/°Rankine^4

T_a = air temperature at a level 6 feet above the water surface, °F

R_L = reflectivity of the water surface for atmospheric radiation = 0.03

C_L = cloudiness, fraction of cloud cover

4.5 WATER SURFACE BACK RADIATION

The third source of radiation transfer through the air-water interface is long-wave back radiation from the water surface, H_b, which represents a loss of heat from the water. It can be seen from Table IV-1 that back radiation accounts for a substantial portion of the heat loss from a body of water. This loss is expressed by the Stefan-Boltzman Fourth Power Radiation Law for a blackbody as:

$$H_b = 0.97\ \sigma\ (T_s + 460)^4 \qquad \text{IV-29}$$

where

H_b = water surface back radiation flux, Btu/ft^2-hr

T_s = water surface temperature, °F

Equation IV-29 can be linearized over a given temperature range as

$$H_b = \alpha_2 + \beta_2 T_s \qquad \text{IV-30}$$

where

α_2, β_2 = constants defined over the range 35 to 135 °F

In the steady-state temperature solution, this linearized version of the back radiation equation is used to allow the temperature dependent terms to be separated out of the equation. Sets of α_2, β_2 are specified for 21 5°F temperature intervals between 35°F and 135°F. For dynamic simulations the heat flux term calculations are based on the temperature at the beginning of the time step.

4.6 EVAPORATION

A water body also loses heat to the atmosphere by evaporation. Each pound of water that leaves as water vapor carries its latent heat of vaporization (approximately 1050 BTU at 60°F) plus its sensible heat. This significant heat loss due to evaporation can be expressed as:

$$H_e = \gamma H_L E + H_v \qquad \text{IV-31}$$

where

γ = specific weight of the water being evaporated, lb/ft^3

H_L = latent heat of vaporization, Btu/lb, given by

$H_L = 1084 - 0.5\ T_s$

E = evaporation rate, ft/hr

H_v = sensible heat loss Btu/ft^2-hr

The evaporation rate, E, is most often expressed as

$$E = (a + bW)(e_s - e_a) \qquad \text{IV-32}$$

where

a,b = constants

W = wind speed, in mph, measured 6 feet above the water surface

e_s = saturation vapor pressure of the air, in. of Hg, at the temperature of the water surface, as given by

$$e_s = 0.1001 \exp (0.03\ T_s) - 0.0837$$

and

e_a = water vapor pressure, in. of Hg, at a height of 6 feet above the water surface, given as

$$e_a = e_{wb} - 0.000367\ P_a\ (T_a - T_{wb})\ (1.0 + \frac{T_{wb} - 32}{1571}) \qquad \text{IV-34}$$

where

e_{wb} = saturation vapor pressure, in. of Hg, at the wet bulb temperature from the expression

$$e_{wb} = 0.1001 \exp (0.03\ T_{wb}) - 0.0837 \qquad \text{IV-35}$$

P_a = local barometric pressure, in. of Hg

T_{wb} = wet bulb air temperature, °F

T_a = dry bulb air temperature, °F

The literature contains a wide range of values for the evaporation constants a and b. Roesner (1969) reports that a good average value of a would be 6.8 x 10^{-4} ft/hr-in. of Hg, while b would best be represented by 2.7 x 10^{-4} ft/hr-in. of Hg.-mph.

To linearize the variation of evaporation rate with surface water temperature T_s, equation IV-34 is approximated over 5°F intervals as:

$$e_s = \alpha_1 + \beta_1 T_s \qquad \text{IV-36}$$

Sets of α_1, β_1 are specified for twenty-one 5°F intervals between 35°F and 135°F. The linearized evaporation expression is used in the steady-state temperature solution.

The sensible evaporative heat loss can be expressed simply as:

$$H_v = c \gamma E (T_s - T_o) \qquad \text{IV-37}$$

where

c = heat capacity of water = 1 Btu/lb-°F

T_o = reference temperature, °F

Sensible heat loss is very small compared to the other heat loss components in the energy budget and thus is not included in the QUAL2E temperature computation.

4.7 CONDUCTION

Heat that is transferred between the water and the atmosphere due to a temperature difference between the two phases and not related to water vapor exchange is normally called conduction. Using the fact that transfer by conduction is a function of the same variables as evaporation, it is possible to arrive at a proportionality between heat conduction and heat loss by evaporation. This proportionality, known as Bowen's ratio, is expressed as:

$$B = \frac{H_c}{H_e} = C_B \left[\frac{T_s - T_a}{e_s - e_a}\right] \frac{P_a}{29.92} \qquad \text{IV-38}$$

where C_B is a coefficient $\cong$ 0.01.

By using Bowen's ratio, the rate of heat loss to the atmosphere by heat conduction, H_c, can be defined as:

$$H_c = \gamma H_L (a+bW) \left(0.01 \frac{P_a}{29.92}\right) (T_s - T_a) \qquad \text{IV-39}$$

For practical purposes, the ratio $(P_a/29.92)$ can be taken as unity.

4.8 QUAL2E MODIFICATIONS FOR REACH VARIABLE LOCAL CLIMATOLOGY AND TEMPERATURE

Prior versions of QUAL-II and QUAL2E have assumed that the input variables for temperature simulation were uniform over the entire river basin (global inputs). These input variables consist of climatological, geographical, and heat balance information as follows: basin elevation, dust attenuation

coefficient, evaporation coefficients, dry and wet bulb air temperatures, atmospheric pressure, cloud cover, and wind speed. In the current version of QUAL2E most of these inputs, with the exception of the evaporation coefficients are reach variable. Thus, for systems in which variable ambient temperature and climatology may be important, for example in modeling rivers with large changes in elevation, different values for these factors may be supplied for each reach in the river. The overall heat balance computations are performed as described in Sections 4.1-4.7 of this chapter, using the reach specific values of each input variable. When reach variable temperature simulation inputs are used, a detailed temperature and heat balance summary is provided with the QUAL2E final output.

