Water Quality

MIKE ECO Lab WQ Templates

Scientific Description

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CONTENTS

Water Quality
MIKE ECO Lab WQ Templates
Scientific Description

1 Introduction

MIKE ECO Lab is a numerical lab for Ecological Modelling. It is a generic and open tool for customising aquatic ecosystem models to describe for instance water quality and eutrophication. DHI's expertise and know how concerning ecological modelling has been collected in predefined ecosystem descriptions (MIKE ECO Lab templates) to be loaded and used in MIKE ECO Lab. The MIKE ECO Lab templates describe physical, chemical and biological processes related to environmental problems and water pollution. The following is a common description of the DHI supported WQ (water quality) templates:

1. WQSimple.ecolab
2. WQSimpleCOLI.ecolab
3. WQSimpleTandS.ecolab
4. WQSimpleTandSCOLI.ecolab
5. WQNutrients.ecolab
6. WQNutrientsCHL.ecolab

The templates describe the resulting concentrations of a number of variables such as bacteria, which threatens bathing water quality, oxygen depletion due to the release of BOD, excess concentrations of nutrients, chlorophyll-nutrient interactions and degradation of chemical substances. The templates #3 and #4 also include salinity and temperature state variables. Salinity is here treated as a pure conservative component whereas the temperature is controlled by a simple heat balance calculation. The other templates rely on the data provided by the hydrodynamic engine for salinity and temperature; if not calculated, these data have to be provided by the user.

The MIKE ECO Lab is integrated with the advection-dispersion module, which describes the physical transport processes at each grid-point covering the area of interest. Other data required are concentrations at model boundaries, flow and concentrations from pollution sources, water temperature, etc.

The MIKE ECO Lab system solves the process equations using a rational extrapolation method in an integrated two-step procedure with the advection-dispersion module. Only the water quality processes are included in the description and equations explained below.

2 Applications

The water quality templates are used for a range of environmental investigations:

- Studies of hygienic problems related to bacteria from sewage outfalls and other sources.
- Survival of bacteria related to different environmental conditions.
- Oxygen conditions affected by BOD, ammonia and other oxygen consuming substances.
- Spreading, degradation and interaction between the inorganic nutrient: ammonia, nitrite, nitrate and phosphate.
- Evaluation of potential for eutrophication problems related to nutrient levels (nitrogen and phosphorus) and chlorophyll-a.
- Decay of chemical substances and effect evaluation based on resulting concentration levels.

3 Mathematical Formulations

The MIKE 21/3 ECO Lab solves the system of differential equations describing the physical, chemical and biological interactions involved in the survival of bacteria, degradation of organic matter, resulting oxygen conditions and excess levels of nutrients in coastal areas.

The following variables can be modelled using DHI supported WQ templates:

Component	Symbol	Templates
Dissolved BOD	BOD_d	#1 - #6
Suspended BOD	BOD_s	#5
Sedimented BOD	BOD_b	#5
Dissolved oxygen	DO	#1 - #6
Ammonia (NH_4^+-N)	NH_3	#5, #6
Nitrite (NO_2^-- N)	NO_2	#6
Nitrate (NO_3^--N)	NO_3	#5, #6
Phosphorus	PO_4	#5, #6
Chlorophyll (algae)	CHL	#6
Faecal coliforms	C_F	#2, #4, #6
Total coliforms	C_T	#2, #4, #6
Temperature*	T	#3, #4
Salinity*	S	#3, #4

*) if not included as state variables data is provided by the hydrodynamic engine or as user specified value

The processes and concentrations of the parameters are influences by external factors such as incident solar radiation (photosynthesis, coliform bacteria decay) and discharges.

Several combinations of the listed variables are implemented as “model levels” securing maximum flexibility. At the simplest level only BOD and DO are modelled and the most complex level includes all the variables.

In the following equations a bar under a symbol indicates that the value is clipped against 0.0, i.e.

$$\underline{X} == \min\left(0.0\,, X\right)$$

This is done to enhance the numeric stability of the solution.

