LECTURE 26

Computer Methods

Lecture overview: I review some computer-oriented methods for solving oxygen balances with the computer. First I develop the steady-state system response matrix for the Streeter-Phelps framework. Then I provide an introduction to the QUAL2E model. After some historical background, I describe its underlying structure. Then I illustrate its use by applying it to simulate oxygen levels in a stream, with a focus on oxygen depletion due to BOD and SOD.

Although we have touched on some computer methods, to this point our discussion of oxygen modeling has focused on analytical, closed-form solutions. Now we broaden our perspective to show how numerical methods allow us to implement such calculations with the computer. First I describe a matrix approach that has great utility for developing steady-state solutions for linear DO models. Then I provide an introduction to EPA's QUAL2E software package.

26.1 STEADY-STATE SYSTEM RESPONSE MATRIX

In Lecs. 6 and 11 we developed the steady-state-system response matrix as a means to summarize the interactions of loadings and responses for linear water-quality models. Recall that the steady-state mass balances for such systems could be expressed as a set of linear algebraic equations. These equations could then be solved as

$$\{C\} = [A]^{-1}\{W\} \tag{26.1}$$

where $\{C\}$ = vector of unknown concentrations
$\{W\}$ = vector of loadings
$[A]^{-1}$ = matrix inverse or the steady-state-system response matrix

We showed how each element of $[A]^{-1}$ provides the change in concentration in element i due to a unit load change to segment j.

We now illustrate how this idea can be expanded to BOD/oxygen modeling. To do this we limit our analysis to a one-dimensional system with carbonaceous BOD and oxygen. The approach can be easily extended to multidimensional systems, NBOD, or linear representations of nitrification. A steady-state mass balance for CBOD in segment i can be written as

$$\begin{aligned} 0 = {} & W_{Li} + Q_{i-1,i}(\alpha_{i-1,i}L_{i-1} + \beta_{i-1,i}L_i) - Q(\alpha_{i,i+1}L_i + \beta_{i,i+1}L_{i+1}) \\ & + E'_{i-1,i}(L_{i-1} - L_i) + E'_{i,i+1}(L_{i+1} - L_i) - k_{ri}V_iL_i \end{aligned} \tag{26.2}$$

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

$$[A]\{L\} = \{W_L\} \tag{26.3}$$

with a solution

$$\{L\} = [A]^{-1}\{W_L\} \tag{26.4}$$

Now the coefficients of $[A]$ bear scrutiny. They are

$$a_{i,i-1} = \underset{\text{Transport}}{-\alpha_{i-1,i}Q_{i-1,i} - E'_{i-1,i}} \tag{26.5}$$

$$a_{i,i} = \underbrace{\alpha_{i,i+1}Q_{i,i+1} - \beta_{i-1,i}Q_{i-1,i} + E'_{i-1,i} + E'_{i,i+1}}_{\text{Transport}} + \underbrace{k_{ri}V_i}_{\text{Kinetics}} \tag{26.6}$$

$$a_{i,i+1} = \underset{\text{Transport}}{\beta_{i,i+1}Q_{i,i+1} - E'_{i,i+1}} \tag{26.7}$$

All the terms marked "transport" would be identical regardless of the pollutant. Thus the $[A]$ matrix can be divided into two parts, as in

$$[A] = [T] + [k_rV] \tag{26.8}$$

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

Using a similar approach, we can write mass balances for deficit (see Thomann and Mueller 1987). However, because such an approach can lead to errors for systems where saturation is variable (recall our discussion in Lec. 21), we write the mass balance for oxygen,

$$\begin{aligned} 0 = {} & W_{oi} + Q_{i-1,i}(\alpha_{i-1,i}o_{i-1} + \beta_{i-1,i}o_i) - Q_{i,i+1}(\alpha_{i,i+1}o_i + \beta_{i,i+1}o_{i+1}) \\ & + E'_{i-1,i}(o_{i-1} - o_i) + E'_{i,i+1}(o_{i+1} - o_i) - k_{di}V_iL_i \\ & + k_{ai}V_i(o_{si} - o_i) + P_iV_i - R_iV_i - S'_BA_{si} \end{aligned} \tag{26.9}$$

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

$$[B]\{o\} = \{W_o\} + \{PV\} - \{RV\} - \{S'_BA_s\} + \{k_aVo_s\} - \{k_dVL\} \tag{26.10}$$

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where

$$[B] = [T] + [k_a V] \tag{26.11}$$

By collecting terms, we can write the resulting system of equations as

$$[B]\{o\} = \{W_o'\} - [k_d V]\{L\} \tag{26.12}$$

where $\{W_o'\}$ is a matrix containing all the external oxygen sources and sinks,

$$\underset{\substack{\text{External}\\\text{sources}}}{\{W_o'\}} = \underset{\substack{\text{Direct}\\\text{loading}}}{\{W_o\}} + \underset{\substack{\text{Photosynthesis}\\\text{gain}}}{\{PV\}} - \underset{\substack{\text{Respiration}\\\text{loss}}}{\{RV\}} - \underset{\substack{\text{SOD}\\\text{loss}}}{\{S_B'A\}} + \underset{\substack{\text{Reaeration}\\\text{gain}}}{\{k_a V o_s\}} \tag{26.13}$$

Multiplying both sides by the matrix inverse of $[B]$ yields

$$\{o\} = [B]^{-1}\{W_o'\} - [B]^{-1}[k_d V][A]^{-1}\{W_L\} \tag{26.14}$$

or

$$\{o\} = [B]^{-1}\{W_o'\} - [C]^{-1}\{W_L'\} \tag{26.15}$$

where $[C]^{-1}$ is a system response matrix that relates oxygen concentration to BOD loading,

$$[C]^{-1} = [B]^{-1}[k_d V][A]^{-1} \tag{26.16}$$

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

Flow = 1×10^7 m^3 d^{-1}	BOD decay = 0.2 d^{-1}
Width = 1500 m	Reaeration = 0.25 d^{-1}
Depth = 5 m	Saturation = 8 mg L^{-1}
Dispersion = 1×10^7 m^2 d^{-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}.

Solution: (*a*) Using the parameter values, we can write and solve the mass balance equations. The results are displayed in Fig. E26.1.

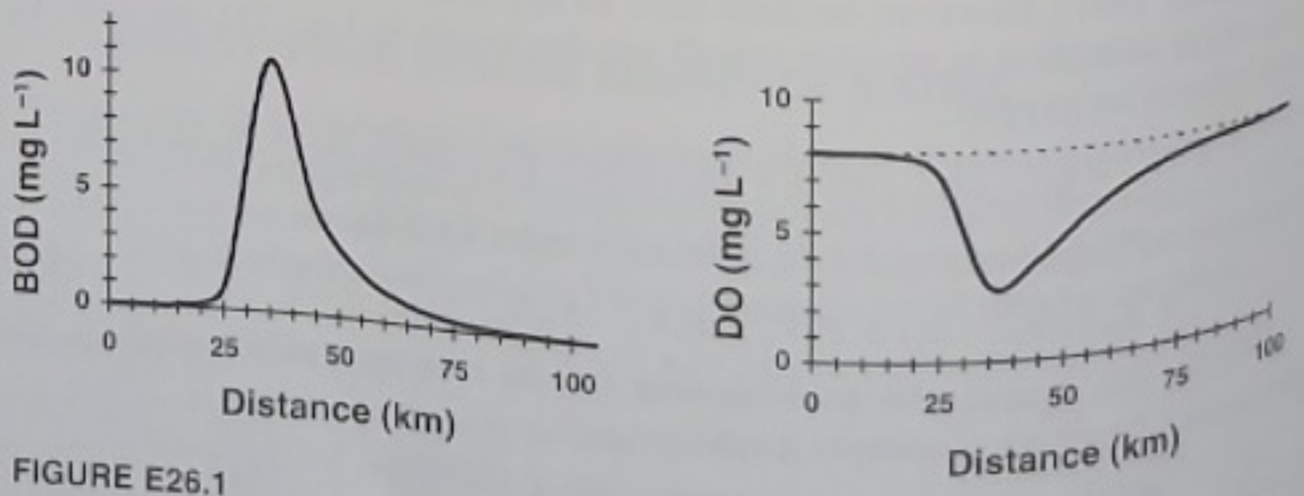

FIGURE E26.1

(*b*) The minimum DO is 2.84 mg L^{-1}. Thus, to bring this value up to 5 mg L^{-1}, we must increase the DO by $\Delta o = 5 - 2.84 = 2.16$ mg L^{-1}. This value can be translated into a load change by using the appropriate value from the matrix inverse,

$$[C]^{-1} = \begin{bmatrix} 1.64E-08 & 2.66E-09 & 3.25E-10 & 3.53E-11 & 3.61E-12 & 3.54E-13 & 3.38E-14 & 3.17E-15 & 2.92E-16 & 2.56E-17 \\ 1.33E-08 & 1.80E-08 & 2.84E-09 & 3.43E-10 & 3.71E-11 & 3.78E-12 & 3.70E-13 & 3.53E-14 & 3.29E-15 & 2.92E-16 \\ 8.12E-09 & 1.42E-08 & 1.81E-08 & 2.85E-09 & 3.44E-10 & 3.72E-11 & 3.78E-12 & 3.70E-13 & 3.53E-14 & 3.17E-15 \\ 4.42E-09 & 8.58E-09 & 1.42E-08 & 1.81E-08 & 2.85E-09 & 3.44E-10 & 3.72E-11 & 3.78E-12 & 3.70E-13 & 3.38E-14 \\ 2.25E-09 & 4.64E-09 & 8.60E-09 & 1.42E-08 & 1.81E-08 & 2.85E-09 & 3.44E-10 & 3.72E-11 & 3.78E-12 & 3.54E-13 \\ 1.11E-09 & 2.36E-09 & 4.65E-09 & 8.60E-09 & 1.42E-08 & 1.81E-08 & 2.85E-09 & 3.44E-10 & 3.71E-11 & 3.61E-12 \\ 5.28E-10 & 1.16E-09 & 2.36E-09 & 4.65E-09 & 8.60E-09 & 1.42E-08 & 1.81E-08 & 2.85E-09 & 3.43E-10 & 3.53E-11 \\ 2.47E-10 & 5.51E-10 & 1.16E-09 & 2.36E-09 & 4.65E-09 & 8.60E-09 & 1.42E-08 & 1.81E-08 & 2.84E-09 & 3.25E-10 \\ 1.14E-10 & 2.57E-10 & 5.51E-10 & 1.16E-09 & 2.36E-09 & 4.64E-09 & 8.58E-09 & 1.42E-08 & 1.80E-08 & 2.66E-09 \\ 5.00E-11 & 1.14E-10 & 2.47E-10 & 5.28E-10 & 1.11E-09 & 2.25E-09 & 4.42E-09 & 8.12E-09 & 1.33E-08 & 1.64E-08 \end{bmatrix}$$