The user has a number of options in specifying the input variables for temperature simulation. Global values may be used (all reaches having the same values for each of the temperature simulation inputs), or different input values may be explicitly specified for each reach in the system. In the case where reach specific values of atmospheric pressure are not known or available, QUAL2E has the capability of estimating the value of atmospheric pressure for each reach from its elevation and air temperature. These estimates are computed from the ideal gas law integrated over the change in elevation relative to a datum (Plate, 1982).

$$P = P_o \, e^{[-(g/RT)(z - z_o)]} \qquad \text{IV-40}$$

Where:

P = atmospheric pressure at elevation z (in Hg),

g = gravitational constant (32.2 ft/sec^2),

R = gas law constant (1715 $ft^2/sec^2\text{-}^oR$),

T = dry bulb air temperature (^oR),

z = elevation of reach (ft),

z_o, P_o = datum elevation and pressure, respectively,

The principal assumptions used in deriving Eq. IV-40 are that air temperature and specific humidity are constant. Thus, the value of the gas constant, R, is that for dry air and the value of dry bulb air temperature, T, is the average of the dry bulb temperatures at elevations z and z_o. Although refinements to this methodology are possible, they were deemed premature until more experience with this option is obtained. If the reach variable values of atmospheric pressure are computed from Eq. IV-40, they are echo-printed with the QUAL2E output.

5. COMPUTATIONAL REPRESENTATION

5.1 PROTOTYPE REPRESENTATION

To expand upon the basic conceptual representation presented in Sections 1 and 2, QUAL2E permits any branching, one-dimensional stream system to be simulated. The first step involved in approximating the prototype is to subdivide the stream system into reaches, which are stretches of stream that have uniform hydraulic characteristics. Each reach is then divided into computational elements of equal length so that all computational elements in all reaches are the same length. Thus, all reaches must consist of an integer number of computational elements.

There are seven different types of computational elements:

1. Headwater element
2. Standard element
3. Element just upstream from a junction
4. Junction element
5. Last element in system
6. Input element
7. Withdrawal element

Headwater elements begin every tributary as well as the main river system, and as such, they must always be the first element in a headwater reach. A standard element is one that does not qualify as one of the remaining six element types. Because incremental flow is permitted in all element types, the only input permitted in a standard element is incremental flow. A type 3 element is used to designate an element on the mainstem that is just upstream of a junction. A junction element (type 4), has a simulated tributary entering it. Element type 5 identifies the last computational element in the river system (downstream boundary); there should be only one element type 5. Element types 6 and 7 represent elements which have inputs (waste loads and unsimulated tributaries) and water withdrawals, respectively.

River reaches, which are aggregates of computational elements, are the basis of most data input. Hydraulic data, reaction rate coefficients, initial conditions, and incremental flow data are constant for all computational elements within a reach.

5.2 FORCING FUNCTIONS

Forcing functions are the user specified inputs that drive the system being modeled. These inputs are specified in terms of flow, water quality characteristics, and local climatology. QUAL2E accommodates four types of hydraulic and mass load forcing functions in addition to local climatological factors--headwater inputs, point sources or withdrawals, incremental inflow/outflow along a reach, and the (optional) downstream boundary concentration.

1. Headwater Inputs - Headwater inputs are typically the upstream boundary conditions at the beginning of the system. They are the conditions required to generate the solution of the mass balance equations for the first computational element in each headwater reach. Headwaters are also the source of water for flow augmentation.

2. Point Sources and/or Withdrawals - These loads are used to represent point source discharges into the system (i.e., sewage and industrial waste, or storm water runoff) and losses from the system resulting from diversions. In QUAL2E point source discharges may represent either raw or treated waste loads. If raw waste loads are used, the effect of treatment can be simulated by applying a specific fractional removal for carbonaceous BOD to each point source load.

3. Incremental Inflow - QUAL2E has the capability to handle flow uniformly added or removed along a reach. The total flow increment along a reach is apportioned equally to all computational elements in the reach. This feature can be used to simulate the effects of non-point source inputs to the system, or the effect of loss of stream flow to the groundwater.

4. Downstream Boundary Concentration (optional) - QUAL2E has the capability of incorporating known downstream boundary concentrations of the water quality constituents into the solution algorithm. This feature is useful in modeling systems with large dispersion in the lower reaches (e.g., estuaries). When downstream boundary concentrations are supplied, the solution generated by QUAL2E will be constrained by this boundary condition. If the concentrations are not provided, the constituent concentrations in the most downstream element will be computed in the normal fashion using the zero gradient assumption (see Section 5.4.3).

Local climatological data are required for the simulation of algae and temperature. The temperature simulation uses a heat balance across the air-water interface and thus requires values of wet and dry bulb air temperatures, atmospheric pressure, wind velocity, and cloud cover. The algal simulation requires values of net solar radiation. For dynamic simulations, these climatological data must be input at regular time intervals over the

course of the simulation and are applied uniformly over the entire river basin. For modeling steady-state temperature and algae, average daily local climatological data are required and may vary spatially over the basin by reach.

5.3 MODEL LIMITATIONS

QUAL2E has been developed to be a relatively general program; however, certain dimensional limitations have been imposed upon it during program development. These limitations are as follows:

Reaches: a maximum of 25

Computational elements: no more than 20 per reach or 250 in total

Headwater elements: a maximum of 7

Junction elements: a maximum of 6

Input and withdrawal elements: a maximum of 25 in total

(Note: These limitations may be modified, if necessary, by the user by altering the PARAMETER statement specifications in file MAIN.VAR of the program and recompiling.

QUAL2E can be used to simulate any combination of the following parameters or groups of parameters.

1. Conservative minerals (up to three at a time)
2. Temperature
3. BOD
4. Chlorophyll a
5. Phosphorus cycle (organic and dissolved)
6. Nitrogen cycle (organic, ammonia, nitrite, and nitrate)
7. Dissolved oxygen
8. Coliforms
9. An arbitrary nonconservative constituent

All parameters can be simulated under either steady-state or dynamic conditions. If either the phosphorus cycle or the nitrogen cycle are not being simulated, the model presumes they will not limit algal growth.

5.4 Numerical Solution Technique

At each time step and for each constituent, Equation II-3 can be written I times, once for each of the I computational elements in the network. Because it is not possible to obtain analytical solutions to these equations under most prototype situations, a finite difference method is used--more specifically, the classical implicit backward difference method (Arden and Astill, 1970; Smith, 1966; and Stone and Brian, 1963).

The general basis of a finite difference scheme is to find the value of a variable (e.g., constituent concentration) as a function of space at a time step n+1 when its spatial distribution at the n^{th} time step is known. Time step zero corresponds to the initial condition. Backward difference or implicit schemes are characterized by the fact that all spatial derivatives ($\partial/\partial x$) are approximated in difference form at time step n+1.

