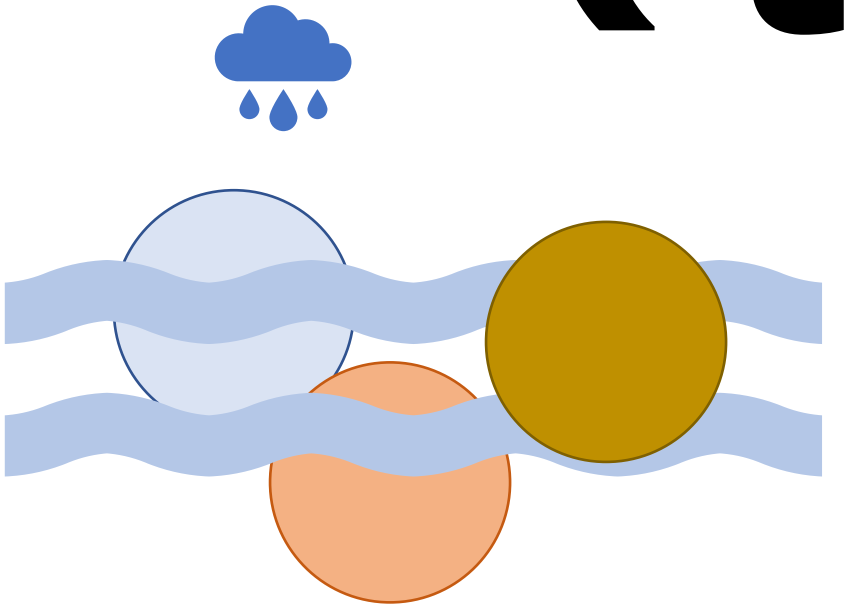
Computer Methods (QUAL 2E)



Steady-State System Response Matrix

The steady-state mass balances for such systems are expressed as a set of linear algebraic equations. These equations are solved as:

$$\{C\} = [A]^{-1}\{W\}$$

Where {C} = vector of unknown concentrations

{W} = vector of loadings

$[A]^{-1}$= matrix inverse of the steady-state system response matrix

Steady-State System Response Matrix

A steady state mass balance for CBOD in segment “i" can be written as

$$0 = W_{Li} + Q_{i-1,i}\left(\alpha_{i-1,i}L_{i-1} + \beta_{i-1,i}L_i\right) - Q\left(\alpha_{i,i+1}L_i + \beta_{i,i+1}L_{i+1}\right)$$
$$+E'_{i-1,i}(L_{i-1} - L_i) + E'_{i,i+1}(L_{i+1} - L_i) - k_{ri}V_iL_i$$

writing this equation for an n-segment system with appropriate upstream and downstream boundary conditions gives:

$$[A]\{L\} = \{W_L\}$$

with a solution:

$$\{L\} = [A]^{-1}\{W_L\}$$

Steady-State System Response Matrix

with a solution:

$$\{L\} = [A]^{-1}\{W_L\}$$

Coefficients of [A} are examined:

$$a_{i,i-1} = \alpha_{i-1,i}Q_{i-1,i} - E'_{i-1,i}$$

Transport

$$a_{i,i} = \underbrace{\alpha_{i,i+1}Q_{i,i+1} - \beta_{i-1,i}Q_{i-1,i} + E'_{i-1,i} + E'_{i,i+1}}_{\text{Transport}} + \underbrace{k_{ri}V_i}_{\text{Kinetics}}$$

$$a_{i,i+1} = \beta_{i-1,i}Q_{i-1,i} - E'_{i,i+1}$$

Transport

Steady-State System Response Matrix

All the transport terms would identical regardless of the pollutant. The [A] matrix can be divided into two parts,

$$[A] = [T] + [k_r V]$$

where [T] is a “transport” matrix identical to matrix [A] but containing only the transport terms, and $[k_r V]$ is a square diagonal matrix containing the terms $k_{ri} V_i$ on the diagonal and 0 elsewhere.