3.1 Oxygen, DO

3.1.1 Oxygen balance

The oxygen balance depends on the chosen complexity level.

Level 1, Oxygen, simple description (templates #1-#4)

$$\frac{dDO}{dt} =$$

$+reaeration$	(only at water surface)
$-\sum \text{BOD decay}$	(1-3 fractions)
$+\text{photosynthesis}$	
$-\text{respiration}$	
$-\text{sediment oxygen demand}$	(only at water bed)

Level 2, Oxygen with nutrients (templates #5, #6)

$$\frac{dDO}{dt} =$$

$+reaeration$	(only at water surface)
$-\text{Y}_1 \cdot \text{nitrification}$	(Y_1: yield factor for oxygen)
$-\sum \text{BOD decay}$	(1-3 fractions)
$+\text{photosynthesis}$	
$-\text{respiration}$	
$-\text{sediment oxygen demand}$	(only at water bed)

3.1.2 Oxygen processes

Reaeration is the process describing the interchange of oxygen between the dissolved oxygen in the water and the atmosphere. The expression includes a saturation level for oxygen in water C_s that depends on the salinity and temperature.

Nitrification is another process influencing the oxygen balance as oxygen is consumed in the nitrification process when transforming ammonia into nitrite.

The oxygen producing photosynthesis process is described relative to a given maximum production at noon and varies with the time of the day and the relative day length.

Respiration from autotroph and heterotrophs is consuming oxygen and described as dependent of the temperature.

The degradation of organic matter is another oxygen consuming process. It is dependent of the temperature, the oxygen concentration and the concentration of organic material. The overall contribution of the BOD decay consists of the sum of all simulated BOD fractions.

The sediment oxygen demand from the degradation of organic material not originating from pollution sources is described separately. The sediment oxygen demand (SOD) is assumed to depend only on the oxygen concentration and the temperature. A Michaelis-Menten expression is used to simulate the processes at low oxygen conditions.

Reaeration

$$reaeration = K_2\ (C_s - DO)$$

Nitrification

$$nitrification = K_4 \cdot \underline{NH_3} \cdot \theta_4^{(T-20)} \cdot \frac{DO}{DO + HS\_nitr}$$

Photosynthesis

$$photosynthesis = sunip * \frac{P_{max}}{H} * F_1(H)$$

Where

$$sunip = \begin{cases} cos\left(2\pi * \frac{\tau}{\alpha}\right), & \tau \in \left[t_{up}, t_{down}\right] \\ 0 & , if\ \tau \notin \left[t_{up}, t_{down}\right] \end{cases}$$

$$F_1(H) = e^{-z*\eta}$$

Respiration

$$respiration = \frac{R_1}{H} \cdot \theta_1^{(T-20)} \frac{\underline{DO}}{DO+mdo}$$

BOD decay (one fraction of BOD)

$$BOD\ decay = K_3 \cdot \underline{BOD} \cdot \theta_3^{(T-20)} \cdot \frac{\underline{DO}}{DO+HS\_BOD}$$

BOD decay (three fractions of BOD)

BOD_d decay$= K_{d3} \bullet \underline{BOD_d} \bullet \theta_{d3}^{(T-20)} \cdot \frac{\underline{DO}}{DO+HS_BOD}$

BOD_S decay$= K_{s3} \bullet \underline{BOD_s} \bullet \theta_{s3}^{(T-20)} \cdot \frac{\underline{DO}}{DO+HS_BOD}$

BOD_b decay$= K_{b3} \bullet \underline{BOD_b} \bullet \theta_{b3}^{(T-20)} \cdot \frac{\underline{DO}}{DO+HS_BOD}$

Sediment oxygen demand

$$sed.oxygen\ demand = \frac{\underline{DO}}{HS\_SOD + DO} \cdot \theta_3{}^{(T-20)}$$

