WQ Templates

Scientific Description

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CONTENTS

WATER QUALITY

Reference

1 Water Quality (MIKE ECO Lab) Reference Manual

1.1 Manual Format

All the descriptions in this Chapter are under headings presented in alphabetical order. A list of the headings for this Chapter is given below.

1.2 A General Description

The Water Quality (WQ) module deals with the basic aspects of river water quality in areas influenced by human activities: e.g. oxygen depletion and ammonia levels as a result of organic matter loadings. The WQ module is coupled to the AD module, which means that the WQ module deals with the transforming processes of compounds in the river and the AD module is used to simulate the simultaneous transport process. The WQ module solves the system of coupled differential equations describing the physical, chemical and biological interactions in the river.

The river water quality can be dealt with at different levels of detail by the model:

1. BOD-DO relationships

2. BOD-DO relationships including exchange with organic matter from the riverbed

3. BOD-DO relationships including nitrification

4. BOD-DO relationships including exchange with the riverbed and nitrification and denitrification

5. BOD-DO relationships including immediate and delayed oxygen demand and exchange with the river bed

6. BOD-DO relationships including all the above mentioned processes

The transport and retention of P, which are optional, can be simulated at all levels.

The decay of bacteria (faecal and total coliforms) can be included at all six modelling levels.

1.3   Biological Oxygen Demand, BOD

General description

The carbonaceous biological oxygen demand is an expression of the water's organic matter content. That is to say the biodegradable part of the organic matter which gives rise to oxygen consumption. The organic matter content is measured by registering the oxygen consumed during the degradation for a period of 5 days. The BOD units are therefore gO_2/m^3.

Degradation in the environment of the organic matter expressed as BOD gives rise to an equivalent consumption of oxygen. The BOD degradation terms will therefore be part of the oxygen balance (see **Dissolved Oxygen**).

Degradation of BOD is also a source of nutrients (nitrogen and phosphorus) since these are part of the organic matter. The inorganic nutrients (ammonia) being products of the BOD degradation can be oxidised and give rise to an additional oxygen consumption (see **Nutrients**).

The oxygen consumption and the nutrient production of the BOD degradation have no direct influence on the BOD degradation and on the mass balance of BOD itself. However, the modelling of BOD is an interrelated part of the dissolved oxygen (DO) modelling and the BOD degradation stops if the water becomes anaerobic, i.e. DO = ZERO. The differential equation(s) describing the BOD variations and the differential equation for oxygen are coupled and solved simultaneously.

The set of two differential equations (one for BOD and one for oxygen) represents the most simple BOD-DO model (model levels 1 and 2).

At a more complex level (model levels 3 and 4), the BOD-DO model can include the production of nutrients during degradation of organic matter as well as the processes changing the oxidation level of the nitrogen. The consequences of these changes in oxidation levels for the oxygen balance are also included. This is described in detail under **Nutrients**. At the most complex levels (model levels 5 and 6) three fractions of BOD are considered: dissolved BOD (BOD_d), suspended BOD (BOD_s) and deposited BOD (BOD_b).

Depending on the chosen **model level** a set of up to seven coupled differential equations are used: oxygen, three fractions of BOD, ammonia, nitrate and temperature. The actual number of differential equations depends on the chosen model level (see **Model Levels**). If modelling of **phosphorus** and/or **coliforms** are chosen, up to four additional differential equations or components are included.

The BOD in treated wastewater will be dissolved and/or suspended. The distribution between these two fractions will depend on the type of treatment plant. The ratio of dissolved BOD to suspended BOD will typically be in the range 1:1.5 - 1:1 for mechanically treated wastewater and around 2:1 for wastewater treated additionally by chemical precipitation.

The degradation of organic matter can be described by first order kinetics. All three fractions of BOD will be subject to decay though possibly at different rates. At **model levels** 5 and 6 a first order decay rate has to be specified for each fraction. The degradation of organic matter is temperature dependent. An Arrhenius expression is used to describe the **temperature dependence** and Arrhenius temperature coefficients are specified for one or three BOD fractions depending on the model level. The input degradation constants must be specified for conditions at 20°C.

In addition to the loss by decay, suspended BOD will be lost by deposition and resuspension from the bottom into the water is assumed to occur. The deposition will stop at water velocities above a certain critical velocity for deposition (U_{crit}) and resuspension will only take place at water velocities above this critical value.

For model levels 5 and 6 resuspension will occur only when the BOD_b-concentration is above a certain critical value. This means that BOD will be resuspended only when there is some BOD at the bed to resuspend. At model levels 2 and 4, the resuspension is assumed to be a zero order process, whereas for model levels 5 and 6 a first order expression is used.

In other words, resuspension of levels 2 and 4 will continue as long as the flow velocity is higher than U_{crit}. No balance for BOD_{sed} is modelled when using levels 2 or 4.

The model constants, which have to be specified for BOD, are summarised below:

Model levels 1-4

K_3 =The degradation constant for organic matter (1/day)

θ_3 =Arrhenius temperature coefficient for decay of organic matter

Model levels 2 and 4

K_3 =The degradation constant for organic matter (1/day)

θ_3 =Arrhenius temperature coefficient for decay of organic matter

K_5 =Deposition rate for BOD (m/day)

S_1 =Resuspension rate (g/m²/day)

V_{crit} =Critical velocity for deposition (m/s)

Model levels 5 and 6

K_{d3} =The degradation constant for dissolved organic matter (1/day)

K_{s3} =The degradation constant for suspended organic matter (1/day)

K_{b3} =The degradation constant for deposited organic matter (1/day)

θ_{d3} =Arrhenius temperature coefficient for dissolved organic matter

θ_{s3} =Arrhenius temperature coefficient for suspended organic matter

θ_{b3} =Arrhenius temperature coefficient for deposited organic matter

S_1 =Resuspension rate for BOD_b (g/m²/day)

K_5 =Deposition rate for BOD_s (m/day)

U_{crit} =Critical velocity for deposition (m/s)

V_{crit} =Critical BOD_b-concentration for resuspension (g/m²/day)

Recommended values

The values of the BOD decay rates depend on the nature of the organic matter. Organic matter can originate from household as well as industrial wastewater. The processes of wastewater treatment plants will also influence the degradability of the effluents. The most readily degradable components will decompose in the treatment plant depending on the processes in the treatment plant in question.

The reported range of BOD decay rates is given by: 0.1 - 1.5 (1/day) (Jørgensen, 1979, see **References**).

The variability of the degradability of industrial wastewater is extensive, ranging from relatively easily degradable waste from food industries to more persistent wastewater from e.g. pulp mills. As examples, the decay rate of BOD for wastewater from a sugar refinery was found to be 0.75 (1/day) (Water Quality Institute, 1984, see **References**) and for a sulphite pulp mill to be 0.25 (1/day) (Nyholm et. al., 1991, see **References**).

Reported ranges of the temperature coefficient for degradation of organic matter in water are 1.02 - 1.09 (Jørgensen, 1979, see **References**). A typical value would be 1.07.

The suspended organic matter (BOD) in the environment at some distance from the outlet point consists of particles in the range 1 - 10 μm. The deposition rates for this range of particles of organic material lie between 0.07 - 0.7 (m/day). A typical value would be 0.2 (m/day) corresponding to a particle size of 5 μm.

Typical values for the resuspension rate of BOD from the bed are difficult to specify. The rate has to be determined by calibrating the model to measured values or from experience of resuspension in similar situations.

Remarks and hints

The first order decay rate for BOD can be estimated from degradation experiments. The standard measurement of BOD is the BOD_5 (after five days). Given the results of intermediate measurements (after 1, 2, 3 and 4 days) and a value that is believed to represent the ultimate BOD level, the decay rate can be extracted. The calculation is based on the equation:

$$BOD_T = BOD_\infty \cdot (1 - e^{-KBOD \cdot T})$$

BOD_T = BOD measured after T days

BOD_∞ = The ultimate BOD value

The principle is illustrated in Figure 1.1.

