Water Quality Modeling and Prediction

The most fundamental human needs for water are for drinking, cooking, and personal hygiene. The quality of the water used to meet these needs must pose no risk to human health. The quality of the water in nature also impacts the condition of all living organisms found in aquatic ecosystems that we depend upon for our own wellbeing. At the same time watersheds and their water bodies serve as convenient sinks for domestic, industrial, and agricultural wastes. Runoff from agricultural and urban lands containing excess nutrients, oils, and solid wastes together with direct point source discharges of wastewaters into water bodies degrades the quality of those water bodies. Water resources management involves the monitoring and management of water quality as much as the monitoring and management of water quantity. Various models can assist in predicting the water quality impacts of alternative land and water management policies and practices. This chapter introduces some approaches to water quality modeling, leaving descriptions of more advanced methods to textbooks devoted solely to this subject.

10.1 Introduction

Water quality management is a critical component of overall integrated water resources management. Most users of water depend on adequate levels of water quality. When these levels are not met, water users must then either pay for water treatment or incur increased risks of using lower quality water. As populations and economies grow, more wastewater pollutants are generated. Many of these are discharged into surface and ground water bodies. Increasingly the major efforts and costs involved in water management are aimed at water quality protection and management. Conflicts among various users of water are increasingly over issues involving water quality.

Natural water bodies are able to serve many uses. One of them is the transport and assimilation of many waterborne wastes. As natural water bodies transport and assimilate wastes, their quality changes. If the quality of water drops to the extent that other uses are adversely impacted, the assimilative capacities of those water bodies have been exceeded with respect to those impacted uses. Water management measures are actions taken to ensure that the total pollutant loads discharged into receiving water bodies do not exceed the waste assimilative capacity of those water bodies and that the quality meets the quality standards set for those waters.

What uses depend on water quality? Almost all one can identify. As everyone knows, all living organisms require water of sufficient quantity and quality to survive. Different aquatic species can tolerate different levels of pollutant concentrations that impact water quality. In much of the developed world it is no longer "safe" to drink natural surface or ground waters. Treatment is usually required before these waters are safe for humans to drink. Treatment is not a practical option for improving the quality of water found in

nature yet this is the water that impacts the health of fish and shellfish and other organisms in natural aquatic ecosystems. Hence the focus in practice is on the use of wastewater treatment facilities to improve the quality of effluents being discharged into natural water bodies.

Standards specifying minimum acceptable levels of quality are commonly set for most ambient waters. Various uses may have their own quality requirements as well. Irrigation water must not be too saline nor contain toxic substances that can be absorbed by the plants or destroy the microorganisms in the soil. Water quality standards for industry can be very demanding, depending on course of the requirements of particular industrial processes.

Domestic wasteloads can contain high concentrations of bacteria, viruses, and other organisms that impact human health. High organic loadings can reduce dissolved oxygen (DO) to levels that can kill parts of the aquatic ecosystem and cause obnoxious odors. Nutrient loadings from both urban and agricultural land runoff can cause excessive algae growth that in turn may degrade the water aesthetically, inhibit boating and swimming, and upon death cause low DO levels. Toxic heavy metals and other micropollutants can accumulate in the bodies of aquatic organisms, including fish, making them unfit for human consumption even if they themselves survive.

Pollutant discharges originate from point to non-point sources. A common approach to controlling point source discharges, such as from stormwater outfalls, municipal wastewater treatment plants or industries, is to impose standards specifying maximum allowable pollutant loads or concentrations in their effluents. This is often done in ways that are not economically efficient or even environmentally effective. Effluent standards typically do not take into account the particular assimilative capacities of the receiving water body. Nevertheless they are relatively easy to monitor and control.

Non-point sources such as agricultural runoff or atmospheric deposition are not as easily controlled and hence it is difficult to apply effluent standards to non-point source pollutants. Pollutant loadings from non-point sources can be much higher than point source loadings. Management of non-point water quality impacts requires a more ambient-focused water quality management program.

The goal of an ambient water quality management program is to establish appropriate standards for water quality in water bodies receiving pollutant loads and then to ensure that these standards are met. Realistic standard setting takes into account the basin's hydrologic, ecological, and land use conditions, the potential uses of the receiving water bodies, and the institutional capacity to set and enforce water quality standards.

Ambient-based water quality prediction and management involves considerable uncertainty. No one can predict what pollutant loadings will be in the future, especially from area-wide non-point sources. In addition to uncertainties inherent in measuring water quality, there are uncertainties in models used to predict the effectiveness of actions taken to meet water quality standards. The models available to help managers predict water quality impacts are relatively simple compared to the complexities of actual water systems. If water quality models are being used to inform those setting standards and permissible waste loadings, these limitations and uncertainties should be understood and addressed.

10.2   Establishing Ambient Water Quality Standards

A first step in setting water quality standards for a water body is to identify the intended uses of that water body, whether a lake, a section of a stream, or areas of an estuary. The most restrictive (in terms of water quality) of the specific desired uses of a water body is termed a *designated use*. Barriers to achieving the designated use are the presence of pollutants or hydrologic and geomorphic changes that impact the quality of the water body.

The designated use dictates the appropriate type of water quality standard. For example, the standards of a water body whose designated use involves human contact recreation should protect humans from exposure to microbial pathogens while swimming, wading, or boating. Other uses might require standards to protect humans and aquatic life including fish, shellfish, and other wildlife from consuming harmful substances.

Standards set upstream may impact the uses of water downstream. For example, the water quality of small headwater streams may affect the ability of a downstream area to achieve a particular designated use such as being "fishable" or "swimmable." In this case, the designated use for the smaller upstream water body may be defined in terms of the achievement of the designated use of the larger downstream water body.

In many areas human activities have sufficiently altered the landscape and aquatic ecosystems to the point where they cannot be restored to their pre-disturbance condition. For example, a reproducing trout fishery in downtown Paris, Philadelphia, Phnom Penh, or Prague may be desired by some, but may not be attainable because of the development history of the areas or the altered hydrologic regimes of the rivers flowing through them. Similarly, health considerations would preclude designating an area for shellfish harvesting near the outfall of a sewage treatment plant. Ambient water quality standards must be realistic.

Decisions regarding the appropriate use for water bodies can be informed by the use of water quality prediction models. However, the final standard selection should reflect a social consensus made in consideration of the current condition of the watershed, its pre-disturbance condition, the advantages derived from a certain designated use, and the costs of achieving the designated use.

10.2.1 Water Use Criteria

The designated use is a qualitative description of a desired condition of a water body. A criterion is a measurable indicator surrogate for use attainment. The criterion may be positioned at any point in the causal chain of boxes shown in Fig. 10.1.

Box 1 of Fig. 10.1 contains information about the pollutant discharges, e.g., from a treatment plant or in runoff (e.g., biological oxygen demand, ammonia (NH_3), pathogens, and suspended sediments). Effluent standards specifying maximum permissible loadings may apply to these pollutant loadings. Criteria in Boxes 2 and 3 are possible measures of ambient water quality conditions. Box 2 includes measures of a water

Fig. 10.1 Factors considered when determining designated use and associated water quality standards
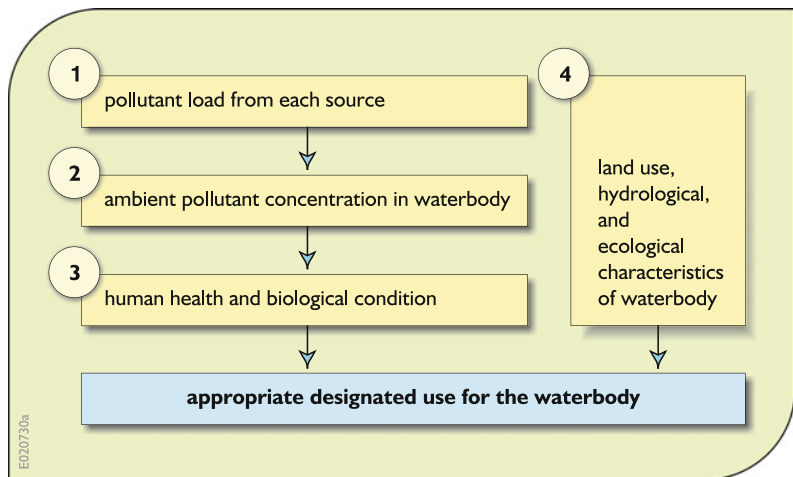
quality parameter such as DO, pH, nitrogen concentration, suspended sediment, or temperature. Criteria closer to the designated use (e.g., Box 3) include more combined or comprehensive measures of the biological community as a whole, such as the condition of the algal community (chlorophyll *a*) or a measure of contaminant concentration in fish tissue. Box 4 represents criteria that are associated with sources of pollution other than pollutants. These criteria might include measures such as flow timing and pattern (a hydrologic criterion), abundance of nonindigenous taxa, some quantification of channel modification (e.g., decrease in sinuosity), etc. (NRC 2001).

The more precise the statement of the designated use, the more accurate the criterion will be as an indicator of that use. For example, the criterion of fecal coliform count may be a suitable criterion for water contact recreation. The maximum allowable count itself may differ among water bodies that have water contact as their designated use, however.

Surrogate indicators are often selected for use as criteria because they are easy to measure and in some cases are politically appealing. Although a surrogate indicator may have appealing attributes, its usefulness can be limited unless it can be logically related to a designated use.

As with setting designated uses, the connections among water bodies and segments must be considered when determining criteria. For example, where a segment of a water body is designated as a mixing zone for a pollutant discharge, the criterion adopted should assure that the mixing zone use will not adversely affect the surrounding water body uses. Similarly, as previously discussed, the desired condition of a small headwater stream may need to be chosen as it relates to other water bodies downstream. Thus, an ambient nutrient criterion may be set in a small headwater stream to ensure a designated use downstream, even if there are no local adverse impacts resulting from the nutrients in the small headwater stream. Conversely, a high fecal coliform criterion may be permitted upstream of a recreational area if the fecal load dissipates before the flow reaches that area.

10.3 Water Quality Model Use

Monitoring data are the preferred form of information for identifying impaired waters. Model predictions might be used in addition to or instead of monitoring data for several reasons

1. Modeling could be feasible in some situations where monitoring is not.
2. Integrated monitoring and modeling systems could provide better information than monitoring or modeling alone for the same total cost. For example, regression analyses that correlate pollutant concentration with some more easily measurable factor (e.g., streamflow) could be used to extend monitoring data for preliminary planning purposes. Models can also be used to determine preliminary probability distributions of impairment that can help direct monitoring efforts and reduce the quantity of monitoring data needed for making listing decisions at a given level of reliability (see Chaps. 7 and 9).
3. Modeling can be used to assess (predict) future water quality situations resulting from different management strategies. For example, assessing the improvement in water quality after a new wastewater treatment plant begins operating, or the effect of increased industrial growth and effluent discharges.

A simple, but useful, modeling approach that may be used in the absence of monitoring data is "dilution calculations." In this approach the rate of pollutant loading from point sources in a water body is divided by the stream flow to give a set of estimated pollutant concentrations that may be compared to the standard. Simple dilution calculations assume conservative movement of pollutants. Thus, the use of dilution calculations will tend to be conservative and lead to higher than actual concentrations for decaying pollutants. Of course one could include a best estimate of the effects of decay processes in the dilution model.

Combined runoff and water quality prediction models link stressors (sources of pollutants and pollution) to responses. Stressors include human

activities likely to cause impairment, such as the presence of impervious surfaces in a watershed, cultivation of fields close to the stream, over-irrigation of crops with resulting polluted return flows, the discharge of domestic and industrial effluents into water bodies, installing dams and other channelization works, introduction of nonindigenous taxa, and over-harvesting of fishes. Indirect effects of humans include land cover changes that alter the rates of delivery of water, pollutants, and sediment to water bodies.

Direct and indirect environmental effects of human activities can include

- alterations in physical habitat,
- modifications in the seasonal flow of water,
- changes in the food base of the system,
- changes in interactions within the stream biota, and
- release of contaminants (conventional pollutants) (Karr 1990; NRC 1992, 2001).

Ideally, models designed to manage water quality should consider all five types of alternative management measures. The broad-based approach that considers these five features provides a more integrative approach to reduce the cause or causes of degradation (NRC 1992).

Models that relate stressors to responses can be of varying levels of complexity. Sometimes, models are simple qualitative conceptual representations of the relationships among important variables and indicators of those variables. More quantitative models can be used to make predictions about the assimilative capacity of a water body, the movement of a pollutant from various point and non-point sources through a watershed, or the effectiveness of certain best management practices.

10.3.1 Model Selection Criteria

There was a time when if one needed a water quality model, they had to build it. Today there exist a wide range of water quality models for various types of water bodies, and for various contaminants, and hence it makes little sense to build another one if an existing model will suffice. This section discusses criteria that can be used to select a particular model.

Water quality predictive models can include both mathematical expressions and expert scientific judgment. They may be process-based (mechanistic) models or data-based (statistical) models. Quality models used for planning and management should link management options to meaningful response variables (e.g., pollutant sources and water quality standard parameters). They should incorporate the entire "chain" from stressors to responses. Process-based models should be consistent with scientific theory. Model prediction uncertainty should be reported. This provides decision-makers with estimates of the risks of alternative options. To do this requires prediction error estimates (Chap. 6).

Water quality management models should be appropriate to the complexity of the situation and to the available data. Simple water quality problems can be addressed with simple models. Complex water quality problems may or may not require the use of more complex models. Models requiring large amounts of monitoring data should not be used in situations where such data are unavailable. Models should be flexible enough to allow updates and improvements as appropriate based on new research and monitoring data.

Stakeholders need to accept the models proposed for use in any water quality management study. Given the increasing role of stakeholders in water management decision processes, they need to understand and accept the models being used, at least to the extent they wish to. Finally, the cost of maintaining and updating the model during its use must be acceptable.

Although predictions are typically made using mathematical models, there are certainly situations where expert judgment can be just as good. Reliance on professional judgment and simpler models is often acceptable, especially when limited data exist.

Highly detailed models require more time and are more expensive to develop and apply. Complex modeling studies should be undertaken only if warranted by the complexity of the

management problem. More complex modeling will not necessarily assure that uncertainty is reduced, and in fact added complexity can compound problems of uncertainty analyses (Chap. 8).

Placing a priority on process description usually leads to complex mechanistic model development and use over simpler mechanistic or empirical models. In some cases this may result in unnecessarily costly analyses for effective decision-making. In addition, physical, chemical, and biological processes in terrestrial and aquatic environments are far too complex to be fully represented in even the most detailed models. For water quality management, the primary purpose of modeling should be to support decision-making. The inability to completely describe all relevant processes can be accounted for by quantifying the uncertainty in the model predictions.

10.3.2   Model Chains

Many water quality management analyses require the use of a sequence of models, one feeding data into another. For example, consider the sequence or chain of models required for the prediction of fish and shellfish survival as a function of nutrient loadings into an estuary. Of interest to the stakeholders are the conditions of the fish and shellfish. One way to maintain healthy fish and shellfish stocks is to maintain sufficient levels of oxygen in the estuary. The way to do this is to control algae blooms. This in turn requires limiting the nutrient loadings to the estuary that can promote algae growth and blooms, and subsequent DO deficits. The modeling challenge is to link nutrient loading to fish and shellfish survival.

The negative effects of excessive nutrients (e.g., nitrogen) in an estuary are shown in Fig. 10.2. Nutrients stimulate the growth of algae. Algae die and accumulate on the bottom where bacteria consume them. Under calm wind conditions density stratification occurs. Oxygen is depleted in the bottom water. Fish and shellfish may die or become weakened and more vulnerable to disease.

A model consisting of a sequence of conditional probabilities can be defined to predict the probability of shellfish and fish abundance based on upstream nutrient loadings causing problems with fish and shellfish populations into the estuary. These conditional probabilities can be judgmental, mechanistic, and/or statistical. Each conditional probability can be a separate submodel. Assuming each submodel can identify a conditional probability distribution, the probability $\Pr\{C|N\}$ of a specified amount of carbon, C, given some specified loading of a nutrient, say nitrogen, N, equals the probability $\Pr\{C|A\}$ of that given amount of carbon given a concentration of algae biomass, A, times the probability $\Pr\{A|N, R\}$ of that concentration of algae biomass given the nitrogen loading, N, and the river flow, R, times the probability $\Pr\{R\}$ of the river flow, R.

$$\Pr\{C|N\} = \Pr\{C|A\}\Pr\{A|N, R\}\Pr\{R\} \quad (10.1)$$

An empirical process-based model of the type to be presented later in this chapter could be used to predict the concentration of algae and the chlorophyll violations based on the river flow and nitrogen loadings. Similarly to predict the production of carbon based on algae biomass. A seasonal statistical regression model might be used to predict the likelihood of algae blooms based on algal biomass. A cross system comparison may be made to predict sediment oxygen demand. A relatively simple hydraulic model could be used to predict the duration of stratification and the frequency of hypoxia given both the stratification duration and sediment oxygen demand. Expert judgment and fish survival models could be used to predict the shellfish abundance and fishkill and fish health probabilities.

The biological endpoints "shell-fish survival" and "number of fishkills," are meaningful indicators to stakeholders and can easily be related to designated water body use. Models and even conditional probabilities assigned to each link of
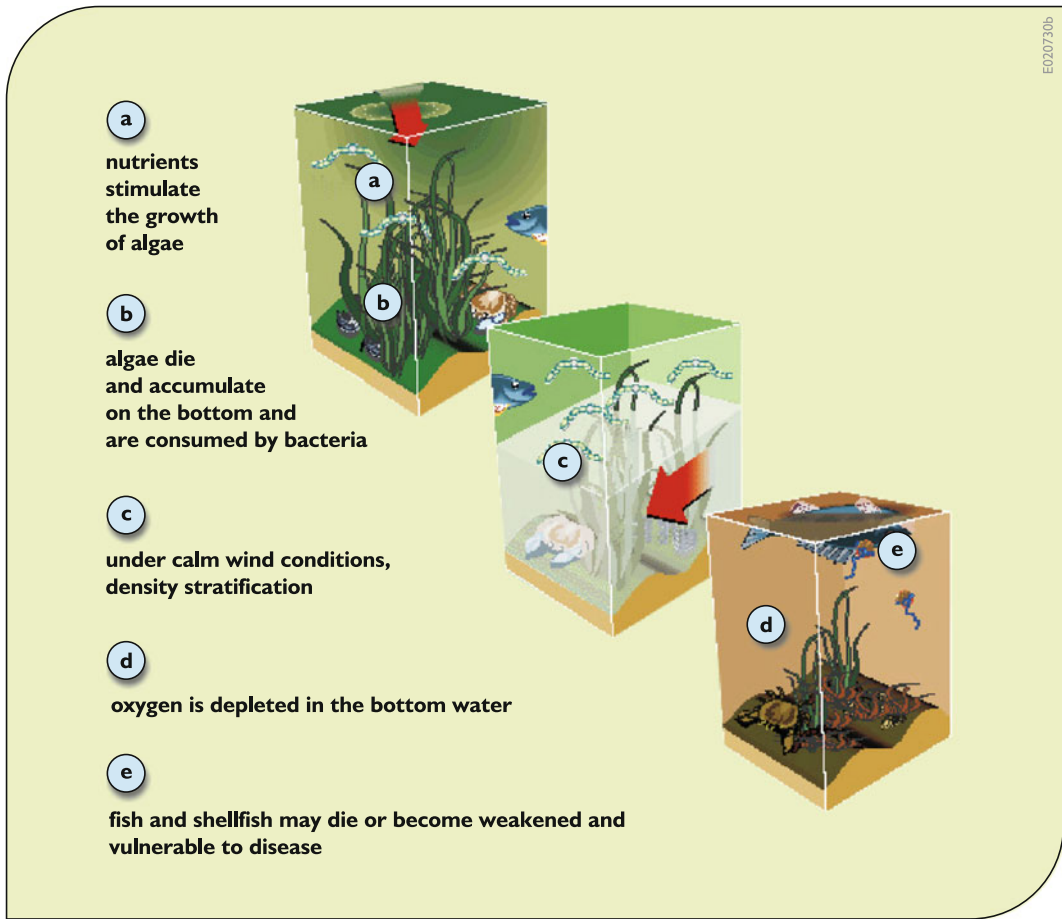
Fig. 10.2 The negative impacts of excessive nutrients in an estuary (NRC 2001)

the network in Fig. 10.3 can reflect a combination of simple mechanisms, statistical (regression) fitting, and expert judgment.