Steady-State System Response Matrix

Writing a similar mass balance for deficit, however we write the mass balance slightly different:

$$0 = W_{oi} + Q_{i-1,i}\left(\alpha_{i-1,i}o_{i-1} + \beta_{i-1,i}o_i\right) - Q_{i,i+1}\left(\alpha_{i,i+1}o_i + \beta_{i,i+1}o_{i+1}\right)$$
$$+E'_{i-1.i}(o_{i-1} - o_i) + E'_{i,i+1}(o_{i+1} - o_i) - k_{di}V_iL_i$$
$$+k_{ai}V_i(o_{si} - o_i) + P_iV_i - R_iV_i - S'_BA_{si}$$

Writing this equation for an n-segment system with appropriate upstream and downstream boundary conditions gives

$$[B]\{o\} = \{W_o\} + \{PV\} - \{RV\} - \{S'_BA_s\} + \{k_AVo_s\} - \{k_dVL\}$$

Steady-State System Response Matrix

$$[B]\{o\} = \{W_o\} + \{PV\} - \{RV\} - \{S'_B A_s\} + \{k_A V o_s\} - \{k_d V L\}$$

where

$$[B] = [T] + [k_a V]$$

by collecting terms, we write the resulting system of equations as

$$[B]\{o\} = \{W'_o\} - [k_d V]\{L\}$$

where $\{W'_o\}$ is a matrix containing all external oxygen sources and sinks

$\{W'_o\}$	$=$	$\{W_o\} +$	$\{PV\}$	$-$	$\{RV\} -$	$\{S'_B A_s\} +$	$\{k_a V o_s\}$
External sources		Direct loading	Photosynthesis gain		Respiration loss	SOD loss	Reaeration gain

EXAMPLE 26.1. MATRIX APPROACH FOR OXYGEN. A one-dimensional estuary has the following characteristics:

Flow = 1×10^7 m^3 d^{-1}
Width = 1500 m
Depth = 5 m
Dispersion = 1×10^7 m^2 d^{-1}

BOD decay = 0.2 d^{-1}
Reaeration = 0.25 d^{-1}
Saturation = 8 mg L^{-1}

The estuary is 100 km long. The boundary conditions at both the upstream and downstream ends are $L = 0$ and $o = o_s$. Loadings of BOD and oxygen of 300,000 and 100,000 kg d^{-1}, respectively, enter the estuary at KP 35. Centered differences were used to approximate space.

(*a*) Calculate the distribution of BOD and oxygen in the estuary using segment sizes of 10 km.

(*b*) Determine the BOD loading reduction needed to raise the minimum oxygen concentration in the estuary to 5 mg L^{-1}.

The QUAL2E Model

QUAL 2E (enhanced QUAL-II model) is capable of simulating up to 15 water quality constituents in dendritic streams that are well-mixed laterally and vertically. It allows for multiple waste discharges, withdrawals, tributary flows, and incremental (distributed) inflows and outflows.

The QUAL2E Model

TABLE 26.1
The 15 constituents that can be simulated by QUAL2E

Dissolved oxygen	Ammonia as N	Coliform bacteria
Biochemical oxygen demand	Nitrite as N	Arbitrary nonconservative constituent
Temperature	Nitrate as N	Conservative constituent I
Algae as chlorophyll *a*	Organic phosphorus as P	Conservative constituent II
Organic nitrogen as N	Dissolved phosphorus as P	Conservative constituent III