The needed value is in the fourth row and the fourth column: $c_{44}^{-1} = 1.81 \times 10^{-8}$ (mg L^{-1})/(g d^{-1}). (Remember, the column location is dictated by the position of the loading and the row by the location of the resulting concentration.) This value can be used to compute

$$\Delta W_L = \frac{2.16 \text{ mg L}^{-1}}{1.81 \times 10^{-8} \dfrac{\text{mg L}^{-1}}{\text{g d}^{-1}}} \left(\frac{\text{kg}}{1000 \text{ g}}\right) = 119{,}337 \text{ kg d}^{-1}$$

Thus the BOD load must be reduced by 40% to meet the oxygen goal.

The matrix approach is predicated on having a linear model. Although this is true for the classic Streeter-Phelps framework, more recent oxygen models include nonlinear terms that preclude the matrix approach. Consequently it might seem that the method outlined in the present section is obsolete. There are three reasons why this isn't necessarily true:

1. Even though nonlinearities appear in models, some of the new mechanisms are not highly nonlinear. Consequently some mechanisms are amenable to linearization via a Taylor-series expansion. For such cases the foregoing approach could be employed without incurring major errors.

(*b*) The minimum DO is 2.84 mg L^{-1}. Thus, to bring this value up to 5 mg L^{-1}, we must increase the DO by $\Delta o = 5 - 2.84 = 2.16 \text{ mg L}^{-1}$. This value can be translated into a load change by using the appropriate value from the matrix inverse,

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1.64\text{E}-08 & 2.66\text{E}-09 & 3.25\text{E}-10 & 3.53\text{E}-11 & 3.61\text{E}-12 \\
1.33\text{E}-08 & 1.80\text{E}-08 & 2.84\text{E}-09 & 3.43\text{E}-10 & 3.71\text{E}-11 \\
8.12\text{E}-09 & 1.42\text{E}-08 & 1.81\text{E}-08 & 2.85\text{E}-09 & 3.44\text{E}-10 \\
4.42\text{E}-09 & 8.58\text{E}-09 & 1.42\text{E}-08 & 1.81\text{E}-08 & 2.85\text{E}-09 \\
2.25\text{E}-09 & 4.64\text{E}-09 & 8.60\text{E}-09 & 1.42\text{E}-08 & 1.81\text{E}-08 \\
1.11\text{E}-09 & 2.36\text{E}-09 & 4.65\text{E}-09 & 8.60\text{E}-09 & 1.42\text{E}-08 \\
5.28\text{E}-10 & 1.16\text{E}-09 & 2.36\text{E}-09 & 4.65\text{E}-09 & 8.60\text{E}-09 \\
2.47\text{E}-10 & 5.51\text{E}-10 & 1.16\text{E}-09 & 2.36\text{E}-09 & 4.65\text{E}-09 \\
1.14\text{E}-10 & 2.57\text{E}-10 & 5.51\text{E}-10 & 1.16\text{E}-09 & 2.36\text{E}-09 \\
5.00\text{E}-11 & 1.14\text{E}-10 & 2.47\text{E}-10 & 5.28\text{E}-10 & 1.11\text{E}-09
\end{matrix}\right.$$

$$\left.\begin{matrix}
3.54\text{E}-13 & 3.38\text{E}-14 & 3.17\text{E}-15 & 2.92\text{E}-16 & 2.56\text{E}-17 \\
3.78\text{E}-12 & 3.70\text{E}-13 & 3.53\text{E}-14 & 3.29\text{E}-15 & 2.92\text{E}-16 \\
3.72\text{E}-11 & 3.78\text{E}-12 & 3.70\text{E}-13 & 3.53\text{E}-14 & 3.17\text{E}-15 \\
3.44\text{E}-10 & 3.72\text{E}-11 & 3.78\text{E}-12 & 3.70\text{E}-13 & 3.38\text{E}-14 \\
2.85\text{E}-09 & 3.44\text{E}-10 & 3.72\text{E}-11 & 3.78\text{E}-12 & 3.54\text{E}-13 \\
1.81\text{E}-08 & 2.85\text{E}-09 & 3.44\text{E}-10 & 3.71\text{E}-11 & 3.61\text{E}-12 \\
1.42\text{E}-08 & 1.81\text{E}-08 & 2.85\text{E}-09 & 3.43\text{E}-10 & 3.53\text{E}-11 \\
8.60\text{E}-09 & 1.42\text{E}-08 & 1.81\text{E}-08 & 2.84\text{E}-09 & 3.25\text{E}-10 \\
4.64\text{E}-09 & 8.58\text{E}-09 & 1.42\text{E}-08 & 1.80\text{E}-08 & 2.66\text{E}-09 \\
2.25\text{E}-09 & 4.42\text{E}-09 & 8.12\text{E}-09 & 1.33\text{E}-08 & 1.64\text{E}-08
\end{matrix}\right]$$

The needed value is in the fourth row and the fourth column: $c_{44}^{-1} = 1.81 \times 10^{-8}$ (mg L^{-1})/(g d^{-1}). (Remember, the column location is dictated by the position of the loading and the row by the location of the resulting concentration.) This value can be used to compute

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1.33\text{E}{-08} & 1.80\text{E}{-08} & 2.84\text{E}{-09} & 3.43\text{E}{-10} & 3.71\text{E}{-11} \\
8.12\text{E}{-09} & 1.42\text{E}{-08} & 1.81\text{E}{-08} & 2.85\text{E}{-09} & 3.44\text{E}{-10} \\
4.42\text{E}{-09} & 8.58\text{E}{-09} & 1.42\text{E}{-08} & 1.81\text{E}{-08} & 2.85\text{E}{-09} \\
2.25\text{E}{-09} & 4.64\text{E}{-09} & 8.60\text{E}{-09} & 1.42\text{E}{-08} & 1.81\text{E}{-08} \\
1.11\text{E}{-09} & 2.36\text{E}{-09} & 4.65\text{E}{-09} & 8.60\text{E}{-09} & 1.42\text{E}{-08} \\
5.28\text{E}{-10} & 1.16\text{E}{-09} & 2.36\text{E}{-09} & 4.65\text{E}{-09} & 8.60\text{E}{-09} \\
2.47\text{E}{-10} & 5.51\text{E}{-10} & 1.16\text{E}{-09} & 2.36\text{E}{-09} & 4.65\text{E}{-09} \\
1.14\text{E}{-10} & 2.57\text{E}{-10} & 5.51\text{E}{-10} & 1.16\text{E}{-09} & 2.36\text{E}{-09} \\
5.00\text{E}{-11} & 1.14\text{E}{-10} & 2.47\text{E}{-10} & 5.28\text{E}{-10} & 1.11\text{E}{-09}
\end{array}\right.$$

$$\left.\begin{array}{ccccc}
3.54\text{E}{-13} & 3.38\text{E}{-14} & 3.17\text{E}{-15} & 2.92\text{E}{-16} & 2.56\text{E}{-17} \\
3.78\text{E}{-12} & 3.70\text{E}{-13} & 3.53\text{E}{-14} & 3.29\text{E}{-15} & 2.92\text{E}{-16} \\
3.72\text{E}{-11} & 3.78\text{E}{-12} & 3.70\text{E}{-13} & 3.53\text{E}{-14} & 3.17\text{E}{-15} \\
3.44\text{E}{-10} & 3.72\text{E}{-11} & 3.78\text{E}{-12} & 3.70\text{E}{-13} & 3.38\text{E}{-14} \\
2.85\text{E}{-09} & 3.44\text{E}{-10} & 3.72\text{E}{-11} & 3.78\text{E}{-12} & 3.54\text{E}{-13} \\
1.81\text{E}{-08} & 2.85\text{E}{-09} & 3.44\text{E}{-10} & 3.71\text{E}{-11} & 3.61\text{E}{-12} \\
1.42\text{E}{-08} & 1.81\text{E}{-08} & 2.85\text{E}{-09} & 3.43\text{E}{-10} & 3.53\text{E}{-11} \\
8.60\text{E}{-09} & 1.42\text{E}{-08} & 1.81\text{E}{-08} & 2.84\text{E}{-09} & 3.25\text{E}{-10} \\
4.64\text{E}{-09} & 8.58\text{E}{-09} & 1.42\text{E}{-08} & 1.80\text{E}{-08} & 2.66\text{E}{-09} \\
2.25\text{E}{-09} & 4.42\text{E}{-09} & 8.12\text{E}{-09} & 1.33\text{E}{-08} & 1.64\text{E}{-08}
\end{array}\right]$$

The needed value is in the fourth row and the fourth column: $c_{44}^{-1} = 1.81 \times 10^{-8}$ (mg L^{-1})/(g d^{-1}). (Remember, the column location is dictated by the position of the loading and the row by the location of the resulting concentration.) This value can be used to compute

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1. Even though nonlinearities appear in models, some of the new mechanisms are not highly nonlinear. Consequently some mechanisms are amenable to linearization via a Taylor-series expansion. For such cases the foregoing approach could be employed without incurring major errors.