Linear regression on

$$\ln\left(\frac{BOD_\infty - BOD_T}{BOD_\infty}\right) versus\, T \tag{1.1}$$

provides the K_{BOD} value. It can very often be assumed that the $BOD_7 \approx BOD_\infty$ as indicated in Figure 1.1. The validity of this assumption can be checked by plotting the measured values as demonstrated in the sketch and/or by studying the regression coefficient (the higher the value the better the validity of the assumption).
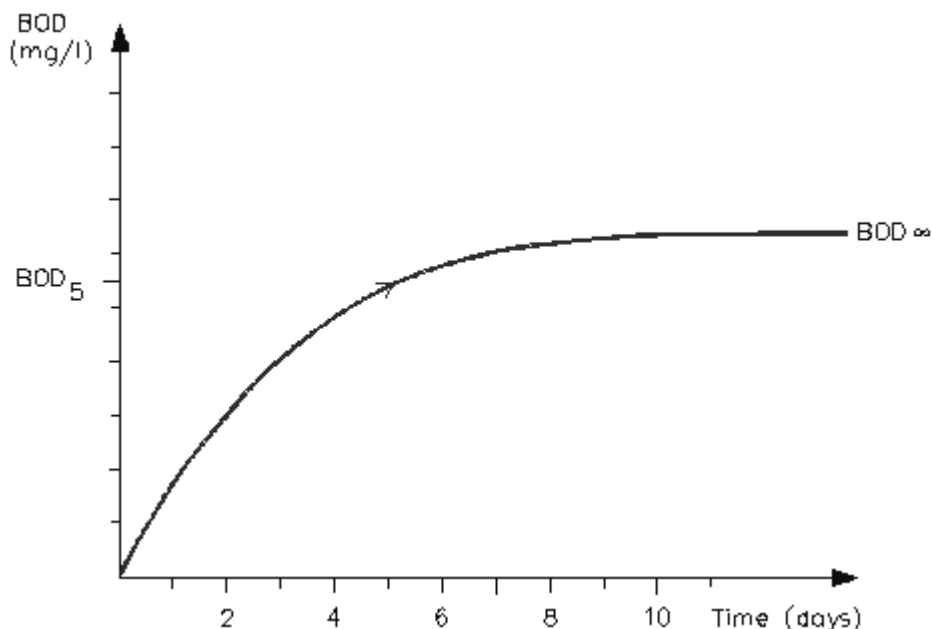
Figure 1.1   Biological oxygen demand as a function of time

1.4   Coliform

General description

Most pathogenic micro-organisms are usually unable to multiply or survive for extensive periods in the aquatic environment. Sedimentation, starvation, sunlight, pH, temperature plus competition with and predation from other micro-organisms are factors involved in the decay of pathogenic bacteria from the aquatic environment.

Eschericia coli (E.coli) is one of the dominant species in faeces from human and warm-blooded animals. The organism itself is normally considered non-pathogenic, but is very often used as indicator for faecal pollution and hence a potential for the presence of real pathogenic organisms.

Two methodologically defined groups of coliforms are distinguished: 'total coliforms' and 'faecal coliforms'. The concept 'total coliforms' may include a wide range of bacterial genera, of which many are not specific of faecal contamination. Although 'faecal coliforms' are more specific it may encompass a number of other bacteria besides E. coli. Experiments with pure cultures of E.coli can therefore not be expected to reproduce exactly the behaviour of neither 'total coliforms' nor 'faecal coliforms'.

Enteric bacteria die-off can be modelled very well by a first order reaction (decay) (Crane & Moore, 1986). However, the die-off rate constant or decay

rate is highly variable due to interaction by environmental factors on bacterial die-off. The main factors are presumably light, temperature and salinity (Mancini, 1978).

The coliform mortality rate (total or faecal) is in MIKE 11 WQ expressed as a row of terms each describing the dependence of the above mentioned environmental factors.

$$K_d = K_{d0} \bullet \theta_s^{(sal)} \bullet \theta_I^{I} \bullet \theta_T^{(T-20)}$$ (1.2)

where

$K_d K_{d0}.\theta_s^{(sal)}.\theta_I^{I}. \theta_T^{(T-20)}$

K_d decay rate of total or faecal coliforms (1/day)

K_{d0} decay rate at 20ºC, a salinity of 0‰ and darkness (1/day)

θ_s salinity coefficient for decay rate

sal salinity (‰)

θ_I light coefficient for decay rate

I light intensity integrated over depth (Kw/m²)

θ_T temperature coefficient for decay rate

T water temperature (ºC)

Model studies as well as field studies have formed the basis for establishing the above equation (Evison, (1988); Gameson, (1986). The experiments of Evison (1988), among other things, concentrated on the effects of light, temperature and salinity. Numerous field studies in British coastal waters reported by Gameson (1986) focused on the role of solar radiation.

Besides the coefficients of the equation above, the model input parameters of the coliform mortality model are the maximum insolation (Kw/m²) at noon (converted from KJ/m² specified in the menu for temperature) and the light attenuation coefficient (1/m) of the water column. The light intensity at a given time of the day is calculated assuming a sinusoidal variation of the light intensity over the day. The mean light intensity is found by integrating over the depth.

Recommended values

A huge amount of data has been examined by Mancini (1978) with the purpose of establishing a mathematical expression for the first order decay rate of coliforms.

The decay rate at 20ºC, fresh water and darkness were estimated at 0.8 (1/day) and the temperature coefficient at 1.07. These values are applied as default values. The value for marine water is calculated automatically from the user specified salinity and salinity coefficient. The light coefficient has been estimated from the field studies of Gameson (1986). The reported light intensities and resulting decay rates (or rather T_{90} values) are shown in Figure 1.2. The T_{90} value (the time elapsed until 90% of the coliforms are dead) is related to the first order decay rate by:

$$K_d = \frac{Ln(10)}{T_{90}} \qquad (1.3)$$

The light coefficient is from the slope of the straight line in Figure 1.2 found to be 1_l = 7.4.

Mancini (1978) also includes a plot of the observed versus calculated decay rates, which is included here. This figure gives a good indication of the range of decay rates to be expected.
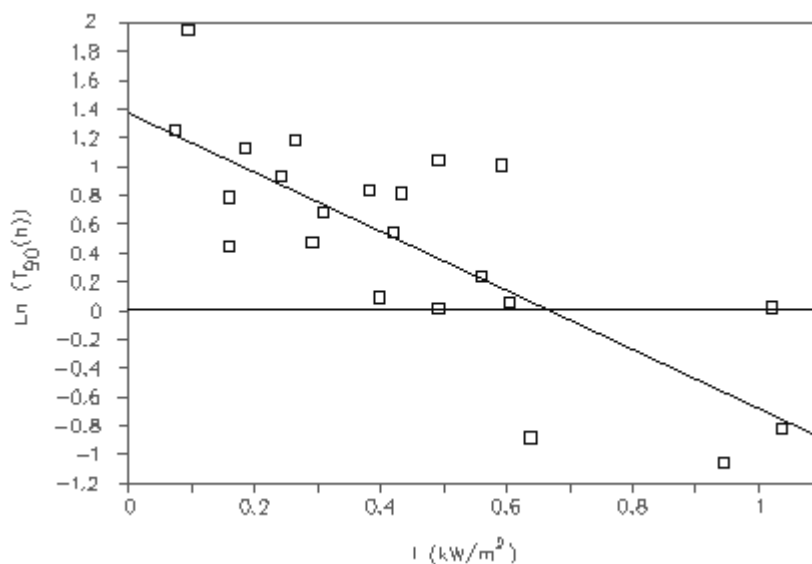
Figure 1.2   Ln(T90) versus light intensity. Data from Gameson (1986)
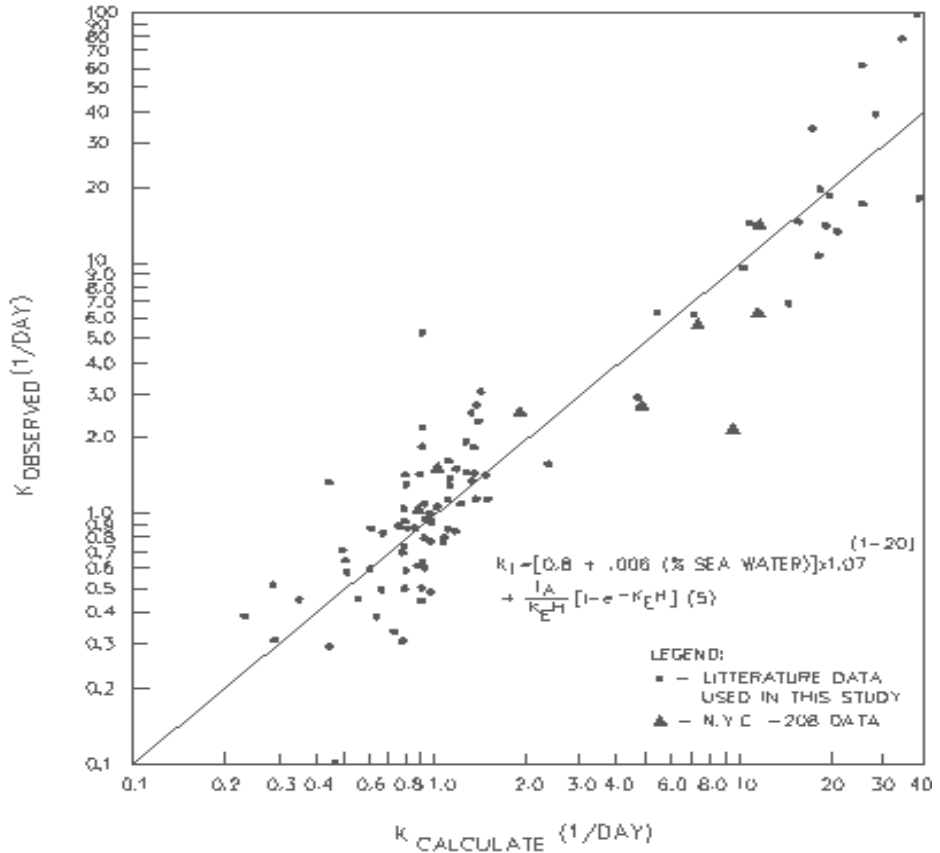
*Figure 1.3   Observed versus calculated coliform mortality rates (from
Mancini, 1978)*