QUAL2E

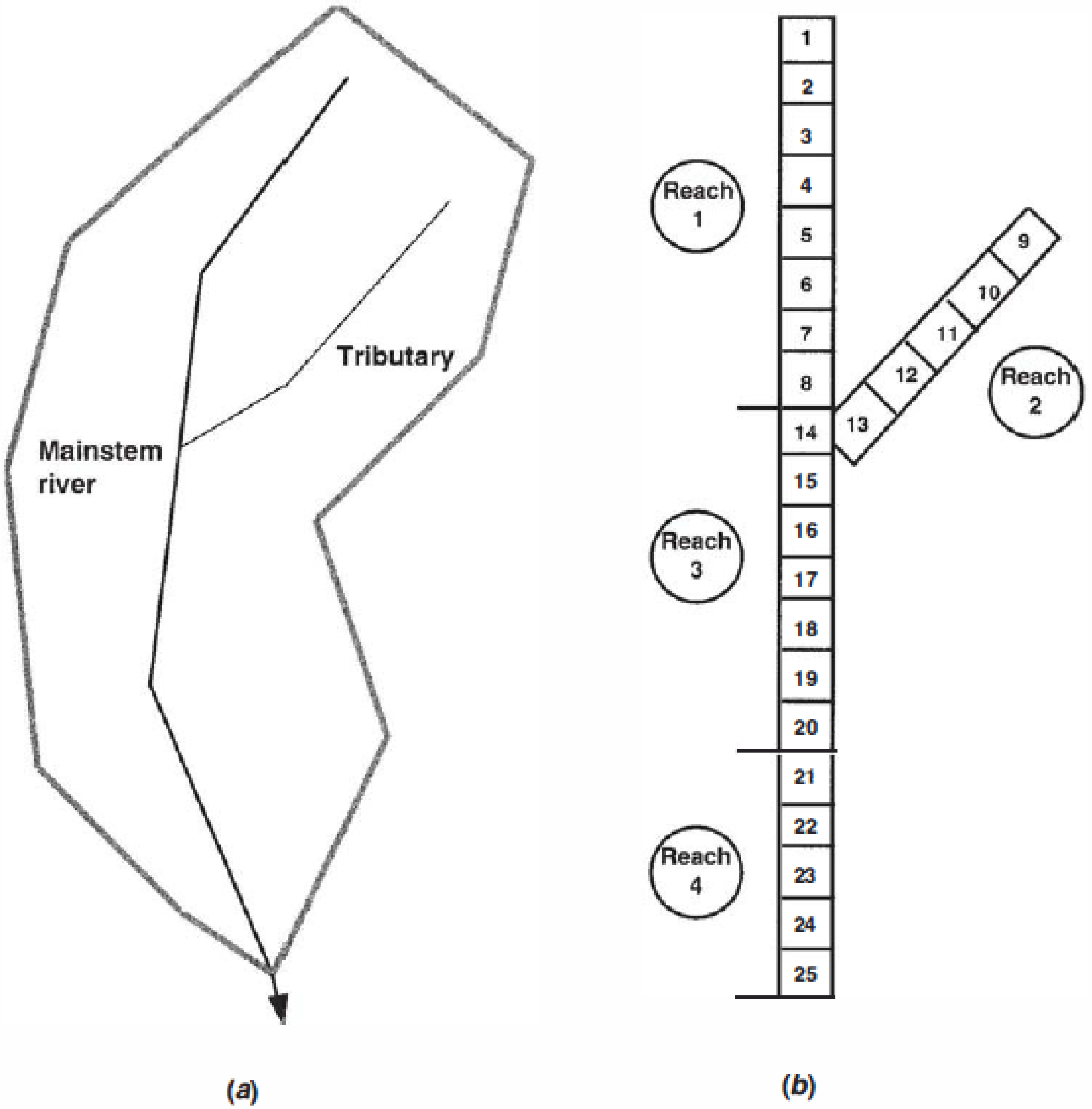


FIGURE 26.1
(*a*) A river basin and (*b*) a QUAL2E representation as reaches and elements.

Spatial Discretization and Model Overview

QUAL2E treats a river as a collection of reaches, each having homogenous hydrogeometric properties.

$$V\frac{\partial c}{\partial t} = \frac{\partial\left(A_c E\frac{\partial c}{\partial x}\right)}{\partial x}dx - \frac{\partial(A_c U_c)}{\partial x}dx + V\frac{dc}{dt} + s$$

Accumulation Dispersion Advection Kinetics External sources/sinks

where V = volume

c = constituent concentration

Ac = element cross-sectional area

E = longitudinal dispersion coefficient

x = distance

U = average velocity

s = external sources (positive) or sinks (negative) of the consitutuent

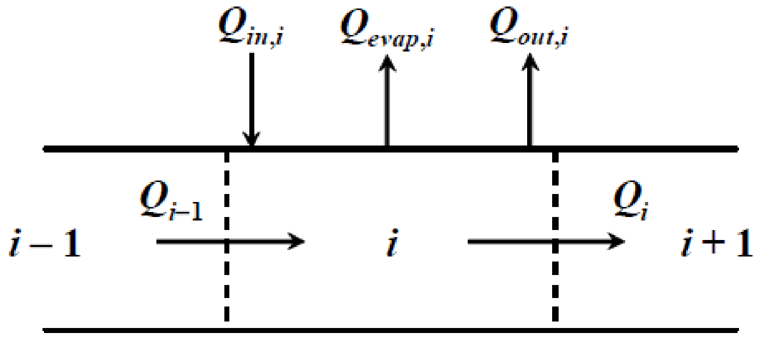
Transport

$$\frac{\partial\left(A_c E \frac{\partial c}{\partial x}\right)}{\partial x} dx - \frac{\partial (A_c U_c)}{\partial x} dx$$

