# 12. Water Quality Modelling and Prediction

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**The most fundamental human needs for water are for drinking, cooking and personal hygiene. To meet these needs, the quality of the water used must pose no risk to human health. The quality of the water in nature also affects the condition of ecosystems that all living organisms depend on. At the same time, humans use water bodies as convenient sinks for the disposal of domestic, industrial and agricultural wastewaters. This of course 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 have been developed to assist in predicting the water quality impacts of alternative land and water management policies and practices. This chapter introduces some of the main principles of water quality modelling.**

## 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, these water users must either pay an additional cost for water treatment or incur at least increased risks of damage or loss. As populations and economies grow, more pollutants are generated. Many of these are waterborne, and hence can end up in surface and groundwater bodies. Increasingly, the major efforts and costs involved in water management are devoted to water quality protection and management. Conflicts among various users of water are increasingly over issues involving water quality as well as water quantity.

Natural water bodies are able to serve many uses, including the transport and assimilation of waterborne wastes. But as natural water bodies assimilate these wastes, their quality changes. If the quality drops to the extent that other beneficial uses are adversely affected, the assimilative capacities of those water bodies have been exceeded with respect to those affected uses. Water quality management measures are actions taken to ensure that the total pollutant loads discharged into receiving water bodies do not exceed the ability of those water bodies to assimilate those loads while maintaining the levels of quality specified by quality standards set for those waters.

What uses depend on water quality? One can identify almost any use. All living organisms require water of sufficient quantity and quality to survive, although different aquatic species can tolerate different levels of water quality. Regrettably, in most parts of the developed world it is no longer safe to drink natural surface or ground waters; they usually need to be treated before they become fit for human consumption. Treatment is not a practical option for recreational bathing, or for maintaining the health of fish, shellfish and other organisms found in natural aquatic ecosystems. Thus, standards specifying minimum acceptable levels of quality are set for most ambient waters. Various other uses have their own standards as well. Irrigation water must not be too saline or contain toxic substances that can be absorbed by the plants or destroy microorganisms in the soil. Water quality standards for industry can be very demanding, depending of course on the particular industrial processes.

Pollutant loadings degrade water quality. High domestic wasteloads can result in high concentrations of bacteria, viruses and other organisms that affect human health. High organic loadings can reduce dissolved oxygen to levels that are fatal to parts of the aquatic ecosystem and cause obnoxious odours. Nutrient loadings from both urban and agricultural land runoff can cause excessive algae growth, which in turn may degrade the water aesthetically and recreationally, and upon death result in low dissolved oxygen levels. Toxic heavy metals and other micro-pollutants 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 and non-point sources. A common approach to controlling point source discharges, such as those 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.

Non-point sources such as agricultural runoff or atmospheric deposition are less easily controlled, and hence it is difficult to apply effluent standards to non-point source pollutants, and their loadings can be much more significant than point source loadings. Management of non-point water quality impacts requires a more ambient-focused water quality management programme.

The goal of an ambient water quality management programme 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 hydrological, ecological and land use conditions, the potential uses of the receiving water body, 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 occur in the future, especially from area-wide non-point sources. In addition to uncertainties inherent in measuring the attainment of water quality standards, there are uncertainties in models used to determine sources of pollution, to allocate pollutant loads, and 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 with the complexities of actual water systems. These limitations and uncertainties should be understood and addressed as water quality management decisions are based on their outputs.

## 2. Establishing Ambient Water Quality Standards

Identifying the intended uses of a water body – whether a lake, a section of a stream or an estuary – is a first step in setting water quality standards for that body. The most restrictive 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 hydrological and geomorphic changes that affect the water quality.

The designated use dictates the appropriate type of water quality standard. For example, a designated use of human recreation should protect humans from exposure to microbial pathogens while swimming, wading or boating. Other uses include those designed to protect humans and wildlife from consuming harmful substances in water, in fish and in shellfish. Aquatic-life uses include the protection and propagation of fish, shellfish and wildlife resources.

Standards set upstream may affect the uses of water downstream. For example, small headwater streams may have aesthetic value but may not be able to support extensive recreational uses. However, their condition may affect the ability of a downstream area to achieve a particular designated use such as 'fishable' or 'swimmable'. In this case, the designated use for the smaller upstream water body may be defined in terms of achieving the designated use of the larger downstream water body.

In many areas, human activities have altered the landscape and aquatic ecosystems to the point where they cannot be restored to their pre-disturbance condition. For example, someone's desire to establish a trout fish-farm in downtown Paris, Phnom Penh, Prague or Pretoria may not be attainable because of the development history of these areas or the altered hydrological regimes of the rivers flowing through them. Similarly, someone might wish to

designate an area near the outfall of a sewage treatment plant for shellfish harvesting, but health considerations would preclude any such use. Ambient water quality standards must be realistic.

Designating the appropriate use for a water body is a policy decision that can be informed by the use of water quality prediction models of the type discussed in this chapter. However, the final standard selection should reflect a social consensus made while bearing in mind the current condition of the watershed, its pre-disturbance condition, the advantages derived from a certain designated use, and the costs of achieving that use.

## 2.1. Water-Use Criteria

The designated use is a qualitative description of the 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 Figure 12.1.

In Box 1 of Figure 12.1 are measures of the pollutant discharge from a treatment plant (such as biological oxygen demand, ammonia ($NH_3$), pathogens and suspended sediments) or the amount of a pollutant entering the edge of a stream from runoff. A criterion at this position is referred to as an effluent standard. Criteria in Boxes 2 and 3 are possible measures of ambient water quality conditions. Box 2 includes measures of a water quality parameter such as dissolved oxygen (*DO*), pH, total phosphorus 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 hydrological criterion), abundance of non-indigenous taxa, or some quantification of channel modification (e.g. a decrease in sinuosity) (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 these 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, the desired condition of a small headwater stream may need to be specified in relation to other water bodies downstream; thus, an ambient nutrient criterion may be set in a small headwater stream to ensure a designated use in a downstream estuary, even if there are no local adverse impacts resulting from the nutrients in the small headwater stream, as previously discussed. 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.
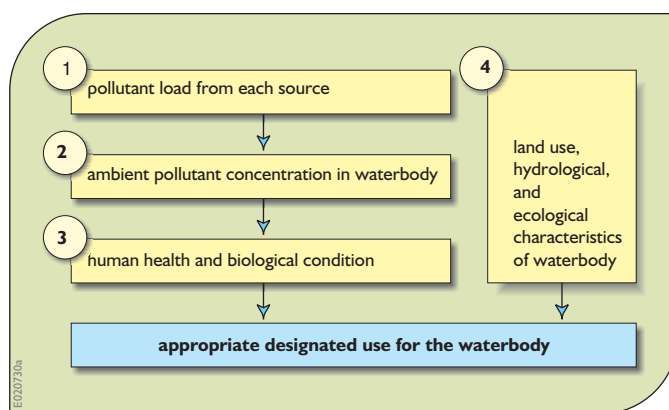


**Figure 12.1.** Factors considered when determining designated use and associated water quality standards.

## 3. Water Quality Model Use

Monitoring data are the preferred form of information for identifying impaired waters (Appendix B). Model predictions might be used in addition to or instead of

monitoring data for several reasons:

- Modelling might be feasible in some situations where monitoring is not.
- Integrated monitoring and modelling systems could provide better information than one or the other alone for the same total cost. For example, regression analyses that correlate pollutant concentration with some more easily measurable factor (such as stream-flow) could be used to extend monitoring data for preliminary listing (of impared status) purposes. Models can also be used in a Bayesian framework 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 Chapter 7).
- Modelling 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 is built, or the effect of increased industrial growth and effluent discharges.

A simple but useful modelling 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 streamflow 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 predict 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 non-indigenous taxa and over-harvesting of fish. Indirect effects of humans include land cover changes that alter the rates of delivery of water, pollutants and sediment to water bodies.

A review of direct and indirect effects of human activities suggests five major types of environmental stressors:

- 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
- 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. A 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, they are simple qualitative conceptual representations of the relationships among important variables and indicators of those variables, such as the statement 'human activities in a watershed affect water quality, including the condition of the river biota'. 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.

## 3.1. Model Selection Criteria

Water quality predictive models include both mathematical expressions and expert scientific judgement. They include process-based (mechanistic) models and data-based (statistical) models. The models should link management options to meaningful response variables (such as 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 options. To do this requires prediction error estimates (Chapter 9).

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, while complex ones 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 do so. Finally, the cost of maintaining and updating the model over time must be acceptable.

Although predictions are typically made with the aid of mathematical models, there are certainly situations where expert judgement can be just as good. Reliance on professional judgement and simpler models is often acceptable, especially when data are limited.

Highly detailed models require more time and are more expensive to develop and apply. Effective and efficient modelling for water quality management may dictate the use of simpler models. Complex modelling studies should be undertaken only if warranted by the complexity of the management problem. More complex modelling will not necessarily ensure that uncertainty is reduced, and in fact added complexity can compound problems of uncertainty analyses (Chapter 9).

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

## 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 limits on the nutrient loadings to the estuary that can cause algae blooms, and subsequent dissolved oxygen deficits. The modelling challenge is to link nutrient loading to fish and shellfish survival.
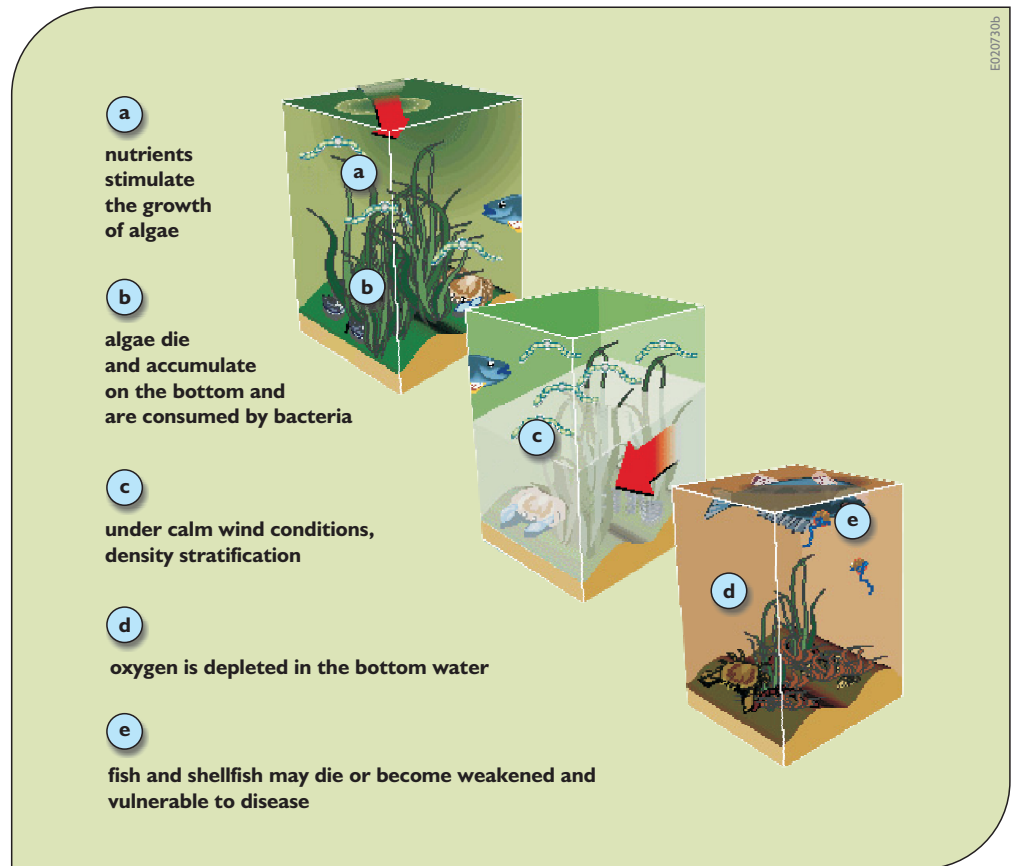
The negative effects of excessive nutrients (e.g. nitrogen) in an estuary are shown in Figure 12.2. Nutrients stimulate the growth of algae. Algae die and accumulate on the bottom, where bacteria consume them. Under calm wind conditions density stratification occurs. Oxygen is depleted in the lower levels of 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 into the estuary that might cause problems for fish and shellfish populations. These conditional probabilities can be judgemental, mechanistic and/or statistical. Each conditional probability can be a separate sub-model. Assuming each sub-model 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, $R$. In other words:

$$Pr\{C | N\} = Pr\{C | A\}Pr\{A | N, R\}Pr\{R\} \qquad (12.1)$$

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 on the basis of the river flow and nitrogen loadings. It could similarly predict the production of carbon, on the basis of 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

**Figure 12.2.** The negative impacts of excessive nutrients in an estuary (NRC, 2001).



a
nutrients stimulate the growth of algae

b
algae die and accumulate on the bottom and are consumed by bacteria

c
under calm wind conditions, density stratification

d
oxygen is depleted in the bottom water

e
fish and shellfish may die or become weakened and vulnerable to disease

predict the duration of stratification and the frequency of hypoxia, given both the stratification duration and sediment oxygen demand. Expert judgement 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 the network in Figure 12.3 can reflect a combination of simple mechanisms, statistical (regression) fitting and expert judgement.

Advances in the mechanistic modelling of aquatic ecosystems have enabled us to include greater process (especially trophic) detail and complexity, as well as to perform dynamic simulations, although 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

modelling (Chapra, 1997; McCutcheon, 1989; Orlob, 1983; Schnoor, 1996; Thomann and Mueller, 1987) as well as the current professional journal literature.

## 3.3. Model Data

Data availability and accuracy are sources 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 that lack of data. Model complexity can give the impression of credibility, but this is usually misleading.

It is often preferable to begin with simple models and then, over time, add additional complexity as justified by the collection and analysis of additional data. This strategy makes efficient use of resources. It targets the effort toward information and models that will reduce
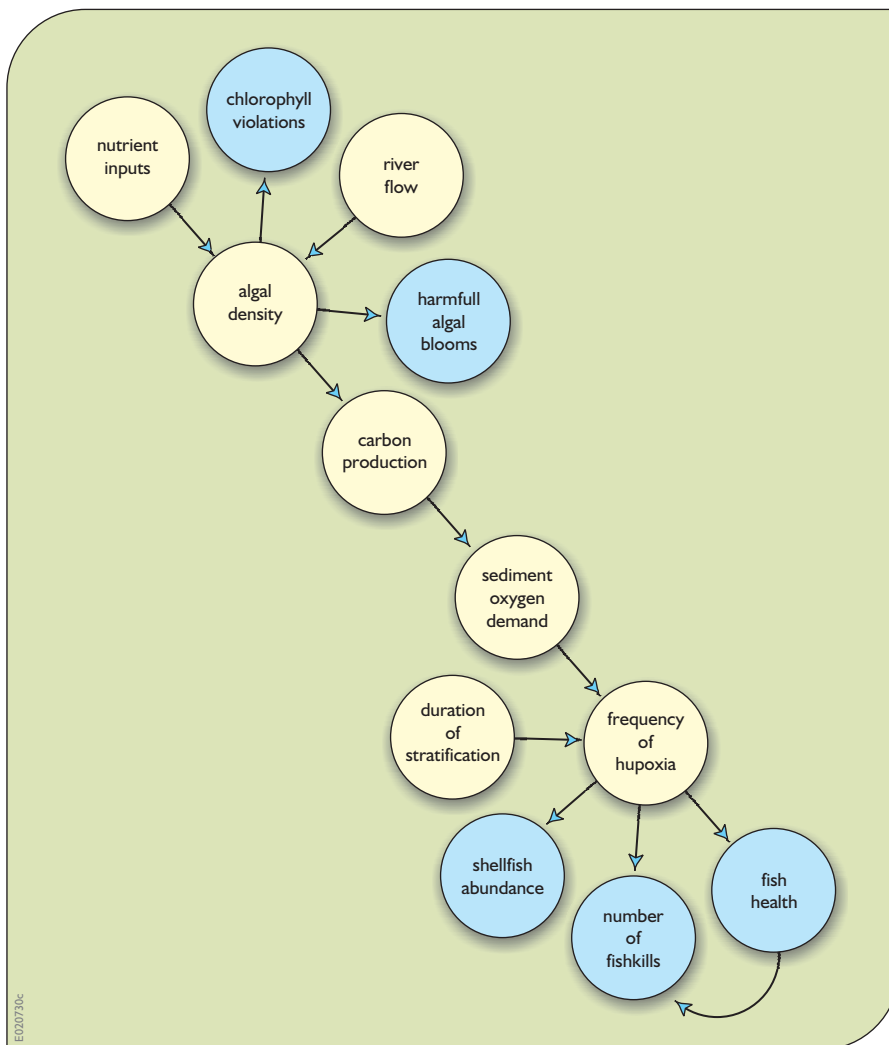
**Figure 12.3.** Cause and effect diagram for estuary eutrophication due to excessive nutrient loadings (Borsuk et al., 2004).

the uncertainty as the analysis proceeds. Models should be selected (simple versus complex) in part on the basis of 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 be 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. a 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, can vary over space and time within the area and time period being simulated, and are typically not known with any precision. Chapter 13 reviews some of these loading models and their limitations.