Advances in mechanistic modeling of aquatic ecosystems have resulted in our ability to include greater process (especially trophic) detail and complexity, as well as to perform dynamic simulations. Still, mechanistic ecosystem models have not advanced to the point of being able to predict community structure or biotic integrity. In this chapter, only some of the simpler mechanistic models will be introduced. More detail can be found in books solely devoted to water quality modeling (Chapra and Reckhow 1983; Chapra 1997; McCutcheon 1989; Thomann and Mueller 1987; Orlob 1983; Schnoor 1996) as well as the current literature.

10.3.3   Model Data

Data availability and accuracy is of concern in the development and use of models for water quality management. The complexity of models used for water quality management should be compatible with the quantity and quality of available data. The use of complex mechanistic models for water quality prediction in situations with little useful water quality data does not compensate for a lack of data. Model complexity can give the impression of credibility but this is not always true.

It is often preferable to begin with simple models and then over time add additional complexity as justified based on the collection and analysis of additional data. This strategy makes
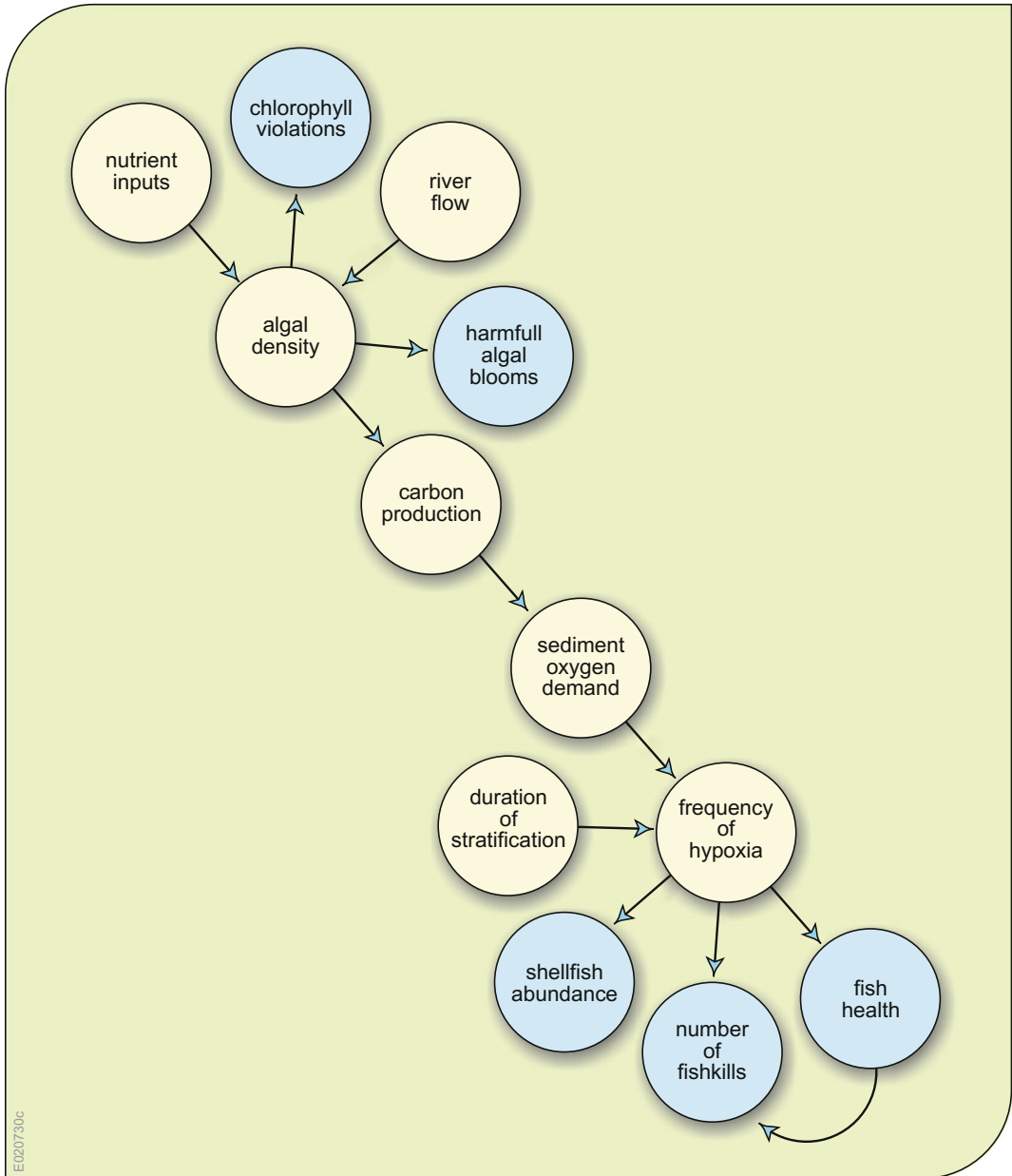
Fig. 10.3 Cause and effect diagram for estuary eutrophication due to excessive nutrient loadings (Borsuk et al. 2001)

efficient use of resources. It focuses efforts toward obtaining information and models that will reduce the uncertainty as the analysis proceeds. Models should be selected (simple vs. complex) in part based on the data available to support their use.

Water quality models of water bodies receiving pollutant discharges require those pollutant loadings as input data. These pollutant discharges can originate from point and non-point sources. Point source discharges are much easier to measure, monitor, and estimate than non-point

source inputs. Non-point discharge data often come from rainfall-runoff models that attempt to predict the quantity of runoff and its constituent concentrations. The reliability of the predictions from these models is not very good, especially if short time periods (e.g., each day or week) are being simulated. Their average values over longer time periods (e.g., each month or year) tend to be more reliable. This is mainly because the short-term inputs to those models, such as constituent loadings on the land and the rainfall within an area, which can vary over space and time within the area and time period being simulated, are typically not known with any precision. Chapter 12 reviews some of these loading models and their limitations.

10.4 Models of Water Quality Processes

Water quality models can be applied to many different types of water systems including streams, rivers, lakes, reservoirs, estuaries, coastal waters, and oceans. The models describe the main water quality processes and typically require the hydrologic and constituent inputs (the water flows or volumes and the pollutant loadings). These models include terms for dispersive and/or advective transport depending on the hydrologic and hydrodynamic characteristics of the water body, and terms for the biological, chemical and physical reactions among constituents. Advective transport dominates in flowing rivers. Dispersion is the predominant transport phenomenon in estuaries subject to tidal action. Lake water quality prediction is complicated by the influence of random wind directions and velocities that often affect surface mixing, currents, and stratification. For this and other reasons, obtaining reliable lake quality predictions is often more difficult than for streams, rivers, and estuaries. In coastal waters and oceans, larges scale flow patterns and tides are the most important transport mechanisms.

As with water quantity modeling, the development and application of water quality models is both a science as well as an art. Each model reflects the creativity of its developer, the particular water quality management problems and issues being addressed, the available data for model parameter calibration and verification, and the time available for modeling and associated uncertainty and other analyses. The fact that most, if not all, water quality models cannot accurately predict what actually happens does not necessarily detract from their value. Even relatively simple models can help managers understand the real-world prototype and estimate at least the relative if not actual change in water quality associated with given changes in the inputs resulting from water and land management policies or practices.

10.4.1 Mass Balance Principles

The basis principle of water quality models is that of mass balance. A water system can be divided into different segments or volumes elements (e.g., stream or river reaches, lake layers, estuary segments), also called "computational cells." For each segment or cell, there must be mass balance for each water quality constituent over time. Most water quality simulation models simulate quality over a consecutive series of discrete time period durations, Δt. Time is divided into discrete intervals and the flows are assumed constant within each of those time period intervals. For each segment and each time period, the mass balance of a substance in a segment can be administrated. Components of the mass balance for a segment include: (1) changes by transport (Tr) into and out of the segment, (2) changes by physical or chemical processes (P) occurring within the segment and (3) changes by sources/discharges to or from the segment (S).

$$M_i^{t+\Delta t} = M_i^t + \Delta t \left(\frac{\Delta M_i}{\Delta t}\right)_{Tr} + \Delta t \left(\frac{\Delta M_i}{\Delta t}\right)_P + \Delta t \left(\frac{\Delta M_i}{\Delta t}\right)_S$$

$$(10.2)$$

The mass balance has the following components:

- the mass in computational cell i at the beginning of a time step t: M_i^t
- the mass in computational cell i at the end of a time step t: $M_i^{t+\Delta t}$
- changes in computational cell i by transport; $\left(\frac{\Delta M_i}{\Delta t}\right)_{Tr}$
- changes in computational cell i by physical, (bio)chemical or biological processes: $\left(\frac{\Delta M_i}{\Delta t}\right)_P$
- changes in computational cell i by sources (e.g., waste loads, river discharges): $\left(\frac{\Delta M_i}{\Delta t}\right)_S$

Transport includes both advective and dispersive transport. Advective transport is the transport by flowing water. Dispersive transport results from concentration differences. Dispersion in the vertical direction is important if the water column is stratified, and dispersion in the horizontal direction can be in one or two dimensions. Dispersion, as defined here, includes the physical concept of molecular diffusion as it represents all transport that is not described by the advective transport.

Processes include physical processes such as reaeration and settling, (bio)chemical processes such as adsorption, transformation, and denitrification and biological processes such as primary production and predation on phytoplankton. Water quality processes convert one substance to another.

Sources include the addition of mass by waste loads and the extraction of mass by intakes. Mass entering over the model boundaries can be considered a source as well. The water flowing into or flowing out of the modeled segment or volume element (the computational cell) is derived from monitoring data or a water quantity (possibly hydrodynamic) model.

To model the transport of substances over space, a water system can be divided into small segments or volume elements. The complete ensemble of all the segments or elements is called the "*grid*" or "*schematization.*" Each computational cell is defined by its volume and its dimensions in one, two, or three directions (Δx, Δy, Δz) depending on the nature of the schematization (1D, 2D, or 3D). Note that the values of Δx, Δy and Δz do not have to be equal. The computational cell can have any rectangular shape. A computational cell can share surface areas with other computational cells, the atmosphere and the bottom sediment or coast line.

The following sections will look at the transport processes in more detail, defining parameters or variables and their units in terms of mass M, length L, and time T.

10.4.1.1   AdvectiveTransport

The advective transport, $T_{x_0}{}^A$ (M T^{-1}), of a constituent at a site x_0 is the product of the average water velocity, v_{x_0} (L T^{-1}), at that site, the surface or cross-sectional area, A (L^2), through which advection takes place at that site, and the average concentration, C_{x_0} (M L^{-3}), of the constituent:

$$T_{x_0}{}^A = v_{x_0} \times A \times C_{x_0} \qquad (10.3)$$

10.4.1.2   Dispersive Transport

The dispersive transport, $T_{x_0}^D$ (M T^{-1}) across a surface area is assumed to be proportional to the concentration gradient $\frac{\partial C}{\partial x}\big|_{x=x_0}$ at site x_0 times the surface area A. Letting D_{x_0} (L^2 T^{-1}), be the dispersion or diffusion coefficient at site x_0:

$$T_{x_0}^D = -D_{x_0} \times A \times \frac{\partial C}{\partial x}\bigg|_{x=x_0} \qquad (10.4)$$

Dispersion is commonly based on Fick's diffusion law. The minus sign reflects the fact that dispersion causes net transport from higher to lower concentrations, so in the opposite direction of the concentration gradient. The concentration gradient is the difference of concentrations per unit length, over a very small distance across the cross section

$$(\partial C/\partial x)|_x = \lim(\Delta x \to 0)$$
$$[(C_{x+0.5\Delta x} - C_{x-0.5\Delta x})/\Delta x] \qquad (10.5)$$

Dispersion coefficients should be calibrated or be obtained from calculations with turbulence models.

10.4.1.3 Mass Transport by Advection and Dispersion

If the advective and dispersive terms are added and the terms at a second surface at site $x_0 + \Delta x$ are included, the one-dimensional equation results

$$M_i^{t+\Delta t} = M_i^t + \Delta t \times \left(v_{x_0} C_{x_0} - v_{x_0 + \Delta x} C_{x_0 + \Delta x} \right.$$
$$\left. - D_{x_0} \frac{\partial C}{\partial x}\bigg|_{x_0} + D_{x_0 + \Delta x} \frac{\partial C}{\partial x}\bigg|_{x_0 + \Delta x} \right) \times A \tag{10.6}$$

or equivalently:

$$M_i^{t+\Delta t} = M_i^t + \Delta t \times \left(Q_{x_0} C_{x_0} - Q_{x_0 + \Delta x} C_{x_0 + \Delta x} \right.$$
$$\left. - D_{x_0} A_{x_0} \frac{\partial C}{\partial x}\bigg|_{x_0} + D_{x_0 + \Delta x} A_{x_0 + \Delta x} \frac{\partial C}{\partial x}\bigg|_{x_0 + \Delta x} \right), \tag{10.7}$$

where Q_{x_0} ($L^3 T^{-1}$) is the flow at site x_0.

If the previous equation is divided by the volume and the time interval Δt, then the following equation results in one dimension.

$$\frac{C_i^{t+\Delta t} - C_i^t}{\Delta t} = \frac{D_{x_0 + \Delta x} \frac{\partial C}{\partial x}\big|_{x_0 + \Delta x} - D_{x_0} \frac{\partial C}{\partial x}\big|_{x_0}}{\Delta x}$$
$$+ \frac{v_{x_0} C_{x_0} - v_{x_0 + \Delta x} C_{x_0 + \Delta x}}{\Delta x} \tag{10.8}$$

Taking the asymptotic limit $\Delta t \to 0$ and $\Delta x \to 0$, the advection–diffusion equation for one dimension results

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial x}\left(D \frac{\partial C}{\partial x} \right) - \frac{\partial}{\partial x}(vC) \tag{10.9}$$

The finite volume computational method for transport can be used to solve the advection–diffusion equation. The accuracy of the method will be related to the size of Δx, A ($=\Delta y\,\Delta z$) and Δt.

By adding terms for transport in the y and z-direction a three-dimensional model is obtained. Taking the asymptotic limit again will lead to a three-dimensional advection–diffusion equation

$$\frac{\partial C}{\partial t} = D_x \frac{\partial^2 C}{\partial x^2} - v_x \frac{\partial C}{\partial x} + D_y \frac{\partial^2 C}{\partial y^2}$$
$$- v_y \frac{\partial C}{\partial y} + D_z \frac{\partial^2 C}{\partial z^2} - v_z \frac{\partial C}{\partial z} + S + f_R(C, t) \tag{10.10}$$

with dispersion coefficients D_j defined for each direction j. If source terms "S" and "f_R" are added as shown in the equation above, the so-called advection–diffusion-reaction equation emerges. The additional terms represent

- Discharges or "waste loads" (S): these source terms are additional inflows of water or mass. As many source terms as required may be added to Eq. 10.10. These could include small rivers, discharges of industries, sewage treatment plants, small waste load outfalls, etc.
- Reaction terms or "processes" (f_R).

Processes can be split into physical processes and other processes. Examples of physical processes are

- settling of suspended particulate matter
- water movement not affecting substances, like evaporation
- volatilization of the substance itself at the water surface.

Examples of other processes are

- biochemical conversions like ammonia and oxygen forming nitrite
- growth of algae (primary production)
- predation by other animals
- chemical reactions.

These processes are described in more detail in the remaining parts of this Sect. 10.4.

Multiplying each term in Eq. 10.9 by the cross-sectional area A (L^2), the expression DA ($\partial C/\partial x$) $- vAC$ for a one-dimensional model, or its equivalent in Eq. 10.10 for a three-dimensional model, is termed the total flux (M T^{-1}). Flux due to dispersion, $DA(\partial C/\partial x)$, is assumed to be proportional to the concentration gradient over distance. Constituents are

transferred by dispersion from higher concentration zones to lower concentrations zones. The coefficient of dispersion D ($L^2 T^{-1}$) depends on the amplitude and frequency of the tide, if applicable, as well as upon the turbulence of the water body. It is common practice to include in this dispersion parameter everything affecting the distribution of C other than advection. The term vAC is the advective flux caused by the movement of water containing the constituent concentration C ($M L^{-3}$) at a velocity rate v ($L T^{-1}$) across a cross-sectional area A.

The relative importance of dispersion and advection depends on how detailed the velocity field is defined. A good spatial and temporal description of the velocity field within which the constituent is being distributed will reduce the importance of the dispersion term. Less precise descriptions of the velocity field, such as averaging across irregular cross sections or approximating transients by steady flows, may lead to a dominance of the dispersion term.

Many of the reactions affecting the decrease or increase of constituent concentrations are often represented by first-order kinetics which assumes that the reaction rates are proportional to the constituent concentration. While higher order kinetics may be more correct in certain situations, predictions of constituent concentrations based on first-order kinetics have often been considered acceptable for natural aquatic systems.

10.4.2   Steady-State Models

Steady state means no change in the concentrations over time. In this case the left-hand side of Eq. 10.9 or 10.10, $\partial C/\partial t$, equals 0. Assume the only sink is the natural decay of the constituent defined as kC where k, (T^{-1}), is the decay rate coefficient or constant. Now Eq. 10.9 becomes

$$0 = D\partial^2 C/\partial x^2 - v\partial C/\partial x - kC \qquad (10.11)$$

Equation 10.11 can be integrated since river reach parameters $A, D, k, v,$ and Q are assumed constant. For a constant loading, W_C ($M T^{-1}$) at

site $x = 0$, the concentration C at any distance x will equal

$$C(x) = \begin{cases} (W_C/Qm)\exp[(v/2D)(1+m)x] & x \leq 0 \\ (W_C/Qm)\exp[(v/2D)(1-m)x] & x \geq 0 \end{cases}$$
$$(10.12)$$

where

$$m = \left(1 + \left(4kD/v^2\right)\right)^{1/2} \qquad (10.13)$$

Note from Eq. 10.13 that the parameter m is always equal or greater than 1. Hence the exponent of e in Eq. 10.12 is always negative. As the distance x increases in magnitude, either in the positive or negative direction, the concentration $C(x)$ will decrease. The maximum concentration C occurs at $x = 0$ and is W_C/Qm.

$$C(0) = W_C/Qm \qquad (10.14)$$

These equations are plotted in Fig. 10.4.

In flowing rivers not under the influence of tidal actions the dispersion is small. Assuming the dispersion coefficient D is 0, the parameter m defined by Eq. 10.13, is 1. When $D = 0$, the maximum concentration at $x = 0$ is W_C/Q.

$$C(0) = W_C/Q \quad \text{if} \ \ D = 0. \qquad (10.15)$$

Assuming $D = 0$ and v, Q and $k > 0$, Eq. 10.12 becomes

$$C(x) = \begin{cases} 0 & x \leq 0 \\ (W_C/Q)\exp[-kx/v] & x \geq 0 \end{cases} \quad (10.16)$$

The above equation for $x > 0$ can be derived from Eqs. 10.12 and 10.13 by noting that the term $(1 - m)$ equals $(1 - m)(1 + m)/(1 + m) = (1 - m^2)/2$ when D is 0. Thus, when D is 0 the expression $(v/2D)(1 - m)x$ in Eq. 10.12 becomes $-kx/v$. The term x/v is sometimes denoted as a single variable representing the time of flow—the time flow Q takes to travel from site $x = 0$ to some other downstream site $x > 0$.