Dispersion Advection

From the previous equation, we note that transport consists of two components: advection and dispersion. Advection refers to the movement of the constituent with water as it flows downstream, the latter relates to the spreading of the constituent due to shear.

Transport: Advection



QUAL2E model assumes steady, nonuniform flow. The term steady flow refers to flow that does not vary temporally. The term nonuniform flow means that it varies spatially. For this characterization a flow balance for element i can be written as:

$$Q_i = Q_{i-1} + Q_{in,i} - Q_{out,i} - Q_{evap,i}$$

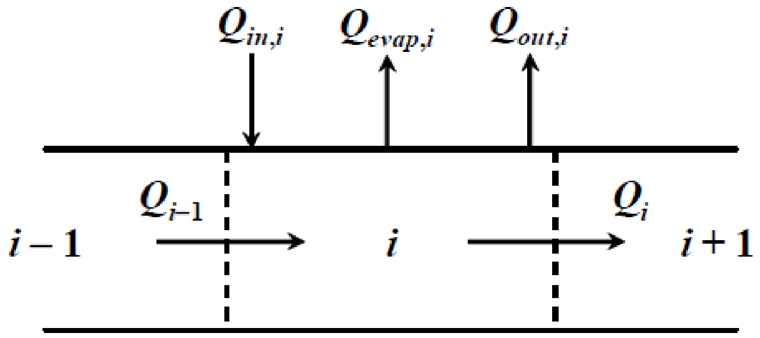
$$Q_{i-1} \pm Q_{x,i} - Q_i = 0$$

where Q_{i-1} = flow from the upstream element

Q_i = outflow from the element

$Q_{x,i}$ = lateral flow into (positive) or out of (negative) the element

Transport: Advection



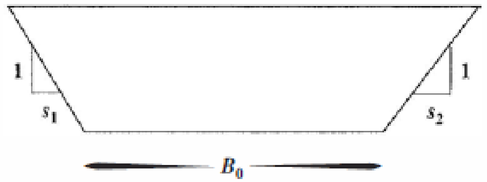
Power Equations can be used to relate mean velocity and depth to flow

$$U = aQ^b$$
$$H = \alpha Q^\beta$$

where H = mean depth and a, b, α, β, are empirical constants that are determined from stage-discharge rating curves. Once velocity has been determined, the cross-sectional area can be calculated from the continuity equation:

$$A_c = \frac{Q}{U}$$

Manning Equation provides relationship between channel and flow



$$Q = \frac{1}{n} A_c R^{2/3} S_e^{1/2}$$

where R= channel's hydraulic radius and S_e = slope of channel's energy gradient line.

Transport: Dispersion

The QUAL2E model uses the following relationship to compute dispersion as a function of the channel's characteristics:

$$E = 3.11KnUH^{5/6}$$

where E= longitudinal dispersion coefficient (m^2s^{-1})

n= channel's roughness coefficient (dimensionless)

U= mean velocity (mps)

H= mean depth (m)

K= a dispersion parameter (dimensionless)

and

$$K = \frac{E}{HU^*}$$

where U* shear velocity (m s^{-1}).

Kinetics

Here we focus on two constituents: carbonaceous BOD (CBOD) and dissolved oxygen.

$$\frac{dL}{dt} = -K_1 L - K_3 L$$

and

$$\frac{do}{dt} = K_2(o_s - o) - K_1 L - \frac{K_4}{H}$$

where L= carbonaceous BOD (mg L^{-1})

K_1= BOD decomposition rate (d^{-1})

K_3 = BOD settling rate (d^{-1})

o = dissolved oxygen concentration (mgL^{-1})

K_2= reaeration rate (d^{-1})

o_s= dissolved oxygen saturation concentration (mgL^{-1})

K_4= sediment oxygen demand (g m^{-2} d^{-1})