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2. Although the Streeter-Phelps model may seem passé, it is still useful where primary and secondary treatment are to be evaluated. Such management contexts still occur in developing countries.
3. The general approach outlined here is useful for other problem contexts beyond oxygen. For example many of the modeling frameworks used to assess toxic substances are linear. Hence the matrix solution techniques are possible and useful.

26.2 THE QUAL2E MODEL

The QUAL2E software package is presently the most widely used computer model for simulating stream-water quality. It is capable of simulating up to 15 water-quality constituents (Table 26.1) in dendritic streams that are well-mixed laterally and vertically. Among its many capabilities it allows for multiple waste discharges, withdrawals, tributary flows, and incremental (that is, distributed) inflows and outflows.

QUAL2E has its roots in the QUAL-I model developed by F. D. Masch and Associates and the Texas Water Development Board (1970). In 1972 Water Resources Engineers, Inc. (now Camp, Dresser and McKee), under contract with the U.S. Environmental Protection Agency, modified and extended QUAL-I to create the first version of QUAL-II. Over the ensuing years the model was upgraded several times (for example Roesner et al. 1981*a*, 1981*b*). The present version (Brown and Barnwell 1987) is known as the "enhanced QUAL-II model" or QUAL2E for short. It is currently maintained by the EPA's Center for Water Quality Modeling in Athens, Georgia.

It should be noted that QUAL2E was originally developed using punch cards as its input media. As the software moved to time-sharing systems and then personal computers, the input files to run the model maintained the data structure of the punch-card input. Recently a user-friendly interface for entering the input file and viewing the results of QUAL2E simulations has been developed and is being distributed (Lahlou et al. 1995). This interface should further enhance the utility and widespread application of this model. Although the interface employs easy-to-use, spreadsheet-like input, it still requires precisely the same information as for the flat-file version. Thus this lecture (as well as later descriptions of QUAL2E applications in Lec. 36) uses the flat-file format. So whether you use the original version or the new interface, our input files provide a concise representation of all the necessary information for performing model simulations with QUAL2E.

TABLE 26.1
The 15 constituents that can be simulated by QUAL2E

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

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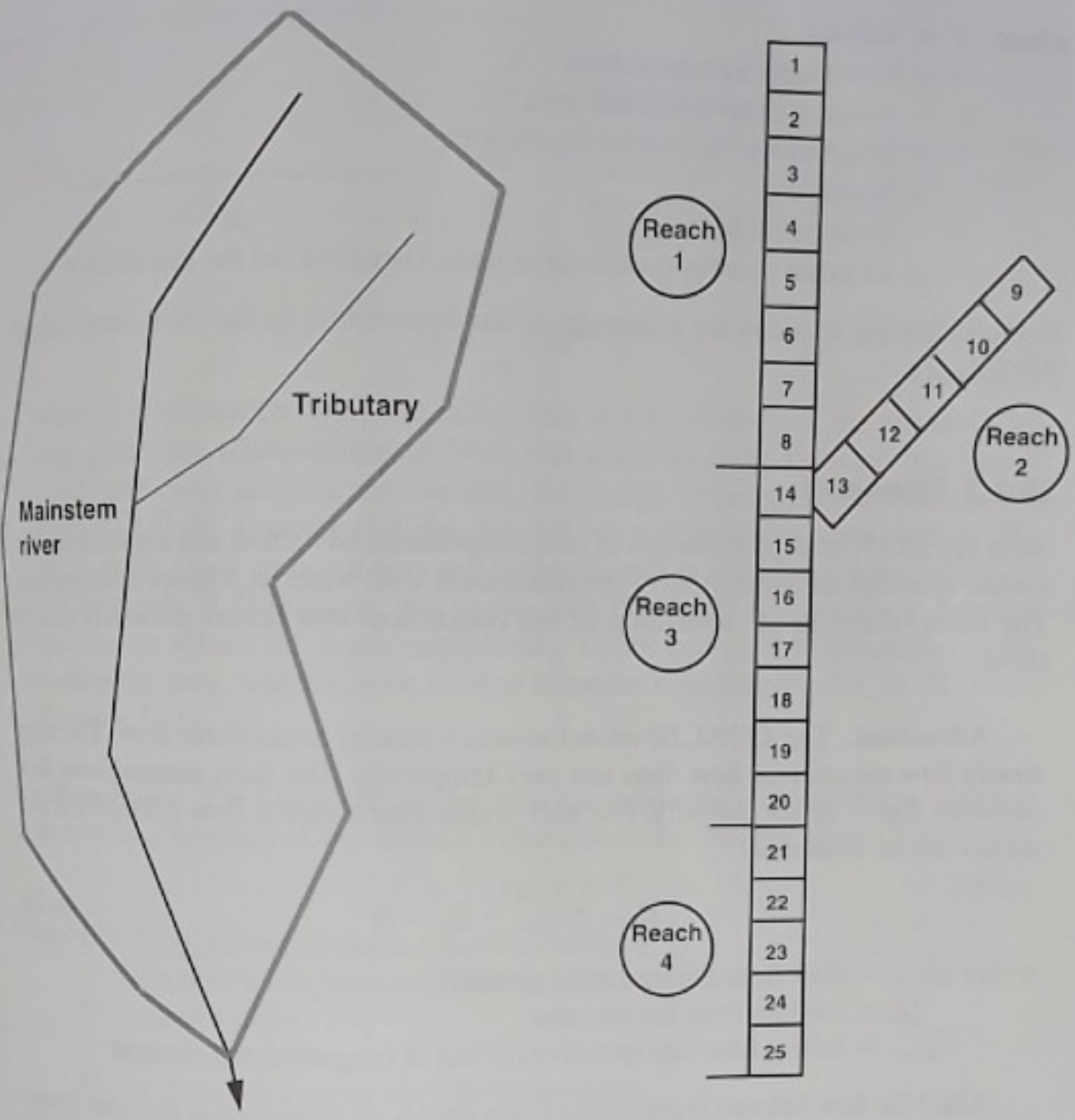
→ EE literature



(a) (b)

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

26.2.1 Spatial Discretization and Model Overview

As depicted in Fig. 26.1, QUAL2E treats a river as a collection of reaches, each having homogeneous hydrogeometric properties. Each reach, in turn, is divided into a series of equal-length computational elements or control volumes.

A mass balance is used to keep track of the water-quality constituents listed in Table 26.1. This balance can be written generally as

$$\underset{\text{Accumulation}}{V\frac{\partial c}{\partial t}} = \underbrace{\underset{\text{Dispersion}}{\frac{\partial\left(A_c E \frac{\partial c}{\partial x}\right)}{\partial x}dx} - \underset{\text{Advection}}{\frac{\partial(A_c U c)}{\partial x}dx}}_{\text{Transport}} + \underset{\text{Kinetics}}{V\frac{dc}{dt}} + \underset{\text{External sources/sinks}}{s} \tag{26.17}$$

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where V = volume
c = constituent concentration
A_c = element cross-sectional area
E = longitudinal dispersion coefficient
x = distance
U = average velocity
s = external sources (positive) or sinks (negative) of the constituent

In the following sections we elaborate on the three terms on the right-hand side of this balance.

26.2.2 Transport

As in Eq. 26.17, transport consists of two components: advection and dispersion. The former specifies the movement of the constituent with water as it flows downstream. The latter relates to the spreading of the constituent that occurs primarily due to shear.

Advection. The QUAL2E model assumes steady, nonuniform flow. The term ***steady flow*** means that flow does not vary temporally. The term ***nonuniform flow*** connotes that it varies spatially. For such a characterization a flow balance for element i can be written as

$$Q_{i-1} \pm Q_{x,i} - Q_i = 0 \tag{26.18}$$

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

Once the flow balance is established, it is necessary to determine the other hydrogeometric characteristics for each element. In particular the resulting water velocity, depth, and cross-sectional area must be established. The relationship of the element's other hydrogeometric characteristics to its flow rate is handled in two ways (recall Lec. 14):

1. Power equations can be used to relate mean velocity and depth to flow,

$$U = aQ^b \tag{26.19}$$

and

$$H = \alpha Q^\beta \tag{26.20}$$

where H = mean depth and a, b, α, and 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

$$A_c = \frac{Q}{U} \tag{26.21}$$

2. The Manning equation provides a means to relate channel characteristics and flow. In metric units,

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→ EE literature

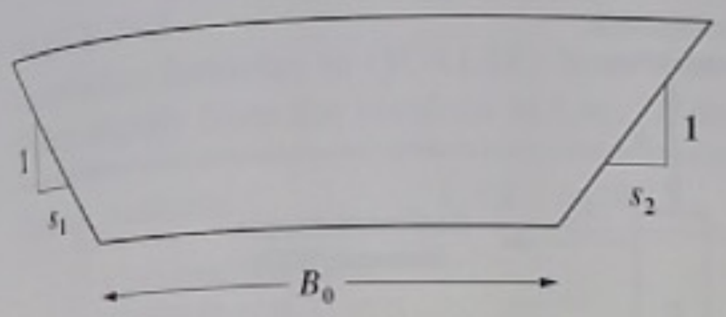

FIGURE 26.2
A trapezoidal channel showing the three parameters needed to uniquely defie the geometry. B_0 = bottom width; s_1 and s_2 = side slopes.

$$Q = \frac{1}{n} A_c R^{2/3} S_e^{1/2} \tag{26.22}$$

where R = channel's hydraulic radius (m) and S_e = slope of the channel's energy grade line (dimensionless). Note that since we have assumed that flow is steady and cross sections are constant, the energy slope is equal to the channel slope. QUAL2E assumes that the channel has a trapezoidal cross section (Fig. 26.2), so the cross-sectional area and hydraulic radius can be expressed as a function of depth. If Q is given, this means that Eq. 26.22 is a nonlinear equation that can be solved for depth numerically. Depth can then be employed to determine the area, which can be used to compute velocity with Eq. 26.21 (recall Example 14.5).