5.4.1 Formulation of the Finite Difference Scheme

The finite difference scheme is formulated by considering the constituent concentration, C, at four points in the mnemonic scheme as shown in Figure V-1.

Three points are required at time n+1 to approximate the spatial derivatives. The temporal derivative is approximated at distance step i.

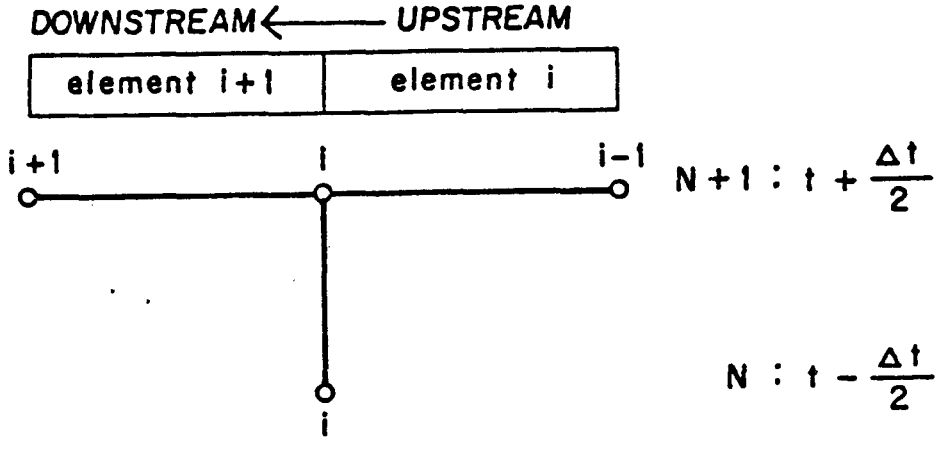

Figure V-1. Classical Implicit Nodal Scheme

Equation II-3 can be written in finite difference form in two steps. First, the advection and diffusion terms are differentiated once with respect to x, giving:

$$\frac{\partial C_i}{\partial t} = \frac{(AD_L \frac{\partial C}{\partial x})_i - (AD_L \frac{\partial C}{\partial x})_{i-1}}{V_i} - \frac{(A\,\bar{u}\,C)_i - (A\,\bar{u}\,C)_{i-1}}{V_i}$$

$$+ \frac{dC_i}{dt} + \frac{s_i}{V_i} \qquad \text{V-1}$$

where

$$V_i = A_i \,\Delta\, x_i$$

Secondly, expressing the spatial derivative of the diffusion terms in finite difference and thence the time derivative of C in finite difference, there results:

$$\frac{C_i^{n+1} - C_1^n}{\Delta t} = \left(\frac{[(AD_L)_i]\, C_{i+1}^{n+1} - [(AD_L)_i]\, C_i^{n+1}}{V_i \,\Delta\, x_i}\right.$$

$$\left. - \frac{[(AD_L)_{i-1}]\, C_i^{n+1} - [(AD_L)_{i-1}]\, C_{i+1}^{n+1}}{V_i \,\Delta\, x_i}\right)$$

$$- \left(\frac{Q_i\, C_i^{n+1} - Q_{i-1}\, C_{i+1}^{n+1}}{V_i}\right) + r_i\, C_i^{n+1} + p_i + \frac{s_i}{V_i} \qquad \text{V-2}$$

In equation V-2, the term dC/dt is expressed as:

$$\frac{dC_i}{dt} = r_i\, C_i^{n+1} + p_i$$

where

r_i = first order rate constant

p_i = internal constituent sources and sinks (e.g., nutrient loss from algal growth, benthos sources, etc.)

Note that the dC/dt for every constituent modeled by QUAL2E can be expressed in this form.

If equation V-2 is rearranged in terms of the coefficients of C_{i-1}^{n+1}, C_i^{n+1}, and C_{i+1}^{n+1}, we obtain the equation:

$$a_i\ C_{i-1}^{n+1} + b_i\ C_i^{n+1} + c_i\ C_{i+1}^{n+1} = Z_i \qquad \text{V-3}$$

where

$$a_i = -\left[(AD_L)_{i-1}\ \frac{\Delta t}{V_i\ \Delta x_i} + \frac{Q_{i-1}\ \Delta t}{V_i}\right]$$

$$b_i = 1.0 + \left[(AD_L)_i + (AD_L)_{i-1}\right]\ \frac{\Delta t}{V_i\ \Delta x_i} + Q_i\ \frac{\Delta t}{V_i} - r_i\ \Delta t$$

$$c_i = -\left[(AD_L)_i\ \frac{\Delta t}{V_i\ \Delta x_i}\right]$$

$$Z_i = C_i^n + \frac{s_i\ \Delta t}{V_i} + p_i\ \Delta t$$

The values of a_i, b_i, c_i, and Z_i are all known at time n, and the C_i^{n+1} terms are the unknowns at time step n+1.

In the case of a junction element with a tributary upstream element, the basic equation becomes:

$$a_i\ C_{i-1}^{n+1} + b_i\ C_i^{n+1} + c_i\ C_{i+1}^{n+1} + d_j\ C_j^{n+1} = Z_i \qquad \text{V-4}$$

where

$$d_j = -\left[(AD)_j\ \frac{\Delta t}{V_i\ \Delta x_i} + \frac{Q_j\ \Delta t}{V_i}\right]$$

j = the element upstream of junction element i

C_j^{n+1} = concentration of constituent in element j at time n+1

It can be seen that the d_j term is analogous to the a_i term. Both terms account for mass inputs from upstream due to dispersion and advection.