As rivers approach the sea, the dispersion coefficient D increases and the net downstream velocity v decreases. Because the flow Q equals the cross-sectional area A times the velocity v,

Fig. 10.4 Constituent concentration distributions along a river or estuary resulting from a constant discharge of that constituent at a single point source in that river or estuary. The *top plot* represents Eq. 10.16, the *middle plot* represents Eq. 10.12, and the *bottom plot* represents Eq. 10.17
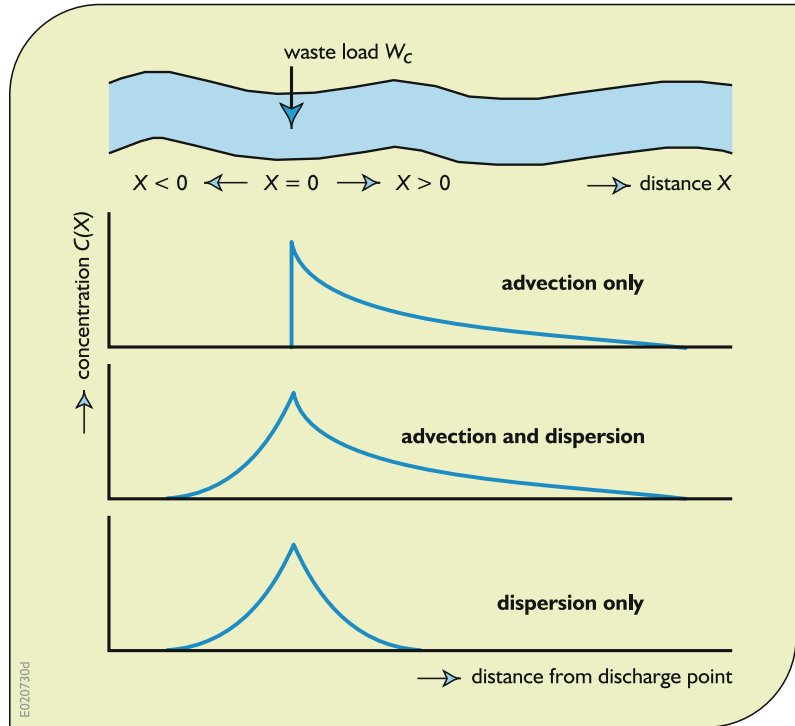
$Q = Av$, and since the parameter m can be defined as $(v^2 + 4kD)^{1/2}/v$, then as the velocity v approaches 0, the term $Qm = Av(v^2 + 4kD)^{1/2}/v$ approaches $2A(kD)^{1/2}$. The exponent $vx(1 \pm m)/2D$ in Eq. 10.12 approaches $\pm x(k/D)^{1/2}$.

Hence for small velocities, Eq. 10.4 becomes

$$C(X) = \begin{cases} \left(W_C/2A(kD)^{1/2}\right)\exp\left[+x(k/D)^{1/2}\right] & x \leq 0 \\ \left(W_C/2A(kD)^{1/2}\right)\exp\left[-x(k/D)^{1/2}\right] & x \geq 0 \end{cases}$$
$$(10.17)$$

Here dispersion is much more important than advective transport and the concentration profile approaches a symmetric distribution, as shown in Fig. 10.4, about the point of discharge at $x = 0$.

Water quality management models are often used to assess the effect of pollutant loadings on ambient waters and to compare the results with specific water quality standards. The above steady state equations can be used to construct such a model for estimating the wastewater removal efficiencies required at each wastewater discharge site that will result in an ambient stream quality that meets the standards along a stream or river.

Figure 10.5 shows a schematic of a river into which wastewater containing constituent C is being discharged at four sites. Assume maximum allowable concentrations of the constituent C are specified at each of those discharge sites. To estimate the needed reduction in these discharges, the river must be divided into approximately homogenous reaches. Each reach can be characterized by constant values of the cross-sectional area, A, dispersion coefficient, D, constituent decay rate constant, k, and velocity, v, associated with some "design" flow and temperature conditions. These parameter values and the length, x, of each reach can differ, hence the subscript index i will be used to denote the particular reach. These reaches are shown in Fig. 10.5.

In Fig. 10.5 each variable C_i represents the constituent concentration at the beginning of reach i. The flows Q represent the design flow conditions. For each reach i the product $(Q_i m_i)$ is represented by $(Qm)_i$. The downstream (forward)
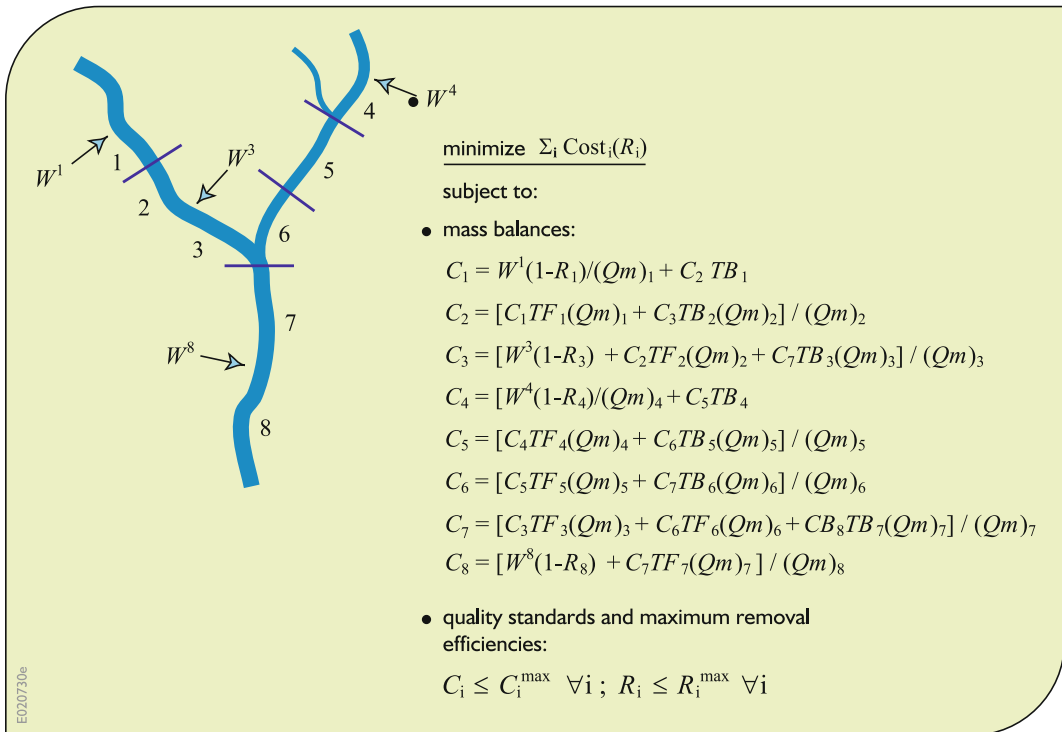
Fig. 10.5 Optimization model for finding constituent removal efficiencies, R_i, at each discharge site i that result in meeting stream quality standards, C_i^{max}, at least total cost

transfer coefficient, TF_i, equals the applicable part of Eq. 10.12,

$$TF_i = \exp[(v/2D)(1-m)x] \qquad (10.18)$$

as does the upstream (backward) transfer coefficient, TB_i.

$$TB_i = \exp[(v/2D)(1+m)x] \qquad (10.19)$$

The parameter m is defined by Eq. 10.13.

Finding the cost solution of a model such as shown in Fig. 10.5 does not mean that the least-cost wasteload allocation plan will be implemented, but such information can help identify the additional costs of other imposed constraints, for example, to ensure equity, or extra safety. Models like this can be used to identify the cost-quality tradeoffs inherent in any water quality management program. Non economic objectives can also be used to obtain other tradeoffs.

The model in Fig. 10.5 incorporates both advection and dispersion. If upstream dispersion under design streamflow conditions is not significant in some reaches, then the upstream (backward) transfer coefficients, TB_i, for those reaches i will equal 0.

10.4.3   Design Streamflows for Setting and Evaluating Quality Standards

In streams and rivers, the water quality may vary significantly depending on the stream or river flow and its quality prior to wastewater discharges. If waste load discharges are fairly constant, a high flow of high quality serves to dilute the waste concentration while contaminant concentrations of low flows may become undesirably high. It is therefore common practice to pick

a more critical low-flow condition for judging whether or not ambient water quality standards are being met. This can also be seen from Eqs. 10.12, 10.14, 10.15, and 10.16. This often is the basis for the assumption that the smaller (or more critical) the design flow, the more likely it is that the stream quality standards will be met in practice. This is not always the case, however.

Different regions of the world use different design low-flow conditions. One example of such a design flow, that is used in parts of North America, is the minimum 7-day average flow expected to be lower only once in 10 years on average. Each year the lowest 7-day average flow is determined, as shown in Fig. 10.6. The sum of each of the 365 sequences of seven average daily flows is divided by 7 and the minimum value is selected. This is the minimum annual average 7-day flow for the year.

These minimum 7-day average flows for each year of record define a probability distribution, whose cumulative probabilities can be plotted. As illustrated in Fig. 10.7, the particular flow on the cumulative distribution that has a 90% chance of being exceeded is the design flow. It is the minimum annual average 7-day flow expected once in 10 years. This flow is commonly called the 7Q10 flow. Analyses have shown that this daily design flow is exceeded about 99% of the time in regions where it is used (NRC 2001). This means that there is on average only about a one percent chance that any daily flow will be less than this 7Q10 flow.

Fig. 10.6 Portion of annual flow time series showing low flows and the calculation of average 7 and 14-day flows
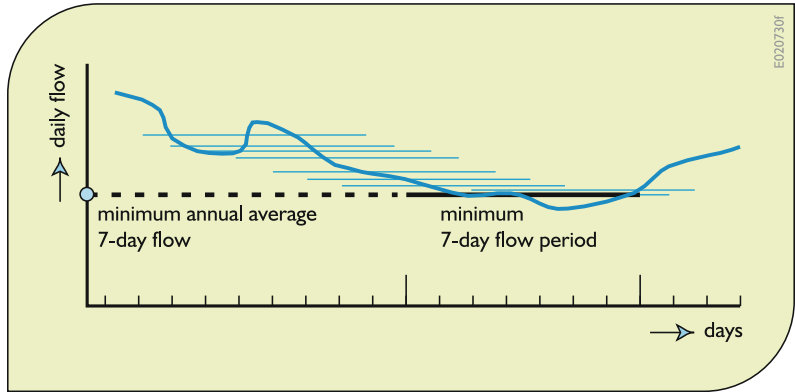
Fig. 10.7 Determining the minimum 7-day annual average flow expected once in 10 years, designated 7Q10, from the cumulative probability distribution of annual minimum 7-day average flows
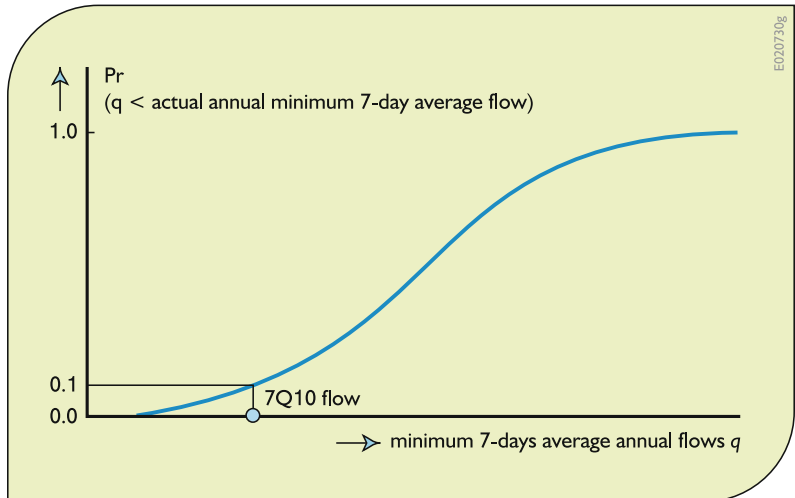
Consider now any one of the river reaches shown in Fig. 10.5. Assume an initial loading of constituent mass, $M/\Delta t$, exists at the beginning of the reach. As the reach flow, Q, increases and the mass loading stays the same, the initial concentration, M/Q, will decrease. However, the flow velocity will increase, and thus the time, Δt, it takes to transport the constituent mass to the end of that reach will decrease. This means less time for the decay of the constituent. Hence it is possible that ambient water quality standards that are met during low flow conditions may not be met under higher flow conditions, conditions that are observed much more frequently. Figure 10.8 illustrates how this might happen. This does not suggest that low flows should not be considered when allocating waste loads, but rather that a simulation of water quality concentrations over varying flow conditions may show that higher flow conditions at some sites are even more critical and more frequent than they are during less frequent low-flow conditions.

Figure 10.8 shows that for a fixed mass of pollutant at $x = 0$, under low flow conditions the more restrictive (lower) maximum pollutant concentration standard in the downstream portion of the river is met, but that same standard is violated under higher flow conditions.
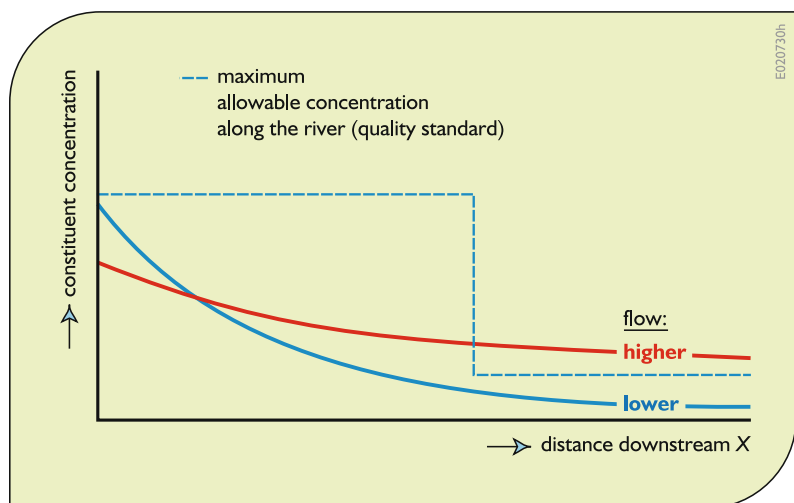
10.4.4   Temperature

Temperature impacts almost all water quality processes taking place in water bodies. For this reason modeling temperature may be important when the temperature varies over the period of interest, or when the discharge of heat into water bodies is to be managed.

Temperature models are based on a heat balance in the water body. A heat balance takes into account the sources and sinks of heat. The main sources of heat in a water body are shortwave solar radiation, longwave atmospheric radiation, conduction of heat from the atmosphere to the water and direct heat inputs. The main sinks of heat are long wave radiation emitted by the water, evaporation, and conduction from the water to atmosphere. Unfortunately, a model with all the sources and sinks of heat requires measurements of a number of variables and coefficients that are not always readily available.

One temperature predictor is the simplified model that assumes an equilibrium temperature T_e (°C) will be reached under steady-state meteorological conditions. The temperature mass balance in a volume segment depends on the water density ρ (g/cm^3), the heat capacity of water, c_p (cal/g/°C), and the water depth h (cm).

Fig. 10.8 Increasing streamflows decreases initial concentrations but may increase downstream concentrations

Assuming the net heat input, $K_H(T_e - T)$ (cal/cm^2/day), is proportional to the difference of the actual temperature, T, and the equilibrium temperature, T_e (°C),

$$\mathrm{d}T/\mathrm{d}t = K_H(T_e - T)/\rho c_p h \qquad (10.20)$$

The overall heat exchange coefficient, K_H (cal/cm^2/day/°C), is determined in units of W/m^2/°C (1 cal/cm^2/day °C = 0.4840 W/m^2/°C) from empirical relationships that include wind velocity U_w (m/s), dew point temperature T_d (°C), and actual temperature T (°C) (Thomann and Mueller 1987).

The equilibrium temperature, T_e, is obtained from another empirical relationship involving the overall heat exchange coefficient, K_H, the dew point temperature, T_d, and the shortwave solar radiation H_s (cal/cm^2/day),

$$T_e = T_d + (H_s/K_H) \qquad (10.21)$$

This model simplifies the mathematical relationships of a complete heat balance and requires less data.

10.4.5   Sources and Sinks

Sources and sinks of water quality constituents include the physical and biochemical processes that are represented by the term S in Eq. 10.10. External inputs of each constituent would have the form W/Q, where W (M T^{-1}) is the loading rate of the constituent and Q represents the flow of water into which the mass of waste W is discharged.

10.4.6   First-Order Constituents

The first-order models are commonly used to predict water quality constituent decay or growth. They can represent constituent reactions such as decay or growth in situations where the time rate of change ($\mathrm{d}C/\mathrm{d}t$) in the concentration C of the constituent, say organic matter that creates a biochemical oxygen demand (BOD), is proportional to the concentration of either the same or another constituent concentration. The temperature-dependent proportionality constant k_c (1/day) is called a rate coefficient or constant. In general, if the rate of change in some constituent concentration C_j is proportional to the magnitude of concentration C_i, of constituent i, then

$$\mathrm{d}C_j/\mathrm{d}t = a_{ij}k_i\theta_i^{(T-20)}C_i, \qquad (10.22)$$

where θ_i is temperature correction coefficient for k_i at 20 °C and T is the temperature in °C. The parameter a_{ij} is the grams of C_j produced ($a_{ij} > 0$) or consumed ($a_{ij} < 0$) per gram C_i. For the prediction of BOD concentration over time, $C_i = C_j = $ BOD and $a_{ij} = a_{BOD} = -1$ in Eq. 10.22. Conservative substances, such as salt, will have a decay rate constant k of 0. The concentration of conservative substances depends only on the amount of water, i.e., dilution.

The typical values for the rate coefficients k_c and temperature coefficients θ_i of some constituents C are in Table 10.1. For bacteria, the first-order decay rate (k_B) can also be expressed in terms of the time to reach 90% mortality (t_{90}, days). The relationship between these coefficients is given by $k_B = 2.3/t_{90}$.

10.4.7   Dissolved Oxygen

DO concentration is a common indicator of the health of the aquatic ecosystem. DO was originally modeled by Streeter and Phelps (1925). Since then a number of modifications and extensions of the model have been made depending on the number of sinks and sources of DO being considered and how processes involving the nitrogen cycle and phytoplankton, are being modeled, as illustrated in Fig. 10.9.

The sources of DO in a water body include reaeration from the atmosphere, photosynthetic oxygen production from aquatic plants, denitrification, and DO inputs. The sinks include oxidation of carbonaceous and nitrogenous material, sediment oxygen demand and respiration by aquatic plants.

Table 10.1 Typical values of the first-order decay rate, k, and the temperature correction factor, θ, for some constituents

constituent	rate constant k		units
total coliform bacteria (freshwater)	1.0-5.5	- a	1/day
total coliform bacteria (sediments)	0.14-0.21	- a	1/day
total coliform bacteria (seawater)	0.7-3.0	- a	1/day
fecal coliform bacteria (seawater)	37-110	- a	1/day
BOD (no treatment)	0.3-0.4	- a	1/day
BOD (activated sludge treatment)	0.05-0.1	- a	1/day
carbofuran	0.03	- b	1/day
DDT	0.0-0.10	- b	1/day
PCB	0.0-0.007	- b	1/day
pentachlorophenol	0.0-33.6	- b	1/day

constituent	θ		units
coliform bacteria (freshwater)	1.07	- b	——
coliform bacteria (saltwater)	1.10	- b	——
BOD	1.04	- a	---

a - Thomann and Mueller (1987)   b - Schnoor (1996)

$$\Delta O_2/\Delta t = \text{loads} + \text{transport} + \text{reaeration}$$
$$+ \text{net primary production} + \text{denitrification}$$
$$- \text{mineralization} - \text{nitrification} - \text{SOD}$$

The rate of reaeration is assumed to be proportional to the difference between the saturation concentration, DO_{sat} (mg/l), and the concentration of DO, DO (mg/l). The proportionality coefficient is the reaeration rate k_r (1/day), defined at temperature $T = 20\ ^\circ C$, which can be corrected for any temperature T with the coefficient $\theta_r^{(T-20)}$. The value of this temperature correction coefficient, θ, depends on the mixing condition of the water body. Values generally range from 1.005 to 1.030. In practice a value of 1.024 is often used (Thomann and Mueller 1987). The reaeration rate constant is a sensitive parameter. There have been numerous equations developed to define this rate constant. Table 10.2 lists some of them.