Dispersion. The QUAL2E model uses the following relationship to compute dispersion as a function of the channel's characteristics (Fischer et al. 1979),

$$E = 3.11 K n U H^{5/6} \tag{26.23}$$

where E = longitudinal dispersion coefficient $(\mathrm{m^2\,s^{-1}})$
n = channel's roughness coefficient (dimensionless)
U = mean velocity (mps)
H = mean depth (m)
K = a dispersion parameter (dimensionless)

defined as

$$K = \frac{E}{HU^*} \tag{26.24}$$

where U^* = shear velocity (m s^{-1}). Equations 26.23 and 26.24 represent circular reasoning. Thus they differ from Eqs. 14.15 and 14.17, which calculate dispersion purely as a function of channel parameters. However, once K is established it provides a formula to compute dispersion as a function of nonuniform flow conditions. It is in this way that K is used in QUAL2E.

26.2.3 Kinetics

To keep this lecture simple we limit the discussion to two constituents: carbonaceous BOD (CBOD) and dissolved oxygen. The kinetics for these constituents are displayed in Fig. 26.3 and can be represented mathematically by

$$\frac{dL}{dt} = -K_1 L - K_3 L \tag{26.25}$$

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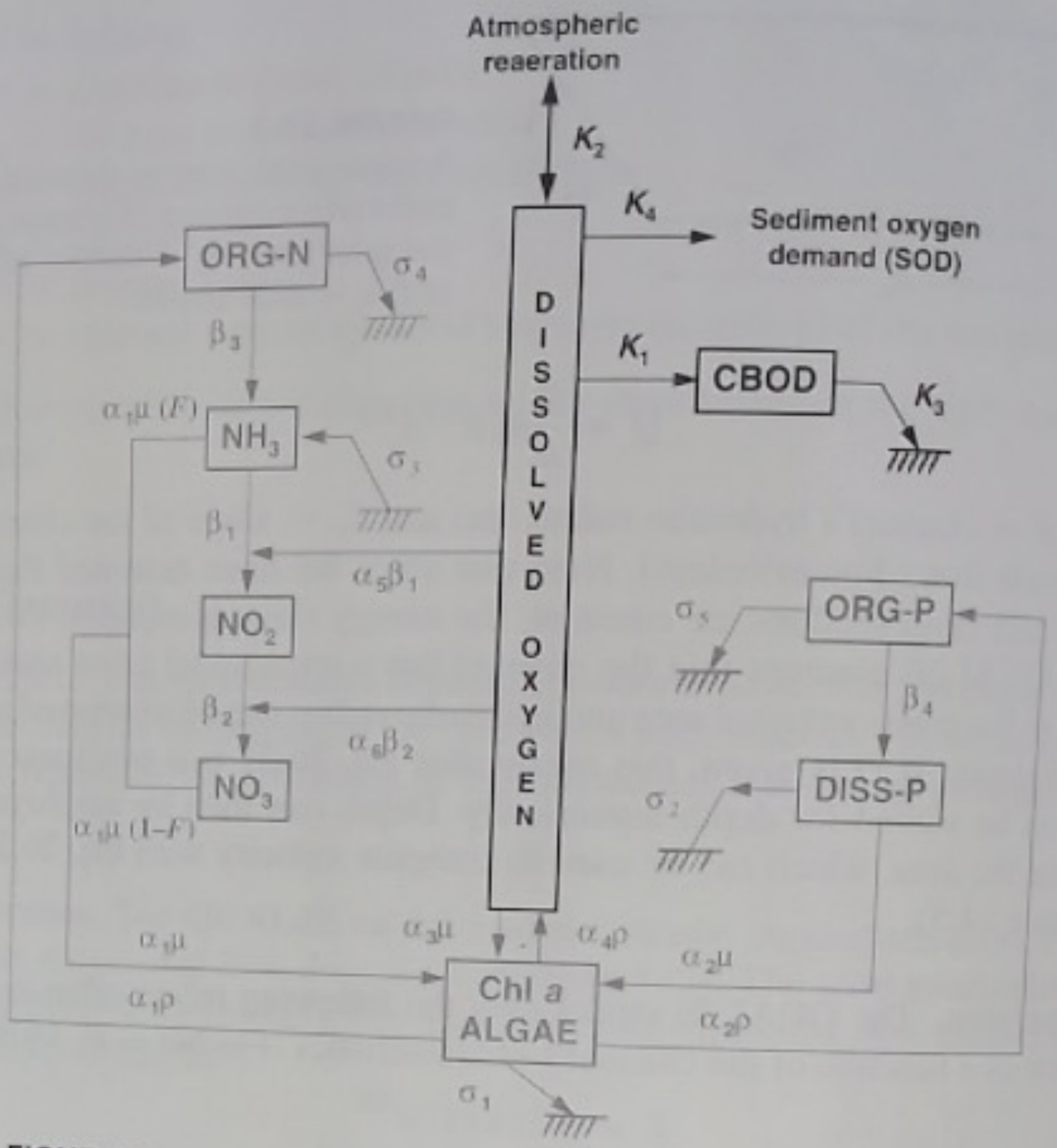

FIGURE 26.3
QUAL2E kinetics. Note that the highlighted constituents and processes are described and modeled in this lecture. We will extend our discussion to the remainder of the diagram in Lec. 36.

and

$$\frac{do}{dt} = K_2(o_s - o) - K_1 L - \frac{K_4}{H} \tag{26.26}$$

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 (mg L^{-1})
K_2 = reaeration rate (d^{-1})
o_s = dissolved oxygen saturation concentration (mg L^{-1})
K_4 = sediment oxygen demand (g m^{-2} d^{-1})

Note that all the rates (the K's) are corrected for temperature by

$$K = K_{20}\theta^{T-20} \tag{26.27}$$

where K = rate at temperature T
K_{20} = rate at 20°C
θ = a temperature correction factor

All the rates in Eqs. 26.25 and 26.26 can be entered directly to QUAL2E. However, the reaeration rate can also be internally calculated using eight different formulas. These formulas are summarized in Table 26.2.

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)

26.2.4 Numerical Algorithm

Now that we have an understanding of the major components of QUAL2E, we can discuss how the model obtains solutions numerically. To do this, Eq. 26.17 can be divided by volume and written as

$$\frac{\partial c}{\partial t} = \frac{\partial\left(A_c E \frac{\partial c}{\partial x}\right)}{A_c \partial x} - \frac{\partial (A_c U c)}{A_c \partial x} + rc + p + \frac{s}{V} \tag{26.28}$$

Observe that we have divided the kinetics into two separate terms,

$$\frac{dc}{dt} = rc + p \tag{26.29}$$

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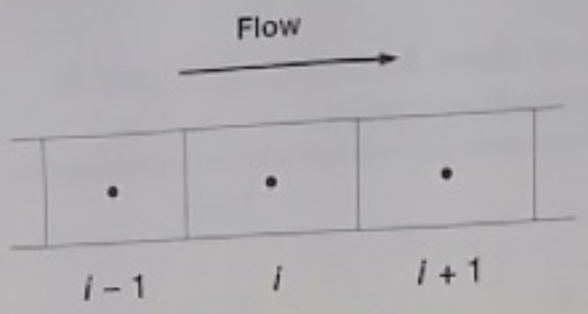

FIGURE 26.4
QUAL2E elements.

The first term on the right denotes those reactions that are linearly dependent on concentration, and the second term denotes internal constituent sources and sinks (for example, benthic sources, nutrient loss from algal growth, etc.). Although some of the latter are constants, others are nonlinear functions of constituent concentrations.

A general representation of the QUAL2E element scheme is shown in Fig. 26.4. Equation 26.28 can be written for element i by using a backward difference, as in

$$\underbrace{\frac{\partial c_i}{\partial t}}_{\text{Acc}} = \underbrace{\frac{\overset{\text{In}}{-\left(A_c E \frac{\partial c}{\partial x}\right)_{i-1}} + \overset{\text{Out}}{\left(A_c E \frac{\partial c}{\partial x}\right)_i}}{V_i}}_{\text{Dispersion}} + \underbrace{\frac{\overset{\text{In}}{(A_c Uc)_{i-1}} - \overset{\text{Out}}{(A_c Uc)_i}}{V_i}}_{\text{Advection}}$$

$$+ \underbrace{r_i c_i}_{\substack{\text{First-order}\\\text{reactions}}} + \underbrace{p_i}_{\substack{\text{Internal}\\\text{sources/sinks}}} + \underbrace{\frac{s_i}{V_i}}_{\substack{\text{External}\\\text{sources/sinks}}} \qquad (26.30)$$

Then backward differences can be used to approximate the remaining spatial derivatives,

$$\frac{\partial c_i}{\partial t} = \frac{(A_c E)(c_{i+1} - c_i)}{V_i \Delta x_i} + \frac{(A_c E)(c_{i-1} - c_i)}{V_i \Delta x_i} + \frac{Q_{i-1} c_{i-1} - Q_i c_i}{V_i} + r_i c_i + p_i + \frac{s_i}{V_i} \qquad (26.31)$$

Finally a backward difference can be applied in time to yield

$$\frac{c_i^{\ell+1} - c_i^\ell}{\Delta t} = \frac{(A_c E)_{i,i+1}(c_{i+1}^{\ell+1} - c_i^{\ell+1})}{V_i \Delta x_i} + \frac{(A_c E)_{i-1,i}(c_{i-1}^{\ell+1} - c_i^{\ell+1})}{V_i \Delta x_i}$$
$$+ \frac{Q_{i-1} c_{i-1}^{\ell+1} - Q_i c_i^{\ell+1}}{V_i} + r_i c_i^{\ell+1} + p_i + \frac{s_i}{V_i} \qquad (26.32)$$

Equation 26.32 can now be reexpressed by collecting terms to yield a linear system

$$e_i c_{i-1}^{n+1} + f_i c_i^{n+1} + g_i c_{i+1}^{n+1} = z_i \qquad (26.33)$$

where

$$e_i = -\left[(A_c E)_{i-1} \frac{\Delta t}{V_i \Delta x_i} + \frac{Q_{i-1} \Delta t}{V_i}\right] \qquad (26.34)$$

$$f_i = 1 + [(A_c E)_{i-1} + (A_c E)_i] \frac{\Delta t}{V_i \Delta x_i} + \frac{Q_i \Delta t}{V_i} - r_i \Delta t \qquad (26.35)$$

$$g_i = -\left[(A_x E)_i \frac{\Delta t}{V_i \, \Delta x_i}\right] \tag{26.36}$$

$$z_i = c_i^n + \frac{s_i \, \Delta t}{V_i} + p_i \, \Delta t \tag{26.37}$$

These equations form a tridiagonal system that can be solved efficiently for concentration as a function of time. Note that the external sources and sinks (the s_i terms) are treated as constants in this formulation. As noted previously, some of these are nonlinear functions of other constituent concentrations. Thus the QUAL2E solution algorithm handles nonlinear terms by treating them as constant contributions to the forcing function that are updated at each time step.

