XII Surface Water Quality Modeling

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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 impacts the condition of ecosystems that all living organisms depend on. At the same time humans use water bodies as convenient receptacles for the disposal of domestic, industrial and agricultural wastewaters which of course degrade their quality. 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 them.

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 then either pay an additional cost of water treatment or incur at least increased risks of some 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 ground water 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. One of them is the transport and assimilation of waterborne wastes. But as natural water bodies assimilate these wastes, their quality changes. If the quality of water drops to the extent that other beneficial uses are adversely impacted, the assimilative capacities of those water bodies have been exceeded with respect to those impacted uses. Water quality management measures are actions taken to insure 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? Almost any use one can identify. All living organisms require water of sufficient quantity and quality to survive. Different aquatic species can tolerate different levels of water quality. Regrettfully, in most parts of the developed world it is no longer ‘safe’ to drink natural surface or ground waters. Treatment is usually required before these waters become safe for humans to drink. Treatment is not a practical option for recreational bathing, and for maintaining the health of fish and shellfish and other organisms found in natural aquatic ecosystems. Thus standards specifying minimum acceptable levels of quality are set for most ambient waters. Various uses have their own standards as well. Irrigation water must not be too saline nor contain various toxic substances that can be absorbed by the plants or destroy the microorganisms in the soil. Water quality standards for industry can be very demanding, depending of course on the particular industrial processes.

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

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

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

The goal of an ambient water quality management program is to establish appropriate standards for water quality in water bodies receiving pollutant loads and then to insure that these standards are met. Realistic standard setting takes into account the basin’s hydrologic, ecological, and land use conditions, the potential uses of the receiving water 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 implementation actions on meeting water quality standards. The models available to help managers predict water quality impacts (such as those outlined in this chapter) are relatively simple compared to the complexities of actual water systems. These limitations and uncertainties should be understood and addressed as water quality management decisions are made 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 areas of an estuary, is a first step in setting water quality standards for that water 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 hydrologic and geomorphic changes that impact the quality of the water body.

The designated use dictates the appropriate type of water quality standard. For example, a designated use of human contact 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 impact the uses of water downstream. For example, small headwater streams may have aesthetic values but they may not have the ability to support extensive recreational uses. However, their condition may affect the ability of a downstream area to achieve a particular designated use such as be “fishable” or “swimmable.” In this case, the designated use for the smaller upstream water body may be defined in terms of the achievement of the designated use of the larger downstream water body.

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

Appropriate use designation 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 in consideration of the current condition of the watershed, its predisturbance condition, the advantages derived from a certain designated use, and the costs of achieving the designated use.

2.1 Water use criteria

The designated use is a qualitative description of a desired condition of a water body. A criterion is a measurable indicator surrogate for use attainment. The criterion may be positioned at any point in the causal chain of boxes shown in Figure 12.1.
Figure 12.1. Factors considered when determining designated use and associated water quality standards.

In Box 1 of Figure 12.1 are measures of the pollutant discharge from a treatment plant (e.g., biological oxygen demand, ammonia (NH$_3$), pathogens, 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, nitrogen concentration, suspended sediment, or temperature. Criteria closer to the designated use (e.g., Box 3) include more combined or comprehensive measures of the biological community as a whole, such as the condition of the algal community (chlorophyll $a$) or a measure of contaminant concentration in fish tissue. Box 4 represents criteria that are associated with sources of pollution other than pollutants. These criteria might include measures such as flow timing and pattern (a hydrologic criterion), abundance of non-indigenous taxa, some quantification of channel modification (e.g., decrease in sinuosity), etc. (NRC, 2001).

The more precise the statement of the designated use, the more accurate the criterion will be as an indicator of that use. For example, the criterion of fecal coliform count may be 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 chosen as it relates to other water bodies downstream. Thus, an ambient nutrient criterion may be set in a small headwater stream to insure 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.

3. Water quality model use

Monitoring data are the preferred form of information for identifying impaired waters (Chapter VI). Model predictions might be used in addition to or instead of monitoring data for two reasons: (1) modeling could be feasible in some situations where monitoring is not, and (2) integrated monitoring and modeling systems could provide better information than monitoring or modeling alone for the same total cost. For example, regression analyses that correlate pollutant concentration with some more easily measurable factor (e.g., streamflow) could be used to extend monitoring data for preliminary listing 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 VIII (A)).

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

Combined runoff and water quality prediction models link stressors (sources of pollutants and pollution) to responses. Stressors include human activities likely to cause impairment, such as the presence of impervious surfaces in a watershed, cultivation of fields close to the stream, over-irrigation of crops with resulting polluted return flows, the discharge of domestic and industrial effluents into water bodies, installing dams and other channelization works, introduction of non-indigenous taxa, and over-harvesting of fishes. Indirect effects of humans include land cover changes that alter the rates of delivery of water, pollutants, and sediment to water bodies.

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, and

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

Models that relate stressors to responses can be of varying levels of complexity. Sometimes, models are simple qualitative conceptual representations of the relationships among important variables and indicators of those variables, 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 nonpoint 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 judgment. They include process-based (mechanistic) models and data-based (statistical) models. The models should link management options to meaningful response variables (e.g., pollutant sources and water quality standard parameters). They should incorporate the entire “chain” from stressors to responses. Process-based models should be consistent with scientific theory. Model prediction uncertainty should be reported. This provides decision-makers with estimates of the risks of options. To do this requires prediction error estimates (Chapter VIII (G)).

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

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

Water quality models can also be classified as either pollutant loading models or as pollutant response models. The former predict the pollutant loads to a water body as a function of land use and pollutant discharges; the latter is used to predict pollutant concentrations and other responses in the water body as a function of the pollutant loads. The pollutant response models are of interest in this chapter.
Although predictions are typically made using mathematical models, there are certainly situations where expert judgment can be just as good. Reliance on professional judgment and simpler models is often acceptable, especially when limited data exist.

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

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

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. To do this one can limit the nutrient loadings to the estuary that can cause algae blooms, and subsequent dissolved oxygen deficits. The modeling challenge is to link nutrient loading to fish and shellfish survival.
Given the current limited understanding of biotic responses to hydrologic and pollutant stressors, models are needed that link these stressors such as pollutant concentrations, changes in land use, or hydrologic regime alterations to biological responses. Some models have been proposed linking chemical water quality to biological responses. One approach aims at describing the total aquatic ecosystem response to pollutant sources. Another approach is to build a simpler model linking stressors to a single biological criterion.

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 bottom water. Fish and shellfish may die or become weakened and more vulnerable to disease.

![Diagram](image)

Figure 12.2. The negative impacts of excessive nutrients in an estuary (Reckhow, 2002).
Figure 12.3  Cause and effect diagram for estuary eutrophication due to excessive nutrient loadings (Borsuk, et al. 2001).

A Bayesian probability network can be developed to predict the probability of shellfish and fish abundance based on upstream nutrient loadings causing problems with fish and shellfish populations into the estuary. These conditional probability models can be a combination of judgmental, mechanistic, and statistical. Each link can be a separate submodel. Assuming each submodel can identify a conditional probability distribution, the probability $Pr\{C\mid N\}$ of a
specified amount of carbon, \( C \), given some specified loading of a nutrient, say nitrogen, \( N \), equals the probability \( \Pr\{C|A\} \) of that given amount of carbon given a concentration of algae biomass, \( A \), times the probability \( \Pr\{A|N,R\} \) of that concentration of algae biomass given the nitrogen loading, \( N \), and the river flow, \( R \), times the probability \( \Pr\{R\} \) of the river flow, \( R \).

\[
\Pr\{C|N\} = \Pr\{C|A\} \Pr\{A|N,R\} \Pr\{R\} \tag{12.1}
\]

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

The biological endpoints “shell-fish survival” and “number of fishkills,” are meaningful indicators to stakeholders and can easily be related to designated water body use. Models and even conditional probabilities assigned to each link of the network in Figure 12.3 can reflect a combination of simple mechanisms, statistical (regression) fitting, and expert judgment.

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

Data availability and accuracy is one source of concern in the development and use of models for water quality management. The complexity of models used for water quality management should be compatible with the quantity and quality of available data. The use of complex mechanistic models for water quality prediction in situations with little useful water quality data does not compensate for a lack of data. Model complexity can give the impression of credibility but this is not usually true. It is often preferable to begin with simple models and then over time add additional complexity as justified based on the collection and analysis of additional data.

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

4. Stream and river models

Models that describe water quality processes in streams and rivers typically include the inputs (the water flows or volumes and the pollutant loadings), the dispersion and/or advection transport terms depending on the hydrologic and hydrodynamic characteristics of the water body, and the biological, chemical and physical reactions among constituents. Advection 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.

The development of stream and river water quality models is both a science as well as an art. Each model reflects the creativity of its developer, the particular water quality management problems and issues being addressed, the available data for model parameter calibration and verification, and the time available for modeling and associated uncertainty and other analyses. The fact that most, if not all, water quality models cannot accurately predict what actually happens does not 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 Steady-state models

For an introduction to model development, consider a one-dimensional river reach that is completely mixed in the lateral and vertical directions. (This complete mixing assumption is common in water quality modeling, but in reality it is often not the case.) The concentration, $C$ (ML$^{-3}$) of a constituent is a function of the rate of inputs and outputs (sources and sinks) of the constituents, of the advection and dispersion of the constituent, and of the various physical, chemical, biological and possibly radiological reactions that affect the constituent concentration.

The concentration, $C(X,t)$, of any constituent discharged at a point along a one-dimensional river reach having a uniform cross-sectional area, $A$ (L$^2$), depends on the time, $t$, and the distance, $X$ (L), along the river with respect to the discharge point, $X = 0$, a dispersion factor, $E$ (L$^2$T$^{-1}$), the net downstream velocity, $U$ (LT$^{-1}$), and various sources and sinks, $S_k$ (ML$^{-3}$T$^{-1}$). At any particular site $X$ upstream ($X<0$) or downstream ($X>0$) from the constituent discharge point in the river, the change in concentration over time, $\partial C/\partial t$, depends on the change, $\partial (\bullet)/\partial X$, in the dispersion, $EA(\partial C/\partial X)$, and advection, $UAC$, in the $X$ direction plus any sources or minus any sinks, $S_k$.

$$\frac{\partial C}{\partial t} = \left(1/A\right) \left[\partial(EA(\partial C/\partial X) – UAC)/\partial X\right] \pm \sum_k S_k \quad (12.2)$$

The expression $EA(\partial C/\partial X) – UAC$ in Equation 12.2 is termed the total flux (MT$^{-1}$). Flux due to dispersion, $EA(\partial C/\partial X)$, is assumed to be proportional to the concentration gradient over distance. Constituents are transferred by dispersion from higher concentration zones to lower concentrations zones. The coefficient of dispersion $E$ 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 $UAC$ is the advective flux caused by the movement of water containing the constituent concentration $C$ at a velocity rate $U$ across a cross-sectional area $A$. 
The relative importance of dispersion and advection depends on how detailed the velocity field is defined. A good spatial and temporal description of the velocity field within which the constituent is being distributed will reduce the importance of the dispersion term. Less precise descriptions of the velocity field, such as averaging across irregular cross sections or approximating transients by steady flows, may lead to a dominance of the dispersion term.

Many of the reactions affecting the decrease or increase of constituent concentrations are often represented by first-order kinetics 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.

4.1.1 Steady-state single constituent models

Steady state means no change over time. In this case the left hand side of Equation 12.2, $\partial C/\partial t$, 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 12.2 becomes

$$0 = E \frac{\partial^2 C}{\partial X^2} - U \frac{\partial C}{\partial X} - kC \quad (12.3)$$

Equation 12.3 can be integrated since river reach parameters $A$, $E$, $k$, and $U$, and thus $m$ and $Q$, are assumed constant. For a constant loading, $WC$ (MT$^{-1}$) at site $X = 0$, the concentration $C$ will equal

$$C(X) = \begin{cases} 
(W_C/Qm) \exp[ (U/2E)(1 + m)X] & X \leq 0 \\
(W_C/Qm) \exp[ (U/2E)(1 - m)X] & X \geq 0 
\end{cases} \quad (12.4)$$

where

$$m = \left( 1 + \frac{4kE}{U^2} \right)^{1/2} \quad (12.5)$$
Note from Equation 12.5 that the parameter \( m \) is always equal or greater than 1. Hence the exponent of \( e \) in Equation 12.4 is always negative. Hence as the distance \( X \) increases in magnitude, either in the positive or negative direction, the concentration \( C(X) \) will decrease. The maximum concentration \( C \) occurs at \( X = 0 \) and is \( W C / Q m \).

\[
C(0) = W C / Q m
\]  
(12.6)
These equations are plotted in Figure 12.4.