The saturation concentration, DO_{sat}, of oxygen in water is a function of the water temperature and salinity [chloride concentration, Cl (g/m^3)], and can be approximated by

$$DO_{sat} = \Big\{14.652 - 0.41022T + (0.089392T)^2$$

$$- (0.042685T)^3\Big\}\{1 - (Cl/100000)\} \quad (10.23a)$$

Table 10.2 Some equations for defining the reaeration rate constant, k_r (1/day)

<div>

units

water and wind velocity (m/s)   **water depth (m)**

k_r = mass transport coefficient for reaeration (m/day) / (water depth)

=   5.026 (water velocity)$^{0.969}$ / (water depth)$^{1.673}$ (Churchill, 1962)

=   3.95 (water velocity)$^{0.5}$ / (water depth)$^{1.5}$ (O'Connor and Dobbiens, 1958)

= (scale factor) 3.95   (water velocity)$^{0.5}$ / (water depth)$^{1.5}$

=   5.344 (water velocity)$^{0.670}$ / (water depth)$^{1.85}$ (Owens, Edwards, Gibb, 1964)

=   5.13 (water velocity)   / (water depth)$^{1.333}$ (Langbien, Durum, 1967)

= { 0.065 (wind velocity)^2 + 3.86 [(water velocity) / (water depth)]$^{0.5}$ } / (water depth)
     (van Pagee 1978, Delvigne 1980)

</div>
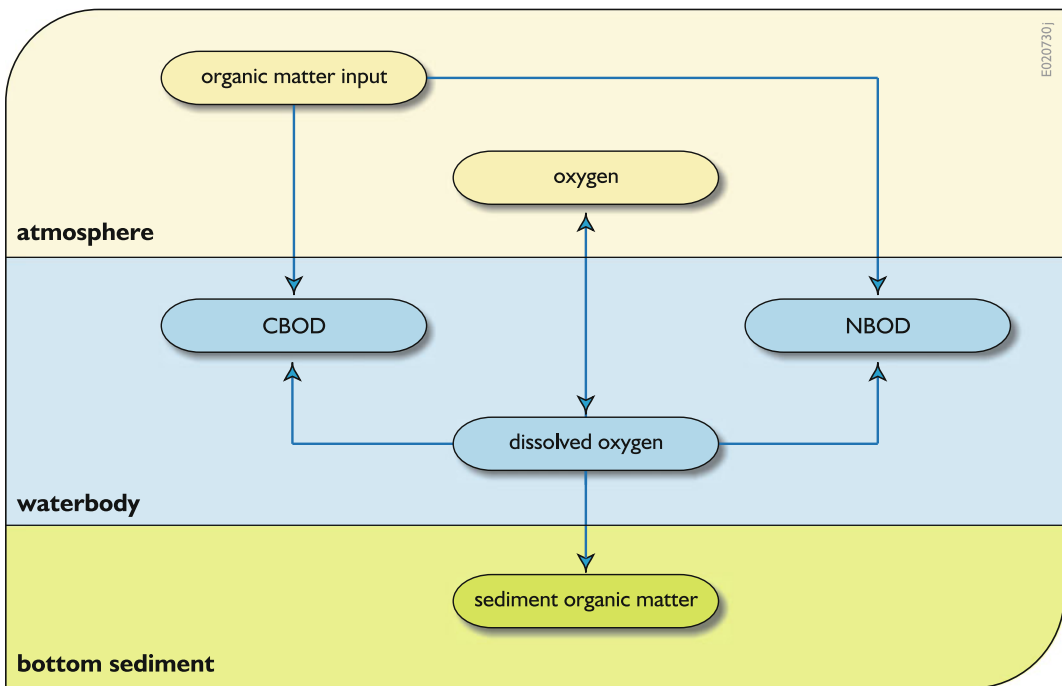
Fig. 10.9 The dissolved oxygen interactions in a water body, showing the decay (satisfaction) of carbonaceous, nitrogenous and sediment oxygen demands and water body reaeration or deaeration (if supersaturated occurs at the air–water interface)

Fig. 10.10 Fitted curve to the saturation dissolved oxygen concentration (mg/l) as a function of temperature (°C)
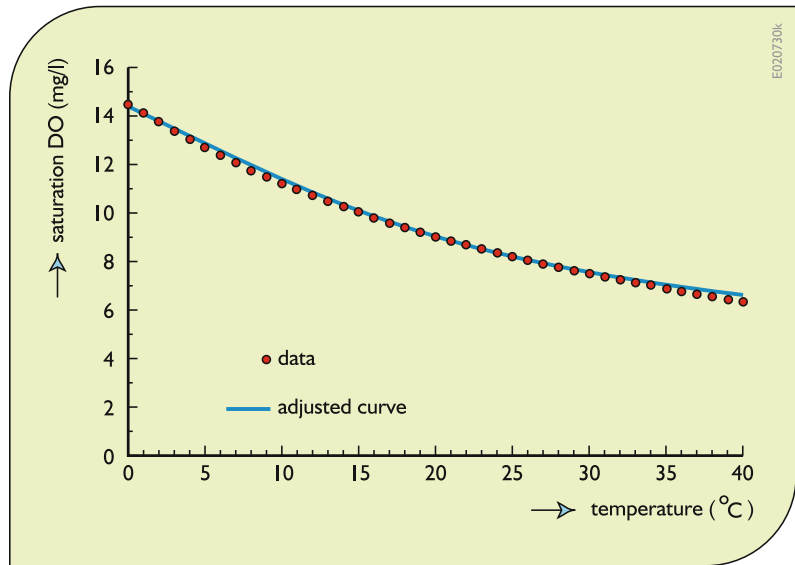
Elmore and Hayes (1960) derived an analytical expression for the DO saturation concentration, DO_{sat} (mg/l), as a function of temperature (T, °C):

$$DO_{sat} = 14.652 - 0.41022T + 0.007991T^2 - 0.000077774T^3$$

$$(10.23b)$$

Fitting a second-order polynomial curve to the data presented in Chapra (1997) results in

$$DO_{sat} = 14.407 - 0.3369T + 0.0035T^2$$

$$(10.23c)$$

as is shown in Fig. 10.10.

Because photosynthesis occurs during daylight hours, photosynthetic oxygen production follows a cyclic, diurnal, pattern in water. During the day, oxygen concentrations in water are high and can even become supersaturated, i.e., concentrations exceeding the saturation concentration. At night, the concentrations drop due to respiration and other oxygen consuming processes.

The biochemical oxygen demand results from carbonaceous organic matter (CBOD, mg/l) and from nitrogenous organic matter (NBOD, mg/l) in the water. There is also the oxygen demand from carbonaceous and nitrogenous organic matter in the sediments (SOD, mg/l/day). These oxygen demands are typically modeled as first-order decay reactions with decay rate constants k_{CBOD} (1/day) for CBOD and k_{NBOD} (1/day) for NBOD. These rate constants vary with temperature, hence they are typically defined for 20 °C. The decay rates are corrected for temperatures other than 20 °C using temperature coefficients θ_{CBOD} and θ_{NBOD}, respectively.

The sediment oxygen demand (SOD) (mg/liter/day) is usually expressed as a zero-order reaction, i.e., a constant demand. One important feature in modeling NBOD is ensuring the appropriate time lag between when it is discharged into a water body and when the oxygen demand is observed. This lag is in part a function of the level of treatment in the wastewater treatment plant.

The DO model with CBOD, NBOD, and SOD is

$$dDO/dt = -k_{CBOD}\theta_{CBOD}^{(T-20)}CBOD - k_{NBOD}\theta_{NBOD}^{(T-20)}NBOD + k_r q_r^{(T-20)}(DO_{sat} - DO) - SOD$$

$$(10.24)$$

$$dCBOD/dt = -k_{CBOD}\theta_{CBOD}^{(T-20)}CBOD \quad (10.25)$$

$$dNBOD/dt = -k_{NBOD}\theta_{NBOD}^{(T-20)}NBOD \quad (10.26)$$

The mean and range values for coefficients included in these DO models are in Table 10.3.

Table 10.3 Typical values of parameters used in the dissolved oxygen models

parameter	value		units
k_r, slow, deep rivers	0.1-0.4	- a	I/day
k_r, typical conditions	0.4-1.5	- a	I/day
k_r, swift, deep rivers	1.5-4.0	- a	I/day
k_r, swift, shallow rivers	4.0-10.0	- a	I/day
k_{CBOD}, untreated discharges	0.35 (0.20-0.50)	- b	I/day
k_{CBOD}, primary treatment	0.20 (0.10-0.30)	- b	I/day
k_{CBOD}, activated sludge	0.075 (0.05-0.10)	- b	I/day
θ_{CBOD}	1.04	- a	—
	1.047	- a	—
	1.04 (1.02-1.09)	- c	—
θ_r	1.024 (1.005-1.030)	- c	---

sediment oxygen demand *	value		units
municipal sludge (outfall vicinity)	4 (2-10)	- c d	$gO_2/m^2/day$
municipal sewage sludge	1.5 (1-2)	- c d	$gO_2/m^2/day$
sandy bottom	0.5 (0.2-1.0)	- c d	$gO_2/m^2/day$
mineral soils	0.07 (0.05-0.1)	- c d	$gO_2/m^2/day$
natural to low pollution	0.1-10.0	- a	$gO_2/m^2/day$
moderate to heavy pollution	5-10	- a	$gO_2/m^2/day$

a - Schnoor (1996)   c - Thomann and Mueller (1987)

b - Chapra (1997)   d - Bowie et al. (1985)

* value has to be divided by the water height (m)

10.4.8   Nutrients and Eutrophication

Eutrophication is the progressive process of nutrient enrichment of water systems. An increase in nutrients leads to an increase in the productivity of the water system that may result in an excessive increase in the biomass of algae or other primary producers such as macrophytes or duck weed. When it is visible on the surface of the

water it is called an algae bloom. Excessive algal biomass could affect the water quality, especially if it causes anaerobic conditions and thus impairs the drinking, recreational, and ecological uses.

The eutrophication component of the model relates the concentration of nutrients and the algal biomass. For example, as shown in Fig. 10.11, consider the growth of algae A (mg/l—not to be confused with area A used in previous equations), depending on phosphate phosphorus, P (mg/l), and nitrite/nitrate nitrogen, N_n (mg/l), as the limiting nutrients. There could be other limiting nutrients or other conditions as well, but here consider only these two. If either of these two nutrients is absent, the algae cannot grow regardless of the abundance of the other nutrient.

The uptake of the more abundant nutrient will not occur.

To account for this, algal growth is commonly modeled as a Michaelis–Menten multiplicative effect, i.e., the nutrients have a synergistic effect. Model parameters include a maximum algal growth rate μ (1/day) times the fraction of a day, f_d, that rate applies (Fig. 10.12), the half saturation constants K_P and K_N (mg/l) (shown as K_c in Fig. 10.13) for phosphate and nitrate, respectively, and a combined algal respiration and specific death rate constant e (1/day) that creates an oxygen demand. The uptake of phosphate, ammonia, and nitrite/nitrate by algae is assumed to be in proportion to their contents in the algae
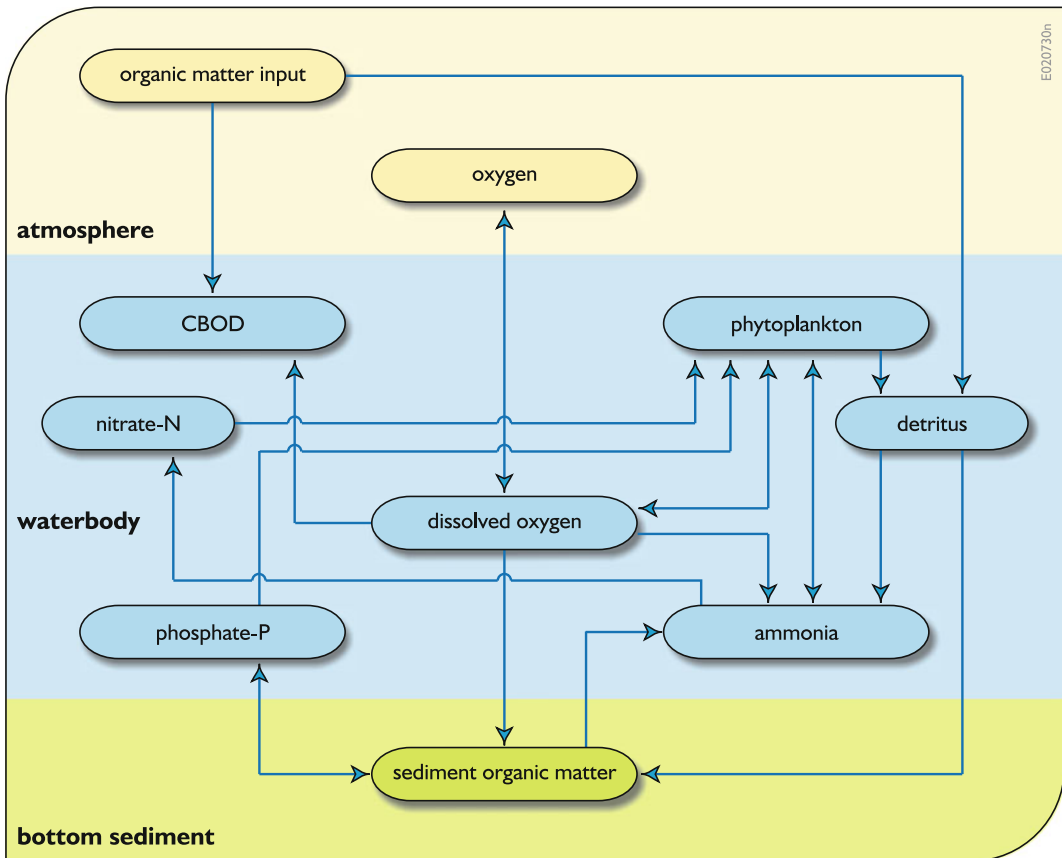

Fig. 10.11 The dissolved oxygen, nitrogen, and phosphorus cycles, and phytoplankton interactions in a water body, showing the decay (satisfaction) of carbonaceous and sediment oxygen demands, reaeration or deaeration of oxygen at the air–water interface, ammonification of organic nitrogen in the detritus, nitrification (oxidation) of ammonium to nitrate–nitrogen and oxidation of organic phosphorus in the sediment or bottom layer to phosphate phosphorus, phytoplankton production from nitrate and phosphate consumption, and phytoplankton respiration and death contributing to the organic nitrogen and phosphorus

Fig. 10.12 Calculation of the fraction, f_d, of the maximum growth rate constant, μ, to use in the algal growth equations. The fraction f_d is the ratio of actual production zone/potential production zone
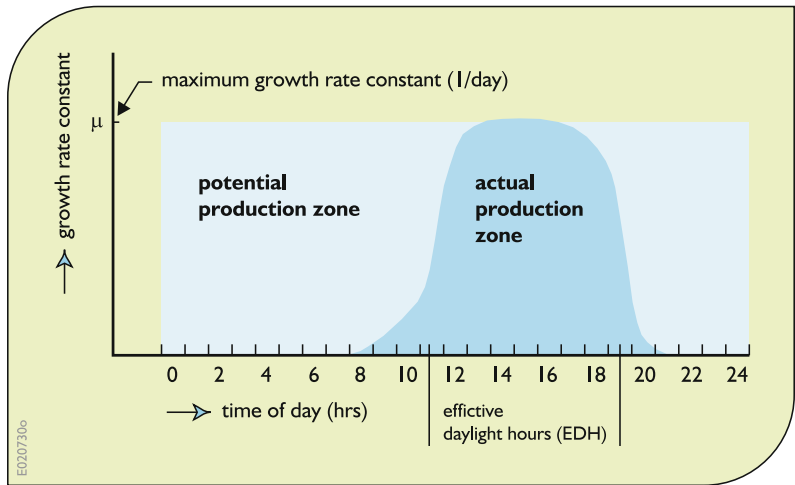
Fig. 10.13 Defining the half saturation constant for a Michaelis–Menten model of algae. The actual growth rate constant $= \mu C/(C + K_C)$
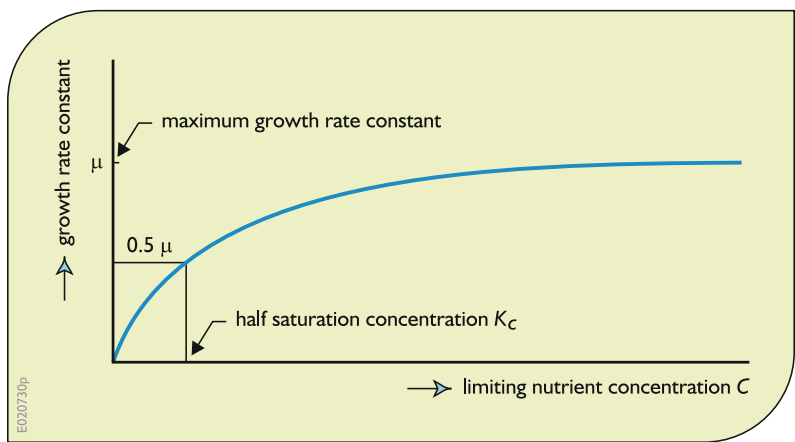
biomass. Define these proportions as a_P, a_A, and a_N, respectively.

In addition to the above parameters, one needs to know the amounts of oxygen consumed in the oxidation of organic phosphorus, P_o, and the amounts of oxygen produced by photosynthesis and consumed by respiration. In the model below, some average values have been assumed. Also assumed are constant temperature correction factors for all processes pertaining to any individual constituent. This reduces the number of parameters needed, but is not necessarily realistic. Clearly other processes as well as other parameters could be added, but the purpose here is to illustrate how these models are developed.

Users of water quality simulation programs will appreciate the many different assumptions that can be made and the large amount of parameters associated with most of them.

The source and sink terms of the relatively simple eutrophication model shown in Fig. 10.11 can be written as follows:

For algae biomass

$$dA/dt = \mu f_d \theta_A^{(T-20)}[P/(P+K_P)][N_n/(N_n+K_N)]A \\ - e\theta_A^{(T-20)}A$$

$$(10.27)$$

For organic phosphorus

$$\mathrm{d}P_\mathrm{o}/\mathrm{d}t = -k_\mathrm{op}\theta_\mathrm{op}^{(T-20)}P_\mathrm{o} \tag{10.28}$$

For phosphate phosphorus

$$\mathrm{d}P/\mathrm{d}t = -\mu f_\mathrm{d}\theta_A^{(T-20)}[P/(P+K_P)][N_\mathrm{n}/(N_\mathrm{n}+K_N)]a_P A \tag{10.29}$$

For organic nitrogen

$$\mathrm{d}N_\mathrm{o}/\mathrm{d}t = -k_\mathrm{on}\theta_\mathrm{on}^{(T-20)}N_\mathrm{o} \tag{10.30}$$

For ammonia–nitrogen

$$\mathrm{d}N_\mathrm{a}/\mathrm{d}t = -\mu f_\mathrm{d}\theta_A^{(T-20)}[P/(P+K_P)][N_\mathrm{n}/(N_\mathrm{n}+K_N)]a_A A \\ + k_\mathrm{on}\theta_\mathrm{on}^{(T-20)}N_\mathrm{o} - k_a\theta_a^{(T-20)}N_\mathrm{a} \tag{10.31}$$

For nitrate–nitrogen

$$\mathrm{d}N_\mathrm{N}/\mathrm{d}t = -\mu f_\mathrm{d}\theta_A^{(T-20)}[P/(P+K_P)][N_\mathrm{n}/(N_\mathrm{n}+K_N)]a_N A \\ + k_a\theta_a^{(T-20)}N_\mathrm{a} - k_n\theta_A^{(T-20)}N_\mathrm{n} \tag{10.32}$$

For DO

$$\mathrm{d}DO/\mathrm{d}t = -k_\mathrm{CBOD}\theta_\mathrm{CBOD}^{(T-20)}CBOD - 4.57k_a\theta_a^{(T-20)}N_\mathrm{a} \\ - 2k_\mathrm{op}\theta_\mathrm{op}^{(T-20)}P_\mathrm{o} + (1.5\,\mu f_\mathrm{d} - 2e)\theta_A^{(T-20)}A \\ + k_r\theta_r^{(T-20)}(DO_\mathrm{sat} - DO) - SOD \tag{10.33}$$

Representative values of the coefficients for this model are in Table 10.4.