3.1.3 Additional expressions

The potential nutrient limitation on photosynthesis is described by a nutrient limitation function:

$$\begin{aligned} &if\ (NH_4 == 0)\ or\ (PO_4 == 0)\ then \\ &\quad F(N,P) = \ 0 \\ &else \\ &\quad F(N,P) = \frac{2}{\frac{IN}{IN + KSN} + \frac{PO_4}{PO_4 + KSP}} \end{aligned}$$

The saturation level for oxygen in water varies with salinity and temperature and is described by the following empiric expression:

$$C_s = 14.652 - 0.0841 \cdot S + T \cdot \begin{Bmatrix} 0.00256 \cdot S - 0.41022 + T \cdot (0.007991 - \\ 0.0000374 \cdot S - 0.000077774 \cdot T) \end{Bmatrix}$$

The rate for the reaeration process K_2 depends on the wind speed W_v, the flow velocity V and the water depth H:

K_2 $= 3.93 \cdot V^{0.5}/H^{1.5} + W/H$ (1/s)

W $= 0.728 \cdot W_v^{0.5} - 0.371 \cdot W_v + 0.0372 \cdot W_v^2$ (m/s)

K_2 is basically a combination of standard O'Connor - Dobbins expression with an additional wind induced aeration (see Banks and Herrera 1977, Thomann and Fritzpatrick 1982).

The photosynthetic oxygen production and the autotrophic respiration vary with the water depth due to the light dependency of the autotrophs. The depth variation is in MIKE 3 modelled using the Lambert Beer Law, which requires a light extinction coefficient for the water to describe the dampening of the light irradiation through the water column. Lambert Beer Law or the light dampening function:

$F_1(H) = e^{-\eta \cdot * z}$

$\eta = \frac{2.3}{SD}$ for templates #1-#5
$\eta = \frac{1.6}{SD}$ for template #6*)

Figure 3.1 shows the principle of the light dampening curve versus the water depth.

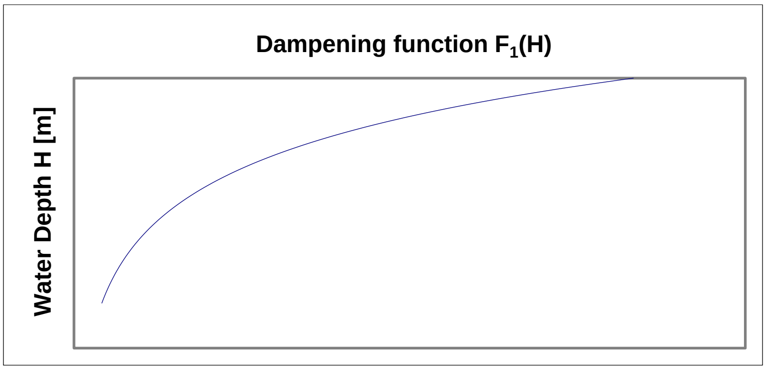

Figure 3.1 The dampening function for light in the water column

*) In template #6 the attenuation coefficient η is assumed to be ~ 69.5% lower as in the other templates #1-#5. If needed, the user provided Secchi disk depth SD can be adjusted accordingly.

3.1.4 Explanation to oxygen expressions

IN = sum of inorganic nitrogen (mg N/l)
KSN = halfsaturation concentration for nitrogen, limitation for photosynthesis by plants and algae (mg N/l)
KSP = halfsaturation concentration for phosphorus, limitation for photosynthesis by plants and algae (mg P/l)
S= salinity (PSU)
T= temperature (°C)
W_v= wind speed (m/s)
H= water depth (m)
V= depth averaged flow velocity (m/s)
NH_3= concentration of ammonia (mg/l)
K_4= nitrification rate at 20°C (1/day)
θ_4= temperature coefficient for nitrification
HS_nitr= halfsaturation concentration for nitrification (mg O_2/l)
Y_1 = yield factor for oxygen
photosynthesis = actual production (g O_2/m^2/day)
P_{max}= maximum production at noon (g O_2/m^2/day)
τ = actual time of the day related to noon
α = actual relative day length
SD = Secchi disc depth [m]
$t_{up,down}$= time for sunrise and sunset
respiration = actual respiration rate of plants, bacteria and (g O_2/m^2/day),
R_1= photosynthetic (autotrophic) respiration rate at 20°C (g O_2/m^2/day)
θ_1= temperature coefficient for photosynthetic respiration/production