Under steady-state conditions, $\frac{\partial C_i}{\partial t} = 0$ in equation V-1. Working through the finite difference approximations and rearranging terms as before, the steady-state version of equation V-3 is derived:

$$a_i\ C_{i-1}^{n+1} + b_i\ C_i^{n+1} + c_i\ C_{i+1}^{n+1} = Z_i \qquad \text{V-5}$$

where

$$a_i = -\left[\frac{(AD_L)_{i-1}}{V_i \Delta x_i} + \frac{Q_{i-1}}{V_i}\right]$$

$$b_i = \left[\frac{(AD_L)_i}{V_i \Delta x_i} + \frac{(AD_L)_{i-1}}{V_i \Delta x_i} + \frac{Q_i}{V_i} - r_i\right]$$

$$c_i = \left[\frac{(AD_L)_i}{V_i \Delta x_i}\right]$$

$$Z_i = \frac{S_i}{V_i} + P_i$$

Note that equation V-5 is the same as equation V-3, with three changes:

- o $\Delta t = 1.0$
- o the constant 1.0 in $b_i = 0.0$
- o the initial concentration C_i^n in $Z_i = 0.0$

5.4.2 Method of Solution

Equations V-3 and V-5 each represent a set of simultaneous linear equations whose solution provides the values of C_i^{n+1} for all i's. Expressed in matrix form, this set of equations appears as:

$$\begin{bmatrix} b_1 & c_1 & & & & \\ a_2 & b_2 & c_2 & & & \\ & a_3 & b_3 & c_3 & & \\ & & \ddots & \ddots & \ddots & \\ & & & a_i & b_i & c_i \\ & & & & \ddots & \ddots \\ & & & & a_{I-1} & b_{I-1} & c_{I-1} \\ & & & & & a_I & b_I \end{bmatrix} \times \begin{bmatrix} C_1^{n+1} \\ C_2^{n+1} \\ C_3^{n+1} \\ \vdots \\ C_i^{n+1} \\ \vdots \\ C_{I-1}^{n+1} \\ C_I^{n+1} \end{bmatrix} = \begin{bmatrix} Z_1 \\ Z_2 \\ Z_3 \\ \vdots \\ Z_i \\ \vdots \\ Z_{I-1} \\ Z_I \end{bmatrix} \qquad \text{V-6}$$

The left matrix is a tri-diagonal matrix. An efficient method that readily lends itself to a computer solution of such a set of equations is:

Divide through the first equation in V-6 by b_1 to obtain:

$$C_1^{n+1} + W_1 C_2^{n+1} = G_1 \qquad \text{V-7}$$

where

$$W_1 = c_1/b_1 \text{ and } G_1 = Z_1/b_1.$$

Combine the expression for b_i (see V-3) and the second equation in V-6 to eliminate a_2 and the result is:

$$C_2^{n+1} + W_2 C_3^{n+1} = G_2 \qquad \text{V-8}$$

where

$$W_2 = \frac{c_2}{b_2 - a_2 W_1} \text{ and } G_2 = \frac{Z_2 - a_2 G_1}{b_2 - a_2 W_1}$$

Combine equation V-8 and the third equation in V-6 to eliminate a_3 and the result is:

$$C_3^{n+1} + W_3 C_4^{n+1} = G_3 \qquad \text{V-9}$$

where

$$W_3 = \frac{c_3}{b_3 - a_3 W_2} \quad \text{and} \quad G_3 = \frac{Z_3 - a_3 G_2}{b_3 - a_3 W_2}$$

Proceed through the equations, eliminating a_i and storing the values of W_i and G_i given by:

$$W_i = \frac{c_i}{b_i - a_i W_{i-1}}, \; i = 2, 3, \ldots, I \qquad \text{V-10}$$

and

$$G_i = \frac{Z_i - a_i G_{i-1}}{b_i - a_i W_{i-1}}, \; i = 2, 3, \ldots, I \qquad \text{V-11}$$

The last equation is solved for C_I^{n+1} by

$$C_I^{n+1} = G_I \qquad \text{V-12}$$

Solve for C_{I-1}^{n+1}, C_{I-2}^{n+1}, . . . , C_1^{n+1} by back substitution.

$$C_i^{n+1} = G_i - W_i C_{i-1}^{n+1}, \; i = I-1, I-2, \ldots, 1 \qquad \text{V-13}$$

5.4.3 Boundary Conditions

In most situations of interest, transport is unidirectional in nature, i.e., there is no significant transport upstream. Therefore, the concentration at some point just upstream from the beginning or end of the stream reach of interest can be used as the boundary condition.

5.4.3.1 Upstream Boundary (Headwater Elements)

For headwater elements there is no upstream, i-1, element. Thus, the headwater driving force is substituted in Equation V-3 for the upstream concentration C_{i-1}. Because the headwater concentrations are fixed, they are incorporated on the right hand side of Equation V-3 in the known term Z_i, for headwater elements as follows.

$$Z_1 = C_1^n + \frac{s_1 \Delta t}{V_1} + p_1 \Delta t - a_1 C_o \qquad \text{V-14}$$

where C_0 is the upstream boundary condition (headwater concentration).

5.4.3.2 Downstream Boundary (Last Element in the System)

QUAL2E has two options for modeling the downstream boundary. One uses a zero gradient assumption; the other incorporates fixed downstream constituent concentrations into the solution algorithm.

Zero Gradient Assumption (Arden and Astill, 1970)--For the last computational element in the system, there is no downstream, i+1, element. At this boundary, a zero gradient assumption is made that replaces C_{i+1} with C_{i-1}. In this manner, the downstream boundary acts as a mirror to produce a zero gradient for the concentration of the constituent variable. The coefficient a_i, therefore, is modified to include the dispersion effect normally found in the coefficient c_i for the last element in the system. Thus, the equation for a_i in V-3 becomes:

$$a_I = -[((AD_L)_{I-1} + (AD_L)_I)\frac{\Delta t}{V_I \Delta x_I} + \frac{Q_{I-1}\Delta t}{V_I}] \qquad \text{V-15}$$

and

$$c_I = 0 \qquad \text{V-16}$$

where I = index of the downstream boundary element

Fixed Downstream Constituent Concentrations--For this boundary option, the user supplies known downstream boundary concentrations C_{LB} for each water quality constituent. Thus, the value of C_{i+1} in Equation V-3 becomes

$$C_{I+1} = C_{LB} \qquad \text{V-17}$$

Because the boundary concentrations are known in this option, they are incorporated on the right hand side of Equation V-3 in the known term Z_i for the downstream boundary element then results as

$$Z_I = C_I^n + \frac{s_I \Delta t}{V_I} + p_I \Delta t - c_I C_{LB} \qquad \text{V-18}$$

6. UNCERTAINTY ANALYSIS WITH QUAL2E

6.1 INTRODUCTION

Uncertainty analysis for model simulations is assuming a growing importance in the field of water quality management. The impetus for this concern is provided by recent public awareness over health risks from improper disposal of toxic wastes as well as by the continuing emphasis within EPA on risk assessment. One of the first steps in the chain of risk assessment is the quantification of the error in predicting water quality. Unfortunately, uncertainty analysis of water quality model forecasts has not received as much attention in practice as has the prediction of expected (average) values.