# 4. Water Quality Model Processes

Water quality models can be applied to many different types of water system, including streams, rivers, lakes, reservoirs, estuaries, coastal waters and oceans. The models describe the main water quality processes, and typically require the hydrological 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 hydrological 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 quality predictions for lakes is often more difficult than for streams, rivers and estuaries. In coastal waters and oceans, large-scale flow patterns and tide are the most important transport mechanisms.

The development and application of water quality models is both a science and 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, the time available for modelling and associated uncertainty, and other considerations. The fact that most, if not all, water quality models cannot accurately predict what actually happens does not 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 management policies or practices.

## 4.1. Mass-Balance Principles

The basic principle of water quality models is that of mass balance. A water system can be divided into different segments or volume elements, also called 'computational cells'. For each segment or cell, there must be a mass balance for each water quality constituent over time. Most water quality simulation models simulate quality over a consecutive series of discrete time periods, $\Delta t$. Time is divided into discrete intervals $t$ 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 defined. Components of the mass balance for a segment include: first, changes by transport ($Tr$) into and out of the segment; second, changes by physical or chemical processes ($P$) occurring within the

segment; and third, changes by sources/discharges to or from the segment ($S$).

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

(12.2)

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. wasteloads, river discharges): $\left(\frac{\Delta M_i}{\Delta t}\right)_S$

Changes by transport include both advective and dispersive transport. Advective transport is 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, differs from the physical concept of molecular diffusion as it stands for all transport that is not advective.

Changes by processes include physical processes such as re-aeration 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.

Changes by sources include the addition of mass by wasteloads 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 modelled segment or volume element (the computational cell) is derived from a water quantity (possibly hydrodynamic) model.

To model the transport of substances over space, a water system is divided in small segments or volume elements. The complete ensemble of all the segments or elements is called the *grid* or s*chematization*. Each computational cell is defined by its volume and its dimensions in one, two or three directions ($\Delta x$, $\Delta y$, $\Delta z$) depending on the nature of the schematization (1D, 2D or 3D). Note that the cell dimensions $\Delta x$, $\Delta y$ and $\Delta z$ do not have to be equal. The computational cell can have any rectangular shape. A computational cell can share surface areas with other cells, the atmosphere, or 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.

### 4.1.1. Advective Transport

The advective transport, $T_{x_0}^A$ (M/T), of a constituent at a site $x_0$ is the product of the average water velocity, $v_{x_0}$ (L/T), 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:

$$T_{x_0}^A = v_{x_0} \times A \times C_{x_0} \tag{12.3}$$

### 4.1.2. Dispersive Transport

The dispersive transport, $T_{x_0}^D$ (M/T), 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), be the dispersion or diffusion coefficient at site $x_0$:

$$T_{x_0}^D = -D_{x_0} \times A \times \frac{\partial C}{\partial x}\bigg|_{x=x_0} \tag{12.4}$$

Dispersion is done according to Fick's diffusion law. The minus sign originates from the fact that dispersion causes net transport from higher to lower concentrations, and 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:

$$\frac{\partial C}{\partial x}\bigg|_x = \lim_{\Delta x \to 0} \frac{C_{x+0.5\Delta x} - C_{x-0.5\Delta x}}{\Delta x} \tag{12.5}$$

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

### 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, a one dimensional equation results:

$$M_i^{t+\Delta t} = M_i^t + \Delta t \times \left( v_{x_0} C_{x_0} - v_{x_0+\Delta x} C_{x_0+\Delta x} \right.$$
$$\left. - D_{x_0} \frac{\partial C}{\partial x}\bigg|_{x_0} + D_{x_0+\Delta x} \frac{\partial C}{\partial x}\bigg|_{x_0+\Delta x} \right) \times A \tag{12.6}$$

or equivalently:

$$M_i^{t+\Delta t} = M_i^t + \Delta t$$
$$\times \left( Q_{x_0} C_{x_0} - Q_{x_0+\Delta x} C_{x_0+\Delta x} - D_{x_0} A_{x_0} \frac{\partial C}{\partial x}\bigg|_{x_0} \right.$$
$$\left. + D_{x_0+\Delta x} A_{x_0+\Delta x} \frac{\partial C}{\partial x}\bigg|_{x_0+\Delta x} \right) \tag{12.7}$$

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

If the previous equation is divided by the volume and the time interval $\Delta t$, then the following equation results in one dimension:

$$\frac{C_i^{t+\Delta t} - C_i^t}{\Delta t} = \frac{D_{x_0+\Delta x}\frac{\partial C}{\partial x}\big|_{x_0+\Delta x} - D_{x_0}\frac{\partial C}{\partial x}\big|_{x_0}}{\Delta x}$$
$$+ \frac{v_{x_0} C_{x_0} - v_{x_0+\Delta x} C_{x_0+\Delta x}}{\Delta x} \tag{12.8}$$

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

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial x}\left( D \frac{\partial C}{\partial x} \right) - \frac{\partial}{\partial x}(vC) \tag{12.9}$$

The finite volume method for transport is a computational method of solving the advection–diffusion equation. The accuracy of the method will be related to the size of $\Delta x$, $A$ ($A = \Delta y \Delta z$) and $\Delta t$.

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

$$\frac{\partial C}{\partial t} = D_x \frac{\partial^2 C}{\partial x^2} - v_x \frac{\partial C}{\partial x} + D_y \frac{\partial^2 C}{\partial y^2} - v_y \frac{\partial C}{\partial y}$$

$$+ D_z \frac{\partial^2 C}{\partial z^2} + v_z \frac{\partial C}{\partial z} + S + f_R(C, t) \qquad (12.10)$$

with dispersion coefficients $D_j$ defined for each direction. 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 'wasteloads' (S): these source terms are additional inflows of water or mass. As many source terms as required may be added to Equation 12.10. These could include small rivers, discharges of industries, sewage treatment plants, small wasteload outfalls and so on.
- Reaction terms or 'processes' ($f_R$).

Processes can be split into physical 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 section.

The expression $D(\partial C/\partial X) - vC$ in Equation 12.9, multiplied by the area $A$, is termed the total flux (M/T). 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 ones. The coefficient of dispersion $D$ (L$^2$/T) 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) across a cross-sectional area $A$ (L$^2$).

The relative importance of dispersion and advection depends on the degree of detail with which 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 that assume 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 found to be acceptable for natural aquatic systems.

## 4.2. Steady-State Models

A steady state means no change over time. If we consider a water body, for example a river, this means there are no changes in the concentrations with time. In this case the left hand side of Equation 12.9, $\partial C/\partial t$, 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 Equation 12.9 becomes

$$0 = D\, \partial^2 C/\partial X^2 - v\partial C/\partial X - kC \qquad (12.11)$$

Equation 12.11 can be integrated, since river reach parameters $A$, $D$, $k$, $v$, and $Q$ are assumed constant. For a constant loading, $W_C$ (M/T) at site $X = 0$, the concentration $C$ at any distance $X$ will equal

$$C(X) = (W_C/Qm) \exp[(v/2D)(1 + m)X] \quad X \le 0$$
$$\quad (W_C/Qm) \exp[(v/2D)(1 - m)X] \quad X \ge 0 \quad (12.12)$$

where

$$m = (1 + (4kD/v^2))^{1/2} \qquad (12.13)$$

Note from Equation 12.12 that the parameter $m$ is always equal to or greater than 1 and that the exponent of $e$ is always negative. Hence, as the distance $X$ increases in magnitude, either in the positive or negative direction, the concentration $C(X)$ will decrease if $k > 0$. The maximum concentration $C$ occurs at $X = 0$ and is $W_C/Qm$.

$$C(0) = W_C/Qm \qquad (12.14)$$

These equations are plotted in Figure 12.4.

In flowing rivers not under the influence of tidal actions the dispersion is usually small. Assuming the dispersion coefficient $D$ is 0, the parameter $m$ defined by Equation 12.13 is 1. Hence, when $D = 0$, the maximum concentration at $X = 0$ is $W_C/Q$.

$$C(0) = W_C/Q \quad \text{if } D = 0. \qquad (12.15)$$

Assuming $D = 0$ and $v$, $Q$ and $k > 0$, Equation 12.12 becomes

$$C(X) = \begin{cases} 0 & X \leq 0 \\ (W_C/Q)\exp[-kX/v] & X \geq 0 \end{cases} \qquad (12.16)$$

The above equation for $X > 0$ can be derived from Equations 12.12 and 12.13 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 Equation 12.12 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 for a distance of $X$.

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 $v$, $Q = Av$, 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 Equation 12.12 approaches $\pm X(k/D)^{1/2}$.

Hence for small velocities, Equation 12.12 becomes

$$C(X) = \begin{cases} (W_C/2A(kD)^{1/2})\exp[+X(k/D)^{1/2}] & X \leq 0 \\ (W_C/2A(kD)^{1/2})\exp[-X(k/D)^{1/2}] & X \geq 0 \end{cases}$$
$$(12.17)$$

Here, dispersion is much more important than advective transport and the concentration profile approaches a symmetric distribution, as shown in Figure 12.4, about the point of discharge at $X = 0$.
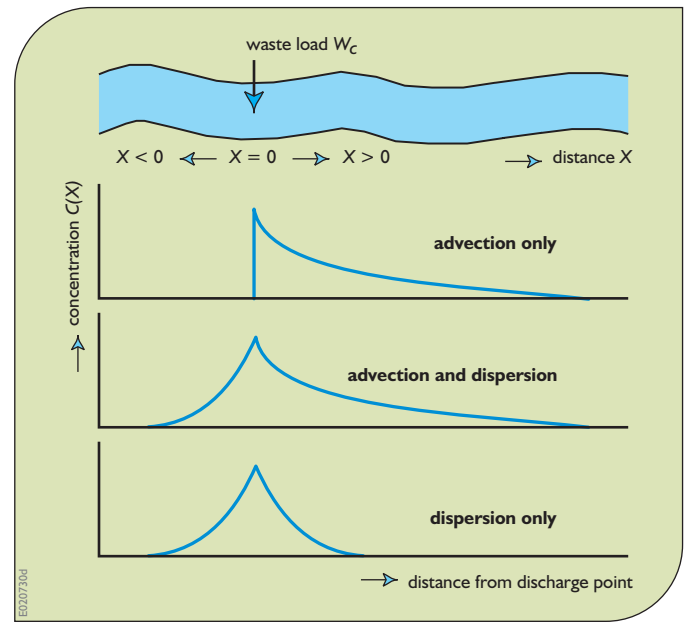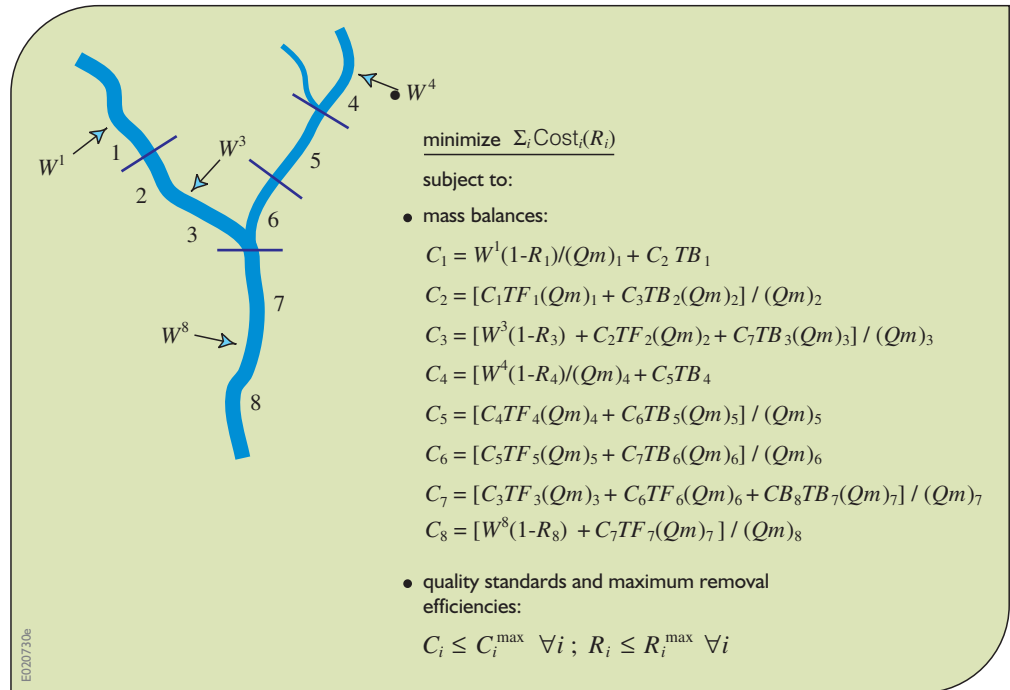


**Figure 12.4.** Constituent concentration distribution along a river or estuary resulting from a constant discharge of that constituent at a single point source in that river or estuary.

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 12.5 shows a schematic of a river into which wastewater containing constituent $C$ is being discharged at four sites. Assume that maximum allowable concentrations of the constituent $C$ are specified at each of those discharge sites. To estimate the necessary 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 parameter values for the particular reach. These reaches are shown in Figure 12.5.

**Figure 12.5.** 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.

In Figure 12.5 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) transfer coefficient, $TF_i$, equals the applicable part of Equation 12.12,

$$TF_i = \exp[(v/2D)(1 - m)X] \qquad (12.18)$$

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

$$TB_i = \exp[(v/2D)(1 + m)X] \qquad (12.19)$$

The parameter $m$ is defined by Equation 12.13.

Solving a model such as the one shown in Figure 12.5 does not mean that the least-cost wasteload allocation plan will be implemented, but least cost solutions can 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 programme. Other than economic objectives can also be used to obtain other tradeoffs.

The model in Figure 12.5 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.

## 4.3. Design Streamflows for Water Quality

In streams and rivers, the water quality may vary significantly, depending on the water flow. If wasteload discharges are fairly constant, a high flow serves to dilute the waste concentration, while where there is a low flow concentrations may become undesirably high. It is therefore common practice to pick a low-flow condition for judging whether or not ambient water quality standards are being met. This can also be seen from Equations 12.12, 12.14, 12.15, and 12.16. 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. 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, which is used in parts of North America, is the minimum seven-day average flow expected once in ten years on average. Each year the lowest seven-day average flow is determined, as shown in Figure 12.6. The sum of each of the 365 sequences of seven average daily flows is divided by seven, and the minimum value is selected. This is the minimum annual average seven-day flow.

These minimum seven-day average flows for each year of record define a probability distribution whose
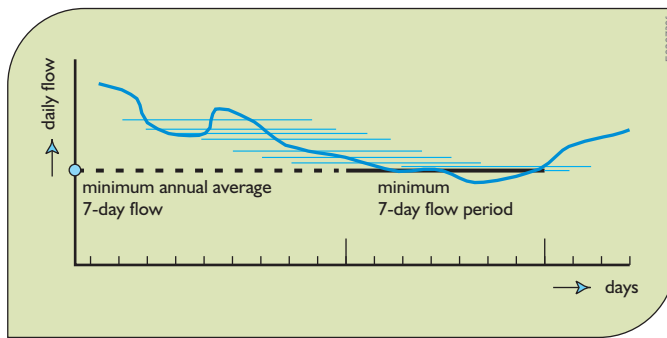
**Figure 12.6.** Portion of annual flow time series showing low flows and the calculation of average seven and fourteen-day flows.



**Figure 12.7.** Determining the minimum seven-day annual average flow expected once in ten years, designated 7Q10, from the cumulative probability distribution of annual minimum seven-day average flows.

cumulative probabilities can be plotted. As illustrated in Figure 12.7, 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 seven-day flow expected once in ten 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 a 1% chance that any daily flow will be less than this 7Q10 flow.

Consider now any one of the river reaches shown in Figure 12.5. Assume an initial amount of constituent mass, $M$, exists at the beginning of the reach. As the reach volume, $Q\Delta t$, increases due to the inflow of less polluted water, the initial concentration, $M/Q\Delta t$, will decrease. However, the flow velocity will increase, and thus the time, $\Delta t$, 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. Thus, wasteload allocations that meet ambient water quality standards during low-flow conditions may not meet them under higher-flow conditions, which are observed much more frequently. Figure 12.8 illustrates how this might happen. This does not suggest low flows should not be considered when allocating wasteloads, 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 are the low-flow conditions.