Because of the growth of phytoplankton cannot occur without nutrients, the eutrophication modeling must be coupled with that of nutrients. Nutrient modeling must include all the different biochemical forms of the nutrients, primarily nitrogen and phosphorus, as well as all the interactions between the different forms. The sum of all these interactions is referred to a "nutrient cycling".

The nitrogen cycle includes ammonium (NH_4–N) and nitrate/nitrite (represented as

Table 10.4 Typical values of coefficients in the eutrophication model

| parameter	value		units
k_N half saturation	10-20	- a	µg N/l
	50-200	- c	µg NO_3/l
	10 (1-20)	- b	µg N/l
k_P half saturation	1-5	- a	µg P/l
	20-70	- c	µg P/l
	10	- b	µg P/l
a_P stoichoimetric ratio	0.012-0.015	- c	mg P/mg A
a_N stoichoimetric ratio	0.08-0.09	- c	mg NO_3/mg A
µ maximum algae growth rate	1.5 (1.0-2.0)	- b	1/day
e death algae rate	0.2-8	- c	1/day
	0.1 (0.05-0.025)	- b	1/day

a - Thomann and Mueller (1987)

b - Schnoor (1996)

c - Bowie et al. (1985)

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NO$_3$–N) as the main forms of dissolved nitrogen in water. Furthermore, nitrogen is present in algae, as well as in detritus, resulting from algae mortality, and in suspended (non-detritus) organic nitrogen. Nitrogen can also be present in different forms in the bottom sediment.

Two important reactions in the nitrogen nutrient cycle are nitrification and denitrification, which affect the flux of ammonium and nitrate in the water column. Nitrification is the conversion of ammonium to nitrite and finally nitrate, requiring the presence of oxygen

$$NH_4{}^+ + 2O_2 \rightarrow NO_3{}^- + H_2O + 2H^+ \quad (10.34)$$
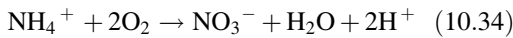
Denitrification is the process occurring during the breakdown (oxidation) of organic matter by which nitrate is transformed to nitrogen gas, which is then usually lost from the water system. Denitrification occurs in anaerobic systems

$$NO_3{}^- \rightarrow N_2 \quad\quad (10.35)$$

The phosphorus cycle is simpler than the nitrogen cycle because there are fewer forms in which phosphorus can be present. There is only one form of dissolved phosphorus, orthophosphorus (also called orthophosphate, PO$_4$–P). Similar to nitrogen, phosphorus also exists in algae, in detritus, and other organic material as well as in the bottom sediment. Unlike nitrogen, there can also be inorganic phosphorus in the particulate phase.

10.4.9 Toxic Chemicals

Toxic chemicals, also referred to as "micropollutants," are substances that at low concentrations can impair the reproduction and growth of organisms including fish and human beings. These substances include heavy metals, many synthetic organic compounds (organic micropollutants), and radioactive substances.

10.4.9.1 Adsorbed and Dissolved Pollutants

An important characteristic of many of these substances is their affinity with the surface areas of suspended or bottom sediments. Many chemicals preferentially sorb onto particulate matter rather than remaining dissolved in water. To model the transport and fate of these substances, the adsorption–desorption process, estimations of the suspended sediment concentration, resuspension from the bottom, and settling are required.

Figure 10.14 depicts the adsorption–desorption and first-order decay processes for toxic chemicals and their interaction in water and sediment. This applies to the water and sediment

Fig. 10.14 Schematic of the adsorption/desorption and decay processes of various toxic chemicals in water bodies and bottom sediments
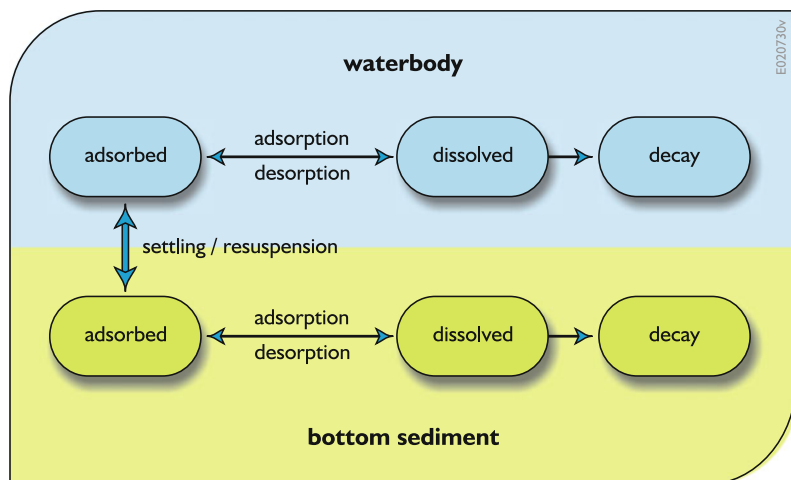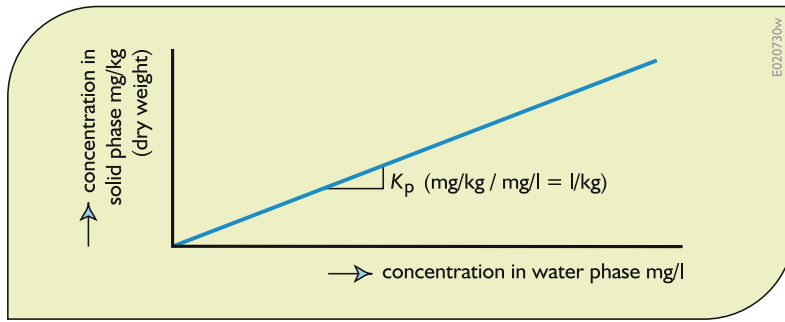
Fig. 10.15 Defining the partition coefficient K_p (liters/kg) as the slope of the fixed ratio between concentrations of a constituent in the water and sediment phases of either a water body or bottom sediments. Different constituents have different partition coefficients, when they apply

phases in both the water body and in the bottom sediments.

The adsorption–desorption model assumes (conveniently but not always precisely) that an equilibrium exists between the dissolved (in water) and absorbed (on sediments) concentrations of a toxic constituent such as a heavy metal or organic contaminant. This equilibrium follows a linear relationship. The slope of that linear relation is the partition coefficient K_p (l/kg). This is shown in Fig. 10.15.

Each partition coefficient K_p (liters per kilogram or l/kg) is defined as the ratio of the particulate concentration C_p' of a micropollutant (mg/kg C) divided by the dissolved concentration C_d' of a micropollutant (mg/l water).

$$K_p = C_p'/C_d' \qquad (10.36)$$

Representative values of partition coefficients K_p are in Table 10.5.

The presence of a micropollutant in water is described by the total concentration (sum of dissolved and particulate concentrations), the total particulate concentration, and the total dissolved concentration for each water and sediment compartment. The particulate and dissolved concentrations are derived from the total concentration and the respective fractions.

Because the fate of most micropollutants is largely determined by adsorption to particulate matter, suspended inorganic and organic matter (including phytoplankton) have to be included in

the model in most cases. It may be necessary to include dissolved organic matter as well.

The adsorbed fractions in the water column are subject to settling. The fractions in the sediment are subject to resuspension. The adsorbed fractions in the sediment can also be removed from the modeled part of the water system by burial.

The rates of settling and resuspension of micropollutants are proportional to the rates for particulate matter. An additional process called bioturbation leads to redistribution of the micropollutant among sediment layers. Bioturbation is caused by physical activity of organisms, and affects both the particulate and dissolved phases but with different rates. Bioturbation is taken into account by means of dispersion coefficients.

For modeling purposes, it is important to know how much of a toxic chemical is present as a dissolved constituent as opposed to adsorbed. Assuming partition coefficients apply to a particular toxic constituent, the concentration, C_w, of that constituent in the water body is divided into a dissolved fraction (f_{dw}) and an absorbed fraction (f_{aw}).

$$C_w = (f_{dw} + f_{aw})C_w \qquad (10.37)$$

In turn, the adsorbed fraction of a micropollutant is composed of the fractions adsorbed to inorganic particulate matter, f_{im}, dead particulate organic matter, f_{poc}, and algae, f_{alg}. The total

Table 10.5 Typical values of partition coefficients in toxic chemical model from Thomann and Mueller (1987)

K_p parameter	value	units
arsenic	10^4	l/kg
heavy metals (Cd,Cu,Cr,Zn)	10^4-10^6	l/kg
benzo(a)pyrene	10^4-10^5	l/kg
lead	10^5-10^6	l/kg
PCB	10^5-10^6	l/kg
plutonium-239	10^4-10^5	l/kg
methoxychlor	10^4	l/kg
napthalene	10^3	l/kg

micropollutant concentration, C_w (mg/m^3) is the sum of all these fractions.

$$C_w = (f_{dw} + f_{im}, + f_{poc} + f_{alg}) C_w \quad (10.38)$$

Considering the simple division into dissolved and adsorbed fractions (f_{dw} and f_{aw}), these fractions depend on the partition coefficient, K_p, and on the suspended sediment concentration, SS (mg/l). The proportions of the total constituent concentration in the water body, C_w, dissolved in the water, DC$_w$ (mg/l), and adsorbed to the suspended sediments, AC$_w$ (mg/l) are defined as

$$DC_w = f_{dw} C_w \quad (10.39)$$

$$AC_w = f_{aw} C_w, \quad (10.40)$$

where the fractions

$$f_{dw} = 1/(1 + K_p SS) \quad (10.41)$$

$$f_{aw} = 1 - f_{dw} = K_p SS/(1 + K_p SS) \quad (10.42)$$

Similarly in the bottom sediments, the dissolved concentration DC$_s$ (mg/l) and adsorbed concentration AC$_s$ (mg/l) are fractions, f_{ds} and f_{as}, of the total concentration C_s (mg/l).

$$DC_s = f_{ds} C_s \quad (10.43)$$

$$AC_s = f_{as} C_s \quad (10.44)$$

These fractions are dependent on the sediment porosity, ϕ, and density, ρ_s (kg/l).

$$f_{ds} = 1/[\phi + \rho_s(1 - \phi)K_p] \quad (10.45)$$

$$f_{as} = 1 - f_{ds}$$
$$= ([\phi + \rho_s(1 - \phi)K_p] - 1)/[\phi + \rho_s(1 - \phi)K_p] \quad (10.46)$$

First-order decay occurs in the water and sediment phases only in the dissolved fraction with decay rate constants k_w and k_s (1/day), respectively. Thus

$$dC_w/dt = -k_w \theta_w^{(T-20)} f_{dw} C_w - f_{aw} C_w S + f_{as} C_s r \quad (10.47)$$

$$dC_s/dt = -k_s \theta_s^{(T-20)} f_{ds} C_s + f_{aw} C_w S - f_{as} C_s r \quad (10.48)$$

In the above two equations the parameter *s* represents the mass of settling sediments (mg/day), *r* the mass of resuspension sediments (mg/day), and θ the temperature correction coefficient of the constituent at temperature *T* = 20 °C. If data are not available to distinguish between the values of the decay rate constants *k* in water and on sediments, they may be assumed to be the same. Similarly for the values of the temperature correction coefficients θ. Suspended solids settling and resuspension can be determined at each day from a sediment model.

10.4.9.2   Heavy Metals
The behavior of heavy metals in the environment depends on their inherent chemical properties. Heavy metals can be divided into different categories depending on their dissolved form and redox (reduction oxidation) status. Some metals, including copper, cadmium lead, mercury, nickel, tin and zinc form free or complexed cations when dissolved in water (e.g., Cu^{2+} or $CuCl^-$). The soluble complexes are formed with negatively charged ions such as chlorine, oxygen, or dissolved organic compounds. These heavy metals also tend to form poorly soluble sulfides under chemically reducing conditions. These sulfides generally settle in bottom sediments and are essentially ecologically unavailable. Other metals such as arsenic and vanadium are present as anions in dissolved form. The differences between groups of metals have important consequences for the partitioning of the metals among several dissolved and particulate phases.

Metals are non-decaying substances. The fate of heavy metals in a water system is determined primarily by partitioning to water and particulate matter (including phytoplankton), and by transport. The partitioning divides the total amount of a pollutant into a 'dissolved' fraction and several 'adsorbed' fractions (as described in Eqs. 10.39–10.42. The fractions of a metal that are adsorbed onto particulate matter are influenced by all the

processes that affect particulate matter, such as settling and resuspension.

Partitioning is described in general by sorption to particulates, precipitation in minerals, and complexation in solution. Complexation with inorganic and organic ligands can be considered explicitly in connection with the other processes. Sorption can be modeled as an equilibrium process (equilibrium partitioning) or as the resultant of slow adsorption and desorption reactions (kinetic formulations). In the latter case, partitioning is assumed to proceed at a finite rate proportional to the difference between the actual state and the equilibrium state.

To describe the fate of certain heavy metals in reducing environments, such as sediment layers, the formation of metal sulfhides or hydroxides can be modeled. The soluble metal concentration is determined on the basis of the relevant solubility product. The excess metal is stored in a precipitated metal fraction.

Sorption and precipitation affect the dissolved metal concentration in different ways. Both the adsorbed and dissolved fractions increase at increasing total concentration as long as no solubility product is exceeded. When it is, precipitation occurs.

10.4.9.3   Organic Mircropollutants
Organic micropollutants generally are biocides (such as pesticides or herbicides), solvents or combustion products and include substances such as hexachlorohexane, hexachlorobenzene, PCB's or polychlorobiphenyls, benzo-a-pyrene and fluoranthene (PAH's or polycyclic aromatic hydrocarbons), diuron and linuron, atrazine and simazine, mevinfos and dichlorvos, and dinoseb.

The short-term fate of organic micropollutants in a water system is determined primarily by partitioning to water and organic particulate matter (including phytoplankton), and by transport. Additional processes such as volatilization and degradation influence organic micropollutant concentrations (this is in contrast to heavy metals which do not decay). Many

toxic organic compounds have decay (or "daughter") products that are equally, if not more, toxic than the original compound. The rates of these processes are concentration and temperature dependent.

Organic micropollutants are generally poorly soluble in water and prefer to absorb to particulate matter in the water, especially particulate organic matter and algae. Therefore, the fractions of a micropollutant adsorbed to inorganic matter, f_{im}, dead particulate organic matter, f_{poc}, the dissolved fraction of a micropollutant, f_d, and algae, f_{alg}, add up to the total micropollutant concentration, C (mg/m^3).

$$C = (f_d + f_{im} + f_{poc} + f_{alg})C \qquad (10.49)$$

The fractions are functions of the partition coefficients K_p [for algae (m^3/g C), for inorganic matter (m^3 g DW^{-1}) and for dead particulate organic matter (m^3/g C)], the individual concentrations C [for algae biomass (g C/m^3), for dissolved (in water) inorganic matter (g/m^3) and for dead particulate organic matter (g C/m^3)], and the porosity ϕ (m^3 water/m^3 bulk). In surface water the value for porosity is 1.

$$f_d = \phi/[\phi + K_{palg}C_{alg} + K_{pim}C_{im} + K_{ppoc}C_{poc}] \qquad (10.50)$$

$$\begin{aligned} f_{im} = &(1 - f_d)K_{pim}C_{im}/[K_{palg}C_{alg} \\ &+ K_{pim}C_{im} + K_{ppoc}C_{poc}] \end{aligned} \qquad (10.51)$$

$$\begin{aligned} f_{poc} = &(1 - f_d)K_{ppoc}C_{poc}/[K_{palg}C_{alg} \\ &+ K_{pim}C_{im} + K_{ppoc}C_{poc}] \end{aligned} \qquad (10.52)$$

$$f_{alg} = (1 - f_d - f_{im} - f_{poc}) \qquad (10.53)$$

In terms of bulk measures, each partition coefficient K_p (see Eq. 10.36) also equals the porosity ϕ times the bulk particulate concentration C_p (mg/m^3 bulk) divided by the product of the dissolved (mg/l bulk) and particulate (mg/m^3 bulk) bulk concentrations, C_d C_s, all times 10^6 mg/kg.

$$K_p = 10^6 \phi\, C_p/(C_d\, C_s) \qquad (10.54)$$

Partitioning can be simulated based on the above equilibrium approach or according to slow sorption kinetics. For the latter, the rate, dC_p/dt, of adsorption or desorption (mg/m^3/day) depends on a first-order kinetic constant k_{sorp} (1/day) for adsorption and desorption times the difference between equilibrium particulate concentration C_{pe} of a micropollutant (mg/m^3 bulk) and the actual particulate concentration C_p (mg/m^3 bulk) of a micropollutant.

$$dC_p/dt = k_{sorp}(C_{pe} - C_p) \qquad (10.55)$$

The kinetic constant for sorption is not temperature dependent. All other kinetic constants for micropollutants are temperature dependent.

Mass balance equations are similar for all micropollutants except for the loss processes.

Metals are conservative substances. They can be transformed into various species either through complexation, adsorption, or precipitation. Organic micropollutants are lost by volatilization, biodegradation, photolysis, hydrolysis, and overall degradation. Most of these processes are usually modeled as first-order processes, with associated rate constants.

The volatization rate, dC_d/dt (mg/m^3/day) of dissolved micropollutant concentrations, C_d (mg/m^3 water) in water depends on an overall transfer coefficient, k_{vol} (m/day), for volatilization and the depth of the water column, H (m).

$$dC_d/dt = -k_{vol} C_d/H \qquad (10.56)$$

The numerator ($k_{vol}\, C_d$) is the volatilization mass flux (mg/m^2/day).

This equation is only valid when the atmospheric concentration is negligibly small, which is the normal situation.

All other loss rates such as biodegradation, photolysis, hydrolysis, or overall degradation (mg/m^3/day) are usually modeled as

$$\mathrm{d}C/\mathrm{d}t = -kC, \qquad (10.57)$$

where C is the total concentration of a micropollutant (mg/m^3), and k is a (pseudo) temperature dependent first-order kinetic rate constant for biodegradation, photolysis, hydrolysis or overall degradation (1/day). This is similar to Eq. 10.22.

10.4.9.4   Radioactive Substances

The fate of most radionuclides such as isotopes of iodine (^{131}I) and cesium (^{137}Cs) in water is determined primarily by partitioning to water and particulate matter (including phytoplankton), by transport, and by decay. Cesium (Ce$^+$) adsorbs to particulate inorganic matter, to dead particulate organic material, and to phytoplankton, both reversibly and irreversibly. The irreversible fraction increases over time as the reversible fraction gradually transforms into the irreversible fraction. Radioactive decay proceeds equally for all fractions. Precipitation of cesium does not occur at low concentrations in natural water systems.

Iodine is only present in soluble form as an anion (IO$_3^-$) and does not adsorb to particulate matter. Consequently, the transport iodine is only subject to advection and dispersion.

Concentrations of radionuclides, C_R (mg/m^3) are essentially conservative in a chemical sense, but they decay by falling apart in other nuclides and various types of radiation. The radioactive decay rate (mg/m^3/day) is usually modeled as a first-order process involving a kinetic radioactive decay constant, k_{dec} (1/day). This kinetic constant is derived from the half-life time of the radionuclide. The initial concentration may be expressed as radioactivity, in order to simulate the activity instead of the concentration. These state variables can be converted into each other using

$$\mathrm{Ac} = 10^{-3}\, N_A\, k_{dec}\, C_R/[86400\ \mathrm{Mw}], \quad (10.58)$$

where Ac = activity of the radionuclide (Bq/m^3/s)
N_A = Avogadro's number (6.02 × 10^{23} mol)
Mw = molecular weight of the radionuclide (g/mole)

10.4.10   Sediments

Sediments in water play an important role in the transport and fate of chemical pollutants in water. Natural waters can contain a mixture of particles ranging from gravel (2–20 mm) or sand (0.07–2 mm) down to very small particles classified as silt or clay (smaller than 0.07 mm). The very fine fractions can be carried as colloidal suspension for which electrochemical forces play a predominant role. Considering the large adsorbing capacities, the fine fraction is characterized as cohesive sediment. Cohesive sediment can include silt and clay particles as well as particulate organic matter such as detritus and other forms of organic carbon, diatoms and other algae. Since flocculation and adsorbing capacities are of minor importance for larger particles, they are classified as non-cohesive sediment.