Kinetics

Note that all K's are corrected for temperature by:

$$K = K_{20}\theta^{T-20}$$

where K= rate at temperature T

K_{20}= rate at 20°C

θ= temperature correction factor

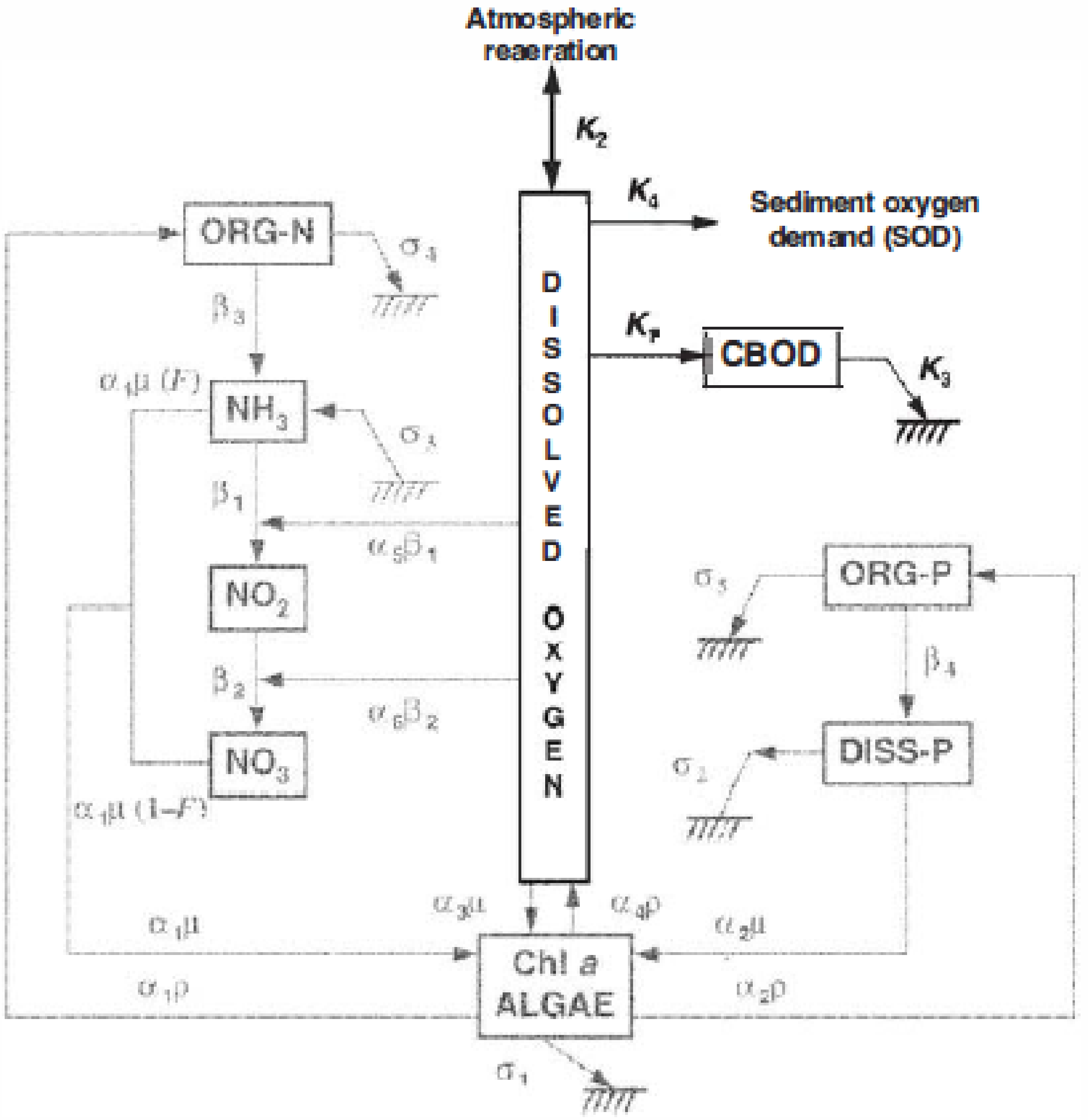


FIGURE 26.3
QUAL2E kinetics. Note that the highlighted constituents and processes are described and modeled in this lecture. We will extend our discussion to the remainder of the diagram in Lec. 36.