Figure 12.8 shows that for a fixed mass of pollutant at $X = 0$, under low-flow conditions the more restrictive
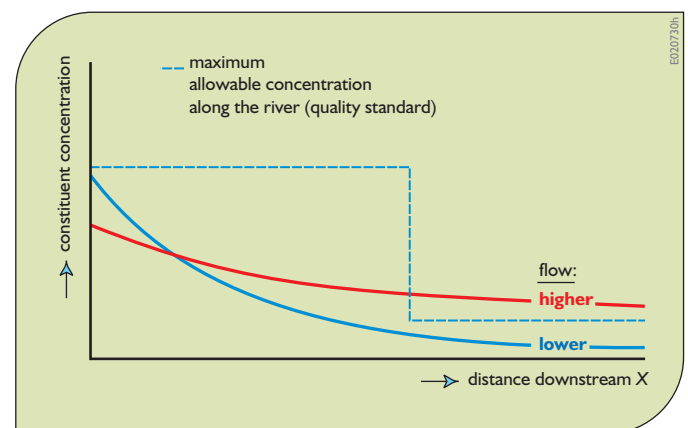


**Figure 12.8.** Increasing the streamflows decreases initial concentrations but may increase downstream concentrations.

(lower) maximum pollutant concentration standard in the downstream portion of the river is met, but that same standard is violated under more frequent higher-flow conditions.

## 4.4. Temperature

Temperature affects almost all water quality processes taking place in water bodies. For this reason, it may be important to model temperature when it may vary substantially 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 short-wave solar radiation, long-wave 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 the 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 $\rho$ (g/cm$^3$), the heat capacity of water, $c_p$ (cal/g/°C), and the water depth $h$ (cm). The net heat input, $K_H(T_e - T)$ (cal/cm$^2$/day), is assumed to be proportional to the difference of the actual temperature, $T$, and the equilibrium temperature, $T_e$ (°C).

$$dT/dt = K_H(T_e - T)/\rho c_p h \qquad (12.20)$$

The overall heat exchange coefficient, $K_H$ (cal/cm$^2$/day/°C), is determined in units of Watts/m$^2$/°C (1 cal/cm$^2$/day/°C = 0.4840 Watts/m$^2$/°C) from empirical relationships that include wind velocity, dew point temperature 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 short-wave solar radiation, $H_s$ (cal/cm$^2$/day),

$$T_e = T_d + (H_s/K_H) \qquad (12.21)$$

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

## 4.5. Sources and Sinks

Sources and sinks of pollutants include wasteloads, and the physical and biochemical processes that alter those wasteloads. External inputs of each constituent would have the form $W/Q\Delta t$ or $W/(A_X\Delta X)$ where $W$ (M/T) is the loading rate of the constituent and $Q\Delta t$ or $A_X\Delta X$ (L$^3$) represents the volume of water into which the mass of waste $W$ is discharged. Constituent growth and decay processes are discussed in the remaining parts of this Section 4.

## 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 (d$C$/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 concentration $C_i$, of constituent $i$, then

$$dC_j/dt = a_{ij}k_i\theta_i^{(T-20)}C_i \qquad (12.22)$$

where $\theta_i$ is the 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 Equation 12.22. 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, that is, dilution.

The typical values for the rate coefficients $k_c$ and temperature coefficients $\theta_i$ of some constituents $C$ are in Table 12.1. 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 $k_B = 2.3/t_{90}$.

## 4.7. Dissolved Oxygen

Dissolved oxygen (DO) concentration is a common indicator of the health of the aquatic ecosystem. DO was originally modelled in the Ohio River (US) by Streeter and Phelps (1925). Since then a number of modifications and extensions of the model have been made relating to the number of sinks and sources of DO being considered, and how processes involving the nitrogen cycle and phytoplankton are being modelled, as illustrated in Figure 12.9.

The sources of DO in a water body include re-aeration from the atmosphere, photosynthetic oxygen production from aquatic plants, denitrification and DO inputs. The

**Table 12.1.** 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)



**Figure 12.9.** The dissolved oxygen interactions in a water body, showing the decay (satisfaction) of carbonaceous, nitrogenous and sediment oxygen demands and water body re-aeration or deaeration (if supersaturation occurs at the air–water interface).

sinks include oxidation of carbonaceous and nitrogenous material, sediment oxygen demand and respiration by aquatic plants.

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

The rate of re-aeration is assumed to be proportional to the difference between the saturation concentration, $DO_{sat}$ (mg/l), and the concentration of dissolved oxygen, $DO$ (mg/l). The proportionality coefficient is the re-aeration rate $k_r$ (1/day), defined at temperature $T = 20\,°C$, which can be corrected for any temperature $T$ with the coefficient $\theta_r^{(T-20)}$. The value of this temperature correction coefficient, $\theta$, 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 re-aeration rate constant is a sensitive parameter. There have been numerous equations developed to define this rate constant. Table 12.2 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

$$DO_{sat} = \{14.652 - 0.41022T + (0.089392T)^2$$
$$- (0.042685T)^3\}\{1 - (Cl/100,000)\} \quad (12.23a)$$

Elmore and Hayes (1960) derived an analytical expression for the $DO$ saturation concentration, $DO_{sat}$ (mg/l), as a function of temperature ($T$, °C):

$$DO_{sat} = 14.652 - 0.41022T + 0.007991T^2$$
$$- 0.000077774T^3 \quad (12.23b)$$

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

$$DO_{sat} = 14.407 - 0.3369T + 0.0035T^2 \quad (12.23c)$$

as is shown in Figure 12.10.

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.
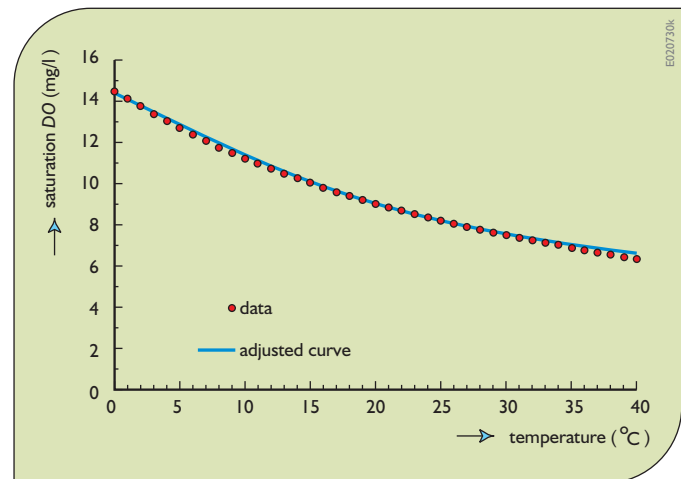
**Figure 12.10.** Fitted curve to the saturation dissolved oxygen concentration (mg/l) as a function of temperature (°C).

**Table 12.2.** Some equations for defining the re-aeration rate constant, $k_r$ (day$^{-1}$).

| 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) | |

One can distinguish between the biochemical oxygen demand from carbonaceous organic matter (*CBOD*, mg/l) in the water, and that 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 modelled 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 $\theta_{CBOD}$ and $\theta_{NBOD}$, respectively.

The sediment oxygen demand *SOD* (mg/l/day) is usually expressed as a zero-order reaction, that is, a constant demand. One important feature in modelling *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 dissolved oxygen (*DO*) model with *CBOD*, *NBOD* and *SOD* is

$$\begin{aligned} dDO/dt = & -k_{CBOD}\theta_{CBOD}^{(T-20)}CBOD \\ & - k_{NBOD}\theta_{NBOD}^{(T-20)}NBOD \\ & + k_r\theta_r^{(T-20)}(DO_{sat} - DO) - SOD \end{aligned} \quad (12.24)$$

$$dCBOD/dt = -k_{CBOD}\theta_{CBOD}^{(T-20)}CBOD \quad (12.25)$$

$$dNBOD/dt = -k_{NBOD}\theta_{NBOD}^{(T-20)}NBOD \quad (12.26)$$

The mean and range values for coefficients included in these dissolved oxygen models are shown in Table 12.3.

## 4.8. Nutrients and Eutrophication

Eutrophication is the progressive process of nutrient enrichment of water systems. The increase in nutrients leads to an increase in the productivity of the water system, which 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. Taking the example shown in Figure 12.11, consider the growth of algae *A* (mg/l), 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 modelled as a Michaelis–Menten multiplicative effect; in other words, the nutrients have a synergistic effect. Model parameters include a maximum algal growth rate $\mu$ (1/day) times the fraction of a day, $f_d$, that rate applies (Figure 12.12), the half saturation constants $K_P$ and $K_N$ (mg/l) (shown as $K_C$ in Figure 12.13) 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 occur in proportion to their contents in the algae 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 Figure 12.11 can be written as follows:

For algae biomass:

$$\begin{aligned} dA/dt = & \mu f_d \theta_A^{(T-20)}[P/(P + K_P)][N_n/(N_n + K_N)] \\ & \times A - e\theta_A^{(T-20)}A \end{aligned} \quad (12.27)$$

For organic phosphorus:

$$dP_o/dt = -k_{op}\theta_{op}^{(T-20)}P_o \quad (12.28)$$

**Table 12.3.** Typical values of parameters used in the dissolved oxygen models.

| parameter | value | | units |
|---|---|---|---|
| $k_r$, slow, deep rivers | 0.1-0.4 | - a | 1/day |
| $k_r$, typical conditions | 0.4-1.5 | - a | 1/day |
| $k_r$, swift, deep rivers | 1.5-4.0 | - a | 1/day |
| $k_r$, swift, shallow rivers | 4.0-10.0 | - a | 1/day |
| $k_{CBOD}$, untreated discharges | 0.35 (0.20-0.50) | - b | 1/day |
| $k_{CBOD}$, primary treatment | 0.20 (0.10-0.30) | - b | 1/day |
| $k_{CBOD}$, activated sludge | 0.075 (0.05-0.10) | - b | 1/day |
| $\theta_{CBOD}$ | 1.04 | - a | — |
|  | 1.047 | - a | — |
|  | 1.04 (1.02-1.09) | - c | — |
| $\theta_r$ | 1.024 (1.005-1.030) | - c | --- |

| sediment oxygen demand * | value | | units |
|---|---|---|---|
| municipal sludge (outfall vicinity) | 4 (2-10) | - c d | g $O_2$ / m$^2$ / day |
| municipal sewage sludge | 1.5 (1-2) | - c d | g $O_2$/ m$^2$/ day |
| sandy bottom | 0.5 (0.2-1.0) | - c d | g $O_2$/ m$^2$/ day |
| mineral soils | 0.07 (0.05-0.1) | - c d | g $O_2$/ m$^2$/ day |
| natural to low pollution | 0.1-10.0 | - a | g $O_2$/ m$^2$/ day |
| moderate to heavy pollution | 5-10 | - a | g $O_2$/ 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)

For phosphate phosphorus:

$$dP/dt = -\mu f_d \theta_A^{(T-20)}[P/(P + K_P)]$$
$$\times [N_n/(N_n + K_N)]a_P A \qquad (12.29)$$

For organic nitrogen:

$$dN_o/dt = -k_{on}\theta_{on}^{(T-20)}N_o \qquad (12.30)$$

For ammonia-nitrogen:

$$dN_a/dt = -\mu f_d \theta_A^{(T-20)}[P/(P + K_P)]$$
$$\times [N_n/(N_n + K_N)]a_A A$$
$$+ k_{on}\theta_{on}^{(T-20)}N_o - k_a\theta_a^{(T-20)}N_a \qquad (12.31)$$

For nitrate-nitrogen:

$$dN_n/dt = -\mu f_d \theta_A^{(T-20)}[P/(P + K_p)]$$
$$\times [N_n/(N_n + K_N)]a_N A$$
$$+ k_a\theta_a^{(T-20)}N_a - k_n\theta_n^{(T-20)}N_n \qquad (12.32)$$

For dissolved oxygen:

$$dDO/dt = -k_{CBOD}\theta_{CBOD}^{(T-20)}CBOD$$
$$- 4.57k_a\theta_a^{(T-20)}N_a - 2k_{op}\theta_{op}^{(T-20)}P_o$$
$$+ (1.5\mu f_d - 2e)\theta_A^{(T-20)}A$$
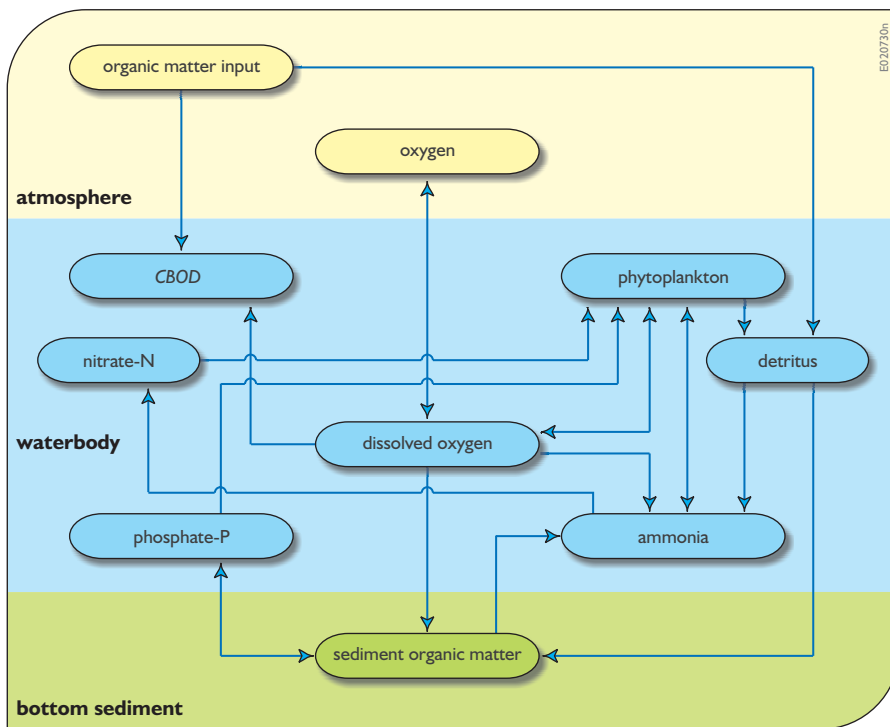$$+ k_r\theta_r^{(T-20)}(DO_{sat} - DO) - SOD \qquad (12.33)$$

**Figure 12.11.** The dissolved oxygen, nitrogen and phosphorus cycles, and phytoplankton interactions in a water body, showing the decay (satisfaction) of carbonaceous and sediment oxygen demands, re-aeration 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.
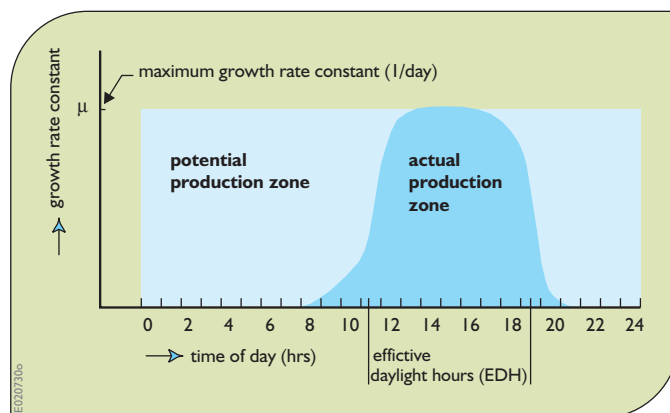


**Figure 12.12.** Calculation of the fraction, $f_d$, of the maximum growth rate constant, $\mu$, to use in the algal growth equations. The fraction $f_d$ is the ratio of actual production zone/potential production zone.



**Figure 12.13.** Defining the half saturation constant for a Michaelis–Menten model of algae. The actual growth rate constant $= \mu C/(C + K_C)$.

Representative values of the coefficients for this model are shown in Table 12.4.

Because the growth of phytoplankton cannot occur without nutrients, the eutrophication modelling must be coupled with that of nutrients. Nutrient modelling 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 $NO_3$-N) as the main forms of dissolved nitrogen in water. Furthermore, nitrogen is present in algae, as well as detritus, resulting from algae mortality, and 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.