Uncertainty analysis has been the subject of much discussion in the ecosystem modeling literature (Rose and Swartzman, 1981 and O'Neill and Gardner, 1979). In the water resources literature, lake eutrophication models have been used to compare various methods of uncertainty analysis (Reckhow, 1979; Scavia et al., 1981; and Malone et al., 1983). The methodologies described in this chapter represent a systematic approach to uncertainty analysis for the general purpose stream water quality model QUAL2E. The objective is to provide some of the tools for incorporating uncertainty analysis as an integral part of the water quality modeling process. The QUAL2E model was chosen for this application because it is a general purpose computer code, widely used by consultants and state regulatory agencies in waste load allocation and other planning activities. The resulting uncertainty model is named QUAL2E-UNCAS.

6.2 QUAL2E-UNCAS

Three uncertainty analysis techniques can be employed in QUAL2E-UNCAS--sensitivity analysis, first order error analysis, or monte carlo simulation. The user is provided this array of options for flexibility, because the methods differ in their assumptions and will not always agree with each other. Discrepancies may be explained by errors in the first order approximation or by errors due to biased variance calculations. Monte carlo simulation has the advantage of output frequency distributions, but it carries a high computational burden. First order error propagation provides a direct estimate of model sensitivity, but that variability is usually more indicative of the variance of model components than of the dynamics of the model structure.

The methodology provided in QUAL2E-UNCAS allows the model user to perform uncertainty analysis with relative ease and efficiently manages the output from the analysis. Although the application is specific to the QUAL2E model, the methodology is general. The preprocessing and postprocessing algorithms used are, in principle, applicable to many water quality models. The preprocessor allows the user to select the variables and/or parameters to be altered, without having to manually restructure the input data set. This task is performed automatically by the preprocessor for as many uncertainty conditions as the user wishes to simulate. The postprocessor stores and manipulates only the output of interest, thus reducing potential voluminous output. The user must select the important variables and locations in the stream network where uncertainty effects are desired for analysis.

6.2.1 Sensitivity Analysis

In normal usage sensitivity analysis is accomplished using a one-variable-at-a-time approach (Duke, 1976). Sensitizing more than one input variable at a time is an attractive method for assessing their interaction effects on the output variable. When many input parameters and variables are altered, however, the number of combinations to be investigated becomes large, thus complicating interpretation of the results. Experimental design strategies can be efficiently applied in this situation to elicit main and interaction effects of input variables.

With the sensitivity analysis option in QUAL2E-UNCAS, the user may vary the inputs singly, in groups, or using factorial design strategies. The input requirements for sensitivity analysis consist of identifying the input variables to be perturbed and specifying the magnitude of the perturbation. The output for each sensitivity simulation consists of the changes (i.e., the sensitivities) in the value(s) of each output variable (ΔY) resulting from the changes in the value(s) of the input variables (ΔX). This output is provided in tabular format, similar to the QUAL2E final summary, except that the table entries are sensitivities rather than the values of the output variables.

QUAL2E-UNCAS also has the capability of assessing the main and interaction effects of input variables on various output variables by sensitizing the inputs according to 2-level factorial design strategies. Currently QUAL2E-UNCAS accommodates only 2-variable (i.e., 2^2) and 3-variable (i.e., 2^3) factorial designs. As in normal sensitivity analysis, the user specifies the names of the input variables to be perturbed and the magnitude of the perturbation. The factorial design computations for main and interaction effects are performed using standard statistical procedures (Box et al., 1978; and Davies, 1967).

Because QUAL2E computes values of each output variable for every computational element in the system, the factorial design output would be voluminous if performed for each element. Thus, the user must specify particular locations (maximum of 5) in the basin where this analysis is to be performed. The critical locations, such as the dissolved oxygen sag point, or the location below the mixing zone of a tributary junction or

point discharge, are usually included among those chosen for analysis.

6.2.2 First Order Error Analysis

First order error analysis utilizes the first order approximation to the relationship for computing variances in multivariate situations. The input variables are assumed to act independently (covariances are ignored) and the model to be linear (the higher order terms of the Taylor expansion are omitted). The first order approximations to the components of output variance is often good (Walker, 1982).

The QUAL2E-UNCAS output for first order error analysis consists of two parts--(a) a tabulation of normalized sensitivity coefficients and (b) a listing of the components of variance. The normalized sensitivity coefficients represent the percentage change in the output variable resulting from a 1 percent change in each input variable, and are computed as follows.

$$S_{ij} = (\Delta Y_j/Y_j)/(\Delta X_i/X_i) \qquad \text{VI-1}$$

where:

S_{ij} = normalized sensitivity coefficient for output Y_j to input X_i,

X_i = base value of input variable,

ΔX_i = magnitude of input perturbation,

Y_j = base value of output variable,

ΔY_j = sensitivity of output variable.

The components of variance for each output variable Y are the percentages of output variance attributable to each input variable X, computed in the following manner.

$$\text{Var}(Y_j) = \sum_i \text{Var}(X_i)(\Delta Y_j/\Delta X_i)^2 \qquad \text{VI-2}$$

where:

$\text{Var}(Y_j)$ = variance of output variable Y_j,

$\text{Var}(X_i)$ = variance of input variable X_i,

Y_j and X_i are as defined in Eq. VI-1.

As can be seen from Eq. VI-2, each term in the summation is a component of the variance of the output variable, Y_j, contributed by the input variable, X_i. The components of the output variance, $Var(Y_j)$, represent a weighting of the input variances, $Var(X_i)$, by the square of the sensitivity of model output to input, $(\Delta Y_j/\Delta X_i)$. Thus, a particular input variable may be a large (small) contributor to the output variance if it has either a large (small) input variance or a large (small) sensitivity coefficient, or both. Performing multiple first order error analyses with differing values of X_i will provide an estimate of the strength of model nonlinearities. Outputs that are linear in X_i will have unchanging sensitivity coefficients, $(\Delta Y_j/\Delta X_i)$, as ΔX_i changes.

In normal applications of first order error analysis, all of the input variables are perturbed. In this manner, the contributions to output variance from all input variables are computed. QUAL2E-UNCAS has the capability, however, of constraining the number of input variables to be included in a first order analysis. This limitation is achieved by allowing the user to specify the generic group of inputs (i.e., "hydraulic variables," "reaction coefficients," "point load forcing functions," etc.) that are to be perturbed in the analysis.