1.5   Day Length

The calculation of the light climate affecting the primary producers in the
water column in ecological models usually consists of two parts, the irradiant
energy at the water surface and, from that, the determination of underwater
light.

At a given latitude and a given day of the year the WQ module of the MIKE 11
system calculates the daily varying irradiant energy at the water surface
based on the day length, i.e. the daily cycle due to the earth's rotation and the
user specified maximum solar insolation at noon.

The day length is calculated based on the variation of total solar radiation at the top of the atmosphere prescribed by Evans and Parslow (1985). They calculate the radiance according to standard trigonometric/astronomical formulae, where declination, i.e. the sun angle at the equator at a given day (L) and day length, (2\) is described as

δ= -0.407 $\cdot$ cos(2$\pi\cdot$T), T = day no/356

2τ= arccos (-tan(δ)$\cdot$tan(ϕ)), ϕ= latitude in radians

1.6 Dissolved Oxygen, DO

General description

The main reason for modelling the dissolved oxygen concentration is to ensure that it is above acceptable levels for biota in the area under consideration.

Oxygen in the aquatic environment is produced by photosynthesis of algae and plants and consumed by respiration of plants, animals and bacteria, BOD degradation, sediment oxygen demand and oxidation of nitrogen compounds. In addition, dissolved oxygen is re-aerated through interchange with the atmosphere.

The variations in the concentration of DO are described differently for each model level. The number of oxygen affecting processes is different and the combination of the processes varies (see also under **Model Levels**). The simplest level describes the oxygen concentration as a function of the naturally occurring processes (photosynthesis, respiration and re-aeration) and degradation of organic matter (BOD). The complexity is then first increased by adding the interaction with the riverbed (by introducing a sediment oxygen demand) and second by including nutrients, e.g. the nitrification of ammonia to nitrate (see also under **Nutrients**). The combination of active state variables and processes included at each model level is described in detail in **Model Levels**.

The processes involved in modelling DO without considering the effects of nutrients are shown in Figure 1.4.

Degradation of the discharged BOD gives rise to an oxygen demand of exactly the same value as in the BOD balance (for details see under **Biological Oxygen Demand**).
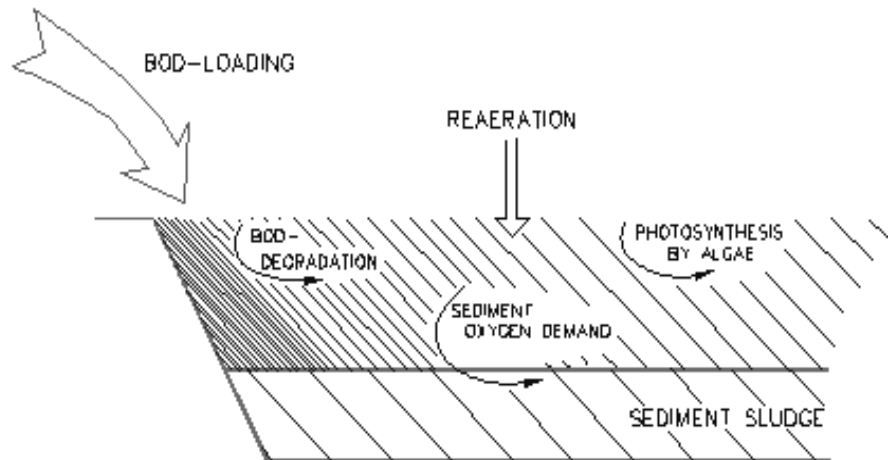
Figure 1.4   Processes involved in basic dissolved oxygen modelling

The sediment has a basic oxygen demand (gO_2/m²/day) from degradation of organic matter besides the oxygen demand from deposited BOD originating from pollution sources. This natural organic matter can include deposited microscopic algae as well as plant material and other organisms. The sediment oxygen demand is temperature dependent described by an Arrhenius expression and the Arrhenius temperature coefficient 1_1 (see **Temperature Dependence)**.

For the simple WQ model at levels 2 and 4 the sediment oxygen demand includes the basic or natural oxygen demand as well as the oxygen demand from deposited BOD originating from pollution sources. At the more complex model levels 5 and 6, the sediment oxygen demand is assumed to be the basic/natural oxygen demand only. The oxygen demand from deposited BOD is taken into account by the state variable for deposited BOD.

The oxygen producing process of photosynthesis by algae and, possibly, macrophytes (if present) is time varying (over the day). The yearly variations follow the light and temperature changes of the year. In addition, there is a diurnal variation, which has its maximum at noon and follows the sinusoidal variation of daily light intensity. The parameter to be specified is the maximum production at noon (gO_2/m²/day) at the relevant time of the year.

Photosynthesis takes place during the day-time only. The actual day length automatically calculated by MIKE 11 depends on the time of the year and the latitude (user specified), (see **Day Length)**.

Concurrent with the oxygen producing photosynthesis is the oxygen consuming respiration by plants, bacteria and animals. Whereas the oxygen produc-

tion only occurs in daytime, the respiration processes continue throughout the day and night. The respiration is temperature dependent described by the Arrhenius expression and an Arrhenius temperature coefficient θ_2. In addition to the temperature coefficient, the respiration rate at 20°C has to be given.

The WQ model at levels 3, 4 and 6 includes the oxygen consumption due to oxidation of ammonia to nitrate (the nitrification process). The nitrification is described as a first order process. The decay of ammonia gives rise to an oxygen demand of two moles of oxygen per mole of nitrogen oxidised. Multiplying this with the moleweights of oxygen (O_2) and nitrogen (N) gives the 'yield' factor describing the amount of oxygen used at nitrification.

The re-aeration process expresses the re-aeration related to the saturation concentration of oxygen. At concentrations lower than the saturation level, oxygen is transferred from the air to the water phase at a specific rate. If the concentration becomes higher than the saturation level, oxygen will similarly be transferred to the air. The re-aeration rate (the transfer rate) is determined from water depth, water velocity and river slope. Due to the large variation in velocity, depth and slope of rivers and streams, six different expressions for the re-aeration constant have been implemented. The user must choose from these. The first expression is recommended for streams, the second for ordinary rivers, the third for rivers with high flow velocities and the fourth, fifth and sixth are expressions to be specified by the user (see also **Processes**). The model calculates the oxygen saturation concentration given the relevant temperature. The equations describing the re-aeration coefficient and the oxygen saturation concentration are given under **Processes**.

The User specified values specific for the oxygen processes are summarised below:

All model levels:

P_{max}=Rate of oxygen production by photosynthesis (gO_2/m²/day).

R_{20} =Respiration rate at 20ºC (gO_2/m²/day).

θ_2 =Arrhenius temperature coefficient for respiration.

B_1 =Sediment oxygen demand; the total oxygen demand for the model levels 2 and 4 and only the basic/natural oxygen demand (gO_2/m²/day) for the model levels 5 and 6.

θ_1 =Arrhenius temperature coefficient for oxygen demand.

Model levels 3, 4 and 6 only:

Y_1 =Factor describing the amount of oxygen consumed by nitrification (gO_2/gNH_3-N).