In flowing rivers not under the influence of tidal actions the dispersion is small. Assuming the dispersion coefficient \( E \) is 0, the parameter \( m \) defined by Equation 12.5, is 1. Hence when \( E = 0 \), the maximum concentration at \( X = 0 \) is \( W C / Q \).

\[
C(0) = W C / Q \quad \text{if } E = 0.
\]  
(12.7)
Assuming \( E = 0 \) and \( U, Q \) and \( k > 0 \), Equation 12.4 becomes

\[
C(X) = \begin{cases} 
0 & X \leq 0 \\
(W C / Q) \exp[-kX/U] & X \geq 0
\end{cases}
\]  
(12.8)
The above equation for \( X > 0 \) can be derived from Equations 12.4 and 12.5 by noting that the term \((1 - m)\) equals \((1 - m)(1 + m)/(1 + m) = (1 - m^2)/2 = -2kE/U \) when \( E = 0 \). The term \( X/U \) in Equation 12.8 is sometimes denoted as a single variable representing the time of flow – the time flow \( Q \) takes to travel from site \( X = 0 \) to some other downstream site \( X \). This equation is plotted in Figure 12.4.

As rivers approach the sea, the dispersion coefficient \( E \) increases and the net downstream velocity \( U \) decreases. Because the flow \( Q \) equals the cross-sectional area \( A \) times the velocity \( U, Q = AU \), and since the parameter \( m \) can be defined as \((U^2 + 4kE)^{1/2}/U \), then as the velocity \( U \) approaches 0, the term \( Qm = AU(U^2 + 4kE)^{1/2}/U \) approaches \( 2A(kE)^{1/2} \). The exponent \( UX(1 \pm m)/2E \) in Equation 3 approaches \( \pm X(k/E)^{1/2} \).
Hence for small velocities, Equation 12.4 becomes

\[
C(X) = \begin{cases} 
\left(\frac{W_C}{2A(kE)^{1/2}}\right) \exp[+X(k/E)^{1/2}] & X \leq 0 \\
\left(\frac{W_C}{2A(kE)^{1/2}}\right) \exp[-X(k/E)^{1/2}] & X \geq 0 
\end{cases}
\]

(12.9)

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.](image)

Most water quality management models are used to find the loadings that meet 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 maximum allowable concentrations of the constituent $C$ are specified at each of those discharge sites. To estimate the needed reduction in these discharges, the river must be divided into approximately homogenous reaches. Each reach can be characterized by constant values of the cross-sectional area, $A$, dispersion coefficient, $E$, constituent decay rate constant, $k$, and velocity, $U$, 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.

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 $(Qm_i)$ is represented by $(Qm)$. The downstream (forward) transfer coefficient, $TF_i$, equals the applicable part of Equation 12.4,

$$
\begin{align*}
\text{minimize} & \quad \Sigma_i \text{Cost}(R_i) \\
\text{subject to:} & \\
\bullet & \text{mass balances:} \\
C_1 &= W^1 (1-R_i) / (Qm)_1 + C_2 \cdot TB_1 \\
C_2 &= [C_1TF_1(Qm)_1 + C_3TB_2(Qm)_2] / (Qm)_2 \\
C_3 &= [W^2 (1-R_2) + C_2TF_2(Qm)_2 + C_4TB_3(Qm)_3] / (Qm)_3 \\
C_4 &= [W^3 (1-R_3) + C_3TF_3(Qm)_3 + C_5TB_4] / (Qm)_4 \\
C_5 &= [C_4TF_4(Qm)_4 + C_5TB_5(Qm)_5] / (Qm)_5 \\
C_6 &= [C_5TF_5(Qm)_5 + C_6TB_6(Qm)_6] / (Qm)_6 \\
C_7 &= [C_6TF_6(Qm)_6 + C_7TF_7(Qm)_7 + CB_7TB_8(Qm)_8] / (Qm)_7 \\
C_8 &= [W^8 (1-R_8) + C_7TF_8(Qm)_8] / (Qm)_8 \\
\bullet & \text{quality standards and maximum removal efficiencies:} \\
C_i & \leq C_i^{\text{max}} \quad \forall i; \ R_i \leq R_i^{\text{max}} \quad \forall i
\end{align*}
$$

Figure 12.5. Optimization model for finding constituent removal efficiencies, $R_i$, at each discharge site $i$ that result in meeting stream quality standards, $C_i^{\text{max}}$, at least total cost.
\[ TF_i = \exp\left(\frac{U}{2E}(1 - m)X\right) \]  
(12.10)

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

\[ TB_i = \exp\left(\frac{U}{2E}(1 + m)X\right) \]  
(12.11)

The parameter \( m \) is defined by Equation 12.5.

Solving a model such as 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 insure equity, or extra safety. Models like this can be used to identify the cost-quality tradeoffs inherent in any water quality management program. 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.

### 4.2 Design streamflows

It is common practice to pick a low flow condition for judging whether or not ambient water quality standards are being met. The rational for this is that the greater the flow, the greater the dilution and hence the lower the concentration of any quality constituent. This is evident from Equations 12.4, 12.6, 12.7, 12.8, and 12.9. 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, that is used in parts of North America, is called the minimum 7-day average flow expected to be lower only once in 10 years on average. Each year the lowest 7-day average flow is determined, as shown in Figure 12.6. The sum of each of the 365 sequences of seven average
daily flows is divided by 7 and the minimum value is selected. This is the minimum annual average 7-day flow.

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

Figure 12.6. Portion of annual flow time series showing low flows and the calculation of average 7 and 14-day flows.
Figure 12.7. Determining the minimum 7-day annual average flow expected once in 10 years, designated 7Q10, from the cumulative probability distribution of annual minimum 7-day average flows.

Consider now any one of the river reaches shown in Figure 12.5. Assume an initial amount of constituent mass, $M$, exists at the beginning of the reach. As the reach flow, $Q$, increases due to the inflow of less polluted water, the initial concentration, $M/Q$, will decrease. However, the flow velocity will increase, and thus the time 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 establishing wasteload allocations that meet ambient water quality standards during low flow conditions may not meet them under higher flow conditions, conditions that 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 waste loads, but rather that a simulation of water quality concentrations over varying flow conditions may show that higher flow conditions at some sites are even more critical and more frequent than are the low flow conditions.

Figure 12.8. Increasing streamflows decreases initial concentrations but may increase downstream concentrations.
Figure 12.8 shows that for a fixed mass of pollutant at $X = 0$, under low flow conditions the more restrictive 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.

4.3 Temperature

Temperature impacts almost all water quality processes taking place in water bodies. For this reason modeling temperature may be important when the temperature can 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 shortwave 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 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 is

$$\frac{dT}{dt} = \frac{K_H(T_e - T)}{\rho c_p h}$$ (12.12)

where $\rho$ is the water density (g/cm$^3$), $c_p$ is the heat capacity of water (cal/g/$°C$) and $h$ is the water depth (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, $T_e$ ($°C$). 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 $U_w$ (m/s), dew point temperature $T_d$ ($°C$) and actual temperature $T$ ($°C$) (Thomann and Mueller 1987).
The equilibrium temperature, $T_e$, is obtained from another empirical relationship involving the overall heat exchange coefficient, $K_H$, the dew point temperature, $T_d$, and the short-wave solar radiation $H_s$ (cal/cm$^2$/day),

$$T_e = T_d + \left( \frac{H_s}{K_H} \right)$$

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

### 4.4 Sources and sinks

Sources and sinks include the physical and biochemical processes that are represented by the terms, $\Sigma_k S_k$, in Equation 12.2. External inputs of each constituent would have the form $W/Q\Delta t$ or $W/(A_X\Delta X)$ where $W$ (MT$^{-1}$) 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.

### 4.5 First-order constituents

The first-order models of 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 ($dC/dt$) 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 we can write this as

$$\frac{dC_j}{dt} = a_{ij} k_i \Theta_i^{(T-20)} C_i$$

(12.14)
where $\theta_i$ is temperature correction coefficient for $k_i$ at 20°C and $T$ is the temperature in °C. The parameter $a_{ij}$ is the grams of $C_j$ produced ($a_{ij} > 0$) or consumed ($a_{ij} < 0$) per gram $C_i$. For the prediction of BOD concentration over time, $C_i = C_j = BOD$ and $a_{ij} = a_{BOD} = -1$ in Equation 12.14.

Conservative substances, such as salt, will have a decay rate constant $k$ of 0.

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 $k_B = 2.3 / t_{90}$.

Table 12.1. Typical values of the first-order decay rate, $k$, and the temperature correction factor, $\theta$, for some constituents.

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

<table>
<thead>
<tr>
<th>constituent</th>
<th>$\theta$</th>
<th>units</th>
</tr>
</thead>
<tbody>
<tr>
<td>coliform bacteria (freshwater)</td>
<td>1.07</td>
<td>b</td>
</tr>
<tr>
<td>coliform bacteria (saltwater)</td>
<td>1.10</td>
<td>b</td>
</tr>
<tr>
<td>BOD</td>
<td>1.04</td>
<td>a</td>
</tr>
</tbody>
</table>

a - Thomann and Mueller (1987)  
b - Schnoor (1996)
4.6 Dissolved oxygen

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

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

![Figure 12.9. The dissolved oxygen interactions in a water body, showing the decay (satisfaction) of carbonaceous, nitrogenous and sediment oxygen demands. Water body reaeration or deaeration if supersaturated occurs at the air-water interface.](image)

The rate of reaeration 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
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

$$DO_{sat} = \{14.652 - 0.41022 T + (0.089392 T)^2 - (0.042685 T)^3\} \{1 - (Cl / 100000)\}$$

(12.15a)

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

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

(12.15b)

Fitting a second-order polynomial curve to the data presented in Chapra (1997) results in:
\[ DO_{\text{sat}} = 14.407 - 0.3369 \, T + 0.0035 \, T^2 \]  

(12.15c)

as is shown in Figure 12.10

![Fitted curve to the saturation dissolved oxygen concentration (mg/l) as a function of temperature (°C).](image)

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

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 modeled as first-order decay reactions with decay rate constants \( k_{CBOD} \) (1/day) for \( CBOD \) and \( k_{NBOD} \) (1/day) for \( NBOD \). These rate constants vary with temperature, hence they are typically defined for 20 °C. The decay rates are corrected for temperatures other than 20 °C using temperature coefficients \( \theta_{CBOD} \) and \( \theta_{NBOD} \) respectively.