The behavior of this fine-grained suspended matter impacts water quality. First, turbidity and its effect on the underwater light is an important environmental condition for algae growth. The presence of suspended sediment increases the attenuation of light in the water column that leads to an inhibition of photosynthetic activity and hence, a reduction in primary production. Second, the fate of contaminants in waters is closely related to suspended solids due to their large adsorbing capacities. Like dissolved matter, sediment is transported by advection and by turbulent motion. In addition, the fate of the suspended cohesive sediment is determined by settling and deposition, as well as by bed processes of consolidation, bioturbation, and resuspension.

10.4.11   Processes in Lakes and Reservoirs

The water quality modeling principles discussed above are applicable to different types of water systems such as streams, rivers, lakes, estuaries, and even coastal or ocean waters. This section presents some of the unique aspects of water quality modeling in lakes. The physical character

and water quality of rivers draining into lakes and reservoirs are governed in part by the velocity and the volume of river water. The characteristics of the river water typically undergo significant changes as the water enters the lake or reservoir, primarily because its velocity reduces. Portions of the sediment and other material carried in the faster flowing water settle out in the basin.

The structure of the biological communities also changes from organisms suited to living in flowing waters to those that thrive in standing or pooled waters. Greater opportunities for the growth of algae (phytoplankton) and the development of eutrophication are present.

Reservoirs typically receive larger inputs of water, as well as soil and other materials carried in rivers than lakes. As a result, reservoirs may receive larger pollutant loads than lakes. However, because of greater water inflows flushing rates are more rapid than in lakes. Thus, although reservoirs may receive greater pollutant loads than lakes, they have the potential to flush out the pollutants more rapidly than do lakes. Reservoirs may therefore exhibit fewer or less severe negative water quality or biological impacts than lakes for the same pollutant load.

The water quality of lakes and reservoirs is defined by

- water clarity or transparency (greater water clarity usually indicates better water quality),
- concentration of nutrients (lower concentrations indicate better water quality),
- quantity of algae (lower levels indicate better water quality),
- oxygen concentration (higher concentrations are preferred for fisheries),
- concentration of dissolved minerals (lower values indicate better water quality), and
- acidity (a neutral pH of 7 is preferred).

Many lakes and reservoirs receive discharges of waste chemical compounds from industry, some with toxic or deleterious effects on humans and/or other water-dependent organisms and products. Some of these pollutants can kill aquatic organisms and damage irrigated crops. Inadequate water purification resulting in the discharge of bacteria, viruses, and other organisms into natural waters can be a primary cause of waterborne disease. Although dangerous to human health worldwide, such problems are particularly severe in developing countries.

There can be major differences between deep and shallow lakes or reservoirs. Deep lakes, particularly in nontropical regions, usually have poorer water quality in lower layers, due to stratification (see Sect. 4.11.3). Shallow lakes do not exhibit this depth differentiation in quality. Their more shallow, shoreline areas have relatively poorer water quality because those sites are where pollutants are discharged and have a greater potential for disturbance of bottom muds, etc. The water quality of a natural lake usually improves as one moves from the shoreline to the deeper central part.

In contrast, the deepest end of a reservoir is usually immediately upstream of the dam. Water quality usually improves along the length of a reservoir, from the shallow inflow end to the deeper, "lake-like" end near the dam, as shown in Fig. 10.16.

Reservoirs, particularly the deeper ones, are also distinguished from lakes by the presence of a longitudinal gradient in physical, chemical, and biological water quality characteristics from the upstream river end to the downstream dam end. Because of this, reservoirs have been characterized as comprising three major zones: an upstream riverine zone, a downstream lake-like zone at the dam end, and a transitional zone separating these two zones (Fig. 10.16). The relative size and volume of the three zones can vary greatly in a given reservoir.

10.4.11.1 Water Quality Changes and Impacts

Dams can produce changes in the downstream river channels below them. These are quite unlike downstream changes from lakes. Because reservoirs act as sediment and nutrient traps, the water at the downstream dam end of a reservoir is typically of higher quality than water entering the reservoir.
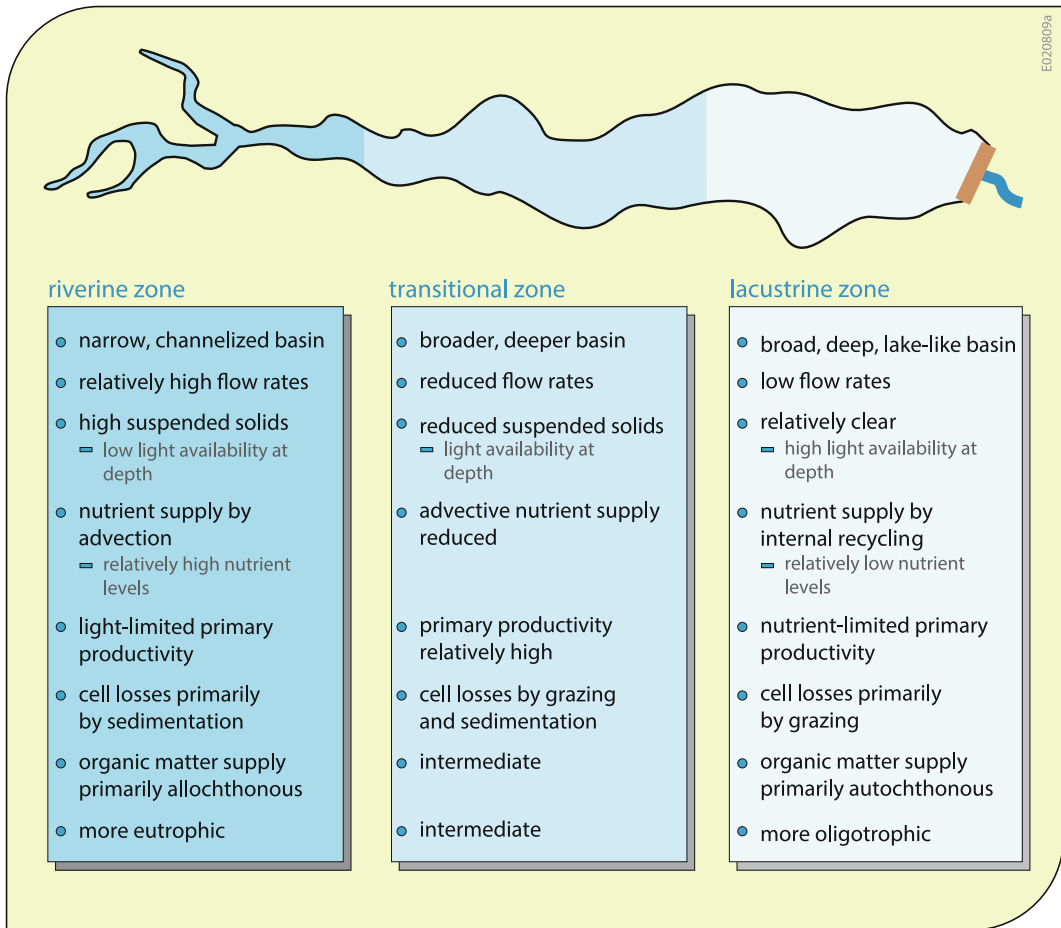
Fig. 10.16 Longitudinal zonation of water quality and other variables in reservoirs

This higher quality water subsequently flows into the downstream river channel below the dam. This is sometimes a problem in that the smaller the quantity of sediments and other materials transported in the discharged water, the greater the quantity that can be picked up and transported as it moves downstream. Because it contains less sediment, the discharged "hungry" water can scour and erode the streambed and banks, picking up new sediment as it continues downstream. This scouring effect can negatively impact the flora, fauna, and biological community structure in the downstream river channel. The removal of sediments from a river by reservoirs also has important biological effects, particularly on floodplains.

Many reservoirs, especially those used for drinking water supplies, have water release or discharge structures located at different vertical levels in their dams (Fig. 10.17). This allows for the withdrawal or discharge of water from different layers within the reservoir, so-called "selective withdrawal." Depending on the quality of the water discharged, selective withdrawal can significantly affect water quality within the reservoir itself, as well as the chemical composition and temperature of the downstream river. Being able to regulate both quantities and qualities of the downstream hydrological regimes can impact both flora and fauna and possibly even the geomorphology of the stream or river.

Fig. 10.17 A multiple outlet reservoir can be better used to regulate the temperature and water quality downstream and possibly the sediment in the reservoir
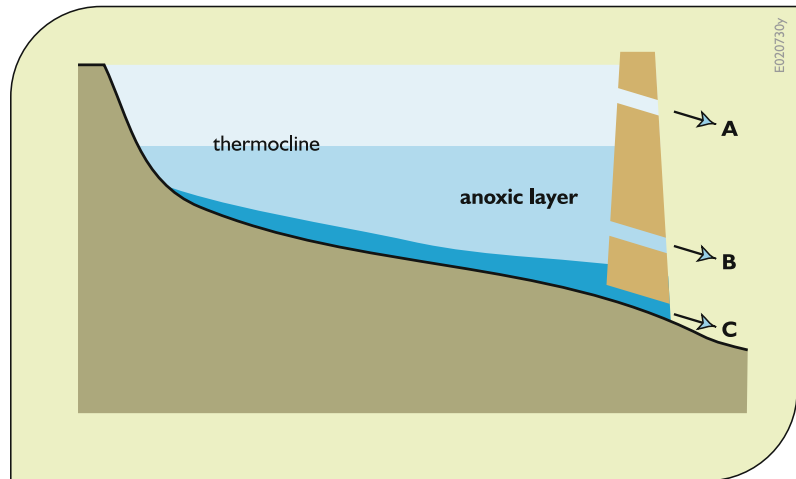
Constructing a reservoir may have significant social and economic implications, including the potential for stimulating urban and agricultural development adjacent to, and below, the reservoir. These activities can have both positive and negative impacts on downstream water quality, depending on the nature and size of development.

Agricultural and urban runoff is often the leading source of pollution in lakes. Healthy lake ecosystems contain nutrients in small quantities from natural sources, but extra inputs of nutrients (primarily nitrogen and phosphorus) adversely impact lake ecosystems. When temperature and light conditions are favorable, excessive nutrients stimulate population explosions of undesirable algae and aquatic weeds. After they die the algae sink to the lake bottom, where bacteria consume DO as they decompose the algae. Fish kills and foul odors may result if dissolved is depleted.

Heavy metals are another major cause of lake quality impairment. Heavy metals accumulate in fish tissue. Since it is difficult to measure heavy metals (e.g., mercury) in ambient water and since they accumulate in fish tissue, fish samples are commonly used to monitor heavy metal contamination. Common sources of heavy metals are "smoke-stack" industries, including power plants, whose airborne discharges of mercury eventually end up in our water supplies.

In addition to nutrients and metals siltation, enrichment by organic wastes that deplete

oxygen and noxious aquatic plants impact lakes and reservoirs. Often, several pollutants and processes impact a single lake. For example, a process such as removal of shoreline vegetation may accelerate erosion of sediment and nutrients into a lake. Extreme acidity (low pH) resulting from acid rain can eliminate fish in isolated lakes. Urban runoff and storm sewers, municipal sewage treatment plants, and hydrologic modifications are also sources of lake pollutants.

10.4.11.2 Lake Quality Models

The prediction of water quality in surface water impoundments is based on mass balance relationships similar to those used to predict water quality concentrations in streams and estuaries. There are also significant problems in predicting the water quality of lakes or reservoirs compared to those of river and estuarine systems. One is the increased importance of wind-induced mixing processes and thermal stratification. Another for reservoirs is the impact of various reservoir-operating policies.

Perhaps the simplest way to begin modeling lakes is to consider shallow well-mixed constant-volume lakes subject to a constant pollutant loading. The flux of any constituent concentration, C, in the lake equals the mass input of the constituent less the mass output less losses due to decay or sedimentation, if any, all divided by the lake volume V (m^3). Given a constant constituent input rate W_C (g/day) of a constituent

having a net decay and sedimentation rate constant k_C (1/day) into a lake having a volume V (m³) and inflow and outflow rate of Q (m³/day), then the rate of change in the concentration C (g/m³/day) is

$$dC/dt = (1/V)(W_C - QC - k_C CV) \quad (10.59)$$

Integrating this equation yields a predictive expression of the concentration $C(t)$ of the constituent at the end of any time period t based in part on what the concentration, $C(t-1)$, was at the end of that previous time period, $t-1$. For a period duration of Δt days,

$$C(t) = [W_C/(Q + k_C V)][1 - \exp\{-\Delta t((Q/V) + k_C)\}]$$
$$+ C(t-1)\exp\{-\Delta t((Q/V) + k_C)\}$$
$$(10.60)$$

The equilibrium concentration, C_e, can be obtained by setting the rate, dC/dt, in Eq. 10.59 to 0. The net result is

$$C_e = W_C/(Q + k_C V) \quad (10.61)$$

The time, t_α, since the introduction of a mass input W_C that is required to reach a given fraction α of the equilibrium concentration (i.e., $C(t)/C_e = \alpha$) is

$$t_\alpha = -V[\ln(1-\alpha)]/(Q + K_C V) \quad (10.62)$$

Similar equations can be developed to estimate the concentrations and times associated with a decrease in a pollutant concentration. For the perfectly mixed lake having an initial constituent concentration $C(0)$, say after an accidental spill, and no further additions, the change in concentration with respect to time is

$$dC/dt = -C(Q + k_C V)/V \quad (10.63)$$

Integrating this equation, the concentration $C(t)$ is

$$C(t) = C(0)\exp\{-t((Q/V) + K_C) \quad (10.64)$$

In this case one can solve for the time t_α required for the constituent to reach a fraction

$(1 - \alpha)$ of the initial concentration $C(0)$ (i.e., $C(t)/C_e = 1 - \alpha$). The result is Eq. 10.62.

Equation 10.60 can be used to form an optimization model for determining the wasteload inputs to this well-mixed lake that meet water quality standards. Assuming that the total of all natural wasteloads $W_C(t)$, inflows and outflows $Q(t)$, and the maximum allowable constituent concentrations in the lake, $C(t)^{max}$, may vary among different within-year periods t, the minimum fraction, X, of total waste removal required can be found by solving the following linear optimization model:

$$\text{Minimize } X \quad (10.65)$$

The following mass balance and constituent concentration constraints apply for each period t :

$$C(t) = [W_C(t)(1 - X)/(Q(t) + k_C V)]$$
$$[1 - \exp\{-\Delta t((Q(t)/V) + k_C)\}]$$
$$+ C(t-1)\exp\{-\Delta t((Q(t)/V) + k_C)\}$$
$$(10.66)$$

$$C(t) \leq C(t)^{max} \quad (10.67)$$

If each period t is a within-year period, and if the waste loadings and flows in each year are the same, then no initial concentrations need be assumed and a steady-state solution can be found. This solution will indicate, for the loadings $W_C(t)$, the fraction X of waste removal that meet the quality standards, $C(t)^{max}$, throughout the year.

10.4.11.3   Stratified Impoundments

Many deep reservoirs and lakes become stratified during particular times of the year. Vertical temperature gradients arise that imply vertical density gradients. The depth-dependent density gradients effectively prevent complete vertical mixing. Particularly in the summer season, two zones may form, an upper volume of warm water called the epilimnion and a lower colder volume called the hypolimnion. The transition zone or boundary between the two zones is called the thermocline (Fig. 10.17).

Because of stratification many models divide the depth of water into layers, each of which is

assumed to be fully mixed. To illustrate this approach without getting into too much detail, consider a simple two-layer lake in the summer that becomes a one-layer lake in the winter. This is illustrated in Fig. 10.18.

Discharges of a mass W_C of constituent C in a flow $Q^{in}(t)$ into the lake in period t have concentrations of $W_C/Q^{in}(t)$. The concentration in the outflows from the summer epilimnion is $C_e(t)$ for each period t in the summer season. The concentration of the outflows from the winter lake as a whole is $C(t)$ for each period t in the winter season. The summer time rates of change in the epilimnion constituent concentrations $C_e(t)$ and hypolimnion concentrations $C_h(t)$ depend on the

mass inflow, $W_C(t)$, and outflow, $C_e(t)Q^{out}(t)$, the net vertical transfer across the thermocline, (v/D_T) $[C_h(t)V_h(t) - C_e(t)V_e(t)]$, the settling on sediment interface, $sH_h(t)\,C_h(t)$, and the decay, $kC_e(t)$:

$$dC_e(t)/dt = (1/V_e(t))\{(W_C(t) - C_e(t)Q^{out}(t)) \\ + (v/D_T)[C_h(t)V_h(t) - C_e(t)V_e(t)]\} \\ - kC_e(t)$$

(10.68)

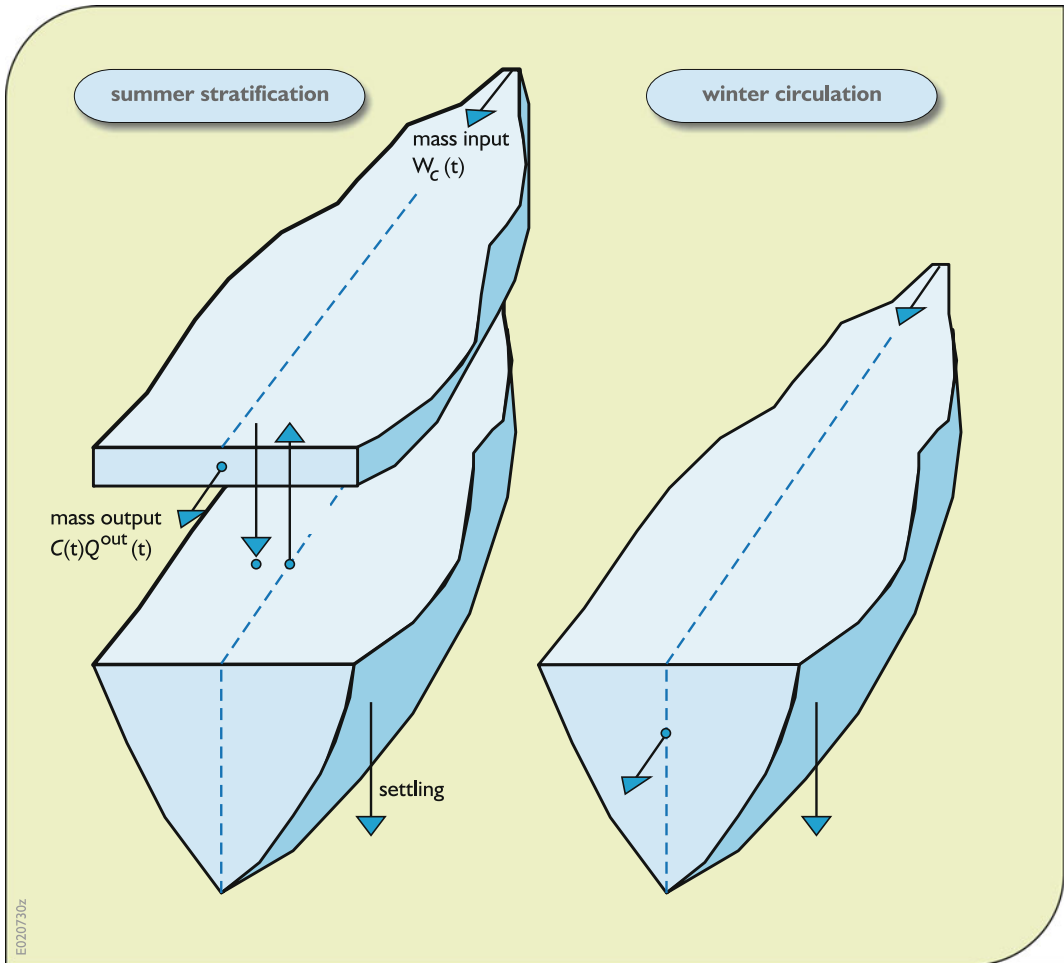$$dC_h(t)/dt = -kC_h(t) \\ - (v/D_T)[C_h(t) - C_e(t)V_e(t)/V_h(t)] \\ - sH_h(t)C_h(t)$$

(10.69)

Fig. 10.18 Lake stratification during summer and complete mixing during winter season

In the above two equations, V_e and V_h (m³) are the time-dependent volumes of the epilimnion and hypolimnion, respectively, k (1/day) is the temperature corrected decay rate constant, v (m/day) is the net vertical exchange velocity that includes effects of vertical dispersion, erosion of hypolimnion, and other processes that transfer materials across the thermocline of thickness D_T (m), s is the settling rate velocity (m/day) and $H_h(t)$ is the average depth of the hypolimnion (m).