TABLE 26.2

Reaeration formulas in QUAL2E. Note that some of these formulas (2, 3, and 4) differ slightly from the versions in Lec. 20 due to rounding errors

Option	Author(s)	K_2 (d^{-1} at 20°C)	Units
1	User-specified value		
2	Churchill et al. (1962)	$5.03\frac{U^{0.969}}{H^{1.673}}$	$\overline{U}$ (m s^{-1}) H (m)
3	O'Connor and Dobbins (1958)	$3.95\frac{U^{0.5}}{H^{1.5}}$	$\overline{U}$ (m s^{-1}) H (m)
4	Owens et al. (1964)	$5.34\frac{U^{0.67}}{H^{1.85}}$	$\overline{U}$ (m s^{-1}) H (m)
5	Thackston and Krenkel (1966)	$24.9\frac{(1+\sqrt{F})u^*}{H}$ where F is the Froude number, $F = \frac{u^*}{\sqrt{gH}}$ and u^* is the shear velocity, $u^* = \sqrt{HS_e g} = \frac{Un\sqrt{g}}{H^{1.67}}$	F (dimensionless) u^* (m s^{-1}) H (m) $\overline{U}$ (m s^{-1})
6	Langbien and Durum (1967)	$5.13\frac{U}{H^{1.33}}$	H (m) $\overline{U}$ (m s^{-1})
7	User-specified power function	aQ^b	Q (cms)
8	Tsivoglou and Wallace (1972); Tsivoglou and Neal (1976)	$c\frac{\Delta H}{t_f}$ where ΔH is change in water-surface elevation in the element, t_f is the flow time in the element, and c is a flow-dependent escape coefficient: $c = 0.36$ for $0.028 \le Q \le 0.28$ cms $c = 0.177$ for $0.708 \le Q \le 85$ cms	c (m^{-1}) ΔH (m) t_f (d)

Numerical Algorithm

We can discuss now how the model obtains solutions numerically. The equation ($V\frac{\partial c}{\partial t} = \frac{\partial\left(A_c E\frac{\partial c}{\partial x}\right)}{\partial x}dx - \frac{\partial(A_c U_c)}{\partial x}dx + V\frac{dc}{dt} + s$) can be divided by volume and written as:

$$\frac{\partial c}{\partial t} = \frac{\partial\left(A_c E\frac{\partial c}{\partial x}\right)}{A_c \partial x} - \frac{\partial(A_c U_c)}{A_c \partial x} + rc + p + \frac{s}{V}$$

observe that we have divided the kinetic into two separate terms

$$\frac{dc}{dt} = rc + p$$

The first term denotes those reactions that are linearly dependent on concentration, the other denotes internal constituent concentrations.

Numerical Algorithm

A general representation of QUAL2E element scheme is written as:

$$\frac{\partial c_i}{\partial t} = \frac{-\left(A_c E \frac{\partial c}{\partial x}\right)_{i-1} + \left(A_c E \frac{\partial c}{\partial x}\right)_i}{V_i} + \frac{(A_c U c)_{i-1} - (A_c U c)_i}{V_i}$$

Acc *In* *Out* *In* *Out*

Dispersion *Advection*

$$+ \quad r_i c_i \quad + \quad p_i \quad + \quad \frac{s_i}{V_i}$$

First –order reactions *Internal sources/sinks* *External sources/sinks*

Numerical Algorithm

Backwards differences can be used to approximate the spatial derivatives:

$$\frac{\partial c_i}{\partial t} = \frac{(A_c E)(c_{i+1} - c_i)}{V_i \Delta x_i} + \frac{(A_c E)(c_{i-1} - c_i)}{V_i \Delta x_i} + \frac{Q_{i-1} c_{i-1} - Q_i c_i}{V_i} + r_i c_i + p_i + \frac{s_i}{V_i}$$