The sediment oxygen demand \( SOD \) (mg/l/day) is usually expressed as a zero-order reaction, i.e. a constant demand. One important feature in modeling \( NBOD \) is insuring the inappropriate time 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

\[
d\frac{DO}{dt} = -k_{CBOD} \theta_{CBOD}^{(T-20)} CBOD - k_{NBOD} \theta_{NBOD}^{(T-20)} NBOD \\
+ k_r \theta_{r}^{(T-20)} (DO_{sat} - DO) - SOD
\]  

(12.16)

\[
d\frac{CBOD}{dt} = -k_{CBOD} \theta_{CBOD}^{(T-20)} CBOD
\]

(12.17)

\[
d\frac{NBOD}{dt} = -k_{NBOD} \theta_{NBOD}^{(T-20)} NBOD
\]

(12.18)

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

Table 12.3. Typical values of parameters used in the dissolved oxygen models.
### 4.7 Nitrogen cycle

Interactions among nitrogen components and dissolved oxygen are shown in Figure 12.12.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>$k_r$, slow, deep rivers</td>
<td>0.1-0.4 a</td>
<td>l/day</td>
</tr>
<tr>
<td>$k_r$, typical conditions</td>
<td>0.4-1.5 a</td>
<td>l/day</td>
</tr>
<tr>
<td>$k_r$, swift, deep rivers</td>
<td>1.5-4.0 a</td>
<td>l/day</td>
</tr>
<tr>
<td>$k_r$, swift, shallow rivers</td>
<td>4.0-10.0 a</td>
<td>l/day</td>
</tr>
<tr>
<td>$k_{CBOD}$, untreated discharges</td>
<td>0.35 (0.20-0.50) b</td>
<td>l/day</td>
</tr>
<tr>
<td>$k_{CBOD}$, primary treatment</td>
<td>0.20 (0.10-0.30) b</td>
<td>l/day</td>
</tr>
<tr>
<td>$k_{CBOD}$, activated sludge</td>
<td>0.075 (0.05-0.10) b</td>
<td>l/day</td>
</tr>
<tr>
<td>$\theta_{CBOD}$</td>
<td>1.04 a</td>
<td>---</td>
</tr>
<tr>
<td></td>
<td>1.047 a</td>
<td>---</td>
</tr>
<tr>
<td></td>
<td>1.04 (1.02-1.09) c</td>
<td>---</td>
</tr>
<tr>
<td></td>
<td>1.024 (1.005-1.030) c</td>
<td>---</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Sediment oxygen demand *</th>
<th>Value</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>Municipal sludge (outfall vicinity)</td>
<td>4 (2-10) c d</td>
<td>gO₂/ m²/ day</td>
</tr>
<tr>
<td>Municipal sewage sludge</td>
<td>1.5 (1-2) c d</td>
<td>gO₂/ m²/ day</td>
</tr>
<tr>
<td>Sandy bottom</td>
<td>0.5 (0.2-1.0) c d</td>
<td>gO₂/ m²/ day</td>
</tr>
<tr>
<td>Mineral soils</td>
<td>0.07 (0.05-0.1) c d</td>
<td>gO₂/ m²/ day</td>
</tr>
<tr>
<td>Natural to low pollution</td>
<td>0.1-10.0 a c d</td>
<td>gO₂/ m²/ day</td>
</tr>
<tr>
<td>Moderate to heavy pollution</td>
<td>5-10 a c d</td>
<td>gO₂/ m²/ day</td>
</tr>
</tbody>
</table>


b - Chapra (1977)  d - Bowie et al. (1985)

* value has to be divided by the water height (m)
Figure 12.12. The dissolved oxygen and nitrogen cycle interactions in a water body, showing the decay (satisfaction) of carbonaceous and sediment oxygen demands, reaeration or deaeration at the air-water interface, ammonification from organic nitrogen in the detritus, nitrification (oxidation) of ammonium to nitrate, phytoplankton production from nitrate consumption, and phytoplankton respiration and death contributing to the organic nitrogen.

An alternative to modeling $N_{BOD}$ is to model the nitrogen cycle and its interactions with oxygen, as illustrated in Figure 12.12. The nitrogen cycle can be represented by a multi-step model including the transformations of organic nitrogen ($N_o$, mg/l), ammonium ($N_a$, mg/l), nitrite and nitrate ($N_n$, mg/l). Ammonium is released during the microbial decomposition of organic matter, a process called the ammonification of organic nitrogen. The microbial oxidation of ammonium into nitrate creates a dissolved oxygen demand. Bacterial nitrification of ammonium $NH_4^+$ to nitrite and then to nitrate, $NO_3^-$, requires two moles (64 grams) of oxygen to one mole (14 grams) of nitrogen, or $64/14 = 4.57$ g$O_2$/g$N$. 

\[ \text{NH}_4^+ + 2 \text{O}_2 \rightarrow \text{NO}_3^- + 2\text{H}_2\text{O} + 2\text{H}^+ \]

or in the presence of bicarbonate,
\[ \text{NH}_4^+ + 2 \text{O}_2 + 2\text{HCO}_3^- \rightarrow \text{NO}_3^- + 2\text{CO}_2 + 3\text{H}_2\text{O} \]

The components \( N_o, N_a, \) and \( N_n \) of the nitrogen cycle incorporated in the model for dissolved oxygen, \( \text{DO}, \text{mg/l} \) with \( \text{CBOD} \) (mg/l) and \( \text{SOD} \) (mg/l/day), involves five equations. The individual rates of transformation of ammonium to nitrite and from nitrite to nitrate are included in the single reaction rate constant \( k_a \) (1/day).

Assuming an aerobic environment (no denitrification), the source and sink terms of the model will include:

For dissolved oxygen:
\[
\frac{d\text{DO}}{dt} = -k_{\text{CBOD}} \theta_{\text{CBOD}}^{(T-20)} \text{CBOD} - 4.57 k_a \theta_a^{(T-20)} N_a + k_r \theta_r^{(T-20)} (\text{DO}_{\text{sat}} - \text{DO}) - \text{SOD} \tag{12.19}
\]

For \( \text{CBOD} \):
\[
\frac{d\text{CBOD}}{dt} = -k_{\text{CBOD}} \theta_{\text{CBOD}}^{(T-20)} \text{CBOD} \tag{12.20}
\]

For organic nitrogen:
\[
\frac{dN_o}{dt} = -k_o \theta_o^{(T-20)} N_o \tag{12.21}
\]

For ammonia-nitrogen:
\[
\frac{dN_a}{dt} = k_o \theta_o^{(T-20)} N_o - k_a \theta_a^{(T-20)} N_a \tag{12.22}
\]

For nitrate-nitrogen:
\[
\frac{dN_n}{dt} = k_a \theta_a^{(T-20)} N_a - k_n \theta_n^{(T-20)} N_n \tag{12.23}
\]

In the above equations \( k_o \) is the organic nitrogen to ammonium decay rate constant (1/day), \( k_a \) the ammonium to nitrite to nitrate decay rate constant (1/day), \( k_n \) the nitrate decay rate constant (1/day). Table 12.4 lists the means and ranges of values for coefficients included in these nitrogen cycle models.

Table 12.4. Typical values of parameters used in the nitrogen cycle models.
4.7.1 Nitrification and denitrification

Ammonia nitrifies to nitrate and nitrate can denitrify to ammonium. Both loss processes have been modeled as either first-order rate governed processes, depending on the dissolved oxygen concentration, or using Michaelis-Menten kinetics. Using the latter, the rates, \( \frac{dN}{dt} \) (gN/m\(^3\)/day) of both processes can be defined as equaling the kinetic constant \( k_{\text{max}} \) (gN/m\(^3\)/day) under ideal conditions times the Michaelis-Menten terms containing the half saturation concentrations, \( K \), for the nutrients (ammonium, \( NH_4 \), or nitrate, \( NO_3 \)) and dissolved oxygen, \( DO \).

Hence for nitrification of ammonium to nitrate,

\[
\frac{dNO_3}{dt} = -\frac{dNH_4}{dt} = \{ k_{\text{max}} \left[ NH_4/(NH_4 + K_{NH4}) \right] [DO/(DO + K_{DO})] \} \tag{12.24}
\]

For denitrification of nitrate to ammonium,

\[
\frac{dNH_4}{dt} = -\frac{dNO_3}{dt} = \{ k_{\text{max}} \left[ NO_3/(NO_3 + K_{NO3}) \right] [1 - (DO/(DO + K_{DO}))] \} \tag{12.25}
\]

Combining these two equations, for the ammonium flux:

\[
\frac{dNH_4}{dt} = k_{\text{max}} \left[ NO_3/(NO_3 + K_{NO3}) \right] [1 - (DO/(DO + K_{DO}))] - \]

### Table: Parameter Values

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>( k_n )</td>
<td>0.05-0.5</td>
<td>- a d</td>
</tr>
<tr>
<td>deep waters</td>
<td>0.1-0.5</td>
<td>- c</td>
</tr>
<tr>
<td>shallow waters</td>
<td>0.1-0.5</td>
<td>- b</td>
</tr>
<tr>
<td>( k_o )</td>
<td>&gt;1</td>
<td>- b</td>
</tr>
<tr>
<td>( k_a )</td>
<td>0.02-0.024</td>
<td>- d</td>
</tr>
<tr>
<td>( \theta_a )</td>
<td>0.003-0.03</td>
<td>- d</td>
</tr>
<tr>
<td>( \theta_f )</td>
<td>1.005-1.030</td>
<td>- c</td>
</tr>
<tr>
<td>a</td>
<td>1.024</td>
<td>- a b</td>
</tr>
<tr>
<td>b</td>
<td>1.024-1.037</td>
<td>- a</td>
</tr>
<tr>
<td>c</td>
<td>1.08</td>
<td>- a</td>
</tr>
<tr>
<td>d</td>
<td>1.08 (1.0548-1.0997)</td>
<td>- c</td>
</tr>
</tbody>
</table>

a - Schnoer (1996)  
b - Chapra (1997)  
c - Thomann and Mueller (1987)  
d - Bowie et al. (1985)
and for the nitrate flux:

\[
\frac{dNO_3}{dt} = k^{max} \{ \frac{NH_4}{(NH_4 + K_{NH_4})}[DO/(DO + K_{DO})] - \frac{NO_3}{(NO_3 + K_{NO_3})}[1 - (DO/(DO + K_{DO}))] \}
\]  \hspace{1cm} (12.27)

Temperature correction constants, not shown in the above equations, may differ.

4.8 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 that may result in an excessive increase in the biomass of algae. When it is visible on the surface of the water it is called an algae bloom. Excessive algal biomass could affect the water quality, especially if it causes anaerobic conditions and thus impairs the drinking, recreational and ecological uses.

The eutrophication component of the model relates the concentration of nutrients and the algal biomass. For example, as shown in Figure 12.12, 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.
Figure 12.12. The dissolved oxygen, nitrogen and phosphorus cycles, and phytoplankton interactions in a water body, showing the decay (satisfaction) of carbonaceous and sediment oxygen demands, reaeration or deaeration of oxygen at the air-water interface, ammonification of organic nitrogen in the detritus, nitrification (oxidation) of ammonium to nitrate-nitrogen and oxidation of organic phosphorus in the sediment or bottom layer to phosphate phosphorus, phytoplankton production from nitrate and phosphate consumption, and phytoplankton respiration and death contributing to the organic nitrogen and phosphorus.
Figure 12.13. Calculating 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: $f_d = (\text{EDH} / 24)$.

To account for this, algal growth is commonly modeled as a Michaelis-Menten multiplicative effect, i.e. the nutrients have a synergistic effect. Model parameters include a maximum algal growth rate $\mu$ (1/day) times the fraction of a day, $f_d$, that rate applies (Figure 12.13), the half saturation constants $K_P$ and $K_N$ (mg/l) (Figure 12.14) 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 in proportion to their contents in the algae biomass. Define these proportions as $a_P$, $a_A$, and $a_N$ respectively.
Figure 12.14. Defining the half saturation constant for a Michaelis-Menten model of algae. The actual growth rate constant = $\mu \frac{C}{(C + K_C)}$.

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 12.12 can be written as follows:

For algae biomass:
$$\frac{dA}{dt} = \mu f_d \theta_A^{(T-20)} \left[ \frac{P}{(P + K_P)} \right] \left[ \frac{N_n}{(N_n + K_N)} \right] A - e \theta_A^{(T-20)} A \quad (12.28)$$

For organic phosphorus:
$$\frac{dP_o}{dt} = -k_{op} \theta_{op}^{(T-20)} P_o \quad (12.29)$$

For phosphate phosphorus:
$$\frac{dP}{dt} = -\mu f_d \theta_A^{(T-20)} \left[ \frac{P}{(P + K_P)} \right] \left[ \frac{N_n}{(N_n + K_N)} \right] a_p A \quad (12.30)$$

For organic nitrogen:
\[
d\frac{dN_o}{dt} = -k_{on} \theta_{on}^{(T-20)} N_o
\]

For ammonia-nitrogen:
\[
d\frac{dN_a}{dt} = -\mu f_d \theta_A^{(T-20)} \left[ \frac{P}{(P + K_P)} \left[ N_w/(N_n + K_N) \right] a_A A \right] \\
\quad + k_{on} \theta_{on}^{(T-20)} N_o - k_a \theta_a^{(T-20)} N_a
\]

For nitrate-nitrogen:
\[
d\frac{dN_n}{dt} = -\mu f_d \theta_A^{(T-20)} \left[ \frac{P}{(P + K_P)} \left[ N_w/(N_n + K_N) \right] a_N A \right] \\
\quad + k_a \theta_a^{(T-20)} N_a - k_n \theta_n^{(T-20)} N_n
\]

For dissolved oxygen:
\[
d\frac{dDO}{dt} = -k_{CBOD} \theta_{CBOD}^{(T-20)} CBOD - 4.57 k_a \theta_a^{(T-20)} N_a - 2 k_{op} \theta_{op}^{(T-20)} P_o \\
\quad + (1.5 \mu f_d - 2 \epsilon) \theta_A^{(T-20)} A + k_r \theta_r^{(T-20)} (DO_{sat} - DO) - SOD
\]

Representative values of the coefficients for this model are in Table 12.5.