R_2=	respiration rate of animals and bacteria (heterotrophic) (g O_2/m^2/day)
θ_2=	temperature coefficient for heterotrophic respiration
$F_1(H)$ =	light dampening function
η=	light extinction coefficient [m^{-1}]
H=	Water depth [m]
BOD =	actual concentration of BOD (mg O_2/l)
K_3=	degradation constant for organic matter at 20°C (l/day)
θ_3=	Arrhenius temperature coefficient
DO =	Actual oxygen concentration (mg O_2/l)
HS_BOD =	Half-saturation oxygen concentration for BOD (mg O_2/l)
BOD_d=	actual concentration of suspended organic matter (mg O_2/l)
BOD_s=	actual concentration of suspended organic matter (mg O_2/l)
BOD_b=	actual amount of sedimented organic matter at the bottom (mg O_2/l)
K_{d3} =	degradation constant for dissolved organic matter at 20°C (l/day). Normally suspended BOD_s will have a slower degradation rate than dissolved BOD_d.
θ_{d3}=	Arrhenius temperature coefficient (dissolved BOD)
K_{s3}=	degradation constant for suspended organic matter at 20 °C (1/day). Normally suspended BOD_s will have a slower degradation rate than dissolved BOD_d.
θ_{s3}=	Arrhenius temperature coefficient (suspended BOD)
K_{b3} =	degradation constant for sedimented organic matter (l/day)
θ_{b3}=	Arrhenius temperature coefficient (sedimented BOD)
HS_SOD=	half-saturation oxygen concentration for SOD (mg O_2/l)
θ_3=	Arrhenius temperature coefficient (SOD)

3.2 Biological Oxygen Demand, BOD_x

The mass balance for organic matter can be described with three equations or one equation depending on the number of fractions chosen for BOD.

3.2.1 Biological oxygen demand balance

One fraction of BOD
The mass balance for organic matter if only one fraction is chosen can be described as

$$\frac{dBOD}{dt} = \text{-BOD decay}$$

Three fractions of BOD
If fractions for dissolved, suspended and sedimented BOD are selected the balances are:

The balance describing the dissolved BOD concentration is:

$$\frac{dBOD_d}{dt} = -BOD_d \textit{ decay}$$

The balance describing the suspended BOD concentration is

$$\frac{dBOD_S}{dt} =$$

- BOD_s decay
+ resuspension
- sedimentation

The balance describing the sedimented BOD concentration is

$$\frac{dBOD_b}{dt} =$$

- BOD_b decay
- resuspension
+ sedimentation

3.2.2 Biological oxygen demand processes

$$BOD\ decay = -K_3 \cdot \underline{BOD} \cdot \theta_3^{(T-20)} \cdot \frac{\underline{DO}}{DO + HS\_BOD}$$

$$BOD_d\ decay = -K_{d3} \cdot \underline{BOD_d} \cdot \theta_{d3}^{(T-20)} \cdot \frac{\underline{DO}}{DO + HS\_BOD}$$

$$BOD_s\ decay = -K_{s3} \cdot \underline{BOD_s} \cdot \theta_{s3}^{(T-20)} \cdot \frac{\underline{DO}}{DO + HS\_BOD}$$

$$BOD_b\ decay = -K_{b3} \cdot \underline{BOD_b} \cdot \theta_{b3}^{(T-20)} \cdot \frac{\underline{DO}}{DO + HS\_BOD}$$

Resuspension, S_1, is assumed where the flow velocity (V) exceeds the critical value (V_1). The resuspension is assumed to be constant in time. At flow velocities smaller than the critical value, sedimentation will occur.

$$resuspension = S_1 \cdot BOD_b / H$$

Sedimentation of BODs is assumed if the flow velocity (V) is below a critical value (V_1). It is described as a first order process.