Finally a backward difference can be applied in time to yield

$$\frac{c_i^{\ell+1} - c_i^{\ell}}{\Delta t} = \frac{(A_c E)_{i,i+1}(c_{i+1}^{\ell+1} - c_i^{\ell+1})}{V_i \Delta x_i} + \frac{(A_c E)_{i-1,i}(c_{i-1}^{\ell+1} - c_i^{\ell+1})}{V_i \Delta x_i} + \frac{Q_{i-1} c_{i-1}^{\ell+1} - Q_i c_i^{\ell+1}}{V_i} + r_i c_i^{\ell+1} + p_i + \frac{s_i}{V_i}$$

QUAL2E Application

TABLE 26.3
Hydrogeometric parameters

Parameter	Units	KP > 100	KP 100–60	KP < 60
Depth	m	1.19	1.24	1.41
	(ft)	(3.90)	(4.07)	(4.62)
Area	m^2	14.71	15.5	18.05
Flow	$m^3\ s^{-1}$	5.787	6.250	7.407
	$m^3\ d^{-1}$	500,000	540,000	640,000
	(cfs)	(204)	(221)	(262)
Velocity	$m\ s^{-1}$	0.393	0.403	0.410
	$m\ d^{-1}$	33,955	34,819	35,424
	(fps)	(1.29)	(1.32)	(1.35)

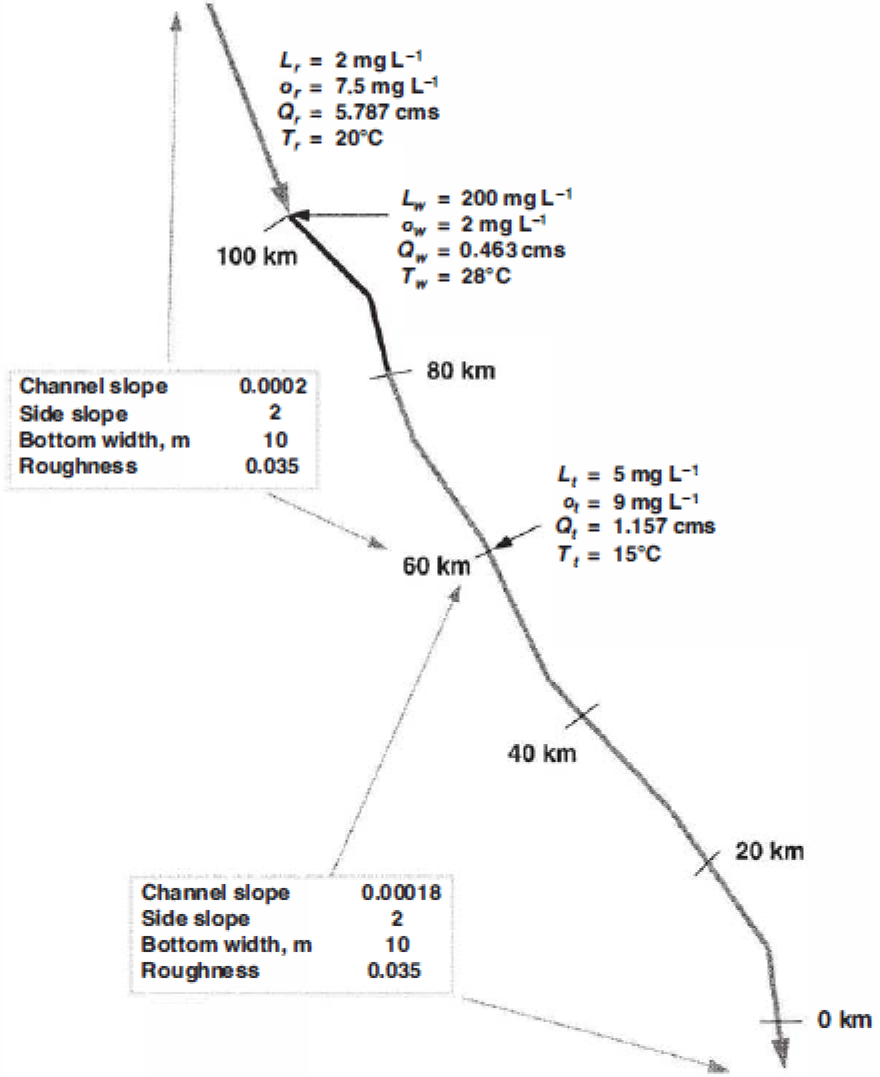


FIGURE 26.5
A stream receiving BOD loadings from a point source and a tributary.