The input requirements for first order error analysis consist of (a) the magnitude of the input perturbation, ΔX_i, and (b) the value of the variance of the input variable, $Var(X_i)$. The value of ΔX_i (default value is 5%, i.e., $\Delta X_i/X_i = 0.05$) is specified by the user and applied uniformly over all inputs for the purpose of computing sensitivities. Default values for the input variances are provided with the QUAL2E-UNCAS model (see Section 6.3); however, users are cautioned to use values appropriate to their modeling application. Finally, as in the factorial design option, the user must choose the locations (maximum of 5) in the basin at which the first order error analysis for the output variables is to be performed.

6.2.3 Monte Carlo Simulation

Monte carlo simulation is a method for numerically operating a complex system that has random components. Input variables are sampled at random from pre-determined probability distributions (with or without correlation) and the distribution of output values from repeated simulations is analyzed statistically. The validity of this method is not affected by nonlinearities in the water quality model.

The monte carlo simulation computations in QUAL2E-UNCAS provide summary statistics and frequency distributions for the state variables at specific locations in the system. The summary statistics include: mean (base and simulated), bias, minimum, maximum, range, standard deviation, coefficient of variation, and skew coefficient. Frequency and cumulative frequency distributions are tabulated in increments of one-half a standard deviation. Comparison of the standard deviation estimates from monte carlo simulations with those from first order error analysis provide an indication of the extent of model nonlinearities. Cumulative frequency distributions are useful in evaluating overall dispersion in the model predictions and in assessing the likelihood of violating a water quality standard.

The input requirements for the monte carlo simulation option in QUAL2E-UNCAS consist of (a) the variance of the input variable, $Var(X_i)$, (b) the probability density function of the input variable, and (c) the number of simulations to be performed. Specification of input variances is done in the same manner as that for first order error analysis. Currently there are two options for the input probability density functions: normal and log-normal. The distribution for each input variable can be specified from either of these options. The default option is the normal distribution. The number of monte carlo simulations must be large enough to avoid large errors in the estimated values of output variance, yet small enough to avoid unduly long computation times. Preliminary experience with UNCAS indicates that about 2000 simulations are required to achieve estimates of output standard deviations with 95% confidence intervals of 5%.

QUAL2E-UNCAS assumes that all inputs act independently. Thus, each input is randomized independently from the others. In normal usage, all input variables are randomized in monte carlo simulation. As in the case of first order error analysis, however, the user may constrain the number of inputs to be varied by specifying that only certain generic groups of inputs be randomized. Lastly, the user must specify the locations (maximum of five) in the basin at which monte carlo simulation results are to be tabulated.

6.3 Input Variable Variances

One of the fundamental requirements for performing uncertainty analyses in water quality modeling is a knowledge of the uncertainty characteristics of the model inputs. Information on model input uncertainty is not widely available in the literature, although recent articles show an increasing tendency to publish such information (Kennedy and Bell, 1986). Three reports (Koenig, 1986; NCASI, 1982; and McCutcheon, 1985) have been examined to compile an uncertainty data base for use with QUAL2E-UNCAS. A summary of this information is shown in Table VI-1. These values represent ranges in the uncertainty of model inputs caused by such factors as spatial variation, temporal variation, sampling error, analytical error, and bias in measurement or estimation technique.

In QUAL2E-UNCAS, uncertainty information is provided in two forms: (a) the value of the variance of the input variables and (b) the specification of a probability density function for each input. The model reads this information, as required, from a data file named "INVAR.DAT." An example of this file, containing a set of default values for all QUAL2E inputs, is provided with the QUAL2E-UNCAS model. These data are consistent with the typical ranges of uncertainty shown in Table VI-1 and are provided only as a guide for beginning the process of estimating the uncertainty associated with QUAL2E input variables. All users are CAUTIONED not to assume that these values are appropriate to all modeling situations. The burden of verifying and confirming input variance estimates for a particular application lies with the user. Efforts to develop a better understanding of input variable uncertainties are continuing.

TABLE VI-1
SUMMARY OF QUAL2E INPUT VARIABLE UNCERTAINTIES

Input Variable or Parameter	QUAL2E Data Type	Relative Standard Deviation, % Low	Typical	High
Algae, Nutrient, Light Coefficients	1A	5	10-20	50
Temperature Coefficients	1B	1	2-5	10
Hydraulic Data	5	1	5-15	50
Temperature/LCD	5A	1	2-10	20
Reaction Coefficients	6	5	10-25	100
Constituent Concentrations	8,10,11			
Temperature		1	2-3	5
DO		2	5-10	15
CBOD		5	10-20	40
N Forms		10	15-30	75
P Forms		10	15-40	75
Algae		5	10-25	50
Coliform		20	25-50	100
Conservative Minerals		1	5-10	15

Summary of data compiled from APHA, 1985; Koenig, 1986; McCutcheon, 1985; and NCASI, 1982a.

In the general case, QUAL2E-UNCAS accepts input variability information in relative rather than absolute units. Thus, the input perturbations for first order error analysis and input variances for first order analysis and monte carlo simulation are supplied as percent perturbation and coefficient of variation, respectively. The transformation equations between relative and absolute units are:

$$\Delta X_i = RP * X_i \qquad \text{VI-3}$$

$$Var(X_i) = (CV_i * X_i)^2 \qquad \text{VI-4}$$

where:

RP = relative perturbation for input variable X_i

CV = coefficient of variation for input variable X_i

X_i = value of input variable used in base case simulation

The specific manner in which the input data requirements are supplied to QUAL2E-UNCAS, including the data file "INVAR.DAT," are described in Appendix B-User Manual for QUAL2E-UNCAS.

6.4 PROGRAMMING STRATEGY IN QUAL2E-UNCAS

QUAL2E-UNCAS has been structured in a manner to minimize the tedious requirements for user adjustments to the QUAL2E input data file used in the base case simulation. The UNCAS portion of QUAL2E-UNCAS consists of two parts: (a) a package of 16 subroutines that perform the necessary book-keeping and computations as well as printing the uncertainty results and (b) one data file to decode and link UNCAS requests with QUAL2E. The user must supply two input data files--the first provides the general specifications for the uncertainty analysis to be performed, and the second contains the input variance information. In addition, during execution, UNCAS creates two disk files for storing and retrieving the simulation information used in computing the uncertainty analysis results. The flow chart for UNCAS in Figure VI-1 shows the relationships among the subroutines and data files. Each component of the UNCAS package and its function is described in the following sections.