Recommended values

The biological processes of photosynthesis and respiration show a yearly variation and, additionally, a diurnal variation of the photosynthetic oxygen production. The model determines the diurnal variation. The user-specified values required are the daily maximum of photosynthesis and the constant respiration (constant over the day). Typical values of oxygen production in the growth season will be 1.75 - 7.0 gO_2/m²/day corresponding to a primary production of 0.5 - 2.0 gC/m²/day. The respiration rate will typically be around 1.0 - 5.0 gO_2/ m²/day. A typical value for the temperature coefficient of respiration will be 1.08 (Jørgensen, 1979, see **References**).

The natural sediment oxygen demand, e.g. the oxygen consumption from organic matter not originating from pollution sources, is typically in the range 0.2 - 1.0 gO_2/m²/day. These values are valid for 'sandy bottom' (Jørgensen, 1979). The same reference states values for 'estuary mud' and 'aged sewage sludge' in the range 1 - 2 gO_2/m²/day, but these types of sediment are definitely affected by pollution sources. A value of 0.5 gO_2/m²/day is recommended for the natural sediment oxygen demand and a value of 1.5 gO_2/m²/day for the total oxygen demand in the lower model levels. A temperature coefficient of 1.07 is typical.

The yield factor for nitrification, i.e. the stoichiometric conditions and the molar weights determine the amount of oxygen consumed by nitrification. Two moles of oxygen are consumed per mole of ammonia oxidised. Multiplying with the molar weight of oxygen (32) and dividing by the molar weight of nitrogen (14) gives a yield factor of 4.57 (gO_2/gNH_3-N).

Remarks and hints

To specify the parameters for oxygen production, respiration rate and sediment oxygen demand, in units of gO_2/m²/day, it is necessary to consider the integrated (or total) value over a typical water column (with 1m² ground area) within the specific model area.

1.7 Faecal Coliforms

See **Coliforms**.

1.8 Integration Routine

The water quality modules of MIKE 11 consist of coupled differential equations. In order to solve these equations taking the interactions between each differential equation into account a numerical integration is applied.

3 different build-in integration routines exist in MIKE 11:

- RKQC: Fifth order Runge-Kutta with Quality Control.

- – RK4: Fourth order Runge-Kutta.
- – EULER: Euler or Linear Solution.

The accuracy (and the computing time) varies for the three integration routines

High accuracy   →   Low accuracy

RKQC ————RK4————EULER

This means that the most accurate result will be calculated when using RKQC (Default routine). However, in many cases the same results are obtained when using the other two routines. The computing time can be reduced at the same time by using RK4 or EULER.

In general, it is recommended to use the RKQC routine. The other two are only applied during the set-up and initial calibration phase.

If the RK4 or the EULER routines are used it is strongly recommended to run an additional simulation with the RKQC routine and compare the two results (RKQC versus RK4/ EULER) before making any conclusions based on the model.

In the case of a very dynamic system with steep gradients in one or more of the components, integration may not be possible with a time step even when using the RKQC routine, and an error message will appear on the screen. Reducing the time step will help in most cases, but sometimes the gradients are so steep that they cannot be solved accurately. The Quality Control of RKQC ensures that all components are calculated within an accuracy of 1 μg/l. Using the second best routine (RK4), where no Quality Control is included, the steep gradients can be solved in a relatively accurate way and RK4 should therefore be used when integration is impossible with the RKQC routine.

1.9 Initial Conditions

User specified

Initial values have to be derived from measurements in the river. In the case of spatial variation along the river, local values can be assigned.

Hot start

Initial values for a simulation can be obtained from an existing result file so long as it is completely and exactly compatible with the new computation.

1.10 Model Levels

General description

Dependent on the nature of the water quality problem under consideration, the model can be adjusted to different levels of detail. The complexity of the model ranges from the simplest version, which includes BOD and DO only, through the introduction of sediment/water interactions and the inclusion of inorganic nitrogen (ammonia and nitrate) to the most complex level, where the BOD is divided into three forms: dissolved, suspended and deposited. The division of BOD into three state variables enables the User to simulate immediate oxygen demand due to degradation of dissolved and suspended organic matter and a delayed oxygen demand due to degradation of the part of the organic matter having settled. This is particularly relevant for the case of sewers and storm sewer overflows (Malmgren-Hansen & Bach, 1991, see **References**).

The use of several model levels, e.g. several levels of detail, maximise the applicability of the model. Thus, the model can be applied to as well simple cases, where the major problem is the oxygen depletion due to degradation of organic matter, as to the most complex cases, where the effects of the different BOD fractions as well as the nutrient effects (e.g. ammonia levels in connection with fish and fish larvae) have to be considered.

Modelling of phosphorus can be included at all six levels. An add-on module for bacterial fate (COLI) can be activated at all levels (see **Coliforms**).

The state variables, processes included and typical problems covered are listed below for each model level. An overview of the state variables and the processes for each level is shown in tabular form.

Model level 1

State variables: BOD, oxygen and temperature.

When calculating the oxygen balance the nitrification component is not included. Suspension and sedimentation are not included in the BOD balance, and only immediate oxygen consumption is taken into account. At this level, the problem understudy relates to oxygen depletion due to discharges of readily degradable organic matter into the river. Phosphorus and coliforms are optional.

Model level 2

State variables: BOD, oxygen and temperature.

As for model level 1, except that here resuspension and deposition are included in the calculation of the BOD balance. Phosphorus and coliforms are optional.

Model level 3

State variables: BOD, oxygen, ammonia, nitrate and temperature.

When calculating the BOD balance, the suspended and deposited components are not applied, only the immediate oxygen demand is considered. When calculating the nitrate balance, the denitrification component is excluded. At this level the effects of ammonia on the oxygen concentration can be studied and so can the concentrations of ammonia itself. When the pH value of the river water is known then the potential concentrations of free ammonium can be estimated. Phosphorus and coliforms are optional.

Model level 4

State variables: BOD, oxygen, ammonia, nitrate and temperature.

As for model level 3, except that all processes concerning these five state variables are included. This means that the denitrification process (a sink for nitrate) is also included. At this level BOD-DO problems including the nitrogen compounds and including the sediment/water interactions can be studied. The BOD is still described by only one state variable. This model level is very applicable to general studies of the effects of discharges from municipal and industrial waste and agricultural run-off. Phosphorus and coliforms are optional.

Model level 5

State variables: dissolved BOD, suspended BOD, BOD at the bottom, oxygen and temperature.

As for model level 2, except that here both immediate and delayed oxygen demand are taken into consideration. At this level the effects of sewer and storm sewer overflows on oxygen depletion can be investigated without considering the nitrogen compounds. Phosphorus and coliforms are optional.

Model level 6

State variables: dissolved BOD, suspended BOD, BOD at the bottom, oxygen, ammonia, nitrate and temperature.

As for model level 4, except that here both immediate and delayed oxygen demand are taken into consideration; i.e. all processes are included. This level is the most complex approach where e.g. the effects of nitrogen compounds (ammonia) on oxygen depletion are included and the concentration of

the nitrogen compounds (ammonia and nitrate) are calculated as well. Phosphorus and coliforms are optional.

Table 1.1   State variables at the different model levels

Model levels	1	2	3	4	5	6
State variables						
Temperature	x	x	x	x	x	x
Oxygen	x	x	x	x	x	x
Ammonia	-	-	x	x	-	x
Nitrate	-	-	x	x	-	x
BOD	x	x	x	x	-	-
Dissolved BOD	-	-	-	-	x	x
Suspended BOD	-	-	-	-	x	x
BOD at the bed	-	-	-	-	x	x
Dissolved P	x	x	x	x	x	x
Particulate P	x	x	x	x	x	x
Faecal Coliforms	x	x	x	x	x	x
Total Coliform	x	x	x	x	x	x

Table 1.2   Process types included at the different model levels

Model levels	1	2	3	4	5	6
Process types						
Re-aeration	x	x	x	x	x	x
Degradation of organic matter						
a) Immediate oxygen demand	x	x	x		-	-
b) Immediate and delayed oxygen demand	-	-	-	-	x	x
Exchange with bottom/sediment	-	x	-	x	x	x
Nitrification	-	-	x	x	-	x
Denitrification	-	-	-	x	-	x

Table 1.2   Process types included at the different model levels

Model levels	1	2	3	4	5	6
Process types						
Phosphorus processes in water	x	x	x	x	x	x
Phosphorus exchange with bottom/sediment	x	x	x	x	x	x
Die-off, Coliforms	x	x	x	x	x	x

1.11   Nutrients

General Description

The nutrients considered are the inorganic forms of nitrogen and phosphorus. All details about phosphorus can be found under the **Phosphorus** heading.

The nitrogen cycle starts with an assimilation of free nitrogen from the atmosphere (e.g. by blue green algae) or uptake by algae and plants of ammonia from the water.