Two forms of the solution are implemented in QUAL2E:

Steady-state. The model is run until it reaches a steady-state. This is the conventional implementation mode for QUAL2E. Thus the time-variable algorithm is a means to an end—the steady-state result (recall our discussion of the backward-time implicit approach in Lec. 13).

Time-variable. The model can also be run in a normal time-variable mode. At present this type of implementation is limited to diurnal simulations.

Now that we have covered the basics of the QUAL2E software package, I'll provide an overview of how it is implemented. However, before doing this I'll introduce a problem context where we will apply the model.

26.2.5 QUAL2E Application

Figure 26.5 shows a river that receives a sewage treatment plant effluent at kilometer point 100 (KP 100) and a tributary inflow at KP 60. Note that the channel is trapezoidal with the characteristics shown. The deoxygenation rate for CBOD is equal to 0.5 d^{-1} at 20°C. For 20 km downstream from the treatment plant there is a CBOD settling removal rate of 0.25 d^{-1}. In addition there is a sediment oxygen demand for this reach of 5 $\text{g m}^{-2}\,\text{d}^{-1}$. Assume that the O'Connor-Dobbins reaeration formula holds and that the stream is at sea level. Values for the channel's geometry and hydraulics are listed in Table 26.3. Kinetic parameters and temperatures are summarized in Table 26.4.

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	$\text{m}^3\,\text{s}^{-1}$	5.787	6.250	7.407
	$\text{m}^3\,\text{d}^{-1}$	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)

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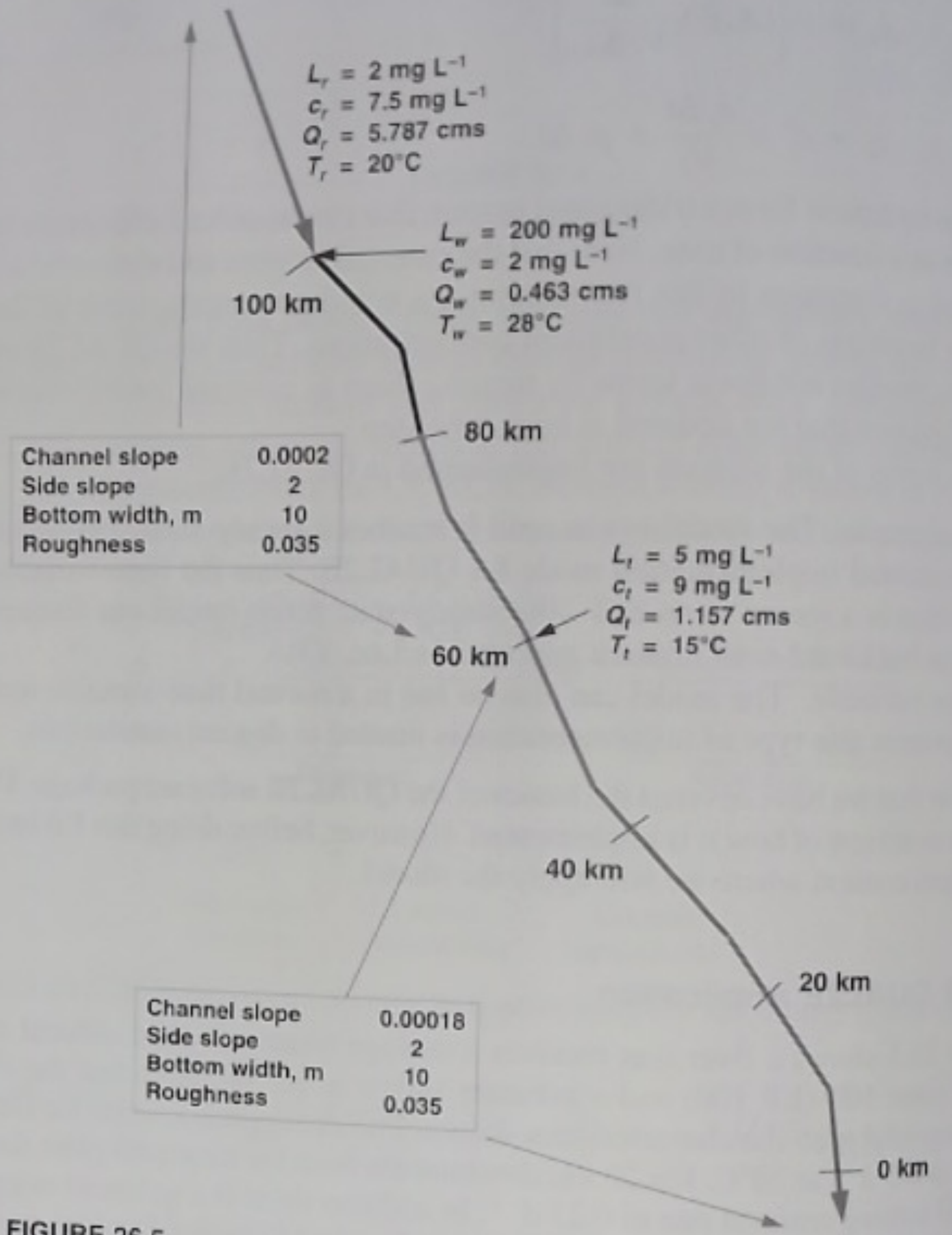

FIGURE 26.5
A stream receiving BOD loadings from a point source and a tributary.

TABLE 26.4
Temperatures and kinetic coefficients

Parameter	KP > 100	KP 100–80	KP 80–60	KP < 60
T (°C)	20	20.59	20.59	19.72
o_s (mg L^{-1})	9.092	8.987	8.987	9.143
k_a (d^{-1})	1.902	1.842	1.842	1.494
k_r (d^{-1})	0.500	0.767	0.514	0.494
k_d (d^{-1})	0.500	0.514	0.514	0.494
k_s (d^{-1})	0.000	0.254	0.000	0.000
SOD (g m^{-2} d^{-1})	0.000	5.175	0.000	0.000

→ EE literature

The first step in using QUAL2E is to develop the spatial segmentation scheme for the system being modeled. This involves dividing the system into reaches of constant hydrogeometric characteristics. These reaches, in turn, consist of equal-length computational elements.

A segmentation scheme used for the present case is depicted in Fig. 26.6. Observe that we have divided the system into six reaches that we will call:

1. MS-HEAD
2. MS100-MS080
3. MS080-MS060
4. MS060-MS040
5. MS040-MS020
6. MS020-MS000

The names for each reach are at the user's discretion and merely serve to identify each reach. We have chosen to use the abbreviation "MS" to designate that we are simulating a "main stem" of a river with no tributaries modeled explicitly. Also notice that we have used distance in kilometers to identify the extent of each reach. However, we have also reversed the sense of the distances. That is, we have measured distance upstream from the downstream end of the system, rather than downstream as in the original problem statement. We have made this modification to make our scheme consistent with the way in which distances must be entered into QUAL2E.

Next, inspection of Fig. 26.6 shows that our scheme consists of 2-km elements. The elements that make up the reach must be numbered in order from the headwater to the most downstream point in the system. In addition the type of each element must be designated. There are seven element types:

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

In the present example we use only four of these types. The first (1) and last (51) elements are type 1 and 5, respectively. Elements 2 and 22 are type 6 because they both receive point inflows. The remainder of the elements are the standard type 2.

Once the system segmentation is defined, we can create a data file to run QUAL2E. The file that conforms to the present problem is shown in Fig. 26.7. Note that the data in this file must be typed exactly as shown (minus lines and shading, of course). This is because QUAL2E is written in FORTRAN 77. Thus each line of input corresponds to an 80-column input-card format that derives from the punched cards used in early FORTRAN programs.

It should be noted that at the time of this book's printing, a user-friendly interface for entering the input file and viewing the results became available (Lahlou et al. 1995). The interface requires precisely the same information as in Fig. 26.7. Thus, whether you employ the original version or the new interface, Fig. 26.7 can serve as a guide for performing the QUAL2E simulation outlined in this lecture.

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Reach name	Reach no.	Element no.	Element type
MS-HEAD	1	1	1
MS100-MS080	2	2	6
		3	2
		4	2
		5	2
		6	2
		7	2
		8	2
		9	2
		10	2
		11	2
MS080-MS060	3	12	2
		13	2
		14	2
		15	2
		16	2
		17	2
		18	2
		19	2
		20	2
		21	2
MS060-MS040	4	22	6
		23	2
		24	2
		25	2
		26	2
		27	2
		28	2
		29	2
		30	2
		31	2
MS040-MS020	5	32	2
		33	2
		34	2
		35	2
		36	2
		37	2
		38	2
		39	2
		40	2
		41	2
MS020-MS000	6	42	2
		43	2
		44	2
		45	2
		46	2
		47	2
		48	2
		49	2
		50	2
		51	5

FIGURE 26.6
The QUAL2E segmentation scheme conforming to the river shown in Fig. 26.5.