Table 12.5. Typical values of coefficients in the eutrophication model.

<table>
<thead>
<tr>
<th>parameter</th>
<th>value</th>
<th>units</th>
</tr>
</thead>
<tbody>
<tr>
<td>(k_N)</td>
<td>10-20</td>
<td>(\mu g N/l)</td>
</tr>
<tr>
<td></td>
<td>50-200</td>
<td>(\mu g NO_3/l)</td>
</tr>
<tr>
<td></td>
<td>10 (1-20)</td>
<td>(\mu g N/l)</td>
</tr>
<tr>
<td>(k_P)</td>
<td>1.5</td>
<td>(\mu g P/l)</td>
</tr>
<tr>
<td></td>
<td>20-70</td>
<td>(\mu g P/l)</td>
</tr>
<tr>
<td>(\alpha_p)</td>
<td>0.012-0.015</td>
<td>mg P/mg A</td>
</tr>
<tr>
<td>(\alpha_N)</td>
<td>0.08-0.09</td>
<td>mg NO_3/mg A</td>
</tr>
<tr>
<td>(\mu)</td>
<td>1.5 (1.0-2.0)</td>
<td>l/day</td>
</tr>
<tr>
<td>(\epsilon)</td>
<td>0.2-8</td>
<td>l/day</td>
</tr>
<tr>
<td></td>
<td>0.1 (0.05-0.025)</td>
<td>l/day</td>
</tr>
</tbody>
</table>

\(a\) - Thomann and Mueller (1987)  
\(b\) - Schnoor (1996)  
\(c\) - Bowie et al. (1985)

4.8.1 An algal biomass prediction model.
An alternative approach to modeling the nutrient, oxygen, and algae parts of an ecological model has been implemented in a simulation model developed by Delft Hydraulics called DELWAQ-BLOOM (Los et al. 1992; WL, 1995; Smits 2001). This model is used to predict algae growth and mortality, oxygen concentrations and nutrient dynamics.

The ecological model DELWAQ-BLOOM has two main tasks. It 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 12.2. 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 four different groups of algae, (phytoplankton (diatoms, and flagellates) or macroalgae (‘attached’ or ‘suspended’ Ulva)), suspended and bottom detritus, oxygen and inorganic phosphorus particulate matter in the bottom sediments.

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

### 4.8.1.1 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 (autolysis), mineralization of detritus in the water column producing inorganic nutrients, and mineralization of detritus in the bottom producing inorganic nutrients. The model accounts for the settling of suspended detritus 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 orthophosphate.
4.8.1.2 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 $Si$). 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:

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

(12.35)

This equation applies in the water column as well as in the bottom sediments, however the mineralization rate constants, $k_C \theta_C^{(T-20)}$, may differ. The concentration of these detritus constituents in the bottom are sometimes expressed in grams per square meter of surface area divided by the depth of the sediment layer.

4.8.1.3 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.

$$dC/dt = -SR_C (C) / Depth$$

(12.36)

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

4.8.1.4 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 mass of these constituents in the water column without changing its volume; hence it increases the concentrations of these constituents in the water column. Assuming a fully mixed active bottom layer, resuspension does not change its concentration. For $C_B$ representing the concentration (grams of dry weight per cubic meter) of resuspended material in the active bottom sediment layer, the flux of constituent concentration in the water column is

$$\frac{dC}{dt} = RR_C \frac{C_B}{H}$$

(12.37)

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

4.8.1.5 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 12.15 shows this nitrogen cycle.
4.8.1.5.1 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 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 \((\text{gN.m}^{-3}.\text{day}^{-1})\) of

\[
dNH_d/dt = -k_{NH4} \theta_{NH4}^{(T-20)} NH_d
\]

Again, \(k_{NH4} \theta_{NH4}^{(T-20)}\) is the temperature corrected rate constant (1/day), and \(NH_d\) 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 there is a gram of nitrate-nitrogen $NO_3-N$ 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:

\[
\text{‘organic matter’} + 2NO_3 \rightarrow N_2 + CO_2 + H_2O
\]

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

\[
\frac{dNO_3}{dt} = -k_{NO_3} \theta_{NO_3}^{(T-20)} NO_3
\]  

(12.39)

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

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.
Equations 12.24 to 12.27 are alternative ways of modeling nitrification-denitrification that are sensitive to the dissolved oxygen levels in the water column.

### 4.8.1.5.2 Ammonia

Ammonia is produced by the autolysis of algae and by the mineralization of organic nitrogen in the water and bottom sediment. Ammonia is converted to nitrate by nitrification. Algae also consume ammonia.

Algae use ammonia and nitrate for growth. Different algae prefer either $NH_3$ or $NO_3$ nitrogen. Upon death they release part of their nitrogen contents as ammonia (autolysis). The remaining nitrogen of dying algae becomes suspended detritus and suspended ‘other organic nitrogen ($OON$)’. Algae can also settle to the bottom. Some algae can be fixed to the bottom, unless wind and water velocities are high enough to dislodge them.

Once in the bottom sediment, algae die and release all their nitrogen contents as ammonium into the water column and to organic nitrogen in the sediment. Algae can be resuspended back into the water column or be buried into a deeper sediment layer.

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. In the water column detritus and organic nitrogen can be mineralized to ammonia or can settle, adding nitrogen to the bottom detritus. 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 mineralization of suspended detritus. The ammonia produced from mineralization is assumed 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 $Si$).

### 4.8.1.6 Phosphorus cycle

The phosphorus cycle (Figure 12.16) 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 12.16. The processes involved in the phosphorus cycle.](image)

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 adsorption/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 the desorption of inorganic phosphorus is assumed to be such.

### 4.8.1.7 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 12.17.

![Figure 12.17. The processes involved in the silica cycle.](image)

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 ($BDetSi$).
4.8.1.8 Summary of nutrient cycles

The nutrient cycles just described are based on the assumption that nutrients can be recycled for 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 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. A considerable portion of the nutrients is 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 modeled as burial. For example, if a nominal value of 0.0025 day$^{-1}$ 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.

4.8.1.9 Algae modeling

Algal processes include its primary production, its mortality from autolysis (producing detritus and inorganic nutrients) and from grazing, its 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 modeling of algae is focused primarily on calculation of its growth and mortality, as well as on its interaction with the nutrient species and its affect on oxygen concentrations.
The basic behavior of algae in surface water can be illustrated by the two diagrams in Figures 12.18 and 12.19. 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.

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**Figure 12.18.** Modeling of diatoms.

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**Figure 12.19.** Modeling of other algae besides diatoms.
4.8.1.9.1 Algae species concentrations

The model BLOOM uses linear programming to find the maximum total net production, or optionally the total biomass, of selected algae species in a certain time-period consistent with the environmental conditions and the existing biomass levels (Los, et al., 1992; Smits 2001). The nutrient and algae biomass concentrations at the beginning of the period are assumed known. The model must be solved for successive time periods in which the nutrient levels and initial biomass concentrations can be changed in accord with the solution of the previous time step.

The total net production or the total biomass of the system is maximized given the availability of nutrients, light and temperature. The optimization procedure distributes the available resources among all chosen algae types yielding a new composition of algae type biomass concentrations.

Typically, BLOOM considers between three and ten representative algae species. For example, consider the following four (groups) of species: diatoms, microflagellates, suspended Ulva, and fixed Ulva. The diatoms can be further divided into two types based on their limiting nutrient or energy. The other algae groups can be divided into three types based on their limiting nutrient or energy. Hence a total of eleven different algae types could be defined in this example.

Denote each distinct specie subtype (from now on called type) by the index $k$. The BLOOM model identifies the maximum 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. The sum of the biomass concentrations over all types $k$ is the total algae biomass concentration. This sum is maximized to identify the potential for algae blooms.

$$\text{Maximize } \sum_k B_k$$

(12.40)

This maximum total concentration does not necessarily indicate whether or not an actual algal bloom will occur. Rather it indicates the potential for an algae bloom.
For each algae type, the requirements for nitrogen, phosphorus and silica (only used 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.m$^{-3}$) of each nutrient in the water column equals the amount in the total living biomass of algae, $\Sigma_k(n_{ik}B_k)$, 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 $i$.

$$\Sigma_k(n_{ik}B_k) + d_i + w_i = C_i$$

The unknown concentration variables $B_k, d_i,$ and $w_i$ are non-negative. All nutrient concentrations $C_i$ are the measured or modeled total concentrations and are assumed to remain constant throughout the time period (e.g., a week in the summer, or a month in the winter) defined for the optimization model. The system is assumed to be in equilibrium over that period.

**4.8.1.9.2 Nutrient recycling**

A certain amount of each algae type $k$ dies in each time step. This takes nutrients out of the live phytoplankton pool. A fraction remains in the in the detritus pool, and the remainder is directly available to grow new algae because the dead cells break apart (a process called 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 is 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, $\frac{dd_i}{dt}$, in the water column equals the increase due to mortality less that which remineralizes and that which settles to the bottom.

$$\frac{dd_i}{dt} = \sum_k (f_k M_k n_{ik} B_k) - m_i d_i - s d_i$$

(12.42)

Assuming steady state conditions, Equation 12.42 equals 0. Both mortality and mineralization rate constants are temperature dependent.

4.8.1.9.3 Competition between species

In (classical) differential equation models competition between algae species depends on net growth rates. When nutrient levels get low, a single half-saturation coefficient of the limiting nutrient can decide the outcome of the competition. In contrast competition between species in BLOOM is determined by the net growth rate constant as a measure for the uptake rate of (limiting) resources by each algae species and by the requirements of each species for each resource.

Occasionally a rapidly growing type of algae can outcompete a slowly growing type even if the latter has a lower requirement for the limiting nutrient. This may happen for example in early spring when potential growth rates of diatoms clearly exceed those of other species. During summer, for example, the Ulva can become dominant under phosphorus limitation even though the potential net growth rates of other species are higher.

4.8.1.9.4 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 $K_k^{\text{max}} (1/\text{m})$ 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 $K_k^{\text{min}}$. The ranges between $K_k^{\text{min}}$ and $K_k^{\text{max}}$ 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

$$KL = \Sigma_k( K_k B_k)$$  \hspace{1cm} (12.43)

Added to this must be the extinction caused by dead cells, $KD$ and the background extinction of the water, $KW$ (1/m).

$$K_k^{\text{min}} \leq KL + KD + KW \leq K_k^{\text{max}}$$  \hspace{1cm} (12.44)

The extinction from dead cells is usually less than half of that from live cells. The amount of dead cells not yet mineralized is, from Equation 12.42, $\Sigma_k(f_p M_k B_k)$. Assuming some fraction $e_d$ (usually between 0.2 and 0.4) of the extinction rate of live cells,

$$KD = e_d \Sigma_k K_k f_p M_k B_k$$  \hspace{1cm} (12.45)

If the total extinction is not within the range for a algae type $k$, 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 modeled by adding three linear constraints for each algae type $k$.

$$KL + KD + KW \leq K_k^{\text{max}} + KM (1 - Z_k)$$  \hspace{1cm} (12.46)

$$KL + KD + KW \geq K_k^{\text{min}} (Z_k)$$  \hspace{1cm} (12.47)

$$B_k \leq BM Z_k$$  \hspace{1cm} (12.48)

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 12.48 wants to set each $Z_k$ value equal to 1, only when the total extinction is outside of the extinction range $K_k^{\text{min}}$ to $K_k^{\text{max}}$ will the $Z_k$ value be forced to 0. Equation 12.48 then forces the corresponding $B_k$ to 0.