In the winter season the lake is assumed to be fully mixed. Thus for all periods t in the winter season the initial concentration of a constituent is

$$C(t) = C_e(t)V_e(t) + C_h(t)V_h(t)/[V_e + V_h] \tag{10.70}$$

$$\begin{aligned} dC(t)/dt = (1/V(t))\{(W_C(t) - C(t)Q^{out}(t)) \\ - \text{decay } kC_e(t) - sH(t)C(t) \end{aligned} \tag{10.71}$$

At the beginning of the summer season, each epilimnion and hypolimnion concentration will be the same.

$$C_e(t) = C(t) \tag{10.72}$$

$$C_h(t) = C(t) \tag{10.73}$$

10.5   Simulation Methods

Most who will be using water quality models will be using simulation models that are commonly available from governmental agencies (e.g., US EPA), universities, or private consulting and research institutions such as the Danish Hydraulics Institute, Wallilngford software or Deltares (Ambrose et al. 1996; Brown and Barnwell 1987; Cerco and Cole 1995; DeMarchi et al. 1999; Ivanov et al. 1996; Reichert 1994; USEPA 2001; WL|Delft Hydraulics 2003).

These simulation models are typically based on numerical methods incorporating a combination of plug flow and continuously stirred reactor approaches to pollutant transport. Users must divide streams, rivers, and lakes and reservoirs into a series of well-mixed segments or volume elements. A hydrologic or hydrodynamic model calculates the flow of water between all the segments and volume elements. In each simulation time step plug flow enters these segments or volume elements from upstream segments or elements. Flow also exits these segments or volume elements to downstream segments or elements. During this time the constituents can decay or grow, as appropriate, depending the conditions in those segments or volume elements. At the end of each time step the volumes and their constituents within each segment or element are fully mixed. The length of each segment or the volume in each element reflects the extent of dispersion in the system.

10.5.1   Numerical Accuracy

As presented in Sect. 10.4, equations describing water quality processes typically include time rate of change terms such as dC/dt. While it is possible to solve analytically some of these differential equations, most water quality simulation models use numerical methods. The purpose of this section is not to explain how this can be done, but rather to point to some of the restrictions placed on the modeler because of these numerical methods.

Consider first the relationship between the stream, river, or lake segments and the duration of time steps, Δt. The basic first-order decay flux, dC/dt (g/m³/day), for a constituent concentration, C, that is dependent on a rate constant, k (1/day), is

$$dC/dt = -kC \tag{10.74}$$

The finite difference approximation of this equation can be written

$$C(t + \Delta t) - C(t) = -C(t)k\Delta t \tag{10.75}$$

or

$$C(t + \Delta t) = C(t)(1 - k\Delta t) \qquad (10.76)$$

This equation can be used to illustrate the restriction placed on the term $k\Delta t$. That term cannot exceed a value of 1 or else $C(t + \Delta t)$ will be negative.

Figure 10.19 is a plot of various values of $C(t + \Delta t)/C(t)$ versus $k\Delta t$. This plot is compared with the analytical solution resulting from the integration of Eq. 10.110, namely

$$C(t + \Delta t) = C(t)\exp\{-k\Delta t\} \qquad (10.77)$$

Reducing the value of Δt will increase the accuracy of the numerical solution. Any value of Δt can be divided by a positive integer n to become $1/n$th of its original value. In this case the predicted concentration $C(t + \Delta t)$ will equal

$$C(t + \Delta t) = C(t)(1 - k\Delta t/n)^n \qquad (10.78)$$

For example if $k\Delta t = 1$, and $n = 2$, the final concentration ratio will equal

$$C(t + \Delta t)/C(t) = (1 - 1/2)^2 = 0.25 \quad (10.79)$$

Compare this 0.25–0.37, the exact solution, and to 0.0, the approximate solution when n is 1. Having $n = 2$ brings a big improvement. If $n = 3$, the concentration ratio will be 0.30, an even greater improvement compared to 0. However no matter what value of n is selected, the predicted concentration will always less than the actual value based on Eq. 10.77, and hence the

error is cumulative. Whenever $\Delta t > n/k$ the predicted concentrations will alternate between positive and negative values, either diverging, converging or just repeating the cycle, depending on how much Δt exceeds n/k. In any event, the predicted concentrations are not very useful.

Letting $m = -n/k\Delta t$, Eq. 10.78 can be written as

$$C(t + \Delta t) = C(t)(1 + 1/m)^{m(-k\Delta t)} \qquad (10.80)$$

As n approaches infinity so does the variable m, and hence the expression $(1 + 1/m)^m$ becomes the natural logarithm base $e = 2.718282$. Thus as n approaches infinity, Eq. 10.80 becomes Eq. 10.77, the exact solution to Eq. 10.74.

10.5.2 Traditional Approach

Most water quality simulation models simulate quality over a period of time. Time is divided into discrete intervals and the water and wastewater flows are assumed constant within each of those time period intervals. Each water body is divided into segments or volume elements and these "computational cells" are considered to be in steady-state conditions within each simulation time period. Advection or plug flow (i.e., no mixing or dispersion) is assumed during each time period. At the end of each period mixing occurs within each segment or volume element to obtain the concentrations in the segment or volume element at the beginning

Fig. 10.19 Plot of numerical approximation (*red line*) based on Eq. 10.77 compared to the true analytical (*blue line*) value obtained from Eq. 10.76
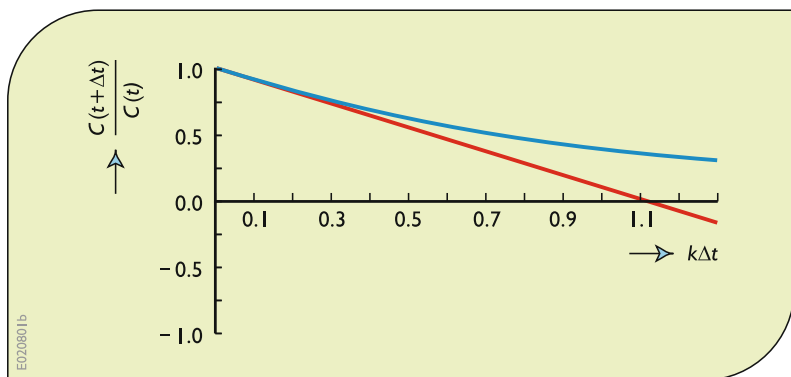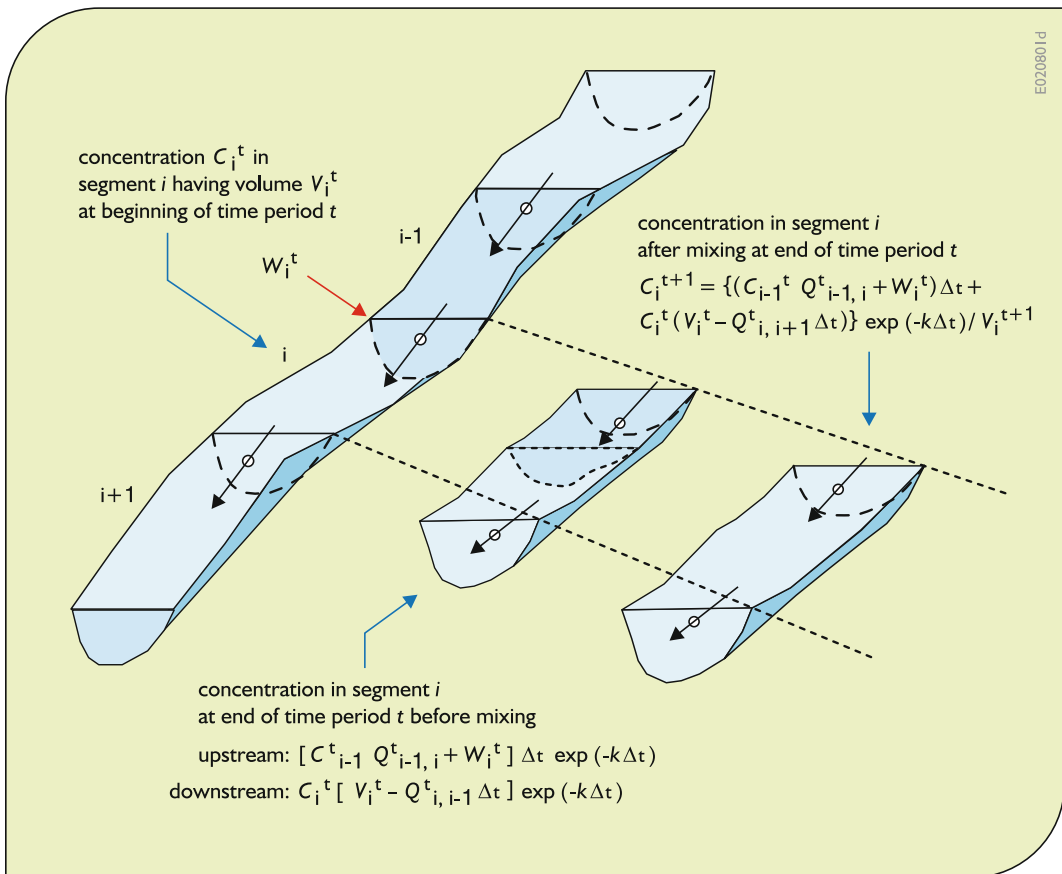
of the next time step. The larger the computational cell the greater is the dispersion.

This method is illustrated in Fig. 10.20. The indices $i − 1$, i and $i + 1$ refer to stream or river reach segments. The indices t and $t + 1$ refer to two successive time periods, respectively. At the beginning of time period t, each segment is completely mixed. During the time interval Δt of period t the water quality model predicts the concentrations assuming plug flow in the direction of flow from segment i toward segment $i + 1$. The time interval Δt is such that the flow from any segment i does not pass through any following segment $i + 1$. Hence at the end of each time period, each segment has some of its original water that was there at the beginning of the period, and its end-of-period concentrations

of constituents, plus some of the immediately upstream segment's water and its end-of-period concentrations of constituents. These two volumes of water and their respective constituent concentrations are then mixed to achieve a constant concentration within the entire segment. This is done for all segments in each time step. Included in this plug flow and then mixing process are the inputs to the reach from point and non-point sources of constituents.

In Fig. 10.20, a mass of waste enters reach i at a rate of W_i^t. The volume in each reach segment is denoted by V and the flows from one segment to the next are denoted by Q. The drawing shown on the left represents a portion of a stream or river divided into well-mixed segments. During a period t waste constituents enter reach segment

concentration C_i^t in segment i having volume V_i^t at beginning of time period t

W_i^t

i-1

concentration in segment i after mixing at end of time period t

$$C_i^{t+1} = \{(C_{i-1}^t\, Q_{i-1,\,i}^t + W_i^t)\Delta t + C_i^t(V_i^t - Q_{i,\,i+1}^t \Delta t)\}\, \exp(-k\Delta t)/\, V_i^{t+1}$$

i

i+1

concentration in segment i at end of time period t before mixing

upstream: $[\, C_{i-1}^t\, Q_{i-1,\,i}^t + W_i^t\,]\, \Delta t\ \exp(-k\Delta t)$

downstream: $C_i^t[\, V_i^t - Q_{i,\,i-1}^t \Delta t\,]\, \exp(-k\Delta t)$

Fig. 10.20 Water quality modeling approach showing a water system schematized into reach segments or 'computational cells'

i from the immediate upstream reach *i* − 1 and from the point waste source. In this illustration, the mass of each of these wastes is assumed to decay during each time period, independent of other wastes in the water. Depending on the types of wastes, the decay, or even growth, processes that take place may be more complex than those assumed in this illustration. At the end of each time period, these altered wastes are mixed together to create an average concentration for the entire reach segment. This illustration applies for each reach segment *i* and for each time period *t*.

The length, Δx_i, of each completely mixed segment or volume element depends on the extent of dispersion. Reducing the length of each reach segment or size of each volume element reduces the dispersion within the entire stream or river. Reducing segment lengths, together with increasing flow velocities, also reduces the allowable duration of each time period *t*. The duration of each simulation time step Δt must be such that flow from any segment or element enters only the adjacent downstream segment or element during that time step. Stated formally, the restriction is

$$\Delta t \leq T_i \qquad (10.81)$$

where T_i is the residence time in reach segment or volume element *i*. For a 1-dimensional stream or river system consisting of a series of segments *i* of length Δx_i, cross-section area A_i and average flow Q_{it}, the restriction is

$$\Delta t \leq \min\{\Delta x_i A_i / Q_{it}; \forall i, t\} \qquad (10.82)$$

If time steps are chosen which violate this condition, then numerical solutions will be in error. The restriction defined by Eq. 10.82 is often termed the "courant condition." It limits the maximum time step value. Since the flows being simulated are not always known, this leads to the selection of very small time steps, especially in water bodies having very little dispersion. While smaller simulation time steps increase the accuracy of the model   they also increase the computational times. Thus, the balance between computational speed and numerical accuracy restricts the model efficiency in the traditional approach to simulating water quality.
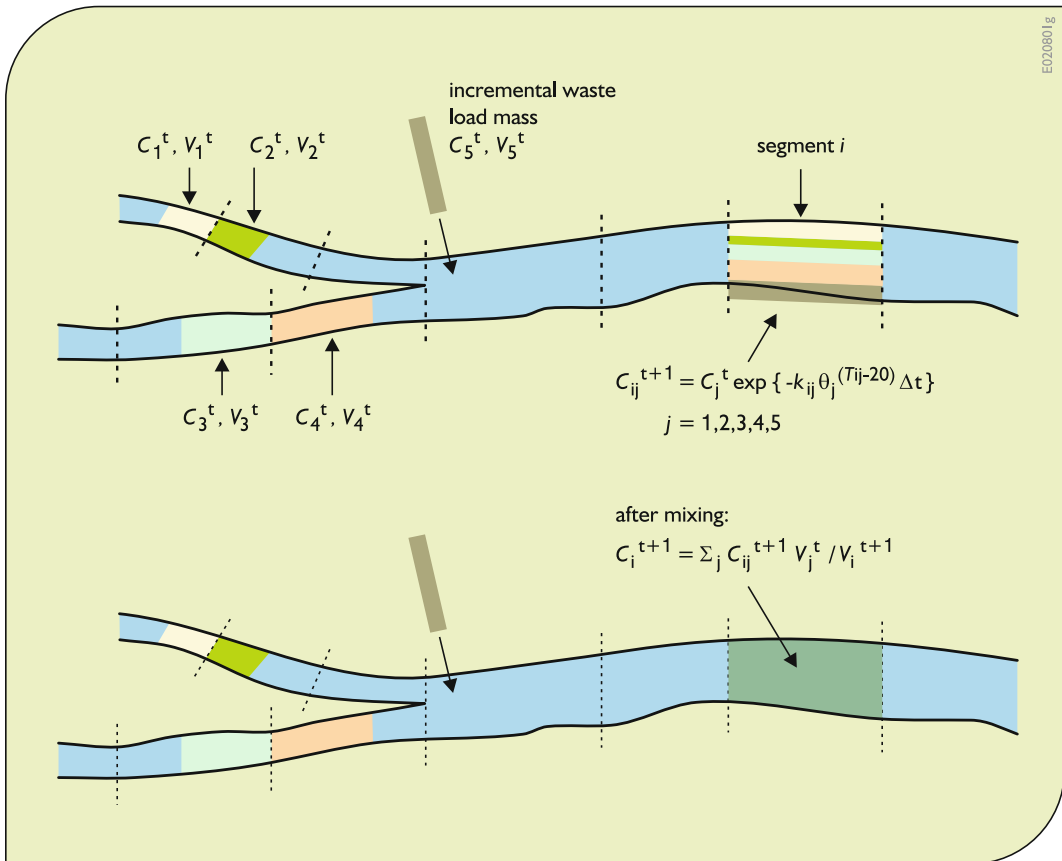
10.5.3   Backtracking Approach

An alternative backtracking approach to water quality simulation eliminates the need to consider the simulation time step duration restriction indicated by Eq. 10.82 (Manson and Wallis 2000; Yin 2002). The backtracking approach permits any simulation time step duration to be used along with any segmenting scheme. Unlike the traditional approach, water can travel through any number of successive segments or volume elements in each simulation time step.

This approach differs from the traditional one in that instead of following the water in a segment or volume element downstream, the system tracks back upstream to find the source concentrations of the contaminants at time *t* that will be in the control volume or segment *i* + 1 at the beginning of time period *t* + 1.

The backtracking process works from upstream to downstream. It starts from the segment of interest, *i*, and finds all the upstream sources of contaminants that flow into segment *i* during time period *t* having a time interval Δt. The contaminants could come from segments in the same river reach or storage site, or from upstream river reach or storage volume segments. They could also come from incremental flows into upstream segments. Flows between the source site and the segment *i* + 1 transport the contaminants from their source sites to segment *i* during the time interval Δt, as shown in Fig. 10.21.

The simulation process for each segment and for each time period involves three steps. To compute the concentration of each constituent in segment *i* at the end of time period *t*, as shown in Fig. 10.21, the approach first backtracks upstream to locate all the contaminant particles at the beginning of period t that will be in the segment *i* at the end of period *t*. This is achieved by finding the most upstream and downstream

$$C_{ij}^{t+1} = C_j^t \exp\{-k_{ij}\theta_j^{(T_{ij}-20)}\Delta t\}$$
$$j = 1,2,3,4,5$$

after mixing:
$$C_i^{t+1} = \Sigma_j C_{ij}^{t+1} V_j^t / V_i^{t+1}$$

Fig. 10.21 The backtracking approach for computing the concentrations of constituents in each reach segment or volume element i during time step duration of Δt

positions of all reach intervals that will be at the corresponding boundaries of segment i at the end of time period t. This requires computing the velocities through each of the intermediate segments or volume elements. Second, the changes in the amounts of the modeled quality constituents, e.g., temperature, organics, nutrients and toxics, are calculated assuming plug flow during the time interval, Δt, using the appropriate differential equations and numerical methods for solving them. Finally, all the multiple incoming blocks of water with their end-of-period constituent concentrations are completely mixed in the segment i to obtain initial concentrations in that segment for the next time step, $t + 1$. This is

done for each segment i in each time period t, proceeding in the downstream direction.

If no dispersion is assumed, the backtracking process can be simplified to consider only the end points of each reach. Backtracking can take place to each end-of-reach location whose time of travel to the point of interest is just equal or greater than Δt. Then using interpolation between end-of-period constituent concentrations at those upstream sites, plus all loadings between those sites and the downstream site of interest, the constituent concentrations at the end of the time period t at the downstream ends of each reach can be computed. This process, like the one involving fully mixed reach segments, must take

into account the possibility of multiple paths from each pollutant source to the site of interest, and the different values of rate constants, temperatures, and other water quality parameters in each reach along those paths.

Figure 10.21 illustrates an example of backtracking involving simple first-order decay processes. Assume contaminants that end up in reach segment i at time the beginning of period $t + 1$ come from J sources with initial concentrations $C_1^t, C_2^t, C_3^t, \ldots, C_J^t$ at the beginning of time period t. Decay of mass from each source j during time Δt in each segment or volume element is determined by the following differential equation:

$$dC_j^t/dt = -k_j\theta_j^{(T-20)}C_j^t \qquad (10.83)$$

The decay rate constant k_j, temperature correction coefficient θ_j and water temperature T are all temporally and spatially varied variables. Their values depend on the particular river reaches and storage volume sites through which water travels during the period t from sites j to segment i.