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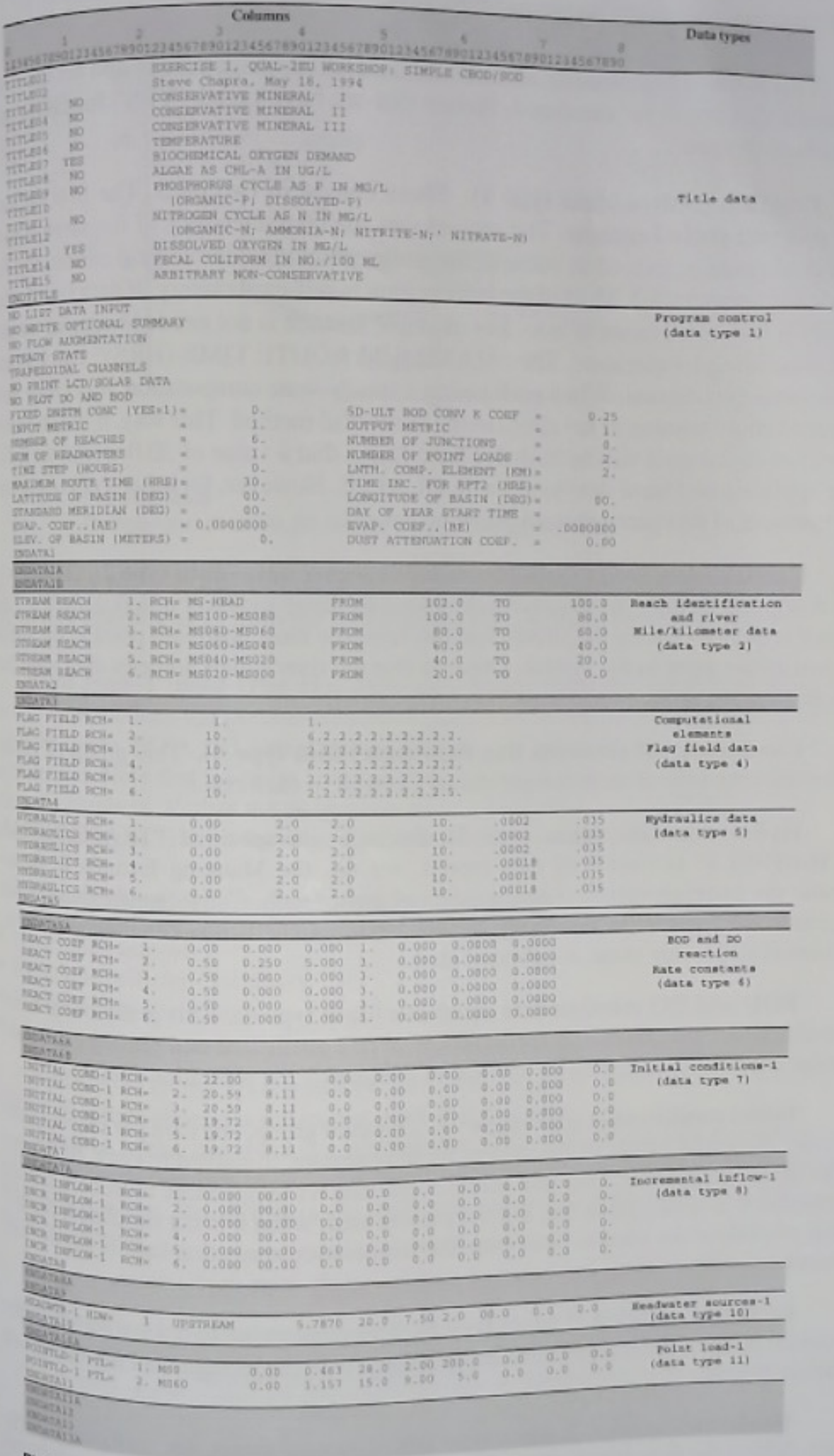
→ EE literature



```
                                Columns
         1         2         3         4         5         6         7         8      Data types
12345678901234567890123456789012345678901234567890123456789012345678901234567890
TITLE01                 EXERCISE 1, QUAL-2EU WORKSHOP: SIMPLE CBOD/SOD
TITLE02                 Steve Chapra, May 18, 1994
TITLE03  NO             CONSERVATIVE MINERAL   I
TITLE04  NO             CONSERVATIVE MINERAL  II
TITLE05  NO             CONSERVATIVE MINERAL III
TITLE06  NO             TEMPERATURE
TITLE07 YES             BIOCHEMICAL OXYGEN DEMAND
TITLE08  NO             ALGAE AS CHL-A IN UG/L
TITLE09  NO             PHOSPHORUS CYCLE AS P IN MG/L
TITLE10                   (ORGANIC-P; DISSOLVED-P)                                  Title data
TITLE11  NO             NITROGEN CYCLE AS N IN MG/L
TITLE12                   (ORGANIC-N; AMMONIA-N; NITRITE-N;' NITRATE-N)
TITLE13 YES             DISSOLVED OXYGEN IN MG/L
TITLE14  NO             FECAL COLIFORM IN NO./100 ML
TITLE15  NO             ARBITRARY NON-CONSERVATIVE
ENDTITLE
NO LIST DATA INPUT                                                              Program control
NO WRITE OPTIONAL SUMMARY                                                        (data type 1)
NO FLOW AUGMENTATION
STEADY STATE
TRAPEZOIDAL CHANNELS
NO PRINT LCD/SOLAR DATA
NO PLOT DO AND BOD
FIXED DNSTM CONC (YES=1)=       0.     5D-ULT BOD CONV K COEF  =     0.25
INPUT METRIC            =       1.     OUTPUT METRIC           =       1.
NUMBER OF REACHES       =       6.     NUMBER OF JUNCTIONS     =       0.
NUM OF HEADWATERS       =       1.     NUMBER OF POINT LOADS   =       2.
TIME STEP (HOURS)       =       0.     LNTH. COMP. ELEMENT (KM)=       2.
MAXIMUM ROUTE TIME (HRS)=      30.     TIME INC. FOR RPT2 (HRS)=
LATITUDE OF BASIN (DEG) =      00.     LONGITUDE OF BASIN (DEG)=      00.
STANDARD MERIDIAN (DEG) =      00.     DAY OF YEAR START TIME  =       0.
EVAP. COEF.,(AE)        = 0.0000000    EVAP. COEF.,(BE)        = .0000000
ELEV. OF BASIN (METERS) =       0.     DUST ATTENUATION COEF.  =     0.00
ENDATA1
ENDATA1A
ENDATA1B
STREAM REACH    1. RCH= MS-HEAD        FROM     102.0   TO     100.0  Reach identification
STREAM REACH    2. RCH= MS100-MS080    FROM     100.0   TO      80.0        and river
STREAM REACH    3. RCH= MS080-MS060    FROM      80.0   TO      60.0  Mile/kilometer data
STREAM REACH    4. RCH= MS060-MS040    FROM      60.0   TO      40.0     (data type 2)
STREAM REACH    5. RCH= MS040-MS020    FROM      40.0   TO      20.0
STREAM REACH    6. RCH= MS020-MS000    FROM      20.0   TO       0.0
ENDATA2
ENDATA3
FLAG FIELD RCH= 1.        1.      1.                                     Computational
FLAG FIELD RCH= 2.       10.      6.2.2.2.2.2.2.2.2.2.                      elements
FLAG FIELD RCH= 3.       10.      2.2.2.2.2.2.2.2.2.2.                  Flag field data
FLAG FIELD RCH= 4.       10.      6.2.2.2.2.2.2.2.2.2.                   (data type 4)
FLAG FIELD RCH= 5.       10.      2.2.2.2.2.2.2.2.2.2.
FLAG FIELD RCH= 6.       10.      2.2.2.2.2.2.2.2.2.5.
ENDATA4
HYDRAULICS RCH= 1.    0.00     2.0   2.0          10.    .0002   .035   Hydraulics data
HYDRAULICS RCH= 2.    0.00     2.0   2.0          10.    .0002   .035    (data type 5)
HYDRAULICS RCH= 3.    0.00     2.0   2.0          10.    .0002   .035
HYDRAULICS RCH= 4.    0.00     2.0   2.0          10.    .00018  .035
HYDRAULICS RCH= 5.    0.00     2.0   2.0          10.    .00018  .035
HYDRAULICS RCH= 6.    0.00     2.0   2.0          10.    .00018  .035
ENDATA5
ENDATA5A
REACT COEF RCH=  1.   0.00   0.000   0.000  1.   0.000  0.0000  0.0000    BOD and DO
REACT COEF RCH=  2.   0.50   0.250   5.000  1.   0.000  0.0000  0.0000     reaction
REACT COEF RCH=  3.   0.50   0.000   0.000  1.   0.000  0.0000  0.0000  Rate constants
REACT COEF RCH=  4.   0.50   0.000   0.000  1.   0.000  0.0000  0.0000   (data type 6)
REACT COEF RCH=  5.   0.50   0.000   0.000  1.   0.000  0.0000  0.0000
REACT COEF RCH=  6.   0.50   0.000   0.000  1.   0.000  0.0000  0.0000
ENDATA6A
ENDATA6B
INITIAL COND-1 RCH=  1.  22.00   8.11   0.0   0.00   0.00   0.00  0.000   0.0  Initial conditions-1
INITIAL COND-1 RCH=  2.  20.59   8.11   0.0   0.00   0.00   0.00  0.000   0.0    (data type 7)
INITIAL COND-1 RCH=  3.  20.59   8.11   0.0   0.00   0.00   0.00  0.000   0.0
INITIAL COND-1 RCH=  4.  19.72   8.11   0.0   0.00   0.00   0.00  0.000   0.0
INITIAL COND-1 RCH=  5.  19.72   8.11   0.0   0.00   0.00   0.00  0.000   0.0
INITIAL COND-1 RCH=  6.  19.72   8.11   0.0   0.00   0.00   0.00  0.000   0.0
ENDATA7
ENDATA7A
INCR INFLOW-1  RCH=  1.  0.000  00.00  0.0  0.0  0.0  0.0  0.0  0.0   0.  Incremental inflow-1
INCR INFLOW-1  RCH=  2.  0.000  00.00  0.0  0.0  0.0  0.0  0.0  0.0   0.    (data type 8)
INCR INFLOW-1  RCH=  3.  0.000  00.00  0.0  0.0  0.0  0.0  0.0  0.0   0.
INCR INFLOW-1  RCH=  4.  0.000  00.00  0.0  0.0  0.0  0.0  0.0  0.0   0.
INCR INFLOW-1  RCH=  5.  0.000  00.00  0.0  0.0  0.0  0.0  0.0  0.0   0.
INCR INFLOW-1  RCH=  6.  0.000  00.00  0.0  0.0  0.0  0.0  0.0  0.0   0.
ENDATA8
ENDATA8A
ENDATA9
HEADWTR-1 HDW=   1  UPSTREAM      5.7870  20.0  7.50 2.0  00.0   0.0   0.0  Headwater sources-1
ENDATA10                                                                    (data type 10)
ENDATA10A
POINTLD-1 PTL=  1. MS0         0.00   0.463  28.0  2.00 200.0  0.0  0.0  0.0  Point load-1
POINTLD-1 PTL=  2. MS60        0.00   1.157  15.0  9.00   5.0  0.0  0.0  0.0  (data type 11)
ENDATA11
ENDATA11A
ENDATA12
ENDATA13
ENDATA13A
```