Degradation of dead organic matter leads to a release of the organic bound nitrogen in the form of ammonia (ammonification). The degrading bacteria, however, utilise some of the nitrogen for their own growth. The rest of the ammonia released by ammonification or discharged from pollution sources can be taken up by plants or nitrified by nitrifying bacteria to nitrate. The nitrate is eventually transformed into free nitrogen by a denitrification process. The principles of this cycle are illustrated in Figure 1.5.
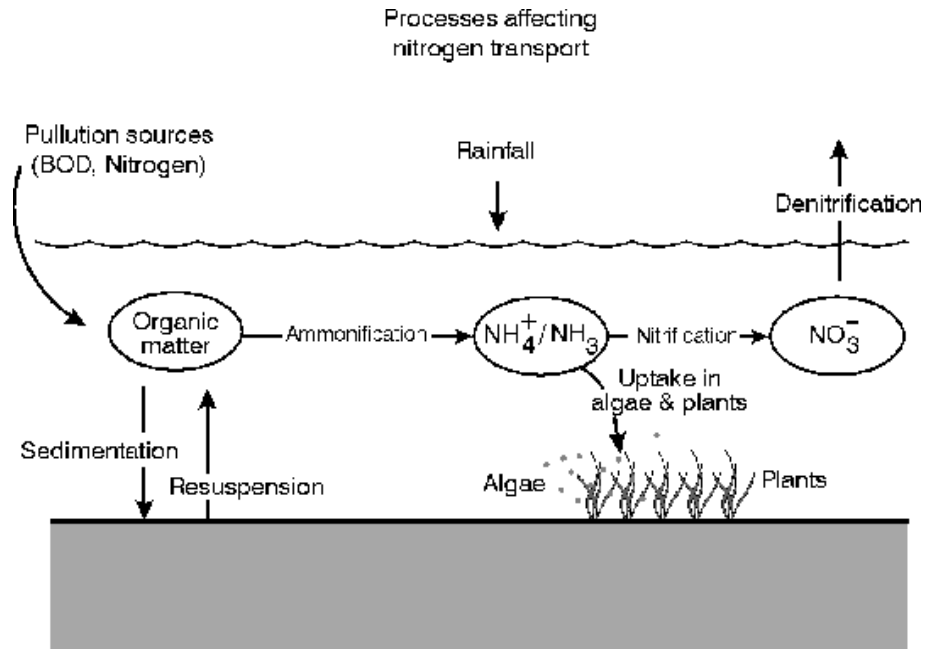
Processes affecting
nitrogen transport

Figure 1.5   Processes affecting nitrogen transport

The assimilation, ammonification and nitrification are all processes taking place in the aerated zones of the water. Denitrification is an anaerobic process requiring anoxic conditions. These conditions can be found in the sediment and in bacteria films on plants.

The processes in the ammonia balance include:

(i)BOD decay, a source of ammonia found by applying a yield factor (gNH_3-N/gO_2) to the BOD decay terms from the BOD balances;

(ii)uptake of nitrogen by bacteria as an integrated part of the BOD decay. The uptake is a constant part of the BOD decay (unit: gNH_3-N/gO_2);

(iii)uptake by plants as part of the photosynthesis and respiration. A constant amount of ammonia is taken up per gram of net production of oxygen (photosynthesis minus respiration). During the night-time the ammonia uptake by plants is assumed to be constant;

(iv)nitrification, the consumption ammonia by a chemical reaction where ammonia is transformed to nitrate. The nitrification process takes place in bacteria films on stones or plant leaves and can

therefore be restricted by the transport resistance through this film. The reaction order of the nitrification can either be chosen as an ordinary first order reaction or a combination of a film resistance and a zero order process, which results in an apparent ½ order process. The modelling of nitrification hereby includes a first order decay constant and an Arrhenius temperature coefficient since the reaction is temperature dependent.

The User specified values for the ammonia processes are summarised below:

Y_d =Yield factor for release of ammonia by ammonification of dissolved BOD.

Y_s =Yield factor for release of ammonia by ammonification of suspended BOD.

Y_b =Yield factor for release of ammonia by ammonification of deposited BOD.

U_1 =Uptake by plants (gNH_3-N/gO_2) during photosynthesis

U_2 =Uptake by bacteria (gNH_3-N/gO_2) during BOD decay

n_1 Order of nitrification reaction

K_4 =Nitrification rate constant (1/day for 1st order process and $(g/m^3)^{½}$/day) for film resisted transport)

θ_4 =Arrhenius temperature coefficient of nitrification

The processes included in the nitrate balance are:

(i)nitrification as a source of nitrate. This is described above as part of the ammonia balance;

(ii)denitrification, by which nitrate is transformed to free atmospheric nitrogen. The denitrification is an anaerobic process taking place in bacteria films on plants and in the sediment. The denitrification is described by a temperature dependent first order reaction or a combination of a transport resistance combined with a first order reaction in the film (resulting in an apparent ½ order reaction). A first or half order decay rate constant for denitrification and an Arrhenius temperature coefficient have to be specified.

The User specified values specific for the nitrate processes are:

n_2=Order of denitrification reaction

K_6 =First or half order denitrification rate (1/day and $(g/m^3)^{½}$/day, respectively)

θ_5 =Arrhenius temperature coefficient for denitrification.

Recommended values

A number of the parameters for the nutrient modelling is determined by stoichiometric conditions. These should not be changed unless direct measurements or other detailed studies indicate the need for other values to be used. These parameters are the uptake of ammonia by plants and bacteria. Recommended values are:

Uptake of ammonia in plants: $0.066 \ gNH_3\text{-}N/gO_2$

and in bacteria: $0.109 \ gNH_3\text{-}N/gO_2$

(Warwick and McDonnel, 1983, see **References**)

The yield factor for release of ammonia by degradation of BOD is dependent on the organic material in question. The organic material will be, in most cases, treated or untreated wastewater. The nitrogen content of wastewater will be dependent on whether the wastewater is treated and on the manner of treatment. Values for raw sewage and for biologically treated wastewater are shown below. The values are estimated from data for a Danish experimental wastewater treatment plant, where all relevant parameters in different stages of the treatment process have been measured frequently. The values are typical for Danish wastewater.

Yield factors for release of ammonia by BOD degradation:

Raw sewage: $0.065 \ gNH_3\text{-}N/gO_2$ (range: 0.01-0.1)

Biologically treated: $0.3 \ gNH_3\text{-}N/gO_2$ (range: 0.1-0.6)

Two reaction rates have to be specified for nitrogen: the nitrification rate and the denitrification rate, along with the corresponding temperature coefficients. For nitrification the reaction rate (first order) will be in the range 0.01-0.3 (1/day). A typical value of 0.05 (1/day) and a temperature coefficient of 1.088 are suggested (Jørgensen, 1979, see **References**). The value of the denitrification rate (first order reaction) will be in the interval 0.05-0.3 (1/day) with a typical value of 0.1 and a temperature coefficient of 1.16 (Jørgensen, 1979, see **References**).

1.12 Oxygen

See Dissolved Oxygen.

1.13 Phosphorus

General Description

The processes influencing the concentration of dissolved phosphorus (OP) are release of inorganic phosphorus, adsorption of dissolved phosphorus, phosphorus uptake by vegetation and degradation of BOD. The processes influencing the concentration of particulate inorganic phosphorus (PP) are its deposition and resuspension and the release and adsorption of dissolved phosphorus. Particulate organic phosphorus is not described explicitly as a state variable, but is related to the concentration of organic material measured as BOD, which in turn is expressed as a function of the BOD decay rate and the suspension and deposition of sediment with attached BOD. The principles of this cycle are illustrated in Figure 1.6.
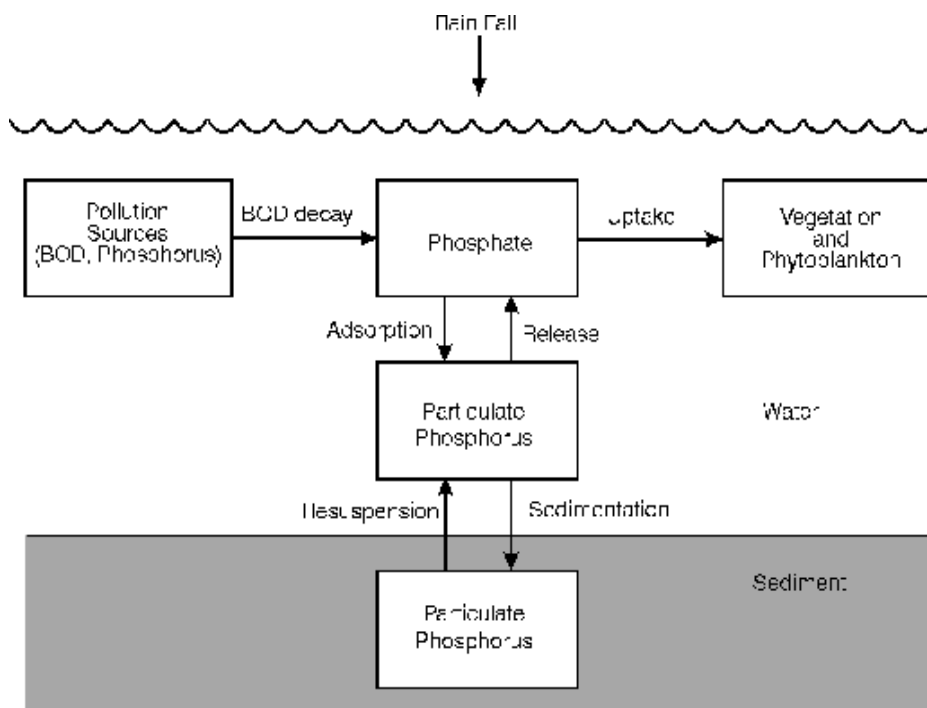