**Table 12.4.** 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 |
| $a_P$ stoichiometric ratio | 0.012-0.015 | - c | mg P/mg A |
| $a_N$ stoichiometric 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)

Nitrification is the conversion of ammonium to nitrite and finally nitrate, requiring the presence of oxygen:

$$NH_4^+ + 2O_2 \rightarrow NO_3^- + 2H_2O + 2H^+ \qquad (12.34)$$

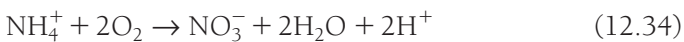Denitrification is the process occurring during the breakdown (oxidation) of organic matter by which nitrate is transformed to nitrogen gas, which is then usually lost from the water system. Denitrification occurs in anaerobic conditions:

$$NO_3^- \rightarrow N_2 \qquad (12.35)$$

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). Like 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.

Further details of the nutrient cycles are given in Section 5.

## 4.9. Toxic Chemicals

Toxic chemicals, also referred to as 'micro-pollutants', 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 micro-pollutants) and radioactive substances.

### 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 surfaces of 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 12.14 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 phases in both the water body and the bottom sediments.

The adsorption–desorption model assumes (conveniently but not always precisely) that an equilibrium exists between the dissolved (in water) and adsorbed (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 $K_p$ (litres/kg). This is shown in Figure 12.15.
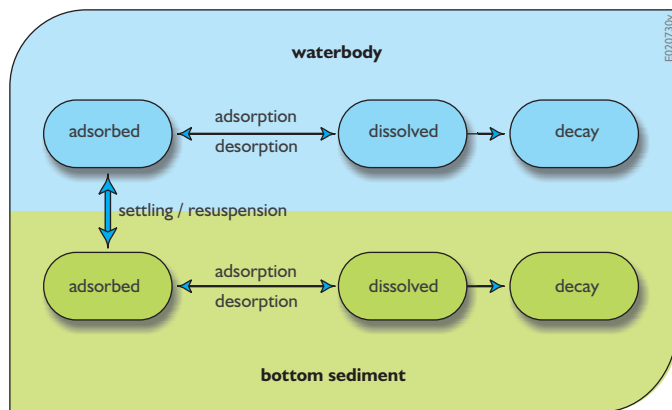
**Figure 12.14.** Schematic of the adsorption/desorption and decay processes of various toxic chemicals in water bodies and bottom sediments.



**Figure 12.15.** Defining the partition coefficient $K_p$ (litres/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.

Each partition coefficient $K_p$ (mg/kgDW/mg/l water or l/kg) is defined as the ratio of the particulate concentration $C'_p$ of a micro-pollutant (mg/kgDW or mg/kgC) divided by the dissolved concentration $C'_d$ of a micro-pollutant (mg/l water).

$$K_p = C'_p/C'_d \tag{12.36}$$

Representative values of partition coefficients $K_p$ are given in Table 12.5.

The presence of a micro-pollutant in a water system 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 micro-pollutants is largely determined by adsorption to particulate matter, suspended inorganic and organic matter (including phytoplankton) has 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 modelled part of the water system by burial.

The rates of settling and resuspension of micro-pollutants are proportional to the rates for particulate matter. An additional process called bioturbation leads to



**Table 12.5.** 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 |

the redistribution of the micro-pollutant among sediment layers. Bioturbation is caused by the physical activity of organisms, and affects both the particulate and dissolved phases but at different rates. Bioturbation is taken into account by means of dispersion coefficients.

For modelling 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 adsorbed fraction $(f_{aw})$;

$$C_w = (f_{dw} + f_{aw})C_w \tag{12.37}$$

In turn, the adsorbed fraction is composed the fractions of a micro-pollutant adsorbed to inorganic particulate

matter, $fim$, dead particulate organic matter, $fpoc$, and algae, $falg$. The total micro-pollutant concentration, $C_w$ (mg/m$^3$) is the sum of all these fractions:

$$C_w = (f_{dw} + fim + fpoc + falg)C_w \qquad (12.38)$$

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

$$DC_w = f_{dw}C_w \qquad (12.39)$$
$$AC_w = f_{aw}C_w \qquad (12.40)$$

where the fractions

$$f_{dw} = 1/(1 + K_pSS) \qquad (12.41)$$
$$f_{aw} = 1 - f_{dw} = K_pSS/(1 + K_pSS) \qquad (12.42)$$

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);

$$DC_s = f_{ds}C_s \qquad (12.43)$$
$$AC_s = f_{as}C_s \qquad (12.44)$$

These fractions are dependent on the sediment porosity, $\phi$, and density, $\rho_s$ (kg/l):

$$f_{ds} = 1/[\phi + \rho_s(1 - \phi)K_p] \qquad (12.45)$$
$$f_{as} = 1 - f_{ds} = ([\phi + \rho_s(1 - \phi)K_p] - 1)/ \\ [\phi + \rho_s(1 - \phi)K_p] \qquad (12.46)$$

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:

$$dC_w/dt = -k_w\theta_w^{(T-20)}f_{dw}C_w \\ - f_{aw}C_wS + f_{as}C_sr \qquad (12.47)$$
$$dC_s/dt = -k_s\theta_s^{(T-20)}f_{ds}C_s \\ + f_{aw}C_wS - f_{as}C_sr \qquad (12.48)$$

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 $\theta$ 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 $\theta$. The settling and resuspension of suspended solids can be determined each day from a sediment model.

### 4.9.2. Heavy Metals

The behaviour of heavy metals in the environment depends on their inherent chemical properties. Heavy metals can be divided into different categories according to their dissolved form and redox 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 sulphides under chemically reducing conditions. These sulphides generally settle in bottom sediments and are essentially unavailable ecologically. 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 Equations 12.39–12.42). 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 modelled 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 sulphides or hydroxides can be modelled. 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.

### 4.9.3. Organic Micro-pollutants

Organic micro-pollutants are generally biocides (such as pesticides or herbicides), solvents or combustion products, and include substances such as hexachlorohexane, hexachlorobenzene, PCBs or polychlorobiphenyls, benzo-a-pyrene and fluoranthene (PAHs or polycyclic aromatic hydrocarbons), diuron and linuron, atrazine and simazine, mevinfos and dichlorvos, and dinoseb.

The short-term fate of organic micro-pollutants 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 micro-pollutant 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 micro-pollutants are generally very poorly soluble in water and prefer to adsorb to particulate matter in the water, especially particulate organic matter and algae. Therefore, the fractions of a micro-pollutant adsorbed to inorganic matter, $fim$, dead particulate organic matter, $fpoc$, the dissolved fraction of a micro-pollutant, $fd$, and algae, $falg$, add up to the total micro-pollutant concentration, $C$ (mg/m$^3$);

$$C = (fd + fim + fpoc + falg)C \tag{12.49}$$

The fractions are functions of the partition coefficients $K_p$ (for algae (m$^3$/gC), for inorganic matter (m$^3$/gDW) and for dead particulate organic matter (m$^3$/gC)), the individual concentrations $C$ (for algae biomass (gC/m$^3$), for inorganic matter (gDW/m$^3$) and for dead particulate organic matter (gC/m$^3$)), and the porosity $\phi$ (m$^3$water/m$^3$bulk). In surface water the value for porosity is 1.

$$fd = \phi/[\phi + Kpalg\ Calg + Kpim\ Cim \\ + Kppoc\ Cpoc] \tag{12.50}$$

$$fim = (1 - fd)\ Kpim\ Cim/ \\ [Kpalg\ Calg + Kpim\ Cim + Kppoc\ Cpoc] \tag{12.51}$$

$$fpoc = (1 - fd)\ Kppoc\ Cpoc/ \\ [Kpalg\ Calg + Kpim\ Cim + Kppoc\ Cpoc] \tag{12.52}$$

$$falg = (1 - fd - fim - fpoc) \tag{12.53}$$

In terms of bulk measures, each partition coefficient $K_p$ (see Equation 12.36) also equals the porosity $\phi$ times the bulk particulate concentration $Cp$ (mg/m$^3$ bulk) divided by the product of the dissolved (mg/l bulk) and particulate (mg/m$^3$ bulk) bulk concentrations, $Cd\ Cs$, all times $10^6$ mg/kg.

$$K_p = 10^6\ \phi Cp/(CdCs) \tag{12.54}$$

Partitioning can be simulated based on the above equilibrium approach or according to slow sorption kinetics. For the latter, the rate, $dCp/dt$, of adsorption or desorption (mg/m$^3$/day) depends on a first order kinetic constant $ksorp$ (day$^{-1}$) for adsorption and desorption times the difference between equilibrium particulate concentration $Cpe$ of a micro-pollutant (mg/m$^3$ bulk) and the actual particulate concentration $Cp$ (mg/m$^3$ bulk) of a micro-pollutant.

$$dCp/dt = ksorp(Cpe - Cp) \tag{12.55}$$

The kinetic constant for sorption is not temperature dependent. All other kinetic constants for micro-pollutants are temperature dependent.

Mass-balance equations are similar for all micro-pollutants except for the loss processes.

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

Volatilization is formulated according to the double film theory. The volatization rate $dCd/dt$ (mg/m$^3$/day) of dissolved micro-pollutant concentrations, $Cd$ (mg/m$^3$ water), in water depends on an overall transfer coefficient, $kvol$ (m/day), for volatilization and the depth of the water column, $H$ (m);

$$dCd/dt = - kvol\ Cd/H \qquad (12.56)$$

The numerator ($kvol\ Cd$) 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 modelled as

$$dC/dt = - kC \qquad (12.57)$$

where $C$ is the total concentration of a micro-pollutant (mg/m$^3$), and $k$ is a (pseudo) temperature-dependent first-order kinetic rate constant for biodegradation, photolysis, hydrolysis or overall degradation (day$^{-1}$).

### 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, with respect to 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 modelled as a first order process involving a kinetic radioactive decay constant, $kdec$ (day$^{-1}$). 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:

$$Ac = 10^{-3}\ N_A kdec C_R /[86400\ Mw] \qquad (12.58)$$

where

$Ac$ = activity of the radionuclide (Bq/m$^3$/s)

$N_A$ = Avogadro's number (6.02 $*$ 10$^{23}$ mole)

$Mw$ = molecular weight of the radionuclide (g/mole).

## 4.10. Sediments

As discussed in the previous section, sediments 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 mm to 20 mm) or sand (0.07 mm to 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 its 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 behaviour of this fine-grained suspended matter affects water quality in several ways. First, turbidity and its effect on the underwater light climate is an important environmental condition for algae growth. The presence of suspended sediment increases the attenuation of light in the water column, which 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.

## 4.10.1. Processes and Modelling Assumptions

From a water quality perspective, the three most important sediment processes are sedimentation, resuspension or 'erosion', and 'burial' of sediment.

The modelling of sedimentation and erosion processes originates in part from the Partheniades–Krone concept (Partheniades, 1962; Krone, 1962). In this concept, the bottom shear stress plays an essential role in defining whether or not sedimentation of suspended particles or erosion of bed material will occur. Sedimentation takes place when the bottom shear stress drops below a critical value. Resuspension occurs when the bottom shear stress exceeds a critical value. The calculation of bed shear stress is discussed in Section 4.10.5.

For purposes of modelling chemical concentrations in the bottom sediment, one or more sediment layers are usually defined. Each sediment layer is assumed homogeneous (well mixed). The density of the layer can vary, depending on the variable sediment layer composition. The porosity within a given layer is assumed constant and user-defined. Water quality models do not generally consider horizontal transport of bed sediments. This horizontal transport would result in a change in the amount of sediment present in the bottom, and hence a change in the thickness of the layer of non-cohesive sediment.

## 4.10.2. Sedimentation

A characteristic feature of cohesive sediments is their ability to form aggregates of flocs that settle to the bottom, in a process called sedimentation. Whether a particle will settle to the bottom depends on its size and density, and the chemical conditions of the surrounding water system. Various laboratory and field measurements show that the suspended matter concentration strongly influences the aggregation process and thereby the settling velocities of the aggregates (Krone, 1962). Strong flocs are denser and have larger settling velocities.

Sediment floc aggregation depends on the chemical and physical properties of the sediment, and on salinity and turbulence. At high sediment concentrations (several g/l) the particles hinder each other, decreasing their settling velocity. Turbulence affects the flocculation and therefore the settling velocity in two opposing ways. Increased turbulence will increase the collisions between

particles, resulting in larger flocs with higher settling velocities, but increased turbulent shear stresses will break up the flocs and decrease their settling velocities.

Sedimentation occurs when the bottom shear stress drops below a critical value. Total shear stress is the sum of the shear stresses induced by flows and wind waves. Sedimentation rates can depend on salinity concentrations.

For any sediment particle $j$ that settles out of the water column, the rate of settling depends on the flow velocity shear stress, $\tau$ (kg/m/sec$^2$), at the bottom surface–water interface, the critical shear stress, $\tau_j$, for the substance $j$, a zero order sedimentation rate, $ZS_j$ (g/m$^2$/day), and the sedimentation velocity, $VS_j$ (m/day), for the settling substance, $C_j$ (g dry wt./m$^3$/day), all divided by the depth, $H$ (m), of settling in the water column.

If the shear stress $\tau$ at the bottom-water interface is less than the critical shear stress $\tau_j$ for the substance $j$, settling is assumed to take place. The rate of decrease of the substance (g dry wt./m$^3$/day) in the water column due to settling is

$$dC_j/dt = -[1 - (\tau/\tau_j)]\,(ZS_j + VS_jC_j)/H \quad \tau \le \tau_j$$

(12.59)

The corresponding flux (g dry wt./m$^2$ of sediment layer area/day) of substance $j$ onto the sediment layer (accretion) is

$$dC_j^{sed}/dt = -(dC_j/dt)\,H \tag{12.60}$$

Sedimentation always results in an increase of the substance settling in the upper sediment bed layer. The quantity of sedimentation in one model time-step cannot exceed the available amount of substance in the water column.

No net resuspension is assumed to take place if sedimentation occurs.

## 4.10.3. Resuspension

If the shear stress $\tau$ exceeds the critical shear stress $\tau_j$ for the type substance $j$, then no net settling takes place. Instead, resuspension can take place (also called 'erosion').

Erosion of cohesive bed material occurs when the bed shear forces exceed the resistance of the bed sediment. The resistance of the bed is characterized by a certain critical erosive strength (bottom shear stress). This critical stress is determined by several factors, such as the chemical

composition of the bed material, particle size distribution and bioturbation. Erosion of sediment is induced by the bed stress due to flow velocities, tidal and wind-induced advective flows, and surface waves. Erosion is directly proportional to the excess of the applied shear stress over the critical erosive bottom shear stress. One formula for erosion of homogeneous beds is based on Partheniades (1962). The erosion/resuspension flux is limited by the available amount of sediment on the sea bed. Typically a one-layer homogeneous bed is assumed.

The rate of resuspension (g dry wt./m$^2$ of bottom layer area/day) of substance $j$ going into the water column depends on these flow velocity shear stresses, a zero-order resuspension flux $ZR$ (g/m$^2$/day) if any, a resuspension rate constant $kR_j$ (day$^{-1}$), and the amount of substance $C_j^{sed}$ in the top sediment layer (g/m$^2$);

$$dC_j/dt = [(\tau/\tau_j) - 1](ZR_j + kR_jC_j^{sed})/H \quad \tau \geq \tau_j$$
$$(12.61)$$

The corresponding flux (g dry wt./m$^2$ sediment layer area/day) of substance $C_j^{sed}$ from the sediment layer area (erosion) is

$$dC_j^{sed}/dt = -(dC_j/dt) H \qquad (12.62)$$

No sedimentation is assumed if resuspension occurs. Resuspension results in a decrease of sediment in the upper sediment bed layer. The sedimentation in one model time step cannot exceed the available amount of substance in the sediment layer. The values of $ZR_j$ and $\tau$ strongly depend on the sediment properties and environmental parameter values.

For water quality considerations, the chemical composition of the resuspending sediment is assumed to be the same as that of the bottom sediment. Resuspension of chemical component concentrations, $N_j$ (g/m$^3$/day), in a substance from the sediment layer is simply the substance, $C^{sed}$ resuspension flux (g dry wt./m$^2$/day) (Equation 12.62) times the fraction, $fr_j$, of component $j$ in the substance divided by the depth, $H$, of water column:

$$dN_j/dt = fr_j(dC^{sed}/dt)/H \qquad (12.63)$$

### 4.10.4. Burial

'Burial' is a term used to convey that bed sediment is no longer available for resuspension because it has been covered by much newer sediment, i.e. it has been buried. This concept is important especially with respect to contaminated sediments, as it implies that buried contaminated sediments are isolated from the overlying water column and no longer pose a threat to the water quality.