Integrating Eq. 10.83 yields:

$$C_j^{t+1} = C_j^t\exp\{-k_j\theta_j^{(T-20)}\Delta t\} \qquad (10.84)$$

Since Δt is the time it takes water having an initial concentration C_j^t to travel to reach i, the values C_j^{t+1} can be denoted as C_{ij}^{t+1}.

$$C_{ij}^{t+1} = C_j^t\exp\{-k_{ij}\theta_j^{(Tij-20)}\Delta t\} \qquad (10.85)$$

In Eq. 10.85 the values of the parameters are the appropriate ones for the stream or river between the source segments j and the destination segment i. These concentrations times their respective volumes, V_j^t, can then be mixed together to define the initial concentration, C_i^{t+1}, in segment i at the beginning of the next time period $t + 1$.

10.5.4   Model Uncertainty

There are two significant sources of uncertainty in water quality management models. One stems from incomplete knowledge or lack of sufficient data needed to estimate the probabilities of various events that might happen. Sometimes it is difficult to even identify possible future events. This type of uncertainty [sometimes called epistemic (Stewart 2000)] stems from our incomplete conceptual understanding of the systems under study, by models that are necessarily simplified representations of the complexity of the natural and socioeconomic systems, as well as by limited data for testing hypotheses and/or simulating the systems.

Limited conceptual understanding leads to parameter uncertainty. For example, there is an ongoing debate about the parameters that can best represent the fate and transfer of pollutants through watersheds and water bodies. Arguably more complete data and more work on model development can reduce this uncertainty. Thus, a goal of water quality management should be to increase the availability of data, improve their reliabilities, and advance our modeling capabilities.

However, even if it were possible to eliminate knowledge uncertainty, complete model prediction certainty in support of water quality management decisions will likely never be achieved until we can predict the variability of natural processes. This is the other significant source of uncertainty in water quality management models. This type of uncertainty arises in systems characterized by randomness. Assuming past observations are indicative of what might happen in the future and with the same frequency, i.e., assuming stationary stochastic processes, we can estimate from these past observations the possible future events or outcomes that could occur and their probabilities. Even if we think we can estimate how likely any possible type of event may be in the future we cannot predict precisely when or to what extent that event will occur.

For ecosystems, we cannot be certain we know even what events may occur in the future, let alone their probabilities. Ecosystems are open systems in which it is not possible to know in advance what all the possible biological outcomes will be. Surprises are not only

possible, but likely. Hence both types of uncertainty, knowledge uncertainty, and unpredictable variability or randomness, cannot be eliminated.

Thus, uncertainty is a reality of water quantity and quality management. This must be recognized when considering the results of water quality management models that relate actions taken to meet the desired water quality criteria and designated uses of water bodies. Chapters 6, 7, and 8 suggests some ways of characterizing this uncertainty.

10.6   Conclusions—Implementing a Water Quality Management Policy

This chapter provides only a brief introduction to some of the relationships contained in water quality models. As can be said for other chapters as well, entire texts, and very good ones, have been written on this subject (see, for example, Chapra and Reckhow 1983; Chapra 1997; McCutcheon 1989; Orlob 1983; Schnoor 1996; Thomann and Mueller 1987). Water quality modeling and management require skill and data. Skill comes with experience.

If accompanied by field data and uncertainty analysis, many existing models can be used to assist those responsible for developing water quality management plans in an adaptive implementation or management framework. Adaptive implementation or management will allow for both model and data improvements over time. Adaptive approaches strive toward achieving water quality standards while relying on monitoring and experimentation to reduce uncertainty. This is often a way one can proceed given the complexity of the real world compared to the predictive models and data and time usually available at the time a water quality analysis is needed. Starting with simple analyses and iteratively expanding data collection and modeling as the need arises is a reasonable approach.

An adaptive management process begins with initial actions that have reasonable chances of succeeding. Future actions must be based on continued monitoring of the water body to determine how it responds to the actions taken. Plans for future regulatory rules and public spending should be subject to revision as stakeholders learn more about how the system responds to actions taken. Monitoring is an essential aspect of adaptive water quality management and modeling.

Regardless of what immediate actions are taken, there may not be an immediate measurable response. For example there may be significant time lags between when actions are taken to reduce nutrient loads and the resulting changes in nutrient concentrations. This is especially likely if nutrients from past activities are bound to sediments or if nutrient-contaminated groundwater has a long residence time before its release to surface water. For many reasons, lags between actions taken and responses must be expected. Water bodies should be monitored to establish whether the "trajectories" of the measured water quality criteria point toward attainment of the designated use.

Waste load allocations will inevitably be required if quality standards are not being met. These allocations involve costs. Different allocations will have a different total costs and different distributions of those costs; hence they will have different perceived levels of fairness. A minimum cost policy may result in a cost distribution that places most of the burden on just some of the stakeholders. But until such a policy is identified one will not know this. An alternative may be to reduce loads from all sources by the same proportion. Such a policy has prevailed in the US over the past several decades. Even though not very cost effective from the point of view of water quality management, the ease of administration and the fulfillment of other objectives must have made such a policy politically acceptable, even though expensive. However, more than these types of waste load allocations policies will be needed for many of

the ecosystem restoration efforts that are increasingly being made. Restoration activities are motivated in part by a recognition of the services ecosystems provide for water quality management.

Our capabilities of including ecosystem components within water quantity and quality management models are at a fairly elementary level. Given the uncertainty, especially with respect to the prediction of how ecosystems will respond to water management actions, together with the need to take actions now, the popular call is for adaptive management. The trial and error aspects of adaptive management based on monitoring and imperfect models may not satisfy those who seek more definitive direction from water quality analysts and their predictive models. Stakeholders and responsible agencies seeking assurances that the actions taken will always work, as predicted, may be disappointed. Even the best predictive capabilities of science cannot assure that an action leading to attainment of designated uses will be initially identified. Adaptive management is a reasonable option in most cases for allowing water quality management programs to move forward in the face of considerable uncertainties.

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Exercises

1. The common version of the Streeter–Phelps equations for predicting biochemical oxygen demand BOD and DO deficit D concentrations are based on the following two differential equations

   (a) $d(BOD)/dt = -K_d(BOD)$

   (b) $dD/dt = K_d (BOD) - K_a D,$

   where K_d is the deoxygenating rate constant (T^{-1}), K_a is the reaeration-rate constant (T^{-1}), and τ is the time of flow along a uniform reach of stream in which dispersion is not significant. Show the integrated forms of (a) and (b).

10.2 Based on the integrated differential equations in Exercise 10.1

   (a) Derive the equation for the distance X_c downstream from a single point source of BOD that for a given streamflow will have the lowest dissolved oxygen concentration.

   (b) Determine the relative sensitivity of the deoxygenation rate constant K_d and the reaeration rate constant K_a on the critical distance X_c and on the corresponding critical deficit D_c. For initial conditions, assume that the reach has a velocity of 2 m/s (172.8 km/day), a K_d of 0.30 per day, and a K_a of 0.4 per day. Assume that the DO saturation concentration is 8 mg/l, the initial deficit is 1.0 mg/l, and the BOD concentration at the beginning of the reach (including that discharged into the reach at that point) is 15 mg/l.

10.3 To account for settling of BOD, in proportion to the BOD concentration, and for a constant rate of BOD addition R due to runoff and scour, and oxygen production ($A > 0$) or reduction ($A < 0$) due to plants and benthal deposits, the following differential equations have been proposed:

   (a) $d(BOD)/d\tau = -(K_d + K_s)(BOD) + R$

   $$\qquad\qquad\qquad\qquad\qquad\qquad (10.86)$$

   (b) $dD/d\tau = K_d(BOD) - K_a D - A,$

   $$\qquad\qquad\qquad\qquad\qquad\qquad (10.87)$$

   where K_s is the settling rate constant (T^{-1}) and τ is the time of flow. Integrating these two equations results in the following deficit equation:

$$D_\tau = \frac{K_d}{K_a - (K_d + K_s)}\left[\left(BOD_0 - \frac{R}{K_d + K_S}\right)\right.$$
$$\{\exp[K_d + K_S] - \exp(-K_a\tau)\}]$$
$$+ \frac{K_d}{K_a}\left\{\left(\frac{R}{K_d + K_s} - \frac{A}{K_d}\right)[1 - \exp(-K_a\tau)]\right\}$$
$$+ D_0\exp(-K_a\tau)$$

$$\qquad\qquad\qquad\qquad\qquad\qquad (10.88)$$

where BOD_o and D_o are the BOD and DO deficit concentrations at $\tau = 0$.

(a) Compare this equation with that found in Exercise 10.1 if Ks, R, and A are 0
(b) Integrate Eq. (10.86) to predict the BOD_τ at any flow time τ.

10.4 Develop finite difference equations for predicting the steady-state nitrogen component and DO deficit concentrations D in a multi-section one-dimensional estuary. Define every parameter or variable used.

10.5 Using Michaelis–Menten kinetics develop equations for

(a) Predicting the time rate of change of a nutrient concentration N (dN/dt) as a function of the concentration of bacterial biomass B;
(b) Predicting the time rate of change in the bacterial biomass B(dB/dt) as a function of its maximum growth rate μ_B^{max}, temperature T, B, N, and the specific-loss rate of bacteria ρ_B; and
(c) Predicting the time rate of change in DO deficit (dD/dt) also as a function of N, B, ρ_B, and the reaeration-rate constant $K_a(T^{-1})$.

How would these three equations be altered by the inclusion of protozoa P that feed on bacteria, and in turn require oxygen? Also write the differential equations for the time rate of change in the concentration of protozoa P(dP/dt).

10.6 Many equations for predicting stream temperature use Eulerian coordinates. The actual behavior of the stream temperature is more easily demonstrated if Lagrangian coordinates (i.e., time of flow t rather than distance X) are used. Assuming insignificant dispersion, the "time-of-flow" rate of temperature change of a water parcel as it moves downstream is

$$dT/d\tau = \lambda(T_E - T)/\rho cD$$

(a) Assuming that λ, D, and T_E are constant over interval of time of flow $t_2 - t_1$, integrate the equation above to derive the temperature T_1 at locations X_1.
(b) Develop a model for predicting the temperature at a point in a nondispersive stream downstream from multiple point sources (discharges) of heat.

10.7 Consider three well-mixed bodies of water that have the following constant volumes and freshwater inflows

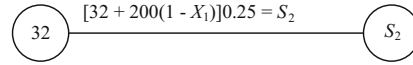| Water body	Volume (m³)	Flow (m³/s)	Displacement time
1	3×10^{12}	3×10^3	3.17 years
2	3×10^8	3×10^2	11.6 days
3	3×10^4	3×10^4	2.8 h

The first body is representative of the Great Lakes in North America, the second is characteristic in size to the upper New York harbor with the summer flow of the Hudson River, and the third is typical of a small bay or cove. Compute the time required to achieve 99% of the equilibrium concentration, and that concentration, of a substance having an initial concentration, and that concentration, of a substance having an initial concentration of 0 (at time = 0) and an input of N (M T^{-1}) for each of the three water bodies. Assume that the decay rate constant K is 0, 0.01, 0.05, 0.25, 1.0, and 5.0 days^{-1} and compare the results.

10.8 Consider the water pollution problem as shown in Figure below. There are two sources of nitrogen, 200 mg/l at site 1 and 100 mg/l at site 2, going into the river, whereas the nitrogen concentration in the river just upstream of site 1 is 32 mg/l.
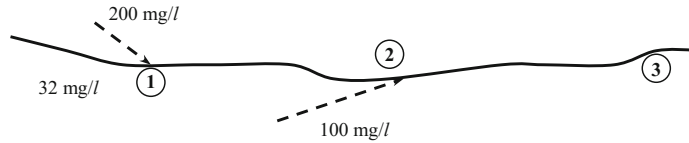
The unknown variables are the fraction of nitrogen removal at each of those sites that would achieve concentrations no greater than 20 and 25 mg/l just upstream of site 2 and at site 3, respectively, at a total minimum cost. Let those nitrogen removal fractions be X_1 and X_2. Assuming unit costs of removal as \$30 and \$20 at site 1 and site 2, respectively, the model can be written as

Minimize $30X_1 + 20X_2$
Subject to : $200(1 - X_1)0.25 + 8 \leq 20$
             $200(1 - X_1)0.15 + 100(1 - X_2)0.60 + 5 \leq 25$
             $X_1 \leq 0.9, X_2 \leq 0.9$

Another way to write the two quality constraints of this model is to define variables S_i $(i = 1, 2, 3)$ as the concentration of nitrogen just upstream of site i. Beginning with a concentration of 32 mg/l just upstream of site 1, the concentration of nitrogen just upstream of site 2 will be

$$[32 + 200(1 - X_1)]0.25 = S_2 \text{ and } S_2 \leq 20.$$

The concentration of nitrogen at site 3 will be

$$[S_2 + 100(1 - X_2)]0.60 = S_3 \text{ and } S_3 \leq 25.$$

This makes the problem easier to solve using discrete dynamic programming. The nodes or states of the network can be discrete values of S_i, the concentration of nitrogen in the river at sites i (just upstream of sites 1 and 2 and at site 3). The links represent the decision variable values, X_i that will result in the next discrete concentration, S_{i+1} given S_i. The stages i are the different source sites or river reaches. A section of the network in stage 1 (reach from site 1 to site 2) will look like

So if S_2 is 20, X_1 will be 0.76; if S_2 is 15, X_1 will be 0.86. For S_2 values of 10 or less X_1 must exceed 0.90 and these values are infeasible. The cost associated with the link or decision will be $30 X_1$.

Setup the dynamic programming network. It begins with a single node representing the state (concentration) of 32 mg/l just upstream of site 1. It will end with a single node representing the state (concentration) 25 mg/l. The maximum possible state (concentration value just upstream of site 2 must be no greater than 20 mg/l. You can use discrete concentration values in increments of 5 mg/l. This will be a very simple network. Find the least-cost solution using both forward and backward moving dynamic programming procedures. Please show your work.

10.9 Identify three alternative sets (feasible solutions) of storage lagoon volume capacities V and corresponding land application areas A and irrigation volumes Q_{2t} in each month t within a year that satisfy a 10 mg/l maximum NO_3–N content in the drainage water of a land disposal system. In addition to the data listed below, assume that the influent nitrogen n_{1t} is 50 mg/l each month, with 10% ($\alpha = 0.1$) of the nitrogen in organic form. Also assume that the soil is a well-drained silt loam containing 4500 kg/ha of organic nitrogen in the soil above the drains. The soil has a monthly drainage capacity d of 60 cm and has a

field capacity moisture content M of 10 cm. Maximum plant nitrogen uptake values N_t^{max} are 35 kg/ha during April till October, and 70 kg/ha during May till September. Finally, assume that because of cold temperatures, no wastewater irrigation is permitted during November till March. December, January, and February's precipitation is in the form of snow and will melt and be added to the soil moisture inventory in March.

removal is required at each discharge site, solve for the least-cost solution given the data in the accompanying table. Can you identify more than one type of model to solve this problem? How would this model be expanded to specifically include both carbonaceous BOD and nitrogenous BOD and non-point waste discharges?

Reach no.	Design BOD load (mg/l)	Present % removal load	Annual costs of various design BOD removal			
			60%	75%	85%	90%
1	248	67	0	22,100	77,500	1,20,600
2	408	30	6,30,000	7,80,000	9,87,000	11,70,000
3	240	30	2,10,000	2,77,500	3,23,000	3,78,000
4	1440	30	4,13,000	5,23,000	6,26,000	6,98,000
6	2180	30	5,00,000	6,38,000	7,90,000	9,00,000
7	279	30	8,40,000	10,72,000	12,32,500	13,50,000

Reach no.	Time of flow (days)	Wastewater discharge (10^3 m³/day)	Entering reach flow (10^3 m³/day)	Total reach flow (10^3 m³/day)	DO saturation conc. (mg/l)	Maximum allowable DO deficit (mg/l)	DO deficit of wastewater (mg/l)	DO Conc at beginning of reach (mg/l)	BOD Conc at beginning of reach (mg/l)	Av. deoxgn rate constant for reach (days^{-1})	Reaeration rate constant days^{-1}
1	0.235	19	5129	5148	10.2	3.2	1	9.5	1.66	0.31	1.02
2	1.330	140	4883	5023	9.95	2.45	1	8	0.68	0.41	0.6
3	1.087	30	10,171	10,201	9	2	1	?	?	0.36	0.63
4	2.067	53	1120	1173	9.7	3.75	1	9.54	1	0.35	0.09
5	0.306	0	11,374	11,374	9	2.5	–	?	?	0.34	0.72
6	1.050	98	11,374	11,472	8.35	2.35	1	–	–	0.35	0.14
7	6.130	155	11,472	11,627	8.17	4.17	1	–	–	0.3	0.02

10.10 Consider the problem of estimating the minimum total cost of waste treatment in order to satisfy quality standards within a stream. Let the stream contain seven homogenous reaches r, reach $r = 1$ being at the upstream end and reach $r = 7$ at the downstream end. Reaches $r = 2$ and 4 are tributaries entering the mainstream at the beginning of 1, 3, 5, 6, and 7. Point sources of BOD enter the stream at the beginning of reaches 1, 2, 3, 4, 6, and 7. Assuming that at least 60% BOD

10.11 Discuss what would be required to analyze flow augmentation alternatives in Exercise 12.8. How would the costs of flow augmentation be defined and how would you modify water quality models to include flow augmentation alternatives?

10.12 Develop a dynamic programming model to estimate the least-cost number, capacity, and location of artificial aerators to ensure meeting minimum allowable DO standards where they would otherwise be

violated during an extreme low-flow design condition in a nonbranching section of a stream. Show how wastewater treatment alternatives, and their costs, could also be included in the dynamic programming model.

10.13 Using the data provided, find the steady-state concentrations C_t of a constituent in a well-mixed lake of constant volume 30×10^6 m^3. The production N_{ti} of the constituent occurs at three sites i, and is constant in each of four seasons in the year. The required fractions of constituent removal P_i at each site i are to be set so that they are equal at all sites i and the maximum concentration in the lake in each period t must not exceed 20 mg/l.

Period, t	Days in period	Flow, Qt (10^3 m^3/day)	Constituent decay rate, constant, Kt (days^{-1})
1	100	90	0.02
2	80	150	0.03
3	90	200	0.05
4	95	120	0.04

Constituent discharge site, i	Constituent production (kg/day)
1	38,000
2	25,000
3	47,000

10.14 Suppose that the solution of a model such as that used in Exercise 10.13, or measured data, indicated that for a well-mixed portion of a saltwater lake, the concentrations of nitrogen ($i = 1$), phosphorus ($i = 2$), and silicon ($i = 3$) in a

particular period t were 1.1, 0.1, and 0.8 mg/l, respectively. Assume that all other nutrients required for algal growth are in abundance. The algal species of concern are three in number and are denoted by $j = 1, 2, 3$. The data required to estimate the probable maximum algal bloom biomass concentration are given in the accompanying table. Compute this bloom potential for all k_i and k equal to 0, 0.8, and 1.0.

Parameter (algae species index j)	Parameter value		
	1	2	3
a_{1j} = mg N/mg dry wt of algae j	0.04	0.01	0.20
a_{2j} = mg P/mg dry wt of algae j	0.06	0.02	0.10
a_{3j} = mg Si/mg dry wt of algae j	0.08	0.01	0.03
D_j = morality and grazing rate constant (days^{-1})	0.6	0.4	0.20
d_j = morality rate constant, (days^{-1})	0.3	0.1	0.10
v = extinction reduction rate constant for dead algae, (days^{-1})	0.07	0.07	0.07
h_j^{max} = max. extinction coef. (m^{-1})	0.07	0.07	0.10
$\eta_j^{min} Z$ = min. extinction coef. (m^{-1})	0.01	0.03	0.03
η_j = increase in extinction coef. per unit increase in mg/l (g/m^3) of dry wt of species j (m^2/g)	0.05	0.164	0.04
Nutrient index i	*1*	*2*	*3*
Nutrient	N	P	Si
μ_i = mineralization rate constant, (days^{-1})	0.02	0.69	0.62