Figure 1.6   Process affecting phosphorus transport

The processes involved in the phosphorus balance are then:

- The release of organic bound phosphorus by degradation of organic matter (BOD) resulting in dissolved phosphate. A yield factor (gP/gO_2) is applied on the BOD decay terms from the BOD balances. This yield factor expresses the phosphorus content of the organic matter.

- Uptake of phosphorus as part of the photosynthesis and respiration. A constant value is multiplied with the net production of oxygen (photosynthesis minus respiration) (unit: gP/gO_2).

- The release of dissolved phosphorus from inorganic particulate bound phosphorus (PP). A rate constant (1/day) and a **Temperature Dependence** are applied in the process description.

- Adsorption of dissolved phosphorus to particles (formation of particulate phosphorus). The process is based on a rate constant (1/day) and a **Temperature Dependence**.

- Resuspension or sedimentation of particulate phosphorus. A critical flow velocity (m/sec) where resuspension = sedimentation in combination with suspension/deposition rates (m/day) are included in the description. If the actual flow velocity exceeds the critical value resuspension takes place (and sedimentation = O). On the other hand, if the velocity is lower than this value sedimentation occurs (and resuspension = O).

The user specified values for the phosphorus processes are summarised below:

Y_3=yield factor (gP/gO_2) for release of inorganic phosphorus by degradation of BOD

U_3=uptake of inorganic phosphorus by plants (gP/gO_2) during photosynthesis

K_7=rate constant (1/day) for release of dissolved phosphorus from particulate phosphorus

θ_7=Arrhenius temperature coefficient of release

K_8=rate constant (1/day) for adsorption of dissolved phosphorus to particulates

θ_8=Arrhenius temperature coefficient of adsorption

S_2=Resuspension rate (m/day) for particulate phosphorus

K_6=Sedimentation rate (m/day) for particulate phosphorus

U_{crit2}=Critical flow velocity (m/sec) for resuspension/sedimentation of particulate phosphorus

Recommended values

The parameter of the phosphorus model is determined by stoichiometric conditions. It should not be changed unless direct measurements or other detailed studies give indication for other values to be used. Recommended value is:

Uptake of phosphorus: $0.0091 \ gP/gO_2$

(Warwick and McDonnel, 1983).

The yield factor for release of phosphorus by degradation of BOD is depending on the organic material in question. The organic material will probably, in most cases, be wastewater, treated or untreated. The phosphorus content of wastewater will be dependent on whether the wastewater is treated and on the way of treatment. Values for raw sewage and for biologically treated wastewater are shown below. The values are estimated using data from a Danish experimental wastewater treatment plant, where all relevant parameters in different stages of the treatment process have been measured frequently. The values are typical for Danish wastewater.

Yield factors for release of phosphorus by BOD degradation:

Raw sewage: $0.014 \ gP/gO_2$ (range: 0.003-0.03)

Biologically treated: $0.06 \ gP/gO_2$ (range: 0.01-0.09)

Processes

The phosphorus processes are calculated simultaneously with the BOD-DO and the Nitrogen processes. The phosphorus processes are:

Release of inorganic phosphorus

Release of dissolved phosphorus from inorganic particulate bound phosphorus, PP:

$$\frac{d \ OP}{dt} = K_7 \bullet PP \bullet \Theta_7^{(T-20)} \tag{1.4}$$

where

K_7 = rate constant for release of dissolved phosphorus

$\theta 1_7$ = Arrhenius temperature coefficient

Adsorption of dissolved phosphorus

$$\frac{d\ OP}{dt} = K_8 \bullet OP \bullet \Theta_8^{(T-20)} \tag{1.5}$$

where

K_8=rate constant for adsorption of dissolved phosphorus

θ_8=Arrhenius temperature coefficient

Phosphorus uptake by vegetation

$$\frac{d\ OP}{dt} = -U_3 \bullet (P-R), \quad \text{if } (P-R) > 0 \quad \text{and} \quad 0, \text{if } (P-R) \le 0 \tag{1.6}$$

where

it is assumed that the growth of vegetation producing 1 g O_2 simultaneously leads to an uptake of 0.00914 g dissolved phosphorus.

U_3=uptake factor

P=photosynthesis

R=respiration

Degradation of BOD

$$\frac{d\ OP}{dt} = + Y_3 \bullet K_3 \bullet BOD \bullet \Theta_3^{(T-20)} \bullet \frac{DO^2}{K_s + DO^2} \tag{1.7}$$

where

Y_3=yield factor describing the amount of dissolved phosphorus released by BOD degradation

The partial differential equation describing the effects of these processes on dissolved phosphorus reads:

$$\frac{dDO}{dt} = +K_7 \bullet PP \bullet \Theta_7^{(T-20)} \quad (desadsorption) \tag{1.8}$$

$$- K_8 \bullet OP \bullet \Theta_8^{(T-20)} \quad (\text{adsorption})$$

$$- U_3 \quad \bullet (P-R) \ (\text{uptake by vegetation})$$

$$+Y_3 \quad \bullet K_3 \bullet BOD \bullet \Theta_3^{(T-20)} \quad (\text{BOD degradation})$$

Particulate Inorganic Phosphorus

The processes influencing the concentration of particulate inorganic phosphorus, PP, are sedimentation and resuspension besides the release and adsorption of dissolved phosphorus described in the previous section. The description of sedimentation and resuspension follows the same approach as in **Processes**.

The partial differential equation describing the effects of different processes on particulate inorganic phosphorus reads:

$$\frac{dDO}{dt} = -K_7 \bullet PP \bullet \Theta_{d3}^{(T-20)} \quad (desadsorption)$$

$$+K_8 \bullet OP \bullet \Theta_8^{(T-20)} \quad (\text{dissolved BOD})$$

$$-S_2 / \text{H} \quad (suspended \text{ BOD})$$

$$+K_6 / \text{H} \bullet PP \quad (sedimentation) \tag{1.9}$$

where

S_2 = resuspension rate for inorganic particulates

K_6 = sedimentation rate for inorganic particulates

H = water depth

1.14 Processes

The WQ module is integrated with the AD module and simulates the reaction processes in multi-compound systems. The WQ module solves the system of differential equations describing the physical, chemical and biological interactions involved in the survival of bacteria, resulting oxygen conditions and excess levels of nutrients in the aquatic environment. The solution is based on a numerical **Integration Routine**.

As a basis for the description of the water quality conditions the AD calculates the conservative transport of the modelled components. The WQ processes in combination with the AD transport give the final result.

Oxygen Processes

A number of processes affect the oxygen concentration:

Re-aeration

$$\frac{dDO}{dt} = K_2(C_s - DO) \tag{1.10}$$

C_s = saturation concentration of DO

= 14.652 + T {-0.41022+T (0.007991-0.000077774T)}

where

T =water temperature (^{0}C)

K_2 =re-aeration constant at 20ºC (1/day)

The six different expressions for K_2 are based upon empirical connections between the re-aeration constant and the flow velocity, the water depth and river slope in the stream. The three first expressions are standard ones, whereas the user may specify the last three.