Burial is a sink for sediments that are otherwise susceptible for resuspension. Assuming a fixed active sediment layer thickness, burial occurs when this thickness is exceeded. Establishing this requires knowledge of the depth, $h_j$ (m/g dry wt/m$^2$) of particle size substance $j$ per unit dry wt per square metre. Hence, if the total depth of the active sediment layer, $\sum_j C_j^{sed}h_j$, is greater than the assumed maximum depth, $D^{max}$ (m), of active sediment layer, then burial will result. The decrease in available sediment substance $j$ will be in proportion to its contribution, $C_j^{sed}h_j$, to the total depth, $\sum_j C_j^{sed}h_j$, of the sediment layer. The burial flux will equal a burial rate constant $k_B$ (day$^{-1}$ and usually set equal to 1) times the amount $C_j^{sed}$ of substance $j$ times the depth ratio times the excess depth ratio, $(\sum_j C_j^{sed}h_j - D^{max})/(\sum_j C_j^{sed}h_j)$.

$$dC_j^{bur}/dt = k_B C_j^{sed}\left[ C_j^{sed}h_j \bigg/ \left(\sum_j C_j^{sed}h_j\right)\right]$$
$$\times \left[\sum_j C_j^{sed}h_j - D^{max}\right] \bigg/ \left(\sum_j C_j^{sed}h_j\right) \qquad (12.64)$$

### 4.10.5. Bed Shear Stress

The bed shear stress directly influences the sedimentation and erosion rates. It depends on the flow (currents) and the wind-generated (and sometimes human-generated) surface waves. For sedimentation–erosion processes, it is usually assumed that the total bed shear stress, $\tau$ (Newton/m$^2$ or kg/m/s$^2$) due to flow, $\tau_{flow}$, and waves, $\tau_{wave}$, are additive:

$$\tau = \tau_{flow} + \tau_{wave} \qquad (12.65)$$

The bed shear stress $\tau_{flow}$ for depth-averaged flow depends on the water density (1,000 kg/m$^3$), the horizontal flow velocity, $U_h$ (m/s), acceleration of gravity, $g$ (9.81 m/s$^2$), and a Chezy coefficient, $Cz$ (m$^{0.5}$/s).

$$\tau_{flow} = 1,000 \ (9.81)U_h^2/Cz^2 \qquad (12.66)$$

The Chezy coefficient, $Cz$ ($m^{0.5}$/s), is defined as a function of water depth, $H$ (m), and bottom roughness length (Nikuradse equivalent roughness length) (m), *Rough* (m), or Manning's roughness coefficient, n (s/$m^{1/3}$):

$$Cz = 18 \log_{10}(12\ H/Rough) \tag{12.67}$$

$$Cz = (H)^{1/6}/n \tag{12.68}$$

Both Nikuradse's roughness coefficient and Manning's roughness coefficient may be changing due to bed load movements. Here (and in most models) they are assumed fixed.

Surface waves are caused by wind stress on the water surface. The magnitude of the waves depends on the wind conditions, wind duration, water depth and bottom friction. Wave fields are commonly described by the significant wave height, significant wave period and wavelength. Waves induce a vertical circular movement (orbital velocity) that decreases with depth. The waves exert friction forces on the bed during propagation.

The magnitude of the bed shear stress, $\tau_{wave}$, due to waves depends on a wave friction factor, $f_w$, the density of water, (1,000 kg/$m^3$) and the effective orbital horizontal velocity at the bed surface, $U_o$.

$$\tau_{wave} = 0.25\ (1,000)\ f_w U_o^2 \tag{12.69}$$

The wave friction factor, $f_w$, and the effective orbital horizontal velocity at the bed surface, $U_o$, are functions of three wave parameters: the significant wave height, $H_s$ (m), the mean wave period, $T_m$ (s), and mean wave length, $L_m$ (m) (see also Figure 12.16). Also required is the depth of water, $H$ (m).

The effective horizontal bottom velocity due to waves is defined as

$$U_o = \pi H_s/[T_m \sinh(2\pi H/L_m)] \tag{12.70}$$

The friction or shear factor, $f_w$, can be calculated in two ways (Monbaliu, et al., 1999). One way is

$$f_w = 0.16\ [Rough/(U_o T_m/2\pi)]^{0.5} \tag{12.71}$$

The other way uses a factor depending on a parameter $A$ defined as

$$A = H_s/[2\ Rough \sinh(2\pi H/L_m)] \tag{12.72}$$

If $A > 1.47$ then

$$f_w = \exp\{-5.977 + 5.123H^{-0.194}\} \tag{12.73}$$

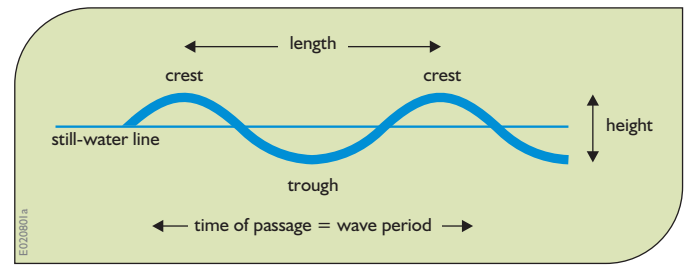Otherwise

$$f_w = 0.32 \tag{12.74}$$



**Figure 12.16. Wave dimensions of significant wave height, period and length.**

## 4.11. Lakes and Reservoirs

The water quality modelling principles discussed above are applicable to all different types of water systems: streams, rivers, lakes, estuaries and even coastal or ocean waters. This section presents some of the unique aspects of water quality modelling in lakes. The physical character and water quality of rivers draining into lakes and reservoirs are governed in part by the velocity and 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. Sediment and other material that were 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. There are greater opportunities for the growth of algae (phytoplankton) and the development of eutrophication.

Reservoirs typically receive larger inputs of water (as well as soil and other materials carried in rivers) than lakes do, and as a result, may receive larger pollutant loads. 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. 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 variables measured within the water basin. Although there are many variables of limnological significance,

water quality is typically characterized on the basis of conditions such as:

- 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)
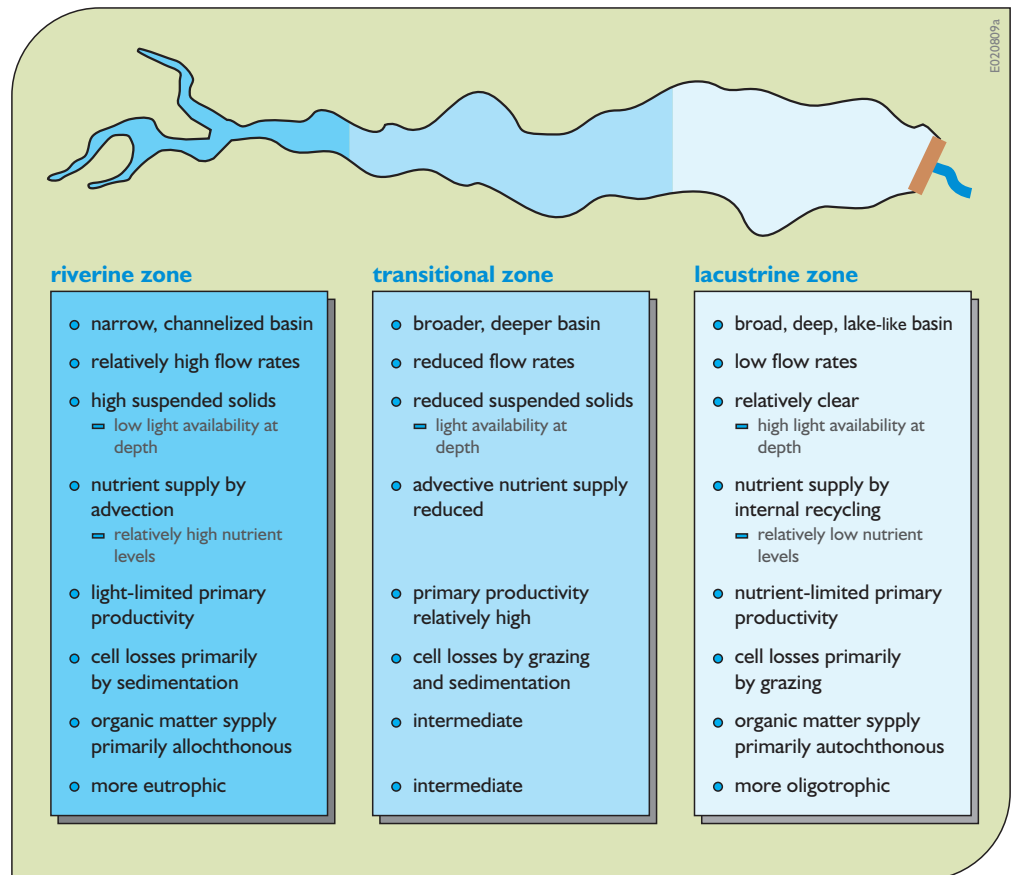- acidity (a neutral pH of 7 is preferred).

Many waste chemical compounds from industry, some with toxic or deleterious effects on humans and/or other water-dependent organisms and products, are discharged into lakes and reservoirs. Some 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 non-tropical regions, usually have poorer water quality in their lower layers, due to stratification (see Section 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 pollutant inputs are discharged and have a greater potential for disturbance of bottom muds and the like. 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 Figure 12.17.

**Figure 12.17.** Longitudinal zonation of water quality and other variables in reservoirs (UNDP, 2000).



**riverine zone**

- narrow, channelized basin
- relatively high flow rates
- high suspended solids
  - low light availability at depth
- nutrient supply by advection
  - relatively high nutrient levels
- light-limited primary productivity
- cell losses primarily by sedimentation
- organic matter sypply primarily allochthonous
- more eutrophic

**transitional zone**

- broader, deeper basin
- reduced flow rates
- reduced suspended solids
  - light availability at depth
- advective nutrient supply reduced
- primary productivity relatively high
- cell losses by grazing and sedimentation
- intermediate
- intermediate

**lacustrine zone**

- broad, deep, lake-like basin
- low flow rates
- relatively clear
  - high light availability at depth
- nutrient supply by internal recycling
  - relatively low nutrient levels
- nutrient-limited primary productivity
- cell losses primarily by grazing
- organic matter sypply primarily autochthonous
- more oligotrophic

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 (Figure 12.17). The relative size and volume of the three zones can vary greatly in a given reservoir.

### 4.11.1. Downstream Characteristics

Constructing a dam can produce dramatic changes in the downstream river channel below it. These are quite unlike downstream changes from lakes. Because reservoirs act as sediment and nutrient traps, the water at the dam end of a reservoir is typically of higher quality than water entering the reservoir. This higher-quality water subsequently flows into the downstream river channel below the dam. This phenomenon 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 it can now pick up and transport. Because it contains less sediment, the discharged water can scour and erode the streambed and banks, picking up new sediment as it continues downstream. This scouring effect can have significant negative impacts on 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 supplies, have water release or discharge structures located at different vertical levels in their dams (Figure 12.18). This allows for the withdrawal or discharge of water from different layers within the reservoir, known as '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 makes it possible to affect both flora and fauna, and possibly even the geomorphology of the stream or river.
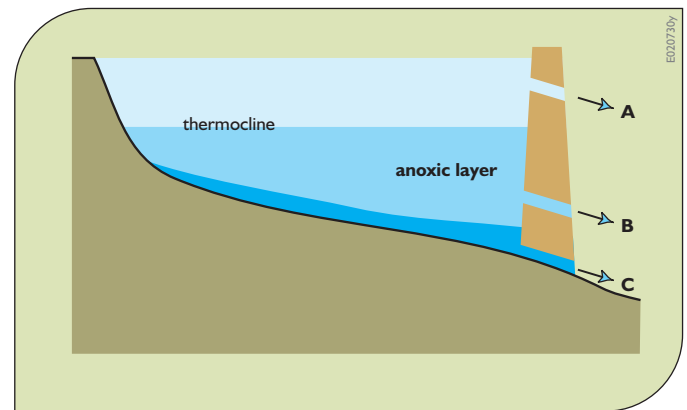


**Figure 12.18.** A multiple-outlet reservoir can be better used to regulate the temperature and water quality downstream.

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.

Agriculture 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) unbalance lake ecosystems. When temperature and light conditions are favourable, excessive nutrients stimulate population explosions of undesirable algae and aquatic weeds. After the algae die, they sink to the lake bottom, where bacteria consume the available dissolved oxygen as they decompose the algae. Fish may die and foul odours may result if dissolved oxygen is depleted.

Heavy metals are another major cause of lake quality impairment. Our knowledge of this is mainly due to the widespread detection of heavy metals in fish tissue samples. Since it is difficult to measure mercury in ambient water, and since it bioaccumulates in fish tissue, fish samples are commonly used to indicate the level of contamination. Common sources of mercury involve atmospheric transport from power-generating facilities and other 'smoke-stack' industries.

In addition to nutrient and metal siltation, enrichment by organic wastes that deplete oxygen and by noxious aquatic plants affect lakes and reservoirs. Often,

several pollutants and processes affect 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 hydrological modifications are also sources of lake pollutants.

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.

### 4.11.2. Lake Quality Models

Perhaps the simplest way to begin modelling 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 $k_C$ (day$^{-1}$) into a lake having a volume $V$ (m$^3$) and inflow and outflow rate of $Q$ (m$^3$/day), then the rate of change in the concentration $C$ (g/m$^3$/day) is

$$dC/dt = (1/V)(W_C - QC - k_CCV) \tag{12.75}$$

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 the previous time period, $t-1$. For a period duration of $\Delta t$ days,

$$C(t) = [W_C/(Q + k_CV)]$$
$$[1 - \exp\{-\Delta t((Q/V) + k_C)\}]$$
$$+ C(t-1) \exp\{-\Delta t((Q/V) + k_C)\} \tag{12.76}$$

The equilibrium concentration, $C_e$, can be obtained by assuming each concentration is equal in Equation 12.76 or by setting the rate in Equation 12.75 to 0, or by setting $C(t-1)$ equal to 0 and letting $\Delta t$ go to infinity in Equation 12.76. The net result is

$$C_e = W_C/(Q + k_CV) \tag{12.77}$$

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

$$t_\alpha = - V[\ln(1 - \alpha)]/(Q + K_CV) \tag{12.78}$$

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

$$dC/dt = - C(Q + k_CV)/V \tag{12.79}$$

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

$$C(t) = C(0) \exp\{- t((Q/V) + K_C) \tag{12.80}$$

In this case, one can solve for the time $t_\alpha$ required for the constituent to reach a fraction $(1 - \alpha)$ of the initial concentration $C(0)$ (that is, $C(t)/C(0) = (1 - \alpha)$). The result is Equation 12.78.

Equation 12.76 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:

Minimize $X$ $\tag{12.81}$

Subject to the following mass-balance and constituent concentration constraints for each period $t$:

$$C(t) = [W_C(t)(1-X)/(Q(t) + k_CV)]$$
$$[1 - \exp\{-\Delta t((Q(t)/V) + k_C)\}]$$
$$+ C(t-1) \exp\{-\Delta t((Q(t)/V) + k_C)\} \tag{12.82}$$

$$C(t) \leq C(t)^{\max} \tag{12.83}$$

If each period $t$ is a within-year period, and if the wasteloadings 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.

### 4.11.3. Stratified Impoundments

Many deep impoundments become stratified during particular times of the year. Vertical temperature gradients arise that imply vertical density gradients. The depth-dependent density gradients in stratified lakes effectively prevent complete vertical mixing. Particularly in the summer season, lakes may exhibit two zones: 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* (Figure 12.18).