4.8.1.9.5 Growth limits
For all algae types $k$ the maximum possible biomass concentration, $B_{k}^\text{max}$ (g dry.m$^{-3}$), at the end of the time interval $\Delta t$ (days) depends on the biomass concentration, $B_k$, (g dry.m$^{-3}$), the maximum gross production rate $P_{gk}^\text{max}$ (day$^{-1}$), the respiration rate constant, $R_k$, (day$^{-1}$), and a time and depth averaged production efficiency factor, $E_k$. Using the net production rate constant, $P_{nk} (= P_{gk}^\text{max} E_k - R_k)$ (day$^{-1}$), for each algae type $k$:

$$B_{k}^\text{max} = B_k^o \exp\{ P_{nk} \Delta t \} \quad (12.49)$$

### 4.8.1.9.6 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, $B_{k}^\text{min}$ (g dry.m$^{-3}$), of type $k$ at the end of time interval $\Delta t$ depends on the initial biomass, $B_k^o$ (g dry.m$^{-3}$), of type $k$ and the specific mortality rate constant, $M_k$ (day$^{-1}$) of type $k$.

$$B_k^\text{min} = B_k^o Z_k \exp\{- M_k \Delta t \} \quad (12.50)$$

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.

$$\sum_{k \text{ of species } j} B_k^\text{min} \leq \sum_{k \text{ of species } j} B_k \leq \sum_{k \text{ of species } j} B_k^\text{max} \quad \forall \text{ species } j \quad (12.51)$$

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. Thus when the minimum biomass of a species drops below this base level, it is set to zero.

### 4.8.1.9.7 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. The model includes the production of oxygen by algae (primary production), and the consumption of oxygen from algal respiration. Oxygen is also consumed by 1) the mineralization of detritus and other organic material (in the water column and bottom sediment), 2) nitrification of ammonia to nitrate, and 3) exchange of oxygen with the atmosphere (e.g. reaeration).

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 $32/12 \text{ gO}_2$ to 1 gC. The net growth of algae produces oxygen at a molar ratio of 1:1, equivalent to a ratio of $32/12 \text{ gO}_2$ to 1 gC. 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 $32/12 \text{ gO}_2$ to 1 gC. The nitrification reaction consumes oxygen at a molar ratio of 2:1, equivalent to a ratio of $64/14 \text{ gO}_2$ to 1 gN. 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 $32/12 \text{ gO}_2$ to 1 gC.

4.8.1.9.7.1 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 $32/12 \text{ gO}_2$ to 1 gC.

4.8.1.9.7.2 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 24-hour day-night cycle. Typically, oxygen concentrations are lowest in the early morning as oxygen is consumed during the night with the processes of algae respiration and organic material mineralization. During the daylight hours, oxygen is produced, and highest values (often supersaturated) are typically found in the late afternoon.
The option to calculate the daily cycle of oxygen has been built into the BLOOM algae model. 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.

In reality, the primary production of algae and the associated production of oxygen are concentrated in the daytime. On the other hand, there are the processes of algae respiration and mineralization of organic matter that consume oxygen continuously. These effects combined cause a rather strong variation of the oxygen concentration in water over a day.

The calculation of variable oxygen concentration is implemented by calculating the actual oxygen production by algae for each hour of 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 nighttime. The hourly oxygen production is combined with the daily averaged oxygen consumption processes to produce an hourly value of oxygen concentration in the water.

4.8.1.9.7.3 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, i.e., 32/12 g\(O_2\) to 1 gC. Total respiration is divided into growth respiration and a 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 depend on the temperature-dependent respiration rate constant, \(k_k^{\text{res}}\theta_k^{\text{res}(T-20)}\) (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 (gC\(_2\).m\(^{-3}\).day\(^{-1}\)) at which carbon in algae is oxidized is

\[
dAlgC_k/dt = k_k^{\text{res}}\theta_k^{\text{res}(T-20)} AlgC_k
\]  

(12.52)
4.9 Toxic chemicals

Toxic chemicals are substances that at low levels can impair the reproduction and growth of fish and human beings. Another important characteristic of these substances is their affinity with the surface areas of sediments. To model this adsorption-desorption process, estimations of the suspended sediment concentration, resuspension from the bottom, and settling are required.

Figure 12.18 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 waterbody and in the bottom sediments.

![Figure 12.18. Schematic of the adsorption/desorption and decay processes of various toxic chemicals in waterbodies and bottom sediments.](image)

The adsorption-desorption model assumes (conveniently but not always precisely) that an equilibrium exists between the dissolved (in water) and absorbed (on sediments) concentrations of a toxic constituent such as a heavy metal or organic contaminant. This equilibrium follows a linear relationship. The slope of that linear relation is the partition coefficient $K_p$ (liters/kg). This is shown in Figure 12.19.
Figure 12.19. Defining the partition coefficient $K_p$ (liters/kg) as the slope of the fixed ratio between concentrations of a constituent in the water and sediment phases of either a water body or bottom sediments. Different constituents have different partition coefficients, when they apply.

Representative values of partition coefficients $K_p$ are in Table 12.6.


<table>
<thead>
<tr>
<th>$K_p$ parameter</th>
<th>value</th>
<th>units</th>
</tr>
</thead>
<tbody>
<tr>
<td>arsenic</td>
<td>$10^4$</td>
<td>l/kg</td>
</tr>
<tr>
<td>heavy metals (Cd,Cu,Cr,Zn)</td>
<td>$10^4-10^6$</td>
<td>l/kg</td>
</tr>
<tr>
<td>benzo(a)pyrene</td>
<td>$10^4-10^5$</td>
<td>l/kg</td>
</tr>
<tr>
<td>lead</td>
<td>$10^5-10^6$</td>
<td>l/kg</td>
</tr>
<tr>
<td>PCB</td>
<td>$10^5-10^6$</td>
<td>l/kg</td>
</tr>
<tr>
<td>plutonium-239</td>
<td>$10^4-10^5$</td>
<td>l/kg</td>
</tr>
<tr>
<td>methoxychlor</td>
<td>$10^4$</td>
<td>l/kg</td>
</tr>
<tr>
<td>naphthalene</td>
<td>$10^3$</td>
<td>l/kg</td>
</tr>
</tbody>
</table>

Assuming partition coefficients apply to a particular toxic constituent, the concentration, $C_w$, of that constituent in the waterbody is divided a dissolved fraction and an absorbed fraction. These fractions $f_{dw}$ and $f_{aw}$, respectively, depend on the partition coefficient, $K_p$, and on the suspended sediment concentration, $SS$ (kg/mg). The proportions of the total constituent concentration in the
waterbody, $C_w$, dissolved in the water, $DC_w$ (mg/l), and adsorbed to the suspended sediments, $AC_w$ (mg/l) are defined as

$$DC_w = f_{dw} C_w$$
$$AC_w = f_{aw} C_w$$

where the fractions

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

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).

$$DC_s = f_{ds} C_s$$
$$AC_s = f_{as} C_s$$

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

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

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

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

In the above two equations the parameter $s$ is the mass of settling sediments (mg/day), $r$ is the mass of resuspension sediments (mg/day), and $\theta$ is the temperature correction coefficient of the constituent at temperature $T = 20^\circ$ 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 $\theta$. Suspended solids settling and resuspension can be determined at each day from a sediment transport model.
4.9.1 Micropollutants

Micropollutants include heavy metals, organic substances and radioactive substances. These three groups of pollutants show basic differences with respect to properties and processes.

Heavy metals can be divided among three subgroups:
1. cadmium, copper, lead, mercury, nickel, tin, zinc;
2. chromium; and
3. arsenic; vanadium.

Subgroup 1 includes the heavy metals that tend to form poorly soluble sulphides at chemically reducing conditions. Chromium and arsenic do not form sulphide precipitates under normal conditions in sediments. However, chromium and vanadium may form oxides and hydroxides. Arsenic and vanadium are present as anions in dissolved form, whereas the other metals form free or complexed cations. The differences between the groups of metals have important consequences for the partitioning of the metals among several dissolved and particulate phases.

Metals are conservative 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. Adsorbed fractions of a metal on particulate matter are influenced by all the processes that affect particulate matter, such as settling and resuspension.

Partitioning is described in general by sorption to particulates, precipitation in minerals, and complexation in solution. Complexation with inorganic and organic ligands can be considered explicitly in connection with the other processes. Sorption can be modeled as an equilibrium process (equilibrium partitioning) or as the resultant of slow adsorption and desorption reactions (kinetic formulations). In the latter case, partitioning is assumed to proceed at a finite rate proportional to the difference between the actual state and the equilibrium state.
To describe the fate of certain heavy metals in reducing environments, such as sediment layers, the formation of metal sulphides or hydroxides can be modeled. The soluble metal concentration is determined on the basis of the relevant solubility product. The excess metal is stored in a precipitated metal fraction.

Sorption and precipitation affect the dissolved metal concentration in different ways. Both the adsorbed and dissolved fractions increase at increasing total concentration as long as no solubility product is exceeded. The dissolved concentration is bounded by precipitation at the level at which a solubility product is exceeded.

### 4.9.2 Organic substances

Organic micropollutants include hexachlorohexane, hexachlorobenzene, PCB’s or polychlorobiphenyls, benzo-a-pyrene and fluoranthene (PAH’s or polycyclic aromatic hydrocarbons), diuron and linuron, atrazine and simazine, mevinfos and dichlorvos, and dinoseb.

The short-term fate of organic micropollutants in a water system is determined primarily by partitioning to water and organic particulate matter (including phytoplankton), and by transport. Additional processes such as volatilization and degradation influence organic micropollutant rates. The rates of these processes are concentration and temperature dependent.

The presence of a micropollutant 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. The latter are calculated from partitioning formulations.

Because the fate of most micropollutants 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 modeled part of the water system by burial.

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

Other transport processes taken into account concern advection and dispersion (including diffusion) between the various compartments in the water column and the sediment layer.

Heavy metals and organic substances can adsorb to particulate inorganic matter, to dead particulate organic matter, and to phytoplankton. The adsorption to particulate matter is described by means of equilibrium or kinetic partitioning, on the basis of a partitioning coefficient. For each particulate phase, a different partition coefficient may apply. The partition coefficient values are dependent on the chemistry of the water (pH and dissolved calcium) and the macrochemical composition of the inorganic matter (binding capacity). These dependencies are often neglected, however.

The fractions of a micropollutant adsorbed to algae, $f_{alg}$, inorganic matter, $f_{im}$, dead particulate organic matter, $f_{poc}$, and the dissolved fraction of a micropollutant, $f_{d}$, add up to the total micropollutant concentration, $C$ (mg.m$^{-3}$).

\[
C = (f_{alg} + f_{im} + f_{poc} + f_{d}) C
\]  
(12.63)

Where the fractions are functions of the partition coefficients $Kp$ (for algae (m$^3$.gC$^{-1}$), for inorganic matter (m$^3$.gDW$^{-1}$) and for dead particulate organic matter (m$^3$.gC$^{-1}$)), 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).
\[ fd = \phi / [ \phi + K_{palg} C_{alg} + K_{pim} C_{im} + K_{ppoc} C_{poc} ] \]  (12.64)

\[ fim = (1 - fd) K_{pim} C_{im} / [K_{palg} C_{alg} + K_{pim} C_{im} + K_{ppoc} C_{poc} ] \]  (12.65)

\[ f_{poc} = (1 - fd) K_{ppoc} C_{poc} / [K_{palg} C_{alg} + K_{pim} C_{im} + K_{ppoc} C_{poc} ] \]  (12.66)

\[ f_{alg} = (1 - fd - fim - f_{poc}) \]  (12.67)

Each partition coefficient \( Kp \) (mg.kg\(^{-1}\)DW/mg.l\(^{-1}\) water or l/kg) is defined as the ratio of the particulate concentration \( C_{p}' \) of a micropollutant (mg.kg\(^{-1}\)DW or mg.kg\(^{-1}\)C) divided by the dissolved concentration \( C_{d}' \) of a micropollutant (mg/l water).

\[ Kp = C_{p}' / C_{d}' \]  (12.68)

In terms of bulk measures, each partition coefficient \( Kp \) also equals the porosity \( \phi \) times the bulk particulate concentration \( C_{p} \) (mg.m\(^{-3}\) bulk) divided by the product of the dissolved (mg.l\(^{-1}\) bulk) and particulate (mg/m\(^{3}\) bulk) bulk concentrations, \( C_{d} C_{s} \), all times \( 10^6 \) mg/kg.

\[ Kp = 10^6 \phi C_{p} / (C_{d} C_{s}) \]  (12.69)

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

\[ dC_{p}/dt = k_{sorp} (C_{pe} - C_{p}) \]  (12.70)
The kinetic constant for sorption is not temperature dependent. All other kinetic constants for micropollutants are temperature dependent.