sedimentation = $K_s \cdot BOD_s / H$

3.2.3 Explanation to BOD expressions

T=	temperature (°C)
K_3=	degradation constant for organic matter at 20°C (l/day)
θ_3=	Arrhenius temperature coefficient
DO =	Actual oxygen concentration (mg O_2/l)
HS_BOD =	Half-saturation oxygen concentration for BOD (mg O_2/l)
BOD=	actual concentration of organic matter (mg O_2/l)
BOD_d=	actual concentration of suspended organic matter mg O_2/l)
BOD_s=	actual concentration of suspended organic matter (mg O_2/l)
BOD_b=	actual amount of sedimented organic matter at the bottom (mg O_2/l)
K_{d3} =	degradation constant for dissolved organic matter at 20°C (l/day). Normally suspended BOD_s will have a slower degradation rate than dissolved BOD_d.
θ_{d3}=	Arrhenius temperature coefficient (dissolved BOD)

K_{s3}= degradation constant for suspended organic matter at 20 °C (1/day). Normally suspended BOD_s will have a slower degradation rate than dissolved BOD_d.

θ_{s3}= Arrhenius temperature coefficient (suspended BOD)

K_{b3} = degradation constant for sedimented organic matter (l/day)

θ_{b3}= Arrhenius temperature coefficient (sedimented BOD)

S_1= resuspension rate for BOD_b (m/day)

K_s= sedimentation rate for BOD_s (m/day)

H= water depth (m)

The processes involved in the mass balances for organic matter is derived from the descriptions of the processes in the oxygen balance except for the description of resuspension and sedimentation of BOD, that is described in 3.2.3.

3.3 Ammonium, NH_3

3.3.1 Ammonium balance

The balance describing the ammonium/ammonia mass balance:

$$\frac{dNH_3}{dt} =$$

$$\begin{aligned}&+ammonium\ yield\ from\ BOD\ \text{decay}\\&-transformation\ of\ ammonium\ to\ nitrate\\&-ammonium\ uptake\ by\ plants\\&-ammonium\ uptake\ by\ bacteria\end{aligned}$$

3.3.2 Ammonium processes

BOD decay

One fraction of BOD

ammonium yield from BOD decay =

$$Y_{BOD} \cdot K_3 \cdot \underline{BOD} \cdot \theta_3^{(T-20)} \cdot \frac{\underline{DO}}{DO+HS\_BOD}$$

Three fractions of BOD

ammonium yield from BOD decay =

$$\begin{aligned}&+Y_b \cdot K_{b3} \cdot \underline{BOD_b} \cdot \theta_{b3}^{(T-20)} \cdot \frac{\underline{DO}}{DO+HS\_BOD}\\&+Y_d \cdot K_{d3} \cdot \underline{BOD_d} \cdot \theta_{d3}^{(T-20)} \cdot \frac{\underline{DO}}{DO+HS\_BOD}\\&+Y_s \cdot K_{s3} \cdot \underline{BOD_S} \cdot \theta_{S3}^{(T-20)} \cdot \frac{\underline{DO}}{DO+HS\_BOD}\end{aligned}$$

Nitrification

The transformation of ammonium to nitrate is described by the following expression:

transformation of ammonium to nitrate =

$$K_4 \cdot \underline{NH_3} \cdot \theta_4^{(T-20)} \cdot \frac{\underline{DO}}{DO+HS\_nitr}$$

Uptake by plants

ammonium uptake by plants = *(template #5)*

$$\begin{aligned}
&if\ (P - R_1) >\ 0.8 * \left(\frac{P_{max}}{H} - R_1\right)\ then\\
&\qquad UN_P * (P - R_1) * \frac{\underline{NH_3}}{NH_3+HS\_NH3}\\
&else\\
&\qquad UN_P * 0.8 * \left(\frac{P_{max}}{H} - R_1\right) * \frac{\underline{NH_3}}{NH_3+HS\_NH3}
\end{aligned}$$

ammonium uptake by plants = *(template #6)*

$$\begin{aligned}
&if\ (P - R_1) >\ 0.8 * \left(\frac{P_{max}}{H} - R_1\right)\ then\\
&\qquad UN_P * (P - R_1) * fnp\\
&else\\
&\qquad UN_P * 0.8 * \left(\frac{P_{max}}{H} - R_1\right) * fnp
\end{aligned}$$