Because of lake 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 Figure 12.19

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 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, $kC_e(t)$:

$$dC_e(t)/dt = (1/V_e(t))\{(W_C(t) - C_e(t)Q^{out}(t)) + (v/D_T)[C_h(t)V_h(t) - C_e(t)V_e(t)]\} - kC_e(t) \tag{12.84}$$

$$dC_h(t)/dt = -kC_h(t) - (v/D_T)[C_h(t) - C_e(t)V_e(t)/V_h(t)] - sH_h(t)C_h(t) \tag{12.85}$$

In the above two equations, $V_e$ and $V_h$ (m$^3$) are the time-dependent volumes of the epilimnion and hypolimnion respectively; $k$ (day$^{-1}$) 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).
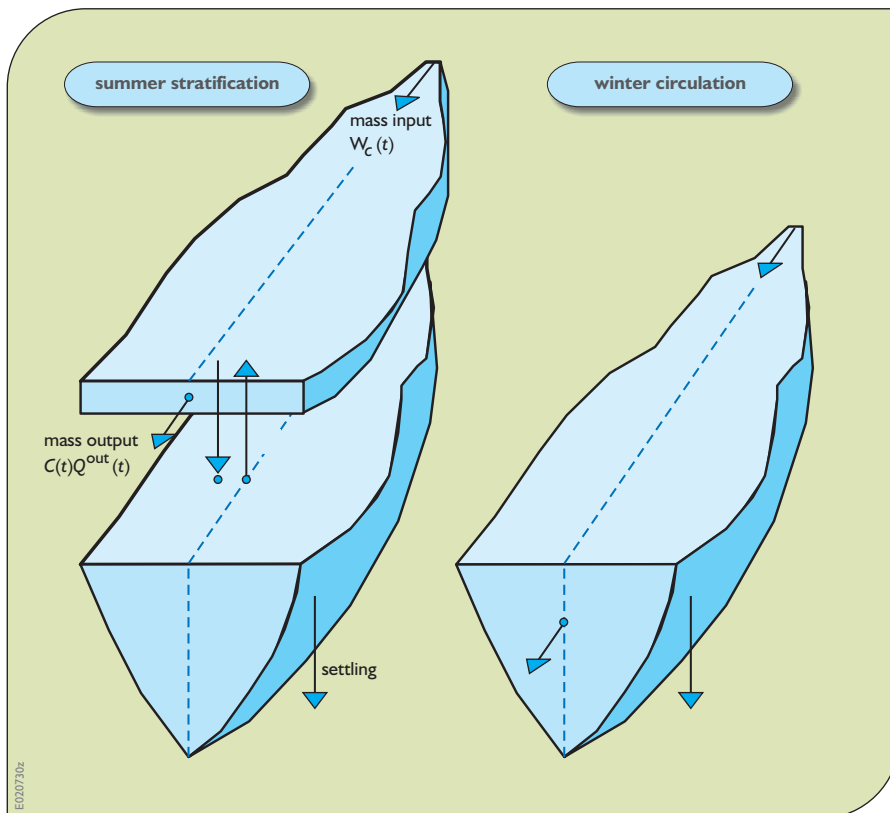


**Figure 12.19.** Lake stratification during summer and complete mixing during winter season.

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:

$$C(t) = C_e(t)V_e(t) + C_h(t)V_h(t)/[V_e + V_h] \qquad (12.86)$$

$$dC(t)/dt = (1/V(t))\{(W_C(t) - C(t)Q^{out}(t)) - kC_e(t) - sH(t)C(t) \qquad (12.87)$$

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

$$C_e(t) = C(t) \qquad (12.88)$$

$$C_h(t) = C(t) \qquad (12.89)$$

# 5. An Algal Biomass Prediction Model

An alternative approach to modelling the nutrient, oxygen and algae parts of an ecological model has been implemented in a simulation model developed by WL | Delft Hydraulics called DELWAQ-BLOOM (Los, 1991; Los et al., 1992; Molen et al., 1994; Smits 2001; WL | Delft Hydraulics, 2003). This model is used to predict algae growth and mortality, oxygen concentrations and nutrient dynamics.

The ecological model DELWAQ-BLOOM calculates the advection and dispersion of constituents (state variables) in the water column, and the water quality and ecological processes affecting the concentrations of the constituents. It is based on a three-dimensional version of the governing Equation 12.10. The focus here will be on the source and sink terms in that equation that define the water quality and ecological processes, mostly related to algae growth and mortality, mineralization of organic matter, nutrient uptake and release, and oxygen production and consumption.

For this discussion, consider three nutrient cycles (nitrogen, N, phosphorus, P, and silica, Si) and five different groups of algae, (phytoplankton (diatoms, flagellates and dinoflagellates) or macroalgae ('attached' or 'suspended' *Ulva*)), suspended and bottom detritus, oxygen and inorganic phosphorus particulate matter in the bottom sediments. Different predefined sets of species are available for marine and freshwater ecosystems.

The model processes relating these substances are all interrelated. However, for clarity, the processes can be grouped into nutrient cycling, algae modelling, and oxygen-related processes.

## 5.1. Nutrient Cycling

The DELWAQ-BLOOM model assumes that algae consume ammonia and nitrate in the water column. It includes the uptake of inorganic nutrients by bottom algae, algae-mortality-producing detritus and inorganic nutrients, mineralization of detritus in the water column producing inorganic nutrients, and mineralization of detritus in the bottom that also produces inorganic nutrients. Optionally the model includes algae species with the ability to take up atomic nitrogen (N-fixation) and detritus (mixotrophic growth). The model accounts for the settling of suspended detritus and algae and inorganic adsorbed phosphorus, resuspension of bottom detritus, release of inorganic bottom nutrients to the water, burial of bottom detritus, nitrification or denitrification depending on the dissolved oxygen concentration, and adsorption/desorption of ortho-phosphate.

## 5.2. Mineralization of Detritus

The oxidation or mineralization of the nutrients in detritus (*DetN*, *DetP*, *DetSi*) and also of detritus carbon (*DetC*) reduces detritus concentrations. The mineralization process consumes oxygen and produces inorganic nutrients ($NH_4$, $PO_4$, and $SiO_2$). The fluxes, $dC/dt$, for these four constituents $C$ (mg/l or g/m$^3$) are assumed to be governed by first order processes whose temperature corrected rate constants are $k_C\theta_C^{(T-20)}$ (1/day). Thus:

$$dC/dt = k_C\theta_C^{(T-20)}C \qquad (12.90)$$

This equation applies in the water column as well as in the bottom sediments, but the mineralization rate constants, $k_C\theta_C^{(T-20)}$, may differ. This rate constant also depends on the stochiometric composition of detritus, relative to the requirements of the bacteria. The concentrations of these detritus constituents in the bottom are usually expressed in grams per square metre of surface area divided by the depth of the sediment layer.

## 5.3. Settling of Detritus and Inorganic Particulate Phosphorus

The rate of settling of nutrients in detritus and inorganic particulate phosphorus out of the water column and on to the bottom is assumed to be proportional to their water column concentrations, $C$. Settling decreases the concentrations of these constituents in the water column.

$$dC/dt = - SR_C(C)/H \qquad (12.91)$$

The parameter $SR_C$ is the settling velocity (m/day) of constituent concentration $C$ and $H$ is the depth (m) of the water column.

## 5.4. Resuspension of Detritus and Inorganic Particulate Phosphorus

The rates at which nutrients in detritus and inorganic particulate phosphorus are resuspended depend on the flow velocities and resulting shear stresses at the bed surface–water column interface. Below a critical shear stress no resuspension occurs. Resuspension increases the masses of these constituents in the water column without changing its volume, and hence increases their concentrations in it. For $C_B$ representing the concentration (grams of dry weight per cubic metre) of resuspended material in

the active bottom sediment layer, the flux of constituent concentration in the water column is

$$dC/dt = RR_C C_B/H \qquad (12.92)$$

where $RR_C$ (m/day) is the velocity of resuspension (depending on the flow velocity) and $H$ is the depth of the water column.

## 5.5. The Nitrogen Cycle

The nitrogen cycle considers the water-column components of ammonia ($NH_4$-N), nitrite and nitrate (represented together as $NO_3$-N), algae (*AlgN*), suspended detritus (*DetN*), and suspended (non-detritus) organic nitrogen (*OON*). In the bottom, sediment bottom detritus (*BDetN*) and bottom diatoms (*BDiatN*) are considered. Figure 12.20 shows this nitrogen cycle.

### 5.5.1. Nitrification and Denitrification

Two important reactions in the nitrogen nutrient cycle are nitrification and denitrification. These reactions affect the flux of ammonia and nitrate in the water column. Given sufficient dissolved oxygen and temperature, nitrifying bacteria in the water column transform ammonium to
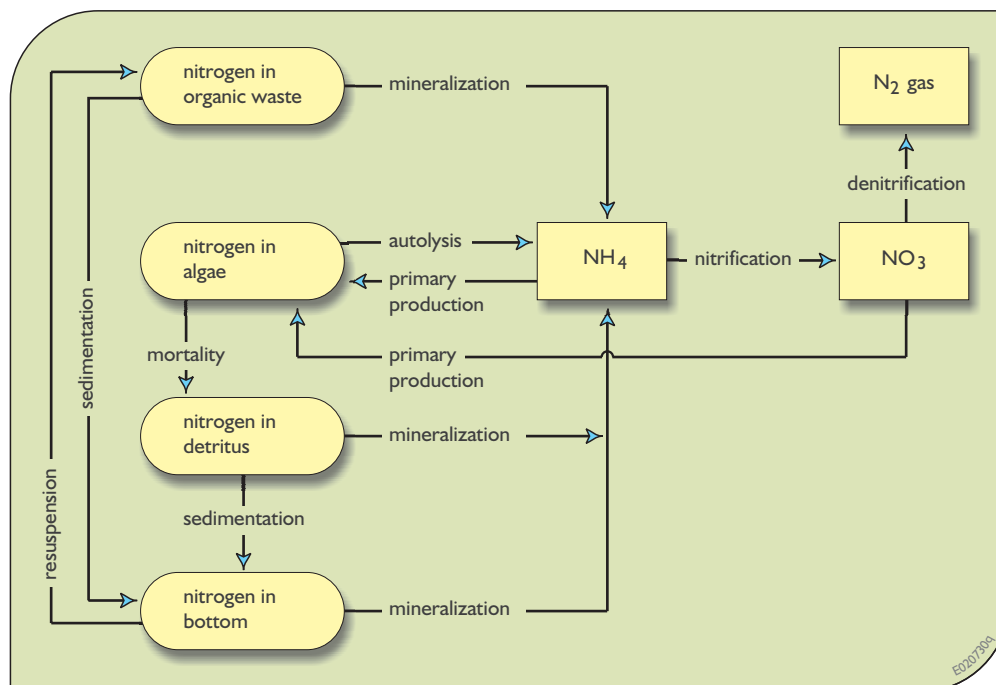


**Figure 12.20.** The nitrogen cycle processes.

nitrite and then nitrate. This can be considered as one reaction,

$$NH_4^+ + 2O_2 \rightarrow NO_3^- + H_2O + 2H^+$$

that occurs at a rate ($gN/m^3$/day) of

$$NH_4/dt = -k_{NH_4}\theta_{NH_4}^{(T-20)}NH_4 \qquad (12.93)$$

Again, $k_{NH_4}\theta_{NH_4}^{(T-20)}$ is the temperature corrected rate constant (1/day), and $NH_4$ is the concentration of nitrogen in ammonium ($gN/m^3$).

Bacterial activities decrease as temperatures decrease. Bacterial activities also require oxygen. The nitrification process stops if the dissolved oxygen level drops below about 2 mg/l or if the temperature $T$ is less than approximately 5 °C.

For each gram of nitrogen in ammonium-nitrogen $NH_4$-N reduced by nitrification, a gram of nitrate-nitrogen $NO_3$-N is produced, consuming 2 moles (64 grams) oxygen per mole (14 grams) of nitrogen (64/14 = 4.57 grams of oxygen per gram of nitrogen). Nitrification occurs only in the water column.

In surface waters with a low dissolved-oxygen content, nitrate can be transformed to free nitrogen by bacterial activity as part of the process of mineralizing organic material. This denitrification process can be written as:

$$\text{'organic matter'} + 2NO_3 \rightarrow N_2 + CO_2 + H_2O \qquad (12.94)$$

Nitrate is (directly) removed from the system by means of denitrification. The reaction proceeds at a rate:

$$dNO_3/dt = -k_{NO_3}\theta_{NO_3}^{(T-20)}NO_3 \qquad (12.95)$$

where $NO_3$ is the concentration of nitrate nitrogen ($gN/m^3$).

This process can occur both in the water column and the sediment, but in both cases results in a loss of nitrate from the water column. Algae also take up nitrate-nitrogen. As with nitrification, denitrification decreases with temperature. The reaction is assumed to stop below about 5 °C.

### 5.5.2. Inorganic Nitrogen

Ammonia is produced when algae die and the cells release their contents into the surrounding water (in a process called autolysis) and by the mineralization of organic nitrogen in the water and bottom sediment. Ammonia is converted to nitrate by nitrification. Algae use ammonia

and nitrate for growth. Different algae prefer either $NH_4$ or $NO_3$ nitrogen. Upon death they release part of their nitrogen contents as ammonia. The remaining nitrogen of dying algae becomes suspended detritus and suspended 'other organic nitrogen' (*OON*). The latter degrades at a much slower rate. Algae can also settle to the bottom. Some macroalgae (*Ulva*) can be fixed to the bottom, unless wind and water velocities are high enough to dislodge them.

Once in the bottom sediment, planktonic algae die and release all their nitrogen contents, as ammonium into the water column and to organic nitrogen in the sediment. In contrast macroalgae and bottom diatoms are attached and are subjected to the normal processes of growth, mortality and respiration.

Suspended detritus and organic nitrogen are formed upon the death of algae. Detritus is also produced by excretion of phyto- and zooplankton and from resuspension of organic matter on and in the sediment. The detritus concentration in the water column decreases by bacterial decay, sedimentation and filtration by zooplankton and benthic suspension feeders.

Bottom detritus is subject to the processes of mineralization, resuspension and burial. Mineralization of bottom detritus is assumed to be slower than that of suspended detritus. The ammonia produced from mineralization is assumed to go directly to ammonia in the water phase. Sedimentation from the water column and mortality of algae in the bottom increase the bottom pool of bottom detritus. The mineralization rate depends on the composition of the detritus, i.e. is a function of the nitrogen/carbon and phosphorus/carbon ratios.

Nitrogen is removed from the system by means of denitrification, a process that occurs under anoxic conditions. Burial is a process that puts the material in a 'deep' sediment layer, and effectively removes it from the active system. This is the only removal process for the other nutrients (P and Si).

### 5.6. Phosphorus Cycle

The phosphorus cycle (Figure 12.21) is a simplified version of the nitrogen cycle. There is only one dissolved pool: orthophosphorus, and only one removal process: burial. However, unlike nitrogen and silica, there is also inorganic phosphorus in the particulate phase (*AAP*).
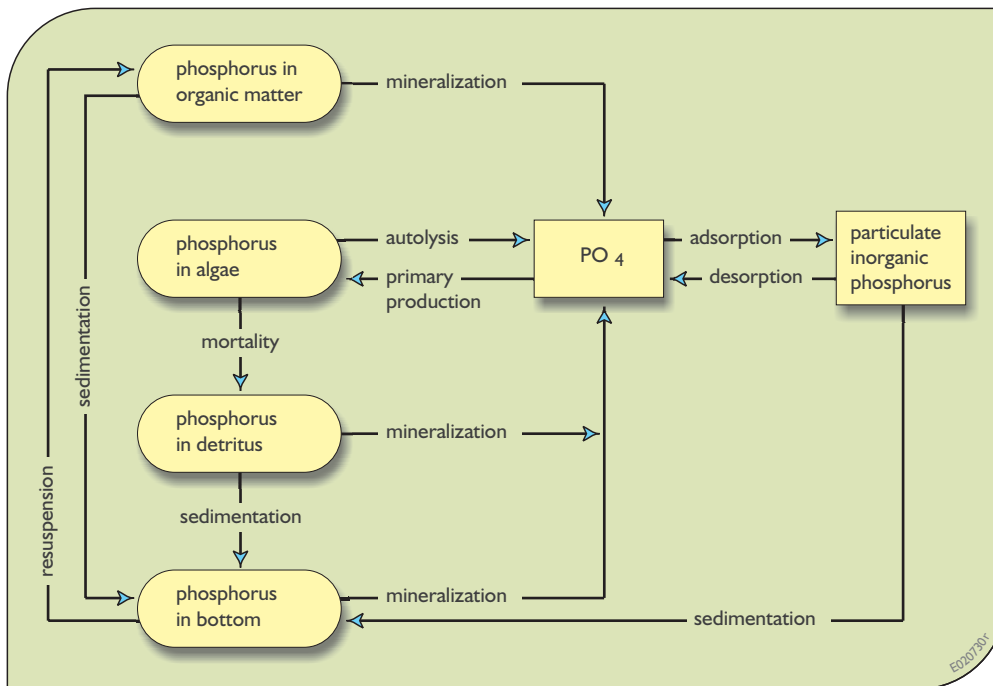
**Figure 12.21.** The processes involved in the phosphorus cycle.

The phosphorus cycle in the water column includes orthophosphate ($PO_4$), algae (*AlgP*), suspended detritus (*DetP*), suspended (non-detritus) organic phosphorus (*OOP*), inorganic adsorbed (available) *P* (*AAP*), and inorganic adsorbed (unavailable) *P* (*UAP*). In the bottom sediment the cycle includes the bottom detritus (*BDetP*) and the bottom inorganic adsorbed *P* (*BAAP*).