1. $K_2 = 27185 * u^{0,931} * h^{-0,692} * I^{1,09}$
2. $K_2 = 3,9 * u^{0,5} * h^{-1,5}$
3. $K_2 = 5,233 * u * h^{-1,67}$
4. $K_2 = a_1 * u^{b1} * h^{c1} * I^{d1}$
5. $K_2 = a_2 * u^{b2} * h^{c2} * I^{d2}$
6. $K_2 = a_3 * u^{b3} * h^{c3} * I^{d3}$

where

K_2= re-aeration constant at 200ºC (1/day)

u= flow velocity (m/s)

h= water depth (m)

I= river slope (m/m)

and where

a_{1-3}= coefficient in the re-aeration expression (proportionality factor)

b_{1-3}= exponent for flow velocity

c_{1-3}= exponent for water depth

d_{1-3}= exponent for river slope

The Thyssen-expression (1) is recommended for application to small streams, the O'Connor-Dubbins-expression (2) to ordinary rivers and the Churchill-expression (3) to rivers with high flow velocities. If a user-defined expression is chosen (4-6) the coefficients a,b,c and d must also be entered.

Nitrification

$$\frac{dNH_3}{dt} = K_4 \bullet NH_3 \bullet \Theta_4^{(T-20)} \bullet \frac{DO^2}{K_s + DO^2} \tag{1.11}$$

or

$$\frac{dNH_3}{dt} = K_4 \bullet NH_3^{\frac{1}{2}} \bullet \Theta_4^{(T-20)} \bullet \frac{DO^2}{K_s + DO^2} \tag{1.12}$$

where

NH_3= concentration of ammonia (mg/l)

K_4= nitrification rate at 20ºC (1/day) or $((mg/l)^{\frac{1}{2}}/day)$

θ_4=Arrhenius temperature coefficient

K_s= half-saturation constant

Photosynthesis

$$P = P_{max} \bullet \cos 2\pi \, (\tau/\alpha), \quad \text{if } \tau \in [t_{up}, t_{down}] \quad 0, \text{if } \tau \notin [t_{up}, t_{down}] \tag{1.13}$$

where

P=actual production (g O_2/m²/day)

P_{max}=maximum production at noon (g O_2/m²/day)

τ=actual time of the day related to noon

α= actual relative **day length**

$t_{up,down}$= time of sunrise and sunset

Respiration

$$R = R_{20} \bullet \Theta_2^{(T-20)} \tag{1.14}$$

where

R= actual respiration rate of plants, bacteria and animals (g O_2/m²/day)

R_{20}= respiration rate at 20ºC (g O_2/m²/day)

$$\theta_2 = \text{Arrhenius temperature coefficient}$$

Oxygen consumption from degradation of dissolved organic matter

$$\frac{dBOD_d}{dt} = K_{d3} \bullet BOD_4 \bullet \Theta_{d3}^{(T-20)} \bullet \frac{DO^2}{K_s + DO^2} \qquad (1.15)$$

where

BOD_d = actual concentration of dissolved organic matter (mg O_2/l)

K_{d3} = degradation constant for dissolved matter at 20ºC (1/day)

θ_{d3} = Arrhenius temperature coefficient

K_s = half-saturation constant

Oxygen consumption from degradation of suspended organic matter

$$\frac{dBOD_s}{dt} = K_{s3} \bullet BOD_s \bullet \Theta_{s3}^{(T-20)} \bullet \frac{DO^2}{K_s + DO^2} \qquad (1.16)$$

where

BOD_s = actual concentration of suspended organic matter (mg O_2/l)

K_{s3} = degradation constant for suspended organic matter at 200ºC (1/day)

θ_{s3} = Arrhenius temperature coefficient

K_s = half-saturation constant

Normally, suspended BOD_s will have a slower degradation rate than dissolved BOD_d.

Oxygen consumption 01 from degradation of deposited organic matter

$$\frac{dBOD_b}{dt} = K_{b3} \bullet BOD_b \bullet \Theta_{b3}^{(T-20)} \bullet \frac{DO^2}{K_s + DO^2} \qquad (1.17)$$

where

BOD_b = actual amount of deposited organic matter at the bottom (mg O_2/l)

K_{b3} = degradation constant for deposited organic matter (1/day)

θ_{b3}= Arrhenius temperature coefficient

K_s =half-saturation constant

Sediment oxygen demand

The sediment oxygen demand from the degradation of organic material **not** originating from pollution sources is described separately.

This sediment oxygen demand (B_1) is assumed to be constant in time.

Oxygen balance

The differential equation describing the effects of these processes on the dissolved oxygen concentration reads:

$$\frac{dDO}{dt} = +K_2 \bullet (C_s - DO)(\text{re-aeration})$$

(1.18)

$$\cdot K_{d3} \bullet BOD_4 \bullet \Theta_{d3}^{(T-20)} \bullet \frac{DO^2}{K_s + DO_2} \ (\text{dissolved BOD})$$

$$\cdot K_{s3} \bullet BOD_s \bullet \Theta_{s3}^{(T-20)} \bullet \frac{DO^2}{K_s + DO_2} \ (\textit{suspended} \ \text{BOD})$$

$$\cdot K_{b3} \bullet BOD_b \bullet \Theta_{b3}^{(T-20)} \bullet \frac{DO^2}{K_s + DO_2} \ (\textit{deposited} \ \text{BOD})$$

$$\cdot Y_1 \bullet K_4 \bullet NH_3 \bullet \Theta_4^{(T-20)} \bullet \frac{DO^2}{K_s + DO_2} \ (\textit{nitrification})$$

or

$$- Y_1 \bullet K_4 \bullet NH_3^{1/2} \bullet \Theta_4^{(T-20)} \bullet \frac{DO^2}{K_s + DO_2}$$

$$\cdot R_{20} \bullet \Theta_2^{(T-20)}(\text{respiration})$$

$$\cdot P \ \ (\text{photosynthesis})$$

$$\cdot B_1 \ \ (\textit{sediment oxygen demand})$$

where the symbols are as before. Y_1 is a yield factor describing the amount of oxygen used at nitrification.

Biological Oxygen Demand Processes

The decay of different fractions of organic matter is derived from the descriptions of the oxygen balance.

Dissolved organic matter

The differential equation describing the BOD_d concentration is:

$$\frac{dBOD_d}{dt} = -K_{d3} \bullet BOD_d \bullet \Theta_{d3}^{(T-20)} \quad \bullet \frac{DO^2}{K_s + DO^2} \; (\text{BOD}_d \; \text{decay}) \qquad (1.19)$$

Suspended organic matter

Deposition
Deposition of BOD_s is assumed to occur if the flow velocity (U) is below a critical value (U_{crit}). It is described as a first order process.

Resuspension
Resuspension, S_1, is assumed to occur where the flow velocity (U) exceeds the critical value (U_{crit}). The resuspension is assumed to be constant in time. At flow velocities smaller than the critical value, deposition will occur as described above.

The differential equation describing the BOD_s concentration is:

$$\frac{dBOD_3}{dt} = -K_{s3} \bullet BOD_s \bullet \Theta_{s3}^{(T-20)} \quad \bullet \frac{DO^2}{K_s + DO^2} \; (\text{BOD}_s \; \text{decay}) \qquad (1.20)$$

$$\vdash S_1 \; /h \; (\text{resuspension})$$

$$\cdot K_5 \bullet BOD_s \; /h \; (\text{deposition})$$

where

S_1 = resuspension rate for BOD_b (g/m^2/day)

K_5 = deposition rate for BOD_s (m/day)

H = water depth (m)

Here $S_1 = 0$, if BOD_b is below a critical value C_r - BOD_b.