6.4.1 UNCAS Subroutines

a. Subroutine UNCAS. Subroutine UNCAS manages the execution of the uncertainty analysis simulations, computations, and output reports for QUAL2E-UNCAS. It calls the appropriate subroutines for reading the uncertainty data files, for screening the input and output variables for consistency and compatibility with the QUAL2E model options selected in

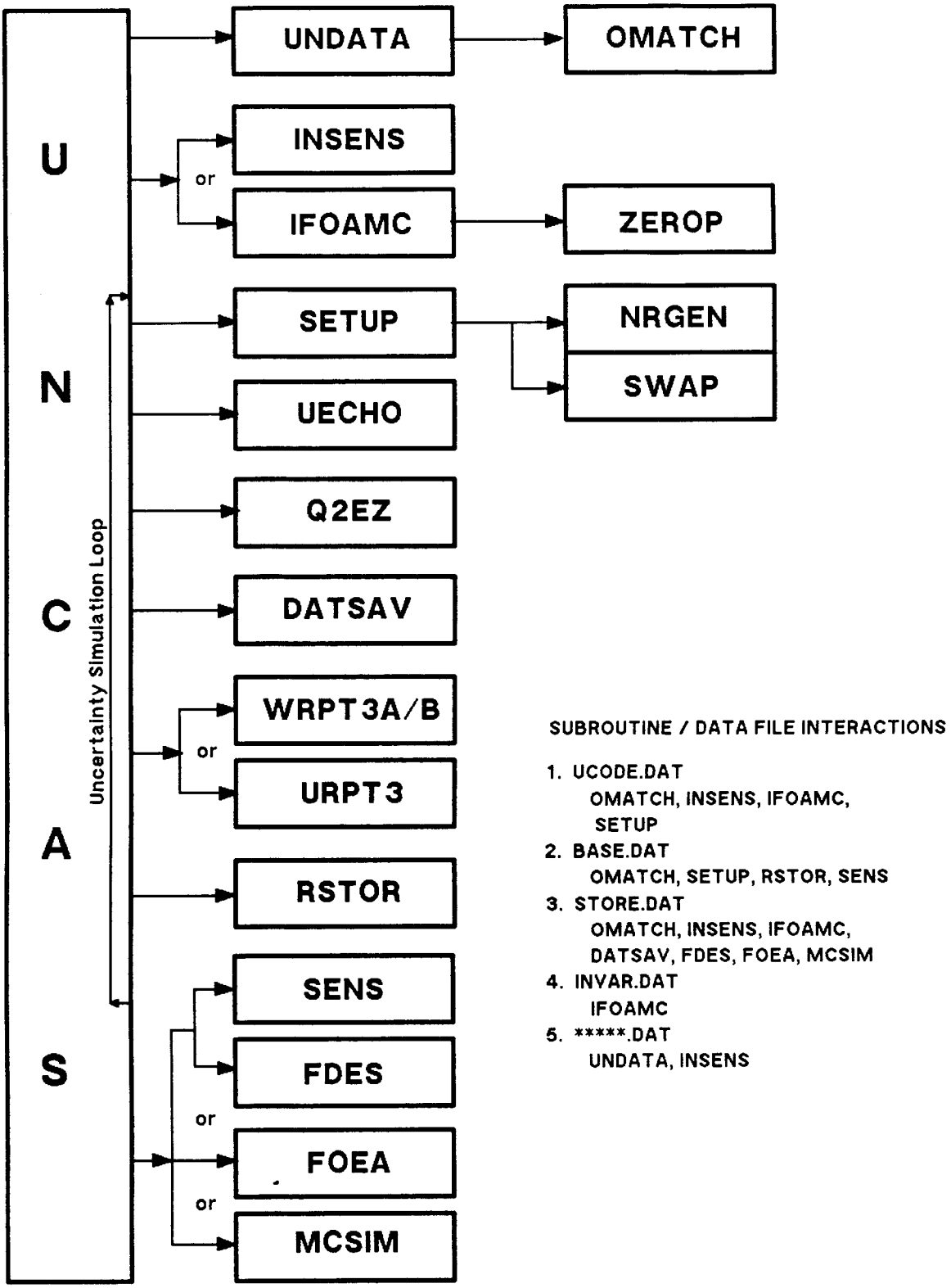

Figure VI-1 UNCAS Flow Diagram and Program Structure

the base case simulation, for performing the uncertainty simulations, and for computing and printing the appropriate uncertainty results.

b. Subroutine UNDATA. This subroutine reads the user-supplied input data file, *****.DAT, which contains the general specifications required for uncertainty analysis. It sets the appropriate flags and conditions for the type of uncertainty analysis to be performed.

c. Subroutine OMATCH. Subroutine OMATCH retrieves, purges, and stores (on disk file) the values of the appropriate output variables from the base case simulation. For sensitivity analysis, it saves the complete output from the base case simulation in the file BASE.DAT. For first order error analysis and monte carlo simulation it stores only the values of the output variables at the locations (maximum of five) in the basin where uncertainty results are desired and only for those that were modeled in the base case simulation (STORE.DAT). These data are subsequently used by subroutines FDES, FOEA, and MCSIM for their respective uncertainty analysis computations.

d. Subroutine INSENS. This subroutine controls the input specifications for sensitivity analysis. It reads the user-supplied input data file, *****.DAT, for the input variables that are to be perturbed for sensitivity analysis. It determines the total number of sensitivity simulations to be performed as well as the levels of all variables to be perturbed in each simulation.

e. Subroutine IFOAMC. Subroutine IFOAMC controls the input specifications for first order error analysis and for monte carlo simulation. It searches through a list of all input variables and purges (a) those variables that are not requested to be perturbed and (b) those input or model options that were not used in the base case simulation.

f. Subroutine ZEROP. This subroutine examines the numerical value of each input variable. If the value is such that the variable is not used in the base simulation (i.e., zero, or 1.0 for a temperature coefficient), the input variable is purged from the uncertainty analysis simulations.

g. Subroutine SETUP. Subroutine SETUP sets up the input condition for the current uncertainty simulation. Using the list of relevant inputs developed in either INSENS or IFOAMC, each input variable is perturbed or randomized as specified. It then calls subroutine SWAP to replace the base case value with the new value of the input variable.