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

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

Volatilization is formulated according to the double film theory. The volatization rate \( \frac{dC_d}{dt} \) (mg.m\(^{-3}\).day\(^{-1}\)) of dissolved micropollutant concentrations, \( C_d \) (mg.m\(^{-3}\) water) in water depends on an overall transfer coefficient, \( k_{vol} \) (m.day\(^{-1}\)), for volatilization and the depth of the water column, \( H \) (m).

\[
\frac{dC_d}{dt} = - \frac{k_{vol} C_d}{H}
\]  \hspace{1cm} (12.71)

The numerator (\( k_{vol} C_d \)) is the volatilization mass flux (mg.m\(^{-2}\).day\(^{-1}\))

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\(^{-1}\)) are usually modeled as

\[
\frac{dC}{dt} = - k C
\]  \hspace{1cm} (12.72)

where \( C \) is the total concentration of a micropollutant (mg.m\(^{-3}\)), and \( k \) is a (pseudo) temperature dependent first order kinetic rate constant for biodegradation, photolysis, hydrolysis or overall degradation (day\(^{-1}\)).
4.9.3 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 adsorbs to particulate matter, both reversibly and irreversibly. Precipitation of cesium does not occur at the low concentrations occurring in natural water systems. Iodine is only present in soluble form as an anion.

Iodine is generally present 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. Cesium ($Ce^+$) can adsorb to particulate inorganic matter, to dead particulate organic material, and to phytoplankton. A part of the adsorbed fraction of cesium in inorganic matter is irreversibly bound. The irreversible fraction increases over time as the reversible fraction gradually transforms into the irreversible fraction, according to first order kinetics. Radioactive decay proceeds equally for all fractions, according to first order kinetics.

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 rate of radioactive decay (mg.m$^{-3}$.day$^{-1}$) is usually modeled as a first order process involving a kinetic radioactive decay constant, $k_{dec}$ (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:

$$Ac = 10^{-3} N_A k_{dec} C_R / [86400 Mw]$$  \hspace{1cm} (12.73)

where

- $Ac =$ activity of the radionuclide (Bq.m$^{-3}$.s$^{-1}$)
- $N_A =$ Avogadro’s number (6.02*10$^{23}$ mole)
- $Mw =$ molecular weight of the radionuclide (g.mole$^{-1}$)

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

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

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

The water quality of lakes and reservoirs is defined by variables measured within the water basin. Although there are many variables of limnological significance, water quality is typically characterized on the basis of such variables as

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

Many waste chemical compounds from industry, some with toxic or deleterious effects on humans and/or water-dependent products, are discharged into lakes and reservoirs. These can kill aquatic organisms and damage irrigated crops. Because of inadequate water purification the
quantity of bacteria, viruses and other organisms in discharged waters are 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 water-bodies, whether lakes or reservoirs. Deep lakes, particularly in non-tropical regions, usually have better water quality in lower layers. Shallow lakes do not exhibit this depth differentiation in quality. Their more shallow, shoreline areas have relatively poorer water quality because they are where pollutant inputs are discharged and areas with a greater potential for disturbance of bottom muds, etc. Thus, the water quality of a natural lake usually improves as one moves from the shoreline to the deeper central part.

![Figure 12.20. Longitudinal zonation of water quality and other variables in reservoirs (UNEP, 2000)](image-url)
In contrast, the deepest end of a reservoir is immediately upstream of the dam so that 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 12.20.

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. Thus, reservoirs have been characterized as comprising three major zones: an upstream riverine zone, a downstream lake-like zone at the dam end, and a transitional zone separating these two zones (Figure 12.20). The relative size and volume of the three zones can vary greatly in a given reservoir.

5.1 Downstream characteristics

Constructing a dam can produce dramatic changes in the downstream river channel below the dam that 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 can be picked up and transported as it moves downstream. Because it contains less sediment the discharged water can scour and erode the streambed and banks as it picks 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.
Figure 12.21. A multiple outlet reservoir can be better used to regulate the temperature and water quality downstream.

Many reservoirs, especially those used for drinking supplies, have water release or discharge structures located at different vertical levels in their dams (Figure 12.21). This allows for the withdrawal or discharge of water from different layers within the reservoir, so called “selective withdrawal.” Depending on the quality of the water discharged, selective withdrawal can significantly affect water quality within the reservoir itself, as well as the chemical composition and temperature of the downstream river. The ability to regulate or schedule water and silt discharges also can fundamentally change downstream hydrological regimes, affecting both flora and fauna.

Constructing a reservoir to protect downstream areas from floods often has significant social and economic implications, including the potential for stimulating urban and agricultural development adjacent to, and below, the reservoir. This can have both positive and negative impacts on 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
favorable, excessive nutrients stimulate population explosions of undesirable algae and aquatic weeds. The algae sink to the lake bottom after they die, where bacteria consume the available dissolved oxygen as the bacteria decompose the algae. Fish kills and foul odors may result if dissolved oxygen is depleted.

Heavy metals are another major cause of lake quality impairment. This is mainly due to the widespread detection of mercury in fish tissue samples. It is difficult to measure mercury in ambient water so fish samples are usually used to indicate mercury contamination, since mercury bioaccumulates in fish tissue. The mercury problem is complex because it involves atmospheric transport from power-generating facilities and other sources.

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

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 differences in the problems of predicting the water quality of lakes or reservoirs compared to those of river and estuarine systems. This is mainly due to the increased importance of wind induced mixing processes and thermal stratification. For reservoirs, it is also due to the impact of various reservoir-operating policies.

### 5.2 Lake quality models

Perhaps the simplest way to begin is to consider shallow well-mixed constant-volume lakes. 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$^3$). Assuming 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 $Q$ (m$^3$/day), then the rate of change in the concentration $C$ (g/m$^3$/day) is

$$\frac{dC}{dt} = (1/V) (W_C - QC - k_C CV) \quad (12.74)$$

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

$$C(t) = \left[ \frac{W_C}{Q + k_C V} \right] \left[ 1 - \exp\{-\Delta t((Q/V) + k_C)\} \right] + C(t-1) \exp\{-\Delta t((Q/V) + k_C)\} \quad (12.75)$$

The equilibrium concentration, $C_e$, can be obtained by assuming each concentration is equal in Equation 12.75 or by setting the rate in Equation 12.74 to 0, or by setting $C(t-1)$ equal to 0 and letting $\Delta t$ go to infinity in Equation 12.75. The net result is

$$C_e = \frac{W_C}{Q + k_C V} \quad (12.76)$$

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

$$t_\alpha = - \frac{V \ln(1 - \alpha)}{(Q + k_C V)} \quad (12.77)$$

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, from Equation 12.45, is

$$\frac{dC}{dt} = - C (Q + k_C V) / V \quad (12.78)$$
Integrating this equation, the concentration \( C(t) \) is

\[
C(t) = C(0) \exp\{- t ((Q/V) + K_C) \} \quad (12.79)
\]

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 \( C(0) \) (i.e., \( C(t)/C_e = 1 - \alpha \)). The result is Equation 12.77.

Equation 12.75 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, \( C(t)^{\text{max}} \), may vary among different within-year periods \( t \), the least uniform fraction of waste removal required at all source sites can be found by solving the following linear optimization model:

Minimize \( X \) \quad (12.80)

Subject to the following constraints for each period \( t \):

\[
C(t) = \left[ \frac{W_C(t)(1-X)}{(Q(t) + k_C V)} \right] \left[ 1 - \exp\{-\Delta t((Q(t)/V) + k_C)\} \right] + C(t-1) \exp\{-\Delta t((Q(t)/V) + k_C)\} \quad (12.81)
\]

\[
C(t) \leq C(t)^{\text{max}} \quad (12.82)
\]

If each period \( t \) is a within-year period, and if the first period follows the last period, then no initial concentrations need be assumed and the steady state solution will indicate, for the loadings \( W_C(t) \), the fraction \( X \) of waste removal that meet the quality standards, \( C(t)^{\text{max}} \), throughout the year.

5.3 Stratified impoundments

Many lakes become stratified during particular times of the year. When stratified the depth-dependent temperature gradients 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. Their different densities prevent complete mixing between the two zones. The transition zone or boundary between the two zones is called the thermocline.

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 12.22.

Figure 12.22. Lake stratification during summer and complete mixing during winter season.

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
$C_c(t)$ 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 $C_h(t)$ are:

$$\frac{dC_e(t)}{dt} = \left( \frac{1}{V_e(t)} \right) \{ \text{mass inflow } W_c(t) - \text{mass outflow } C_c(t)Q_{out}^{t_e(t)} \} + \text{net vertical transfer across thermocline } \left( \frac{v}{D_T} \right) [C_h(t)V_h(t) - C_e(t)V_e(t)] - \text{decay } kC_e(t) \quad (12.83)$$

$$\frac{dC_h(t)}{dt} = - \text{decay } kC_h(t) - \text{net vertical transfer across thermocline } \left( \frac{v}{D_T} \right) [C_h(t) - C_e(t)V_e(t)/V_h(t)] - \text{settling on sediment interface } sH_h(t) C_h(t) \quad (12.84)$$

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).

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:

$$C(t) = C_e(t)V_e(t) + C_h(t)V_h(t) / [V_e + V_h] \quad (12.85)$$

$$\frac{dC(t)}{dt} = \left( \frac{1}{V(t)} \right) \{ \text{mass inflow } W_c(t) - \text{mass outflow } C(t)Q_{out}^{t_e(t)} \} - \text{decay } kC_c(t) - \text{settling } sH(t) C(t) \quad (12.86)$$

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

$$C_e(t) = C(t) \quad (12.87)$$

$$C_h(t) = C(t) \quad (12.88)$$
6. Sediment

The production and transportation of sediment in a watershed and water body are influenced by a complex set of geomorphic processes that vary in time and space. The erosion processes include soil detachment caused by rain and overland flow; rill erosion and transport; gully erosion; channel degradation and bank erosion; surficial gravity erosion and, wind erosion. Erosion also occurs on a larger scale episodically due to channel bank and hill slope failures, landsliding, forest fires, and debris flows. Land use practices such as logging and clearing, grazing, road construction, agriculture, and urbanization activities also affect sediment production and delivery from a watershed. Sediment production may vary significantly with long-term cycles in drainage system development and rejuvenation.

On very small scales of time and space, erosion rate is roughly equivalent to sediment yield. However, for larger basins, as the area and time scales to be considered increase, transport and deposition processes influence both the sediment yield and the timing of sediment discharge from a basin. Deposition occurs at the base of steep slopes; in lakes, reservoirs, and wetlands; in river flood plains; and on point bars in stream channels (lateral accretion and bed aggradation).

Episodic and spatially varying processes dominate sediment and water flow, but theories and quantification of these processes are not well developed. Biota play essential roles in the production, transport and storage of sediment and water, but knowledge of biological functions is poorly integrated into quantitative procedures for estimating sediment and water budgets.

A watershed can be divided into major zones or provinces where different sets of physical processes interact to characterize sedimentation processes. There are three physiographic zones suggested in literature: production zone or sediment source area; transfer zone and, deposition zone or sediment sink area. Development of basin sediment budgets and yield estimates requires an understanding of how these zones or provinces connect and the approximate quantities of materials entering and leaving each zone for the expected range of flow conditions.
For the purpose of estimating sediment production, important processes can be roughly divided into three categories of sheet and rill erosion, gully and channel erosion, and mass wasting processes. The relative magnitudes of each category depend on the soils, geomorphic, hydrologic and land use characteristics of the basin.

Sediment yield is the amount of sediment passing a specified channel location. It is influenced by a number of geomorphic processes. It may be substantially less than the amount actually eroded in the basin. Sediment yield typically expressed as the total sediment volume delivered to a specified location in the basin divided by the effective drainage area above that location for a specified period of time. Sediment yield typically has the units of cubic meters/square kilometer/year or metric tons or English tons per year. However often it is necessary to estimate yield from a watershed from individual storm events of specified frequency (e.g., 5-, 25-, 50-, or 100-year events). These individual event yields are reported as metric tons or cubic meters per event. In some watersheds, single event sediment yields often exceed average annual values by several orders of magnitude.

Spatial and temporal variations in physical and biological features of the watershed make estimation of sediment yield an extremely difficult and imprecise task. As discussed in more detail in Chapter XII, important variables include soils and geology, relief, climate, vegetation, soil moisture, precipitation, drainage density channel morphology, and human influences. Dominant processes within a watershed may be entirely different between physiographic or ecological provinces, and may change with time. The problem becomes even more complex when grain size distributions and sediment yield for particular events must be estimated for input to sedimentation transport simulation models. There is no widely accepted procedure for computing basin sediment yield and grain size distribution directly from watershed characteristics without measured information.