Deposited organic matter

The differential equation describing the BOD_b at the bottom is:

$$\frac{dBOD_b}{dt} = -K_{b3} \bullet BOD_b \bullet \Theta_{b3}^{(T-20)} \quad \bullet \frac{DO^2}{K_s + DO^2} \;(\text{BOD}_b \text{ decay})$$ (1.21)

$$-S_1 \; BOD_b \;/\text{h (resuspension)}$$

$$+K_s \bullet BOD_s \;/\text{h (deposition)}$$

Ammonium Processes

The differential equation describing the ammonium/ammonia reactions is:

$$\frac{dNH_3}{dt} = +Y_b \bullet K_{b3} - BOD_b \bullet \Theta_{b3}^{(T-20)} \quad \bullet \frac{DO^2}{K_s + DO_2}$$ (1.22)

$$+ \; Y_d \bullet K_{d3} - BOD_d \bullet \Theta_{d3}^{(T-20)} \quad \bullet \frac{DO^2}{K_s + DO_2} \;(\text{B}OD$$

$$+ \; Y_s \bullet K_{s3} - BOD_s \bullet \Theta_{s3}^{(T-20)} \quad \bullet \frac{DO^2}{K_s + DO_2} \quad \text{decay})$$

$$- \; K_4 \bullet NH_3 \bullet \Theta_4^{(T-20)} \quad \bullet \frac{DO^2}{K_s + DO_2} \qquad (\textit{nitrification})$$

or

$$- \; K_4 \bullet NH_3^{1/2} \bullet \Theta_4^{(T-20)} \quad \bullet \frac{DO^2}{K_s + DO_2}$$

$$-0.066 \bullet (P - R) \quad \text{(uptake by plants)}$$

$$-K_{b3} \bullet BOD_b \bullet \Theta_{s3}^{(T-20)} \quad \bullet \frac{DO^2}{K_s + DO_2} \quad \text{(uptake}$$

$$-0.109 \bullet K_{d3} \bullet BOD_d \bullet \Theta_{s3}^{(T-20)} \quad \bullet \frac{DO^2}{K_s + DO_2} \quad \text{by bac-}$$

$$-0.109 \bullet K_{s3} \bullet BOD_s \bullet \Theta_{s3}^{(T-20)} \bullet \frac{DO^2}{K_s + DO_2} \qquad \textit{teria})$$

Y_b = nitrogen content in deposited organic matter
(mg NH_3-N/mg BOD)

Y_d = nitrogen content in dissolved organic matter
(mg NH_3-N/mg BOD)

Y_s = nitrogen content in suspended organic matter (mg NH_3-N/mg BOD)

The BOD decay term equals the BOD decay term in the oxygen and BOD balances except for the yield factor Y. Y is the amount of ammonium, which is released during BOD decay. K_4 is the nitrification rate, P the photosynthesis rate and R the respiration rate. During the night-time the ammonium uptake by plants is assumed to be constant.

Nitrate Processes

The reactions influencing the nitrate concentration are given by:

$$\frac{dNO_3}{dt} = +K_4 \bullet NH_3 \bullet \Theta_4^{(T-20)} \bullet \frac{DO^2}{K_s + DO_2}, \quad \text{or (nitrification)} \tag{1.23}$$

$$K_4 \bullet NH_3^{1/2} \bullet \Theta_4^{(T-20)} \bullet \frac{DO^2}{K_s + DO_2}$$

$$-K_6 \bullet NO_3 \bullet \Theta_5^{(T-20)}, \quad \text{or (denitrification)}$$

$$K_6 \bullet (NO_3)^{1/2} \bullet \Theta_5^{(T-20)}$$

where

K_6 = denitrification rate (1/day) or ((g/m³)$^{1/2}$/day)

θ_5 = Arrhenius temperature coefficient

The nitrification term is the same as that described in the oxygen differential equation.

Temperature Processes

$$\frac{dT}{dt} = \text{insolation} - radiation, \quad \text{if } t \in [t_{up}, t_{down}] \tag{1.24}$$

$$-\text{Radiation}, \quad \text{if } t \notin [t_{up}, t_{down}]$$

where

T = actual temperature

θ = actual time of the day

t_{up}, t_{down} = time of sunrise and sunset

t = time

The insolation term is described with a sine function with the maximum around noon. The radiation is assumed constant.

Coliform Processes

See **Coliforms**.

Phosphorus Processes

See **Phosphorus**.

1.15   Solution Scheme

The mass balance for the parameters involved are calculated for all grid-points at all time steps using a rational extrapolation method in an integrated four-step procedure with the AD-module.

1. Calculation of Advection/Dispersion at time n+1 returned as: $C_{n+1,AD}$
2. Calculation of Advection/Dispersion gradient: $LC_{n+1,AD} = (C_{n+1,AD} - C_{n,AD})$ / Lt
3. Calculation of Water Quality at time step n+1 returned as $C_{n+1,WQ}$
4. Integration of $LC_{n+1,WQ} = LC_{n+1,WQ} + LC_{n+1,AD}$

The final result C_{n+1}, returned from the **Integration Routine**, is thereby calculated as a numerical integration of the time step gradients from both the Advection/Dispersion and from the Water Quality differential equations.

The results give a resolution in space and time depending on the details of the chosen grid and the time step used. A fine grid should always be used in stretches where rapid changes are expected, eg. around outlets from larger sewer systems with a high pollution load.

1.16   Temperature Dependence

A large number of reactions in the environment are temperature dependent. Reactions involving biological elements are directly affected due to the increased biological activity at higher temperatures. Other reactions can also increase with increasing temperatures partly owing to the higher molecular activity.

The temperature function (Arrhenius expression) is centred around 20ºC, having the unity value there, then it changes in the same direction as the temperature:

$$f(T) = \Phi^{(T-20)}$$

(1.25)

where T is the temperature and Φ is the temperature coefficient.

1.17 Total Coliforms

See **Coliforms**.

1.18 Nomenclature

a_{1-3}coefficients, re-aeration

b_{1-3}coefficients, re-aeration

B_1sediment oxygen demand; total for simple model, basic/natural for complex model

$BOD_{b,d,s}$ actual concentration of organic matter, deposited at the bottom, dissolved or suspended

c_{1-3}coefficients, re-aeration

Cconcentration (arbitrary unit)

$C_s$saturation concentration of dissolved oxygen

d_{1-3}coefficients, re-aeration

hwater depth

Iriver slope

Ilight intensity integrated over depth (kW/m²)

Klinear decay coefficient s^{-1}

$K_a$adsorption rate for dissolved organic matter BOD_d, -1

$K_{b3,d3,s3}$ degradation constant at 20ºC for deposited, dissolved or suspended organic matter

$K_d$decay rate of total or faecal coliforms (1/day)

K_{d0}decay rate at 20ºC, a salinity of 0‰ and darkness (1/day)

K_2re-aeration constant

K_3degradation constant at 20ºC (1/day)

K_4nitrification rate at 20ºC (1/day)

K_5deposition rate for suspended organic matter, BOD_s, (m/day)

K_6 denitrification rate, (1/day)

K_6 sedimentation rate (m/day) for particulate phosphorus

K_7 rate constant (1/day) for release of dissolved phosphorus from particulate phosphorus

K_8 rate constant (1/day) for adsorption of dissolved phosphorus to particulates

K_s Half-saturation constant, BOD decay and nitrification

n time level

n_1 order of nitrification (1 or ½)

n_2 order of denitrification

p actual production

p_{max} rate of oxygen production by photosynthesis ($gO_2/m^2/day$)

R actual respiration rate of plants, bacteria and animals ($GO_2/m^2/day$)

R_{20} respiration rate at 20ºC ($gO_2/m^2/day$)

sal salinity (‰)

S_1 resuspension rate for deposited organic matter ($g/m^2/day$)

S_2 resuspension rate (m/day) for particulate phosphorus

t actual time

$t_{up,down}$ time of sunrise and sunset

T temperature

T water temperature (ºC)

u flow velocity

u_1 uptake by plants ($gNH_3\text{-}N/gO_2$) during photosynthesis

u_2 uptake by bacteria ($gNH_3\text{-}N/gO_2$) during BOD decay

u_3 uptake of phosphate by plants (gP/gO_2) during photosynthesis

U_{crit} critical flow velocity (m/sec) for resuspension/ sedimentation for particulate phosphorus

U_{crit2}Critical flow velocity (m/sec) for resuspension/sedimentation of particulate phosphorus

$y_{b,d,s}$yield factor for release of ammonia by ammonification of deposited, dissolved or suspended BOD /$mgNH_3$-N/mg BOD)

$y_{b2,d2,s2}$ yield factor for release of phosphate by degradation of deposited, dissolved or suspended BOD

$Y_{b,d,s}$nitrogen content in deposited, dissolved and suspended organic matter

Y_1yield factor: amount of oxygen used during nitrification ($g0_2$/gNH_3-N)

Y_3yield factor (g P/gO_2) for release of inorganic phosphorus by degradation of BOD

$\Theta_{b3,d3,s3}$ Arrhenius temperature coefficient for deposited, dissolved or suspended organic matter

$\Theta_s$salinity coefficient for decay rate

$\Theta_l$light coefficient for decay rate

$\Theta_T$temperature coefficient for decay rate

Θ_1Arrhenius temperature coefficient for oxygen demand

Θ_2Arrhenius temperature coefficient for respiration

Θ_3Arrhenius temperature coefficient for decay of organic matter

Θ_4Arrhenius temperature coefficient for nitrification

Θ_5Arrhenius temperature coefficient for denitrification

ΘArrhenius temperature coefficient of release

Θ_8Arrhenius temperature coefficient of adsorption

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