h. Subroutine SWAP. This subroutine swaps the newly perturbed or randomized value of the input variable(s) for the base value(s). Swapping is done in memory by input data type and EQUIVALENCED arrays. Base case values are either saved in memory (sensitivity or first order options) or stored in the disk file BASE.DAT (monte carlo).

i. Subroutine NRGEN. This subroutine generates either normally or log-normally distributed random numbers for each input variable to be randomized in a monte carlo simulation. It uses a machine-specific random number generator.

j. Subroutine UECHO. Subroutine UECHO prints, as intermediate output, the input conditions of the current uncertainty simulation. This output includes the name of the input variable being altered and its base and perturbed value. This output is optional.

k. Subroutine Q2EZ. This subroutine is not new to UNCAS. It is that portion of the QUAL2E model that performs the simulation computations (see Figure I-1).

l. Subroutine DATSAV. This subroutine stores the appropriate output variables from each uncertainty simulation on the disk file STORE.DAT, for later processing by FDES, FOEA, or MCSIM.

m. Subroutines WRPT3A and WRPT3B. These subroutines are from the QUAL2E model, and write the final output summary for an UNCAS simulation. This output is optional and is not available in the monte carlo option.

n. Subroutine URPT3. Subroutine URPT3 writes a limited intermediate output summary of each uncertainty simulation. The summary consists of a comparison of (a) the steady state convergence characteristics for temperature and algae and (b) the base and new values of the output variables at the locations specified. This output is optional and is available only for the sensitivity analysis using factorial design and first order error analysis.

o. Subroutine RSTOR. This subroutine restores the value of the perturbed input to its base case value after completion of an uncertainty simulation. Thus, it prepares the input data for the next UNCAS simulation.

p. Subroutine SENS. Subroutine SENS writes the UNCAS final report for the sensitivity analysis option. It is similar in format to the QUAL2E output produced by subroutines WRPT3A/B, but consists of the change in output variable (sensitivity) resulting from the input perturbations of the sensitivity analysis.

q. Subroutine FDES. This subroutine performs the analysis of a factorially designed set of sensitivity analysis simulations. It writes the UNCAS final report for the factorial design, including the main and interaction effects of the sensitized input variables on each output variable at the user specified locations in the basin.

r. Subroutine FOEA. Subroutine FOEA performs the computations and writes the UNCAS final report for the first order error analysis option. The output consists of the normalized sensitivity coefficient matrix and the components of variance analysis for all inputs affecting each output variable at the user-specified locations in the basin.

s. Subroutine MCSIM. This subroutine performs the computations and writes the UNCAS final report for the monte carlo simulation option. The output consists of summary statistics, including base and simulated mean, bias, minimum, maximum, range, standard deviation, coefficient of variation, and skew coefficient as well as the frequency distribution (in one-half standard deviation steps) for each output variable at the user-specified locations in the basin.

6.4.2 Internal UNCAS DATA Files

a. File UCODE.DAT. This internal data file is supplied with the UNCAS package. It is a master file that contains information for identifying, matching, and screening the inputs to be modified in an UNCAS simulation. It also serves as the primary information source for linking UNCAS requests to the QUAL2E input data file.

b. File BASE.DAT. This internal data file stores information for the base case simulation. In the sensitivity analysis option, it stores the values of all the output variables for the QUAL2E base simulation. In the monte carlo simulation option, it stores the base values of the input variables that have been randomized. This data file is not used with the first order error analysis option.

c. File STORE.DAT. This internal data file stores the values of output variables at the user-specified locations for the base simulation and for each uncertainty simulation. When all uncertainty simulations are completed, these data are then used for the appropriate uncertainty output computations, i.e., factorial design for the sensitivity analysis option, or normalized sensitivity coefficients and components of variance for the first order error analysis option, or summary statistics and frequency distributions for the monte carlo option.

6.4.3 User-Supplied UNCAS Data Files

a. File INVAR.DAT. This data file contains the uncertainty information for each input varable in QUAL2E. These data consist of the variable name, its coefficient of variation, and its probability density function. An example of this file, containing a set of default data, is provided with the UNCAS package. Instructions for adjusting the uncertainty inputs to user specifications are provided in Appendix B--User Manual for QUAL2E-UNCAS.

b. File*****.DAT. This data file, named and prepared by the user, contains the general requirements for performing a QUAL2E-UNCAS simulation. This information consists, in part, of specifying the uncertainty analysis option, the type of intermediate output, any constraints on input variables to be modified, the output variables and locations for computing and printing uncertainty results, the number of monte carlo simulations, and the magnitude of the input variable perturbation. Instructions for assembling this data file are provided in Appendix B--User Manual for QUAL2E-UNCAS.

6.5 LIMITATIONS AND CONSTRAINTS FOR QUAL2E-UNCAS

Because of the general purpose nature of the QUAL2E and UNCAS computer codes, there are a few constraints in using the models that arise from the program structure and bookkeeping strategies used. These limitations are related to the level of detail the modeler may use in perturbing specific input variables.

1. Reach or Source Variable Inputs and Forcing Functions. In QUAL2E-UNCAS, input variables are treated in the general case rather than individually. For example, if the user wishes to perform uncertainty analysis on the CBOD rate coefficient, or the point load flows, then all input values (over the entire basin) of the rate coefficient and flows are perturbed. UNCAS does not have the capability of perturbing only one (or a few) of these inputs; i.e., the value of the CBOD rate coefficient in reach 3 or the flows for the second and fourth point loads. In short, the user specifies the name of the variable to be perturbed and the magnitude of the perturbation, then all values of that input variable are modified by the amount specified.

2. First Order Error Analysis. In first order error analysis, the user specifies the magnitude of the input perturbation, ΔX, for computing sensitivity coefficients. UNCAS applies this value of ΔX uniformly to all input variables. The modeler is not allowed to use one value of ΔX for one group of inputs and another value for a different group of inputs. (Note: The variance of each input variable can be specified uniquely, but as stated in subsection 1, that variance applies equally to all values of the variable in the basin.)

3. Input Variables Having a Numerical Value of Zero. Input variables whose values are determined by QUAL2E-UNCAS to be zero (either blanks in the input data file or an actual input value of zero) are assumed to be non-modeled inputs. Those variables will not be perturbed in any UNCAS simulation, and thus will not contribute to the uncertainty of the modeled output.