Sediment transport is influenced primarily by the action of wind and water, and deposition occurs in a number of locations where energy for transport becomes insufficient to carry eroded sediments. Colluvial deposits, floodplain, and valley deposits, channel aggradation, lateral channel accretion, and lake and reservoir deposits are examples of typical geomorphic deposition
processes. The stability and longevity of sediment deposits vary. Lake and reservoir deposits tend to be long-term, whereas some channel and floodplain deposits may be remobilized by the next large scale flood event, only to be deposited downstream. The spatial and temporal variability of sediment production, transport and deposition greatly complicates the task of estimating sediment yield from a watershed.

Natural waters flowing at less than flood stages contains 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 the large adsorbing capacities, the fine fraction is characterized as cohesive sediment. Since flocculation and adsorbing capacities are of minor importance for larger particles, they are classified as non-cohesive sediment. The next two sections will focus on these two forms of sediment.

6.1 Cohesive sediment

The quantification of cohesive sediment transport is necessary before one can quantify the transport of particulate fractions of substances. Cohesive suspended matter is considered as silt and clay particles ranging in size from several microns up to about 70 microns. These soil particles are easily brought into suspension.

The behavior of this fine-grained suspended matter plays an important role in the water quality. Firstly, turbidity and its effect on the under-water 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. Secondly, 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.
The modeling of sedimentation and erosion processes originates in part from the Partheniades-Krone concept (Partheniades, 1962 and 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.

6.2 Non-cohesive sediment

Particles sizes of non-cohesive material are larger than those of cohesive sediment, and are in the order of 0.1 mm and more (sandy). The behavior of this sandy sediment transport is of major importance in coastal engineering problems related to morphological changes. The transport of sediment particles can be in the form of bed-load and suspended load, depending on the size of the bed material and the local instantaneous flow conditions (van Rijn, 1984). The transport of particles via rolling, sliding and jumping (saltating) is called bed load transport and this motion is exclusively determined by the effective bed shear stress that is assumed to be dominated by gravity forces. The bed load transport takes places in a thin layer above the bottom. The suspended load is that part of the total load that is moving without continuous contact with the bed as a result of the agitation of fluid turbulence.

Whether there is merely a bed load or a suspended load depends primarily on the intensity of the water movement. There is a critical velocity below which no movement occurs. If the velocity increases bottom transport is initiated to develop ripples and dunes. At higher velocities, sediment grains come into suspension and suspended loads starts. There are many models in the literature describing the transport of bed and suspended sediment loads. Here the transport formulation for the total load of Engelund and Hansen (1967) is discussed. This model is relatively simple and has shown good performance in numerous field and laboratory experiments. There are many others as discussed by Shen and Julien (1993) and in Chapter XII.

There are various ways to model the bottom sediment and related sedimentation and erosion processes. It is common to define two sediment layers at the bottom of the water column. These
sediment layers are not subject to advective and dispersive transport as is the overlying water column segment. The depths of these two sediment layers can either be fixed or variable.

In a variable-layer depth option, the thickness of the upper sediment layer can increase or decrease due to addition of sediment from sedimentation or loss of sediment from erosion. If the sediment layer exceeds its maximum defined thickness, then sediment is transported down to the underlying layer by the process of burial. In this option, it is possible for the upper sediment layer to be completely eroded. If this happens, sedimentation and erosion processes will occur on the lower layer.

In the fixed layer depth option, the thicknesses of the sediment layer(s) are fixed. If sedimentation occurs to the upper layer, then sediment is transferred downward by burial. If erosion to the upper layer occurs, then sediment is transported upward by ‘digging’. In this case, the resuspension of sediment is unlimited.

6.3 Process and model assumptions

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

The transport rate of non-cohesive sediment is determined by the local instantaneous flow conditions. This is commonly assumed for bed load transport. For suspended transport it implies that the time and length scales of the flow variation are much larger than the adaptation time and adaptation length of the sediment concentration respectively. The transport of such sediment is not related to the flow field in the same way as for dissolved substances and hence no dispersion or diffusion is applied.

Cohesive sediment can include silt and clay particles as well as particulate organic matter such as detritus carbon (DetC), other organic carbon (OOC), diatoms (Diat), non-diatom algae (Green)
and organic carbon from BOD loads \((BODC)\). The sediment layer is homogeneous (well mixed). The density of the layer can vary depending on the variable sediment layer composition. The porosity within a given layer is constant and user-defined.

Non-cohesive sediments are modeled as inactive substances. They comprise the bed load. Their horizontal transport rate results in a change of the amount of sediment present in the bottom and hence a change in the thickness of the layer of non-cohesive sediment.

Sedimentation occurs when the bottom shear stress is 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.

The composition of the resuspending sediment is the same as that of the bottom sediment. The resuspension flux can be assumed limited based on the available amount of sediment in a sediment layer, or unlimited. Resuspension flux is zero if the water depth becomes too small.

6.3.1 Mass balances

Mass balance equations provide the change of a concentration (or mass when multiplied with a volume) over a known time step in a segment compartment. They are different for the water column and the sediment layer. The mass balance equations for concentrations, \(C_j\) \((g \text{ dry wt./m}^3)\), of suspended organic or inorganic matter of various types \(j\) in the water column involve inputs, transport, resuspension and settling.

6.3.1.1 Settling

A characteristic feature of cohesive sediments is the ability to form aggregates of flocs that settle to the bottom. Whether a particle will settle to the bottom depends upon its size and density and the chemical conditions of the surrounding water system. Sedimentation is the process describing the settling of particles. 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.

The aggregation of flocs strongly depends on the chemical and physical properties of the sediment, salinity and turbulence. At high sediment concentrations (several g/l) the particles hinder each other, resulting in a decrease of the settling velocity. Turbulence is an important parameter because it affects the flocculation and therefore the settling velocity in two opposing ways. On the one hand an increase in turbulence will increase the collisions between particles, resulting in larger flocs with high settling velocities. On the other hand, it results in turbulent shear stresses that can break up the flocs and decrease the settling velocity.

For any substance $j$ 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

$$\frac{dC_j}{dt} = -\frac{1 - (\tau/\tau_j)}{(ZS_j + VS_j C_j) / H}$$

$$\tau \leq \tau_j$$

(12.89)

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

$$\frac{dC_{j\text{sed}}}{dt} = -\frac{dC_j}{dt} H$$

(12.90)
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.

6.3.1.2 Resuspension

If the shear stress $\tau$ is exceeds the critical shear stress $\tau_j$ for the type substance $j$ then no net settling takes place. Instead resuspension can take place.

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 $C_{j,\text{sed}}$ in the top sediment layer (g/m$^2$).

$$ \frac{dC_j}{dt} = \left( \frac{\tau}{\tau_j} - 1 \right) \left( ZR_j + kR_j C_{j,\text{sed}} \right) / H \quad \tau \geq \tau_j \quad (12.91) $$

The corresponding flux (g dry wt./m$^2$ sediment layer area /day) of substance $C_{j,\text{sed}}$ from the sediment layer area (erosion) is
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 $Z_R$ and $\tau$ strongly depend on the sediment properties and environmental parameter values.

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 12.92) times the fraction, $fr_j$, of component $j$ in the substance divided by the depth, $H$, of water column.

$$\frac{dN_j}{dt} = fr_j \frac{dC_{sed}}{dt} / H$$  \hspace{1cm} (12.93)

### 6.3.2 Armoring

The capacity of water to carry suspended sediments is usually in excess of the actual amounts being carried. This can be due to limited source material or due to armoring. Armoring occurs when larger particle size sediments cover smaller sediment size particles, and the flow velocity shear stress is insufficient to resuspend this top layer of larger particle sizes. Hence they protect or prevent these smaller size particles from being resuspended. Modeling the armoring process would require keeping track of just how much and when different particle sizes were deposited, and where they were deposited. Simpler models usually assume, obviously incorrectly, that the sediment layer is a homogenous mixture of all the existing sediment substances. Given this assumption, one approximate approach is to compute a weighted average critical shear stress value for all substances, including the bed load non-cohesive substances, rather than apply separate critical shear stresses, $\tau_j$, for each type of substance $j$. This average critical shear stress, $\tau_{crit}$, could be defined based on the proportion of substances, by weight, in the active sediment layer.

$$\tau_{crit} = \Sigma_j \frac{\tau_j \ C_j^{sed}}{\Sigma_j \ C_j^{sed}}$$  \hspace{1cm} (12.94)
This average critical shear stress would replace each substances critical shear stress, $\tau_j$, in only the resuspension Equations 12.91.

As flows increase, so do their velocities. In addition the area over which the water flows increases, and these new areas may not have been armored by decreasing flows in previous periods. Stream banks are typical sources of sediment for increasing flows. This suggests that average critical shear stresses may vary depending on the flow simply because the lateral distribution of sediment sizes in the active bottom layer is not uniform. If the sediment sizes are decreasing as the wetted perimeter of the channel increases, then the average critical shear stress decreases. Model developers can make adjustments to account for this in different ways, depending on the number of spatial dimensions being modeled.

### 6.3.3 Burial

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. This requires knowing the depth, $h_j$ (m/g dry wt/m$^2$) of particle size substance $j$ per unit dry wt per square meter. Hence if the total depth of the active sediment layer, $\Sigma_j C_j^{sed} h_j$, 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, $\Sigma_j C_j^{sed} h_j$, 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, $\Sigma_j C_j^{sed} h_j - D_{max})/ (\Sigma_j C_j^{sed} h_j)$.

$$\frac{dC_j^{bur}}{dt} = k_B C_j^{sed} \left[ C_j^{sed} h_j / (\Sigma_j C_j^{sed} h_j) \right] \left[ \Sigma_j C_j^{sed} h_j - D_{max}) / (\Sigma_j C_j^{sed} h_j) \right] \quad (12.95)$$

### 6.3.4 Bed shear stress

The bed shear stress is an essential quantity that directly influences the sedimentation and erosion rates. It depends on the flow (currents) and the wind (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, \( \tau_{\text{flow}} \), and waves, \( \tau_{\text{wave}} \), are additive:

\[
\tau = \tau_{\text{flow}} + \tau_{\text{wave}} \tag{12.96}
\]

The bed shear stress \( \tau_{\text{flow}} \) for depth-averaged flow depends on the water density (1000 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).

\[
\tau_{\text{flow}} = 1000 \times 9.81 \times \frac{U_h^2}{Cz^2} \tag{12.97}
\]

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), \( \text{Rough} \) (m), or Manning’s roughness coefficient, \( n \) (m\(^{-1/3}\).s\(^{1}\)).

\[
Cz = 18 \log_{10}(12 H/\text{Rough}) \tag{12.98}
\]
\[
Cz = (H)^{1/6} / n \tag{12.99}
\]

Both Nikuradse’s roughness coefficient as well as Manning’s roughness coefficient can 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 at the bed during propagation.
The magnitude of the bed shear stress, $\tau_{\text{wave}}$, due to waves depends on a wave friction factor, $f_w$, the density of water, $(1000 \text{ kg/m}^3)$ and the effective orbital horizontal velocity at the bed surface, $U_o$.

$$\tau_{\text{wave}} = 0.25 \times 1000 \times f_w \times U_o^2$$  \hspace{1cm} (12.100)

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). Also required is the depth of water, $H$ (m).