A reaction specific to the phosphorus cycle is the adsorbtion/desorption of particulate inorganic phosphorus. Inorganic phosphorus can be present in the aquatic environment in a dissolved form and adsorbed to inorganic particles, such as calcium or iron. The transition from one form into another is not a first order kinetic process, yet in many models desorption of inorganic phosphorus is assumed to be such.

## 5.7. Silica Cycle

The silica cycle is similar to the phosphorus cycle except that there is no adsorption of silica to inorganic suspended solids. Silica is only used by diatoms, so uptake by algae depends on the presence of diatoms. The silica cycle is shown in Figure 12.22.

The silica cycle in the water column includes dissolved silica (*Si*), diatoms (*Diat*), suspended detritus (*DetSi*), and suspended (non-detritus) organic silica (*OOSi*). In the

bottom sediment the cycle includes the bottom detritus (*BDetSi*).

## 5.8. Summary of Nutrient Cycles

The nutrient cycles just described are based on the assumption that nutrients can be recycled an infinite number of times without any losses other than due to transport, chemical adsorption, denitrification and burial. This is an over-simplification of the organic part of the
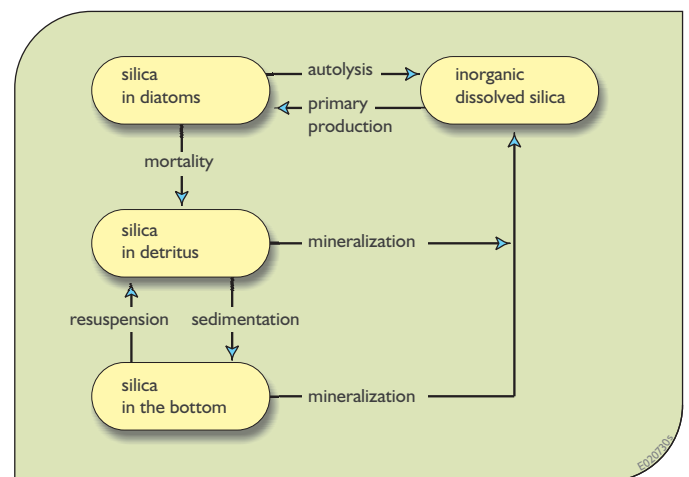


**Figure 12.22.** The processes involved in the silica cycle.

nutrient cycles. The elementary composition of living algae cells is a complicated function of their characteristics as well as the environmental conditions. Upon dying, the algae cell contents are released into the surrounding water. As the cell breaks apart, many of the nutrients are in a form that makes them instantly available for algae cell growth (autolysis). The remaining material consists of more or less degradable substances. Most of this material is mineralized either in the water or at the bottom, but a small portion degrades very slowly if at all. Most of this material settles and is ultimately buried. Resuspension delays but does not stop this process by which nutrients are permanently removed from the water system.

For simplicity, all possible removal processes are lumped into a single term, which is modelled as burial. For example, if a nominal value of 0.0025 per day is used, this means that 0.25% of the bottom amount is buried each day.

The same formulation is used for all three nutrients. Whether or not this is correct depends on the actual removal process. If deactivation is mainly burial into deeper layers of the sediment, there is no reason to distinguish between different nutrients. Other processes such as chemical binding, however, may deactivate phosphorus, but not nitrogen or silica.

## 5.9. Algae Modelling

Algal processes include primary production, mortality (producing detritus and inorganic nutrients) and grazing, settling to become bottom algae and the resuspension of bottom algae, the mortality of bottom algae to bottom detritus, and the burial of bottom algae.

The basic behaviour of algae in surface water can be illustrated by the two diagrams in Figures 12.23 and 12.24. These show the nutrient and carbon fluxes for diatoms and other algae. Diatoms are distinguished from other algae in that they need silicate to grow.

### 5.9.1. Algae Species Concentrations

The module BLOOM II computes phytoplankton within DELWAQ-BLOOM. It is based upon the principle of competition between different species. The basic variables of this module are called 'types'. A type represents the
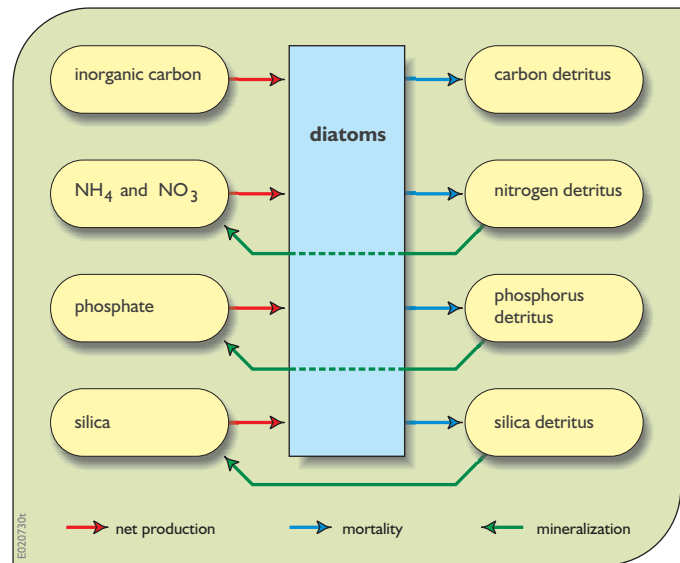


**Figure 12.23.** Modelling of diatoms.
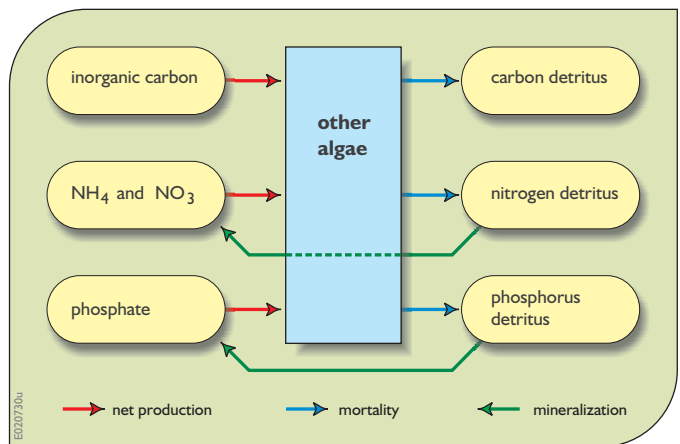


**Figure 12.24.** Modelling of other algae besides diatoms.

physiological state of a species. Usually a distinction is made between three different types: an *N*-type for nitrogen limitation, a *P*-type for phosphorus limitation and an *E*-type for light energy limitation, whose nutrient content is high (luxury uptake). The solution algorithm of the model considers all potentially limiting factors and first selects the one that is most likely to become limiting. It then selects the best-adapted type for that limitation. The suitability of a type (its fitness) is determined by the ratio of its requirement for that particular resource and its growth rate in equal proportion. This means that a type can become dominant either because it needs a

comparatively small amount of a limiting resource (it is efficient) or because it grows rapidly (it is opportunistic).

Now the algorithm considers the next potentially limiting factor and again selects the best-adapted phytoplankton type. This procedure is repeated until it is impossible to select a new pair of a type and limiting factor without violating (that is, over-exhausting) some limiting factor. Thus the model seeks the optimum solution consisting of $n$ types and $n$ limiting factors. To that purpose, it uses linear programming. Typically, BLOOM II considers between three and ten representative algae species and six to fifteen types.

As a further refinement BLOOM II takes the existing biomasses of all phytoplankton types into account. These are the result of growth, loss processes and transport during the previous time steps. Thus, the optimization algorithm does not start from scratch.

As they represent different physiological stages of the same species, the transition of one type to another is a rapid process with a characteristic time step in the order of a day. The equations of the model are formulated in a way that allows such a rapid shift between types of the same species. A transition between different species is a much slower process as it depends on mortality and net growth rates.

It is interesting that the principle just described, by which each phytoplankton type maximizes its own benefit, effectively means that the total net production of the phytoplankton community is maximized.

Denote each distinct species subtype (from now on called type) by the index $k$. The BLOOM II module identifies the optimum concentration of biomass, $B_k$, of each algae type $k$ that can be supported in the aquatic environment characterized by light conditions and nutrient concentrations. Using the net growth rate constant $Pn_k$, it will

$$\text{Maximize} \sum_k Pn_k B_k \qquad (12.96)$$

The sum of the biomass concentrations over all types $k$ is the total algae biomass concentration.

For each algae type, the requirements for nitrogen, phosphorus and silica (used only by diatoms) are specified by coefficients $n_{ik}$, the fraction of nutrient $i$ per unit biomass concentration of algae type $k$.

The total readily available concentration, $C_i$ (g/m³) of each nutrient in the water column equals the amount in

the total living biomass of algae, $\sum_k(n_{ik}B_k)$, plus the amount incorporated in dead algae, $d_i$, plus that dissolved in the water, $w_i$. These mass-balance constraints apply for each nutrient $i$.

$$\sum_k(n_{ik}\, B_k) + d_i + w_i = C_i \qquad (12.97)$$

The unknown concentration variables $B_k$, $d_i$ and $w_i$ are non-negative. All nutrient concentrations $C_i$ are the modelled (optionally measured) total concentrations and are assumed to remain constant throughout the time period (typically a day).

### 5.9.2. Nutrient Recycling

A certain amount of each algae type $k$ dies in each time step, and this takes nutrients out of the live phytoplankton pool. Most of it remains in the detritus and other organic nutrient pools; a smaller fraction (in the order of 30%) is directly available to grow new algae because the dead cells break apart (autolysis) and are dissolved in the water column. Detritus may be removed to the bottom or to the dissolved nutrient pools at rates in proportion to its concentration. Needed to model this are the mortality rate, $M_k$ (day$^{-1}$), of algae type $k$; the fraction, $f_p$, of dead phytoplankton cells that is not immediately released when a cell dies; the remineralization rate constant, $m_i$ (day$^{-1}$), of dead phytoplankton cells; the fraction, $n_{ik}$, of nutrient $i$ per unit biomass concentration of algae type $k$; and the settling rate constant, $s$ (day$^{-1}$), of dead phytoplankton cells.

The rate of change in the nutrient concentration of the dead phytoplankton cells, $dd_i/dt$, in the water column equals the increase due to mortality less that which remineralizes and that which settles to the bottom;

$$dd_i/dt = \sum_k(f_p M_k n_{ik} B_k) - m_i d_i - s d_i \qquad (12.98)$$

Both mortality and mineralization rate constants are temperature dependent.

### 5.9.3. Energy Limitation

Algae absorb light for photosynthesis. Energy becomes limiting through self-shading when the total light absorption of algae, called light extinction, exceeds the maximum at which primary production is just balanced

by respiration and mortality. For each algae type $k$ there exists a specific extinction value $K_k^{\max}$ (1/m) at which this is the case. The light intensity can also be too high, which means the total extinction is too low (photo-inhibition) for growth. This specific extinction value is $K_k^{\min}$. The ranges between $K_k^{\min}$ and $K_k^{\max}$ differ for different algal types $k$. Letting $K_k$ (m$^3$/m/gdry) represent the specific light absorbing extinction constant for living material of algae type $k$, the total extinction due to all living algae is

$$KL = \sum_k (K_k B_k) \qquad (12.99)$$

Added to this must be the extinction caused by dead cells, $KD$, and the background extinction of the water, $KW$ (1/m). As defined here, $KW$ includes the extinction by inorganic suspended matter and humic substances.

$$K_k^{\min} \le KL + KD + KW \le K_k^{\max} \qquad (12.100)$$

In an alternate formulation used in DELWAQ-BLOOM, the total light extinction coefficient in the water column (in m$^{-1}$) is the sum of background extinction ($K_b$, water and non-modelled substances) and extinction due to detritus ($K_{det}$), inorganic material ($K_{im}$), dissolved organic matter or 'yellow substances' ($K_{dom}$) and phytoplankton ($K_{phyt}$):

$$\text{Extinction} = K_b + K_{det} + K_{im} + K_{dom} + K_{phyt} \qquad (12.101)$$

The extinction from each component is calculated by its concentration multiplied by its specific extinction coefficient.

The ratio between the various extinction components is highly site specific. In general it also varies seasonally. The amount of dead cells not yet mineralized is, from Equation 12.98, $\sum_k (fpM_k B_k)$. Assuming some fraction $e_d$ (usually between 0.2 and 0.4) of the extinction rate of live cells,

$$KD = e_d \sum_k K_k fpM_k B_k \qquad (12.102)$$

If the total extinction is not within the range for an algae type $k$, then its concentration $B_k$ will be zero. To ensure that $B_k$ is 0 if the total extinction is outside of its extinction range, a 0, 1 binary (integer) unknown variable $Z_k$ is needed for each algae type $k$. If $Z_k$ is 1, $B_k$ can be any non-negative value; if it is 0, $B_k$ will be 0. This is modelled by adding three linear constraints for each algae type $k$.

$$KL + KD + KW \le K_k^{\max} + KM (1 - Z_k) \qquad (12.103)$$

$$KL + KD + KW \ge K_k^{\min} (Z_k) \qquad (12.104)$$

$$B_k \le BMZ_k \qquad (12.105)$$

where $KM$ and $BM$ are any large numbers no less than the largest possible value of the total extinction or biomass concentration, respectively. Since the objective of maximizing the sum of all $B_k$ together with Equation 12.105 is to set each $Z_k$ value equal to 1, it is only when the total extinction is outside of the extinction range $K_k^{\min}$ to $K_k^{\max}$ that the $Z_k$ value will be forced to 0. Equation 12.105 then forces the corresponding $B_k$ to 0.

### 5.9.4. Growth Limits

For all algae types $k$, the maximum potential biomass concentration, $B_k^{\max}$ (g dry/m$^3$), at the end of the time interval $\Delta t$ (days) depends on the initial biomass concentration, $B_k$, (g dry/m$^3$); the maximum gross production rate, $Pg_k^{\max}$ (day$^{-1}$); the respiration rate constant, $R_k$ (day$^{-1}$); and a time and depth averaged production efficiency factor, $E_k$. Mortality is not included in this computation. Using the net production rate constant, $Pn_k$ ($= Pg_k^{\max} E_k - R_k$) (day$^{-1}$), for each algae type $k$:

$$B_k^{\max} = B_k^0 \exp\{Pn_k \Delta t\} \qquad (12.106)$$

This condition is taken into account by the optimization algorithm. For types with an initial biomass of zero, a small base level is used instead in order to allow previously absent species to start growing.

### 5.9.5. Mortality Limits

As in the case of growth, the mortality of each algae species is also constrained to prevent a complete removal within a single time step. The minimum biomass value of a species is obtained when there is no production, but only mortality. The minimum biomass, $B_k^{\min}$ (g dry/m$^3$), of type $k$ at the end of time interval $\Delta t$ depends on the initial biomass, $B_k^0$ (g dry/m$^3$), of type $k$ and the specific mortality rate constant, $M_k$ (day$^{-1}$), of type $k$.

$$B_k^{\min} = B_k^0 Z_k \exp\{-M_k \Delta t\} \qquad (12.107)$$

These maximum and minimum values are computed for each individual algae type. However, the model sums each of these maximum and minimum values over all subtypes

within each species and applies it to the total biomass of the species. This way the maximum possible mortality cannot be exceeded, but transitions between limit types remain possible.

$$\sum_{k \text{ of species } j} B_k^{\min} \leq \sum_{k \text{ of species } j} B_k \leq \sum_{k \text{ of species } j} B_k^{\max} \quad \forall \text{ species } j$$

(12.108)

As mortality is computed according to a negative exponential function, the minimum biomass level is always positive; in other words, a species can never disappear completely. For computational purposes, the minimum biomass of a species is set to zero if it drops below some small threshold base level. It is conceivable that the amount of biomass, which should minimally be maintained according to Equation 12.108 exceeds the amount permitted according to the available amount of light energy (12.100). If this happens, Condition (12.100) is dropped.

### 5.9.6. Oxygen-Related Processes

The oxygen concentration in the water column depends in part on the biochemical and physical processes that either produce or consume oxygen. For the algae the model includes the production of oxygen (primary production), and its consumption through respiration. Oxygen is also consumed by the mineralization of detritus and other organic material (in the water column and bottom sediment), nitrification of ammonia to nitrate, and exchange of oxygen with the atmosphere (e.g. re-aeration).

The mineralization of carbon detritus in the water column and bottom consumes oxygen at a molar ratio of 1:1, equivalent to a ratio of 32/12 g $O_2$ to 1 g C. The net growth of algae produces oxygen at a molar ratio of 1:1, equivalent to a ratio of 32/12 g $O_2$ to 1 g C. The mineralization of organic carbon in waste and carbon detritus in the water column and bottom consumes oxygen at a molar ratio of 1:1, equivalent to a ratio of 32/12 g $O_2$ to 1 g C. The nitrification reaction consumes oxygen at a molar ratio of 2:1, equivalent to a ratio of 64/14 g $O_2$ to 1 g N. For all algae, oxygen is produced during photosynthesis. The net growth of algae produces oxygen at a molar ratio of 1:1, equivalent to a ratio of 32/12 g $O_2$ to 1 g C.