FIGURE 26.7
QUAL2E input file.

10.

Title data. These specify identification information for the run and set the constituents that are to be simulated. Notice that we have typed "YES" for BOD and dissolved oxygen.

Program control (data type 1). These consist of two parts. The first defines the program control options. The second sets the characteristics of the stream system configuration as well as some of the geographical/meteorological conditions for modeling temperature. Most of the information is self-explanatory. If data is not necessary it is omitted or set to zero. For example latitude is not needed because we are not simulating temperature. The "MAXIMUM ROUTE TIME (HRS)" entry bears additional explanation. When performing a steady-state computation, this entry sets the maximum number of iterations of the numerical method. This way, if the solution does not converge it will be halted. I have found that a value of 30.0 works well for the applications I have developed with QUAL2E. However, for other systems some adjustment of this parameter might be necessary.

Reach identification and river mile/kilometer data (data type 2). The cards in this group identify the stream reach system by name and river mile/kilometer. The latter is done by listing the stream reaches from the most upstream point to the most downstream point in the system. Observe that the river mile/kilometer data must be in descending order.

Computational elements flag field data (data type 4). This group of cards identifies the type of each computational element in each reach.

Hydraulics data (data type 5). Because we specified "TRAPEZOIDAL CHANNELS" in card 5 of data type 1, we use the Manning formula to determine the hydrogeometric characteristics of each reach. Consequently these cards include the parameters necessary for the Manning coefficient calculation (that is, channel slope, side slope, roughness, etc.).

BOD and DO reaction rate constants (data type 6). This group of cards includes reach information on the BOD decay rate coefficient and settling rate, sediment oxygen demand, and the method of computing the reaeration coefficient.

Initial conditions–1 (data type 7). This card group, one card per reach, establishes the initial values of the system for temperature, dissolved oxygen, BOD, and the three conservative minerals. Initial conditions for temperature must be specified whether it is simulated or not. For the present case, when it is not simulated, the initial conditions are used to determine the temperature correction factors for the rate constants. Other values can be set at zero for steady-state applications.

Incremental inflow–1 (data type 8). Even though we will not simulate incremental inflows, these cards must be included. As in our example, all the values can be set to zero.

Headwater sources–1 (data type 10). This card group, one card per headwater, defines the flow, temperature, dissolved oxygen, BOD, and conservative mineral concentrations of the headwater. Note that the headwater numbers are not the same

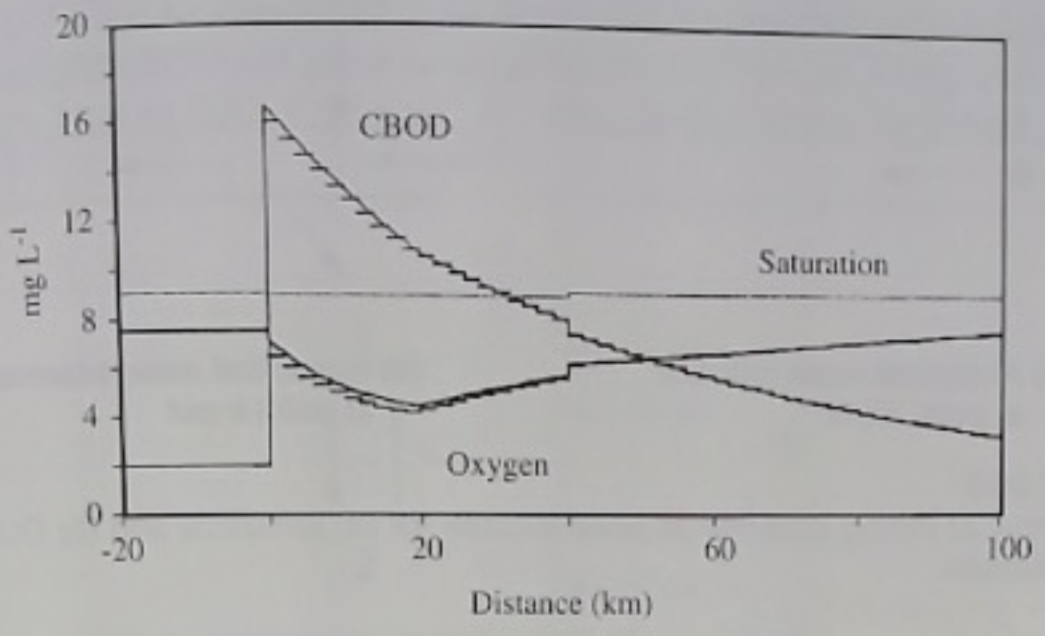


FIGURE 26.8
Comparison of QUAL2E output with analytical solution.

as either the reach or element numbers. Rather the headwaters are numbered consecutively (starting at 1) from the farthest upstream headwater.

Point load–1 (data type 11). This card group, one card per point source or withdrawal, defines the percent treatment, inflow or withdrawal, temperature, dissolved oxygen, BOD, and conservative mineral concentrations of each point load or withdrawal. Note that the point load numbers are not the same as either the reach or element numbers. Rather the point sources or withdrawals are numbered consecutively (starting at 1) from the most upstream to the most downstream.

Model output. The output for this run consists of

- Hydraulics summary
- Reaction coefficient summary
- Water-quality variables
- Dissolved oxygen data

A plot of the QUAL2E output for CBOD and oxygen is shown in Fig. 26.8. The QUAL2E results generally follow the analytical solution.

However, notice that there is a discrepancy at KP 100. This is due to the finite-difference approximation used in QUAL2E. Let us look at CBOD to understand what is happening. Recall that in the analytical solution, a mass balance is made at the mixing point,

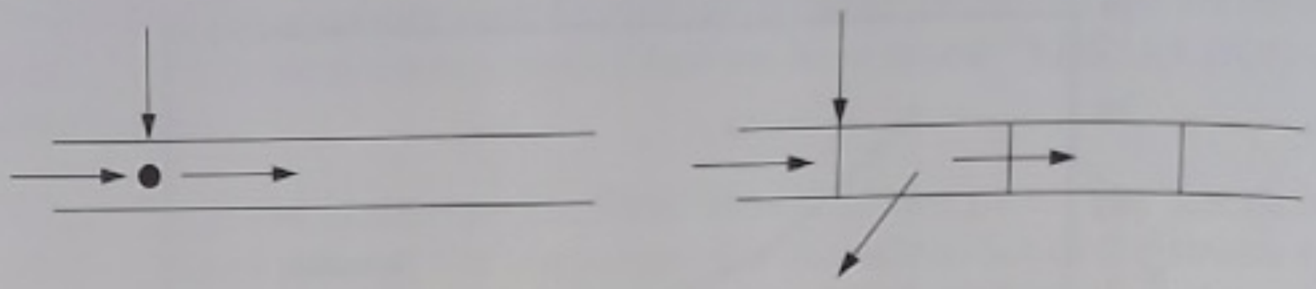
$$Q_r L_r + Q_w L_w - (Q_r + Q_w) L_0 = 0$$

which can be used to calculate (Fig. 26.9*a*)

$$L_0 = \frac{40{,}000(200) + 500{,}000(2)}{540{,}000} = 16.667 \text{ mg L}^{-1}$$

which then decays downstream according to

$$L = 16.667 e^{-\frac{0.514+0.254}{34.819} x}$$



(*a*) Analytical mass balance at point input

(*b*) Numerical mass balance at point input

FIGURE 26.9
Comparison of mixing schemes at point sources for (*a*) analytical and (*b*) QUAL2E mass balances.

Thus at 1 km the value of BOD will have dropped to

$$L = 16.667e^{-\frac{0.767}{34{,}819}1000} = 16.304 \text{ mg L}^{-1}$$

In contrast, for QUAL2E, the loading is introduced into a well-mixed element (Fig. 26.9*b*). Therefore a mass balance must now include the sources and sinks for the volume,

$$Q_r L_r + Q_w L_w - (Q_r + Q_w)L_0 - (K_1 + K_3)VL = 0$$

which can be used to calculate

$$L_0 = \frac{40{,}000(200) + 500{,}000(2)}{540{,}000 + (0.76)31.01 \times 10^3} = 15.98 \text{ mg L}^{-1}$$

Thus there is a discrepancy because of the finite discretization at the mixing point. As discussed in more general terms in Sec. 11.7, care should be taken to ensure that the element size is small enough that such errors do not have a significant impact on the application of the model for decision making.