The effective horizontal bottom velocity due to waves is defined as

$$U_o = \pi \times H_s / [T_m \sinh(2\pi H/L_m)]$$  \hspace{1cm} (12.101)

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

$$f_w = 0.16 \left[ \frac{\text{Rough}}{U_o T_m / 2\pi} \right]^{0.5}$$  \hspace{1cm} (12.102)

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

$$A = H_s / [2 \times \text{Rough} \sinh(2\pi H/L_m)]$$  \hspace{1cm} (12.103)

If $A > 1.47$ then

$$f_w = \exp\{-5.977 + 5.123 H^{-0.194}\}$$  \hspace{1cm} (12.104)
Otherwise

\[ f_w = 0.32 \]  \hspace{1cm} (12.105)

### 6.4 Non-cohesive total bed load transport

A sediment transport formula is an algebraic equation relating the sediment rate with the flow parameters. One commonly used formulae is that of Engelund and Hansen (1967). Bed load transport is based on the local flow conditions at the water-bed surface interface. For non-cohesive material having a median particle size of \( D_{50} \) (m), the rate of transport (cubic meters of material passing over a meter of distance in a second, \( \text{m}^3/\text{m/s} = \text{m}^2/\text{s} \)) is assumed to be

\[
S = 0.05 \frac{U^3}{(D_{50} g^2 \Delta \rho^2)}
\]  \hspace{1cm} (12.106)

where the bed or friction velocity is

\[
U_b^2 = C \left[ \frac{\tau}{1000 \, g} \right]^{0.5}
\]  \hspace{1cm} (12.107)

And the parameter \( \Delta \rho \) is the ratio of the difference in specific densities of the bed material and water divided by the specific density of bed material (kg/m\(^3\)).

\[
\Delta \rho = \left( \frac{\rho_{\text{bed}} - \rho_{\text{water}}}{\rho_{\text{bed}}} \right)
\]  \hspace{1cm} (12.108)

Bedload transport results in a change of the amount of non-cohesive particles present in the bottom layer. The change in non-cohesive sediment volume, \( \Delta V_{\text{bed}} \) (m\(^3\)) over a bottom area of \( A_b \) (m\(^2\)) in a segment will be the difference between the incoming and outgoing sediment rates times the length, \( L \), of the segment times the length of the time period, \( \Delta t \).

\[
\Delta V_{\text{bed}} = (S_{\text{in}} - S_{\text{out}}) L \Delta t
\]  \hspace{1cm} (12.109)
This change can be represented by a change in thickness of this material in the bottom layer. It will depend on the porosity of the material, $\phi$, as well as the difference between the incoming and outgoing bedload. Denoting the thickness change as $\Delta D_{\text{bed}}$ (m),
\[
\Delta D_{\text{bed}} = \left[ \frac{1}{1 - \phi} \right] \frac{\Delta V_{\text{bed}}}{A_b}
\] (12.110)

A mass balance of relative bed depths and material can now be written. Defining $D_{\text{bed}}(t)$ $V_{\text{bed}}(t)$ (m$^3$) as the relative bed load depth and volume, respectively of non-cohesive material in a segment at the beginning of period $t$,
\[
D_{\text{bed}}(t+1) = D_{\text{bed}}(t) + \Delta D_{\text{bed}}
\] (12.111)
\[
V_{\text{bed}}(t+1) = V_{\text{bed}}(t) + \Delta V_{\text{bed}}
\] (12.112)

7. **Simulation methods**

Most who will be using water quality models will be using simulation models that are commonly available from governmental agencies, universities, or institutions such as the Danish Hydraulics Institute or Delft Hydraulics (Ambrose et al. 1995; Brown and Barnwell, 1987; Cerco and Cole 1995; DeMarchi, et al. 1999; Ivanov et al. 1996; Reichert, 1994; USEPA 2001). These simulation models are typically based on numerical methods and 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. In each simulation time step plug flow enters these segments or volume elements from upstream segments or elements. Flow also exits these segments or volume elements to downstream segments or elements. During this time the constituents can decay or grow, as appropriate given 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 determines the extent of dispersion in the system.
7.1 Numerical accuracy

Water quality simulation models based on physical, biological and chemical processes typically include time rate of change terms such as \( \frac{dC}{dt} \). While it is possible to solve analytically some of these differential equations, most water quality simulation models use numerical methods. The purpose of this section is not to explain how this can be done, but rather to point to some of the restrictions placed on the modeler because of these numerical methods. First we focus on the relationship between the stream, river, or lake segments and the duration of time steps, \( \Delta t \).

Consider the basic first-order decay flux \( \frac{dC}{dt} \) (g/m\(^3\)/day) for a constituent concentration \( C \) that is dependent on a rate constant \( k \) (day\(^{-1}\)).

\[
\frac{dC}{dt} = -kC
\]  
(12.113)

The finite difference approximation of this equation can be written

\[
C(t+\Delta t) - C(t) = -k\Delta t
\]  
(12.114)

or

\[
C(t+\Delta t) = C(t) (1 - k\Delta t)
\]  
(12.115)

This equation shows up the restriction placed on the term \( k\Delta t \). This term cannot exceed a value of 1 or else \( C(t+\Delta t) \) will be negative.

Figure 12.24 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 12.113, namely:

\[
C(t+\Delta t) = C(t) \exp\{-k\Delta t\}
\]  
(12.116)
Reducing the value of $\Delta t$ will increase the accuracy of the solution. Hence for whatever value of $\Delta t$, it can be divided by a positive integer $n$ to become $1/n$ of its original value. In this case the predicted concentration $C(t+\Delta t)$ will equal

$$C(t+\Delta t) = C(t) \left(1 - \frac{k\Delta t}{n}\right)^n \quad (12.117)$$

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

$$\frac{C(t+\Delta t)}{C(t)} = (1 - \frac{1}{2})^2 = 0.25 \quad (12.118)$$

Compare this to 0.37, the exact solution, and 0.0, the approximate solution when $n$ is 1. A big improvement. If $n = 3$, the concentration ratio will be 0.30, an even greater improvement compared to 0. No matter what value of $n$ is selected, the predicted concentration is always less than the actual value based on Equation 12.116, 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 12.117 can be written as
\[ C(t+\Delta t) = C(t) \left(1 + \frac{1}{m}\right)^{m(-k\Delta t)} \]  

(12.119)

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 12.119 becomes Equation 12.116, the exact solution to Equation 12.113.

### 7.2 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 segments or volume elements 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 12.25. 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 flow from any segment \( i \) does not pass through any following segment \( i+1 \). Hence at the end of each time period each segment has some of its original water, 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 give constant concentrations within the segment. This is done for all segments. Included in this plug flow and then mixing process are the inputs to the reach from point and non-point sources of constituents.
Figure 12.25 Water quality modeling approach involving plug flow during a time interval $\Delta t$ followed by complete mixing of each segment at the end of the period.

In Figure 12.25, a mass of waste enters reach $i$ at a rate of $W_i^t$. The volume in each reach segment is denoted by $V$ and the flows from one segment to the next are denoted by $Q$. The drawing shown on the left represents a portion of a stream or river divided into well-mixed segments. During a period $t$ segment $i$ receives waste constituents from the immediate upstream reach $i-1$ and from the point waste source. In this illustration, the mass of each of these wastes is assumed to decay during each time period, independent of other wastes in the water. Depending on the types of wastes, the decay, or even growth, processes may be more complex than those assumed in this illustration. At the end of each period these decayed 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 lengths of each segment or element reduces the dispersion. Reducing segment lengths, together with increasing flow velocities, also reduces the allowable duration of each time period \( t \). The duration of each simulation time step \( \Delta t \) 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:

\[
\Delta t \leq T_i
\]  

(12.120)

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:

\[
\Delta t \leq \min \{ \Delta x_i A_i / Q_{it} \; ; \; \forall i,t \}
\]  

(12.121)

If time steps are chosen which violate this condition, then numerical solutions will be in error. The restriction defined by Equation 12.121 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 simulate water quality.

### 7.3 Backtracking approach

An alternative Lagrangian or backtracking approach to water quality simulation eliminates the need to consider the simulation time step duration restriction, Equation 12.121 (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 inversely upstream to find the sources at time \( t \) of the contaminant particles 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 at an upstream node site. The combination of flows between the source site and the segment \( i+1 \) transports the contaminants from the source site to segment \( i \) during the time interval \( \Delta t \), as shown in Figure 12.26.

To compute the concentration in segment \( i+1 \) at the beginning of time period \( t+1 \), the simulation process for each segment and for each time period involves three steps.
Figure 12.26. The backtracking approach for computing the concentrations of constituents in each reach segment or volume element $i$ during time step duration of $\Delta t$.

To compute the concentration of each constituent in segment $i$ at the end of time period $t$, as shown in Figure 12.26, 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 $t$. This requires computing the velocities through each of the intermediate segments or volume elements. Secondly, the changes in the amounts of the modeled quality constituents, i.e., temperature, organics, nutrients and toxics, are calculated assuming plug flow during the time interval, $\Delta t$, using the appropriate differential equations and numerical methods for solving them. Finally, all the multiple incoming blocks of water with their end-of-period constituent concentrations are completely mixed in the segment $i$ to obtain initial concentrations in that segment for the next
time step, \( t+1 \). This is done for each segment \( i \) in each time period \( t \), proceeding in the downstream direction.

If no dispersion is assumed, the backtracking process can be simplified to consider only the end points of each reach. Backtracking can take place to each end-of-reach location whose time of travel to the point of interest is just equal or greater than \( \Delta t \). 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 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 12.26 illustrates an example of backtracking involving simple first-order decay processes. Assume contaminants that end up in reach segment \( i \) at time the beginning of period \( t+1 \) come from \( J \) sources with initial concentrations \( C_{1t}^i, C_{2t}^i, C_{3t}^i, \ldots, C_{Jt}^i \) 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:

\[
dC_j^t/dt = -k_j \theta_j^{(T-20)} C_j^t
\]  

(12.122)

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 water travels during the period \( t \) from sites \( j \) to segment \( i \).

Integrating Equation 12.122 yields:

\[
C_j^{t+1} = C_j^t \exp\{-k_j \theta_j^{(T-20)} \Delta t\}
\]  

(12.123)

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 \( C_{ij}^{t+1} \).
\[ C_{ij}^{t+1} = C_j^t \exp \left\{ -k_{ij} \theta^{(T_{ij} - 20)} \Delta t \right\} \]

(12.124)

In Equation 12.124 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 \(t+1\).

8. **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 is sometimes called epistemic (Stewart, 2000). It stems from our incomplete conceptual understanding of the systems under study, by models that are necessarily simplified representations of the complexity of the natural and socioeconomic systems, as well as by limited data for testing hypotheses and/or simulating the systems.

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

However, even if it were possible to eliminate knowledge uncertainty, complete certainty in support of water quality management decisions will likely never be achieved until we can predict the variability of natural processes. This type of uncertainty arises in systems characterized by randomness. From past observations we assume we know the possible events or outcomes that could occur and their probabilities. While we think we know 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 one cannot know in advance what all the possible biological outcomes will be. Surprises are possible. Hence both types of uncertainty, knowledge uncertainty and unpredictable variability or randomness, cannot be eliminated.

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

9. Conclusions – Implementing a water quality management policy

This chapter provides only a brief introduction to water quality modeling. As can be said for other chapters as well, entire texts, and good ones, have been written on this subject (see, for example, Chapra 1997; McCutcheon 1989; Orlob 1983; Schnoor 1996; Thomann and Mueller, 1987). Water quality modeling and management demands skill and data. Skill comes with experience. Sufficient skill will not be gained by just working with the material introduced in this chapter. This chapter is only 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. Adaptive approaches strive toward achieving water quality standards while relying on monitoring and experimentation to reduce uncertainty. It often is the only way one can proceed given the complexity of the real world compared to the predictive models available and compatible with the data and time available for analyses. Starting with
simple analyses and iteratively expanding data collection and modeling as the need arises is a reasonable approach.

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

Regardless of what immediate actions are taken, there may not be an immediate measurable response. There may be significant time lags between when actions are taken to reduce nutrient loads and the resulting changes in nutrient concentrations. This is especially likely if nutrients from past activities are 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 “trajectory” of the measured water quality criterion points toward attainment of the designated use.

Waste load allocations will inevitably be required if quality standards are not being met. These allocations involve costs. Different allocations will have a different total cost and a different distribution of those costs; hence they will have different perceived levels of fairness. A minimum cost policy may result in a cost distribution that places most of the burden on just some of the stakeholders. But until such a policy is identified one will not know this. An alternative may be to reduce loads from all sources by the same proportion. Such a policy has prevailed in the US over the past several decades. Even though not very cost effective from the point of view of water quality management, the ease of administration and the fulfillment of other objectives must have made such a policy politically acceptable. However, more than these waste load allocations policies will be needed for many of the ecosystem restoration efforts that are increasingly undertaken. Restoration activities are motivated in part by the services ecosystems provide for water quality management.
Our capabilities of including ecosystem components within water quantity and quality management models are at a fairly elementary level. Given the uncertainty, especially with respect to the prediction of how ecosystems will respond to water management actions, together with the need to take actions now, much 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 assure that an action leading to attainment of designated uses will be initially identified. Adaptive management is the only reasonable option in most cases for allowing a water quality management program to move forward in the face considerable uncertainties.

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