### Bottom Oxygen

The mineralization of organic material in the bottom sediment consumes oxygen, which must be supplied from the water column. The process consumes oxygen at a molar ratio (oxygen to carbon) of 1:1, equivalent to a ratio of 32/12 g $O_2$ to 1 g C.

### Daily Oxygen Cycle

Because oxygen is produced by the photosynthesis of algae during the daylight hours, there is a natural variation of oxygen concentrations over the twenty-four-hour day–night cycle. Typically, oxygen concentrations are lowest in the early morning as oxygen is consumed during the night through the processes of algae respiration and organic material mineralization. During the daylight hours, oxygen is produced, and the highest values (often supersaturated) are typically found in the late afternoon. When biomasses are high, these variations may be large enough to cause low oxygen conditions during the night or in the early morning.

In the traditional BLOOM calculation, the water quality processes are all calculated for a daily averaged situation. This is reflected by the choice of the input parameters for the light model: the daily averaged solar radiation and the day length. Reducing the time step would be the most straightforward way to include diurnal variations. The drawback, however, is a considerable increase in computation time. Thus an alternative approach has been adopted in the model. The total daily rate of primary production is computed first. Next, this production is distributed over the day. The model takes into account the day length, and oxygen production begins in the first daylight hour. Oxygen production increases during the morning, levels off at a (user-defined) maximum value for a period in the middle of the day, and decreases during the afternoon. There is no oxygen production during the night-time. The hourly oxygen production is combined with the daily averaged oxygen consumption processes and the re-aeration to produce an hourly value of oxygen concentration in the water.

### Maintenance Respiration

Respiration in algae is a process in which organic carbon is oxidized, using oxygen to produce energy. The process occurs throughout the day and results in oxygen

consumption at a rate of 32 grams of oxygen per 12 grams of carbon: 32/12 g $O_2$ to 1 g C. Total respiration is divided into growth and maintenance respiration. Maintenance respiration is a first-order temperature dependent process. Species growth respiration is accounted for when calculating the net primary production. Maintenance respiration, and thus the amount of oxygen consumed, is governed by the temperature-dependent respiration rate constant, $k_k^{res}\theta_k^{res(T-20)}$ (day$^{-1}$), the temperature, $T$ (°C), of the water (higher respiration at higher temperatures), and the concentration of algae biomass, $AlgC_k$. Each algae type can have a different respiration rate. Hence, the rate (g$C_2$/m′/day) at which carbon in algae is oxidized is

$$dAlgC_k/dt = k_k^{res}\theta_k^{res(T-20)}AlgC_k \qquad (12.109)$$

# 6. Simulation Methods

Most of those who will be using water quality models will be using simulation models that are commonly available from governmental agencies (e.g. USEPA), universities, or private consulting and research institutions such as the Danish Hydraulics Institute, Wallingford software or WL | Delft Hydraulics (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 that incorporate 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 hydrological or hydrodynamic model calculates the flow of water between all of these. In each simulation time step, plug flow enters these segments or volume elements from upstream segments or elements. Flow also exits from them to downstream segments or elements. During this time the constituents can decay or grow, as appropriate, depending on 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.

## 6.1. Numerical Accuracy

Water quality simulation models based on physical, biological and chemical processes typically include time rate of change terms such as d$C$/d$t$. While it is possible to solve some of these differential equations analytically, 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 modeller because of these numerical methods.

Consider first the relationship between the stream, river or lake segments and the duration of time steps, $\Delta t$. The basic first-order decay flux, d$C$/d$t$ (g/m$^3$/day), for a constituent concentration, $C$, that is dependent on a rate constant, $k$ (day$^{-1}$), is:

$$dC/dt = -kC \qquad (12.110)$$

The finite difference approximation of this equation can be written

$$C(t+\Delta t) - C(t) = -C(t)k\Delta t \qquad (12.111)$$

or

$$C(t+\Delta t) = C(t)(1 - k\Delta t) \qquad (12.112)$$

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 12.25 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 Equation 12.110, namely:

$$C(t+\Delta t) = C(t)\exp\{-k\Delta t\} \qquad (12.113)$$

Reducing the value of $\Delta t$ will increase the accuracy of the numerical solution. Hence, for whatever value of $\Delta t$, it 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

$$C(t+\Delta t) = C(t)(1 - k\Delta t/n)^n \qquad (12.114)$$

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

$$C(t+\Delta t)/C(t) = (1 - 1/2)^2 = 0.25 \qquad (12.115)$$

Compare this 0.25 to 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
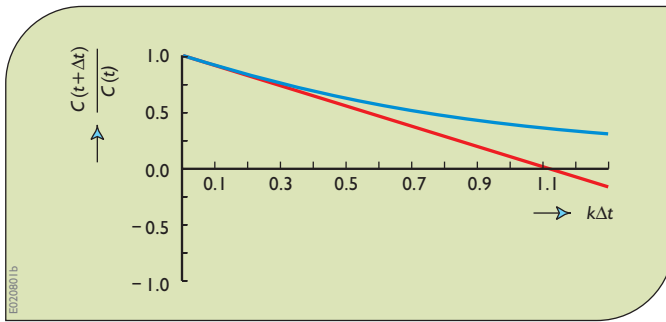
**Figure 12.25.** Plot of numerical approximation (red line) based on Equation 12.112 compared to the true analytical (blue line) value obtained from Equation 12.113.

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 be less than the actual value based on Equation 12.113, 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 $\Delta t$ exceeds $n/k$. In any event, the predicted concentrations are not very useful.

Letting $m = -n/k\Delta t$, Equation 12.114 can be written as

$$C(t + \Delta t) = C(t)(1 + 1/m)^{m\,(-k\Delta t)} \qquad (12.116)$$

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, Equation 12.114 becomes Equation 12.113, the exact solution to Equation 12.110.

## 6.2. Traditional Approach

Most water quality simulation models simulate quality over a consecutive series of discrete time periods. Time is divided into discrete intervals and the flows are assumed constant within each of those time period intervals. Each water body is divided into segments or volume elements, and these 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 of the next time step.

This method is illustrated in Figure 12.26. 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 $\Delta t$ 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 $\Delta t$ 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 the 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 Figure 12.26 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 on the left represents a portion of a stream or river divided into well-mixed segments. During a period $t$, waste constituents enter segment $i$ 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 waste, 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, $\Delta x_i$, 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

**Figure 12.26.** Water quality modelling approach showing a water system schematized into computational cells.
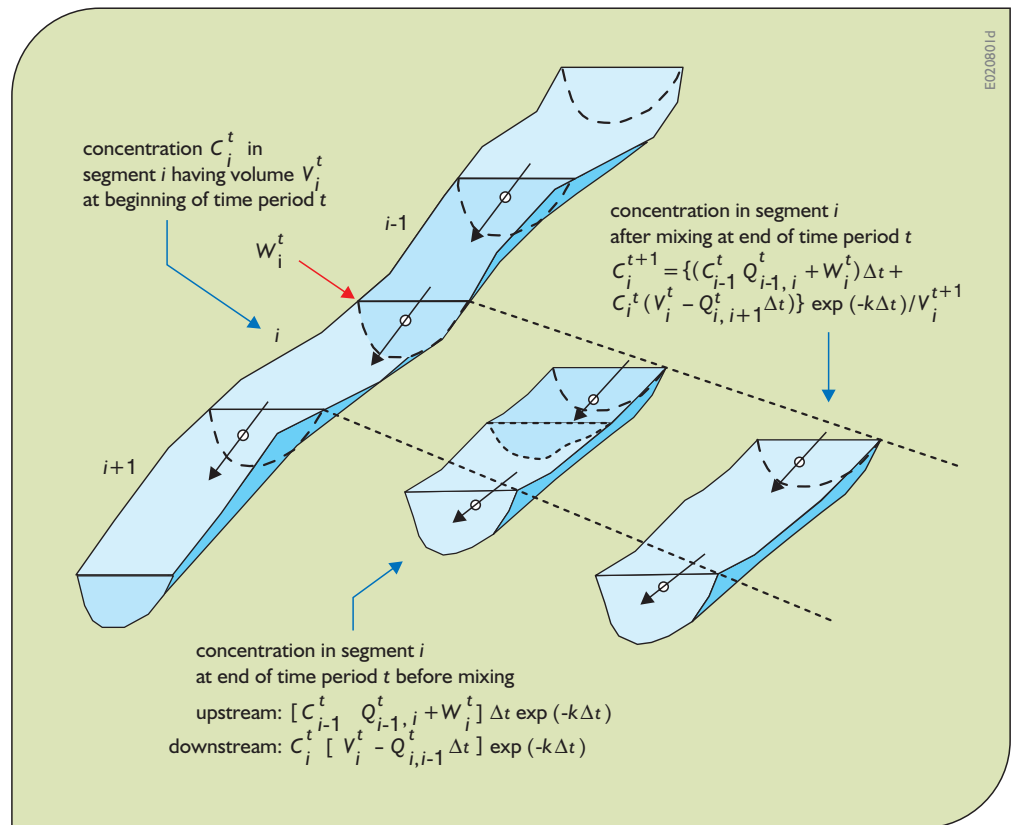
increasing flow velocities, also reduces the allowable duration of each time period $t$. The duration of each simulation time step $\Delta t$ must be such that flow from any segment or element enters only the adjacent downstream segment or element during that time step. Stated formally, the restriction is:

$$\Delta t \leq T_i \qquad (12.117)$$

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 $\Delta x_i$, cross section area $A_i$ and average flow $Q_{it}$, the restriction is:

$$\Delta t \leq \min\{\Delta x_i A_i / Q_{it}; \quad \forall i, t\} \qquad (12.118)$$

If time steps are chosen that violate this condition, then numerical solutions will be in error. The restriction defined by Equation 12.118 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 output, 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.

## 6.3. Backtracking Approach

An alternative Lagrangian or backtracking approach to water quality simulation eliminates the need to consider the simulation time-step duration restriction indicated by Equation 12.118 (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 $t$. The contaminants could come from segments in the same river reach or storage site, or from upstream river reaches 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 $\Delta t$, as shown in Figure 12.27.

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 Figure 12.27, 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 positions of all reach intervals that will be at the corresponding boundaries of segment $i$ at the end of time period $t$. To do this requires computing the velocities through each of the intermediate segments or volume elements. Second, the changes in the amounts of the modelled quality constituents, such as temperature, organics, nutrients and toxics, are calculated, assuming plug flow during the time interval, $\Delta t$, and 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 to or greater than $\Delta t$. 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
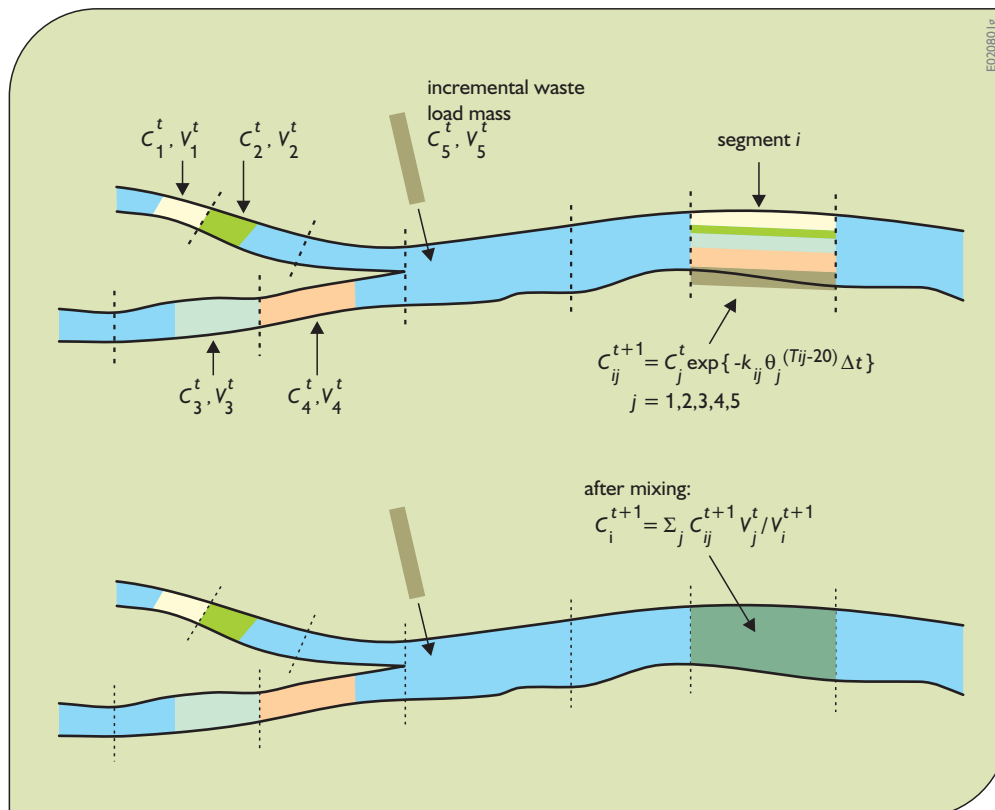


**Figure 12.27.** The backtracking approach for computing the concentrations of constituents in each reach segment or volume element $i$ during time-step duration of $\Delta t$.

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 12.27 illustrates an example of backtracking involving simple first-order decay processes. Assume contaminants that end up in reach segment $i$ at 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 $\Delta t$ in each segment or volume element is determined by the following differential equation:

$$dC_j^t/dt = -k_j\theta_j^{(T-20)}C_j^t \qquad (12.119)$$

The decay rate constant $k_j$, temperature correction coefficient $\theta_j$ 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 the water travels during the period $t$ from sites $j$ to segment $i$.

Integrating Equation 12.119 yields:

$$C_j^{t+1} = C_j^t \exp\{-k_j\theta_j^{(T-20)}\Delta t\} \qquad (12.120)$$

Since $\Delta t$ 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 $C_{ij}^{t+1}$:

$$C_{ij}^{t+1} = C_j^t \exp\{-k_{ij}\theta_j^{(T_{ij}-20)}\Delta t\} \qquad (12.121)$$

In Equation 12.121 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 $t + 1$.

## 6.4. Model Uncertainty

There are two significant sources of uncertainty in water quality management models. One stems from incomplete knowledge or lack of sufficient data 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 socio-economic 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 modelling capabilities.

However, even if it were possible to eliminate knowledge uncertainty, complete certainty in support of water quality management decisions will probably never be achieved until we can predict the variability of natural processes. 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 – in other words, 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, neither type of uncertainty – knowledge uncertainty nor unpredictable variability or randomness – can 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 to actions taken to meet the desired water quality criteria and designated uses of water bodies. Chapter 9 suggests some ways of characterizing this uncertainty.

# 7. Conclusions: Implementing a Water Quality Management Policy

This chapter has provided only a brief introduction to some of the relationships contained in water quality models. As can be said for the other chapters as well, it summarizes a subject on which entire texts, and very good ones, have been written (see, for example, Chapra, 1997; McCutcheon, 1989; Orlob, 1983; Schnoor, 1996; Thomann and Mueller, 1987). Water quality modelling and management demand skill and data. Skill comes with experience. Sufficient expertise will not be gained by working just with the material introduced in this chapter. It serves only as an introduction to surface water quality models, their assumptions and their limitations.

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. Such approaches strive toward achieving water quality standards while relying on monitoring and experimentation to reduce uncertainty. This is often the only way one can proceed, given the complexity of the real world compared to the predictive models and the data and time usually available at the time a water quality analysis is needed. Starting with simple analyses and iteratively expanding data collection and modelling 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 regulation 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 modelling (see Appendix B).

Regardless of what immediate actions are taken, there may not be an immediate measurable response. For example, there may be significant lags between the time 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 tightly 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.

Wasteload allocations will inevitably be required if quality standards are not being met. These involve costs. Different allocations will have 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 United States 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 fulfilment of other objectives must have made such a policy politically acceptable, even though expensive. However, these types of wasteload allocations policies will not in themselves be sufficient for many of the ecosystem restoration efforts that are increasingly being made. Restoration activities are motivated in part by the services ecosystems provide for water quality management.

Our abilities to include 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, long before we can improve these capabilities, 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 ensure that an action that will lead to the attainment of designated uses will be initially identified. Adaptive management is the only reasonable option in most cases for allowing water quality management programmes to move forward in the face of considerable uncertainties.

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