In summary the QUAL2E model provides a convenient tool to implement oxygen balances in stream networks. We will revisit the software in later lectures when we turn to the eutrophication problem in Part V.

PROBLEMS

26.1. Suppose that the following data are available for a vertically stratified estuary (Fig. P26.1):

$$Q_{01} = 4 \times 10^6 \text{ m}^3 \text{ s}^{-1} \quad Q_{32} = 2.5 \times 10^6 \quad Q_{21} = 2.5 \times 10^6 \quad Q_{13} = 6.5 \times 10^6$$

$$E'_{01} = 0 \text{ m}^3 \text{ s}^{-1} \quad E'_{32} = 2.5 \times 10^6 \quad E'_{21} = 1.2 \times 10^6 \quad E'_{13} = 2.5 \times 10^6$$

Determine the steady-state system response matrices for BOD and oxygen if the deoxygenation and reaeration rates are 0.1 and 0.2 d^{-1}, respectively. Use the matrices to determine how much BOD loading can be discharged to segment 1 if a level of

→ EE literature

4 mg L^{-1} must be maintained in all segments. Assume that segments 0 and 3 contain negligible BOD and are at saturated levels of DO ($o_s = 10$ mg L^{-1}). In addition segment 2 has an SOD of 0.1 g m^{-2} d^{-1} and a surface area of 10,000 m^2.

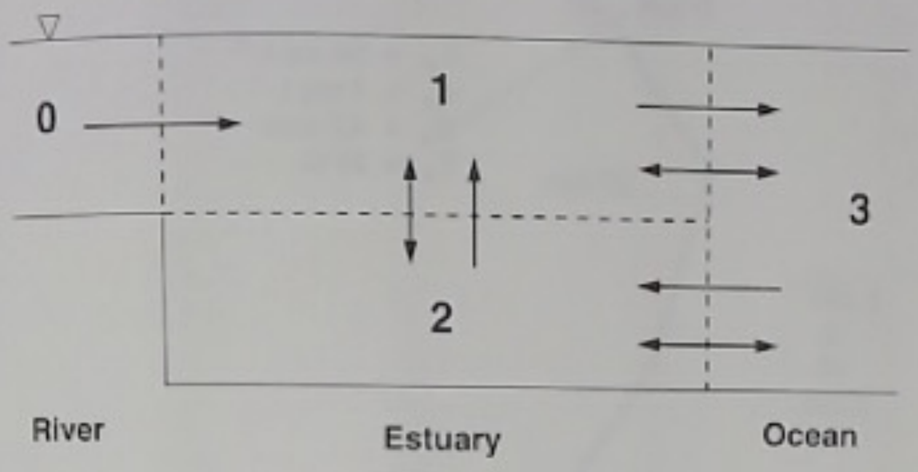


FIGURE P26.1

26.2. A waste source ($Q_w = 1$ cms, $L_w = 25$ mg L^{-1}, $o_w = 2$ mg L^{-1}, $T_w = 25$°C) discharges into a stream ($Q_r = 10$ cms, $L_r = 2$ mg L^{-1}, $o_r = 10$ mg L^{-1}, $T_r = 15$°C). Downstream the stream flows through a rectangular channel with roughness = 0.03, channel slope = 0.0005, bottom width = 20 m, and a side slope of 3. Use QUAL2E to calculate the profiles of both BOD and oxygen downstream assuming the BOD decays at a rate of 1 d^{-1}. Determine the value and the location of the maximum deficit.

26.3. Use QUAL2E to determine the profiles of BOD and dissolved oxygen for the following sea-level stream:

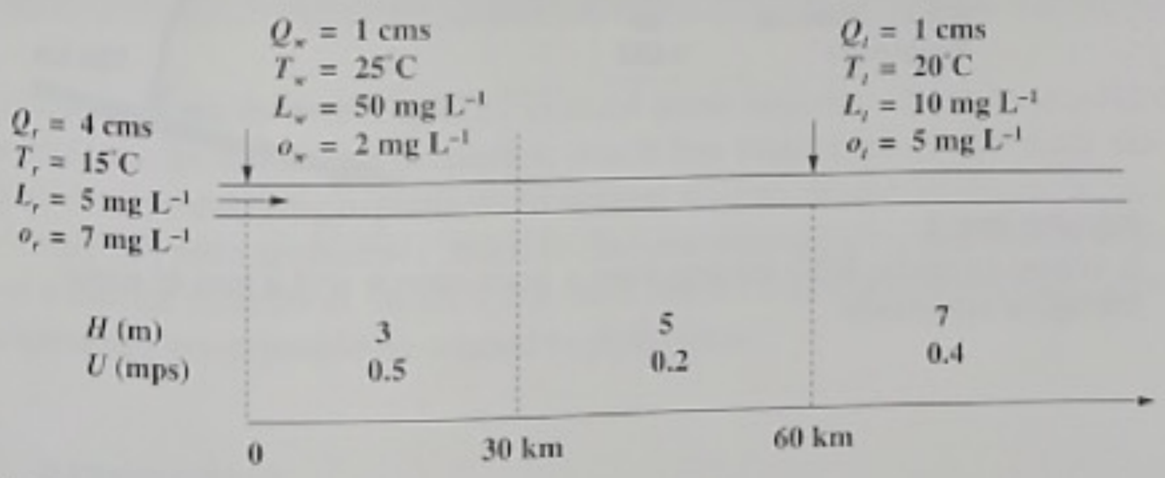


FIGURE P26.3

26.4. Figure P26.4 shows a river that receives a sewage treatment plant effluent at KP 0 and a withdrawal at KP 70. At a distance of 150 km, the stream enters a much larger river. Note that the channel is trapezoidal with the characteristics shown. The deoxygenation rate for CBOD is equal to 1 d^{-1} at 20°C. For 20 km downstream from the treatment plant, there is a CBOD settling removal rate of 2 d^{-1}. In addition there is a sediment oxygen demand for this reach of 4 g m^{-2} d^{-1}. Assume that the Churchill reaeration formula holds, that the stream is at sea level, and that the dispersion constant is zero. Use QUAL2E to simulate the levels of CBOD and oxygen for this case.

#

1024×768 2

1x

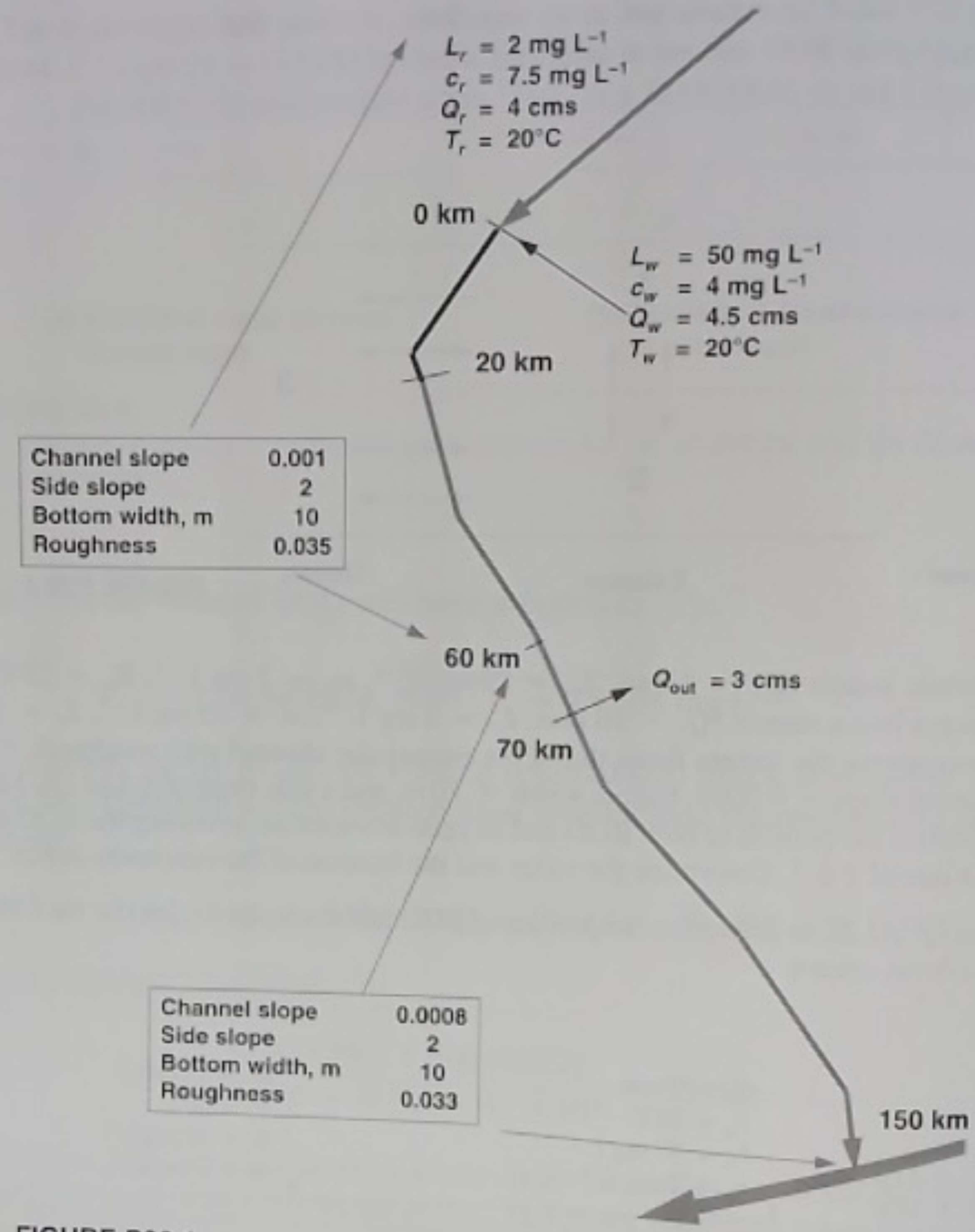


FIGURE P26.4
A stream receiving BOD loading from a point source and a loss of water through a withdrawal.