Uptake of ammonium by bacteria

One fraction of BOD

ammonium uptake by bacteria =

$$UN_b \cdot K_3 \cdot \underline{BOD} \cdot \theta_3^{(T-20)} \cdot \frac{\underline{NH_3}}{NH_3+HS\_NH3}$$

Three fractions of BOD

ammonium uptake by bacteria =

$$\begin{aligned}
&UN_b \cdot K_{b3} \cdot \underline{BOD_b} \cdot \theta_{b3}^{(T-20)} \cdot \frac{\underline{NH_3}}{NH_3 + HS\_NH3}\\
&+UN_b \cdot K_{d3} \cdot \underline{BOD_d} \cdot \theta_{d3}^{(T-20)} \cdot \frac{\underline{NH_3}}{NH_3 + HS\_NH3}\\
&+UN_b \cdot \left(K_{s3} \cdot \underline{BOD_s} \cdot \theta_{s3}^{(T-20)}\right)\Big/ dz \cdot \frac{\underline{NH_3}}{NH_3 + HS\_NH3}
\end{aligned}$$

3.3.3 Explanation to ammonium processes

UN_p= ammonia uptake by plants (mg N/mg O_2)
UN_b= ammonia uptake by bacteria (mg N/mg BOD)
Y_b= nitrogen content in sedimented 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)
F(N,P)= nutrient limitation on the photosynthesis
HS_NH_3= halfsaturation concentration for N uptake by bacteria (mg N/l)

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 at BOD decay. K_4 is the nitrification rate. During the nighttime the ammonium uptake by plants is assumed to be constant. See also explanation to oxygen processes.

3.4 Nitrite, NO_2 (Template #6)

3.4.1 Nitrite balance

Only relevant when nutrients with or without chlorophyll is selected:
The reactions influencing the nitrite mass balance are given by:

$\frac{dNO_2}{dt} =$ *+ transformation of ammonia to nitrite*
- transformation of nitrite to nitrate

3.4.2 Nitrite processes

Template #5:
transformation of ammonia to nitrite = $K_4 \cdot \underline{NH_3} \cdot \theta_4^{(T-20)} \cdot \frac{DO}{DO+HS\_nitr}$

Template #6:
transformation of nitrite to nitrate = $K_7 \cdot \underline{NO_2} \cdot \theta_7^{(T-20)} \cdot \frac{DO}{DO+HS\_nitr}$

3.4.3 Explanation to nitrate processes

NH_3= concentration of ammonia (mg/l)
K_4= nitrification rate at 20°C (1/day)
θ_4= temperature coefficient for nitrification
HS_nitr= halfsaturation concentration for nitrification (mg O_2/l)
NO_2= concentration of nitrite (mg/l)
K_7= specific rate for conversion of nitrite to nitrate at 20°C (1/day)
θ_7 = temperature coefficient for conversion of nitrite to nitrate

3.5 Nitrate, NO_3

3.5.1 Nitrate balance

Only relevant when the option nutrients with or without chlorophyll is selected:
The reactions influencing the nitrite mass balance are given by:

$\frac{dNO_3}{dt} =$ *+ transformation of nitrite to nitrate*
- *denitrification*

3.5.2 Nitrate processes

Template #5:
transformation of nitrite to nitrate = $K_4 \cdot \underline{NH_3} \cdot \theta_4^{(T-20)} \cdot \frac{DO}{DO+HS\_nitr}$

Template #6:

transformation of nitrite to nitrate = = $K_7 \cdot \underline{NO_2} \cdot \theta_7^{(T-20)} \cdot \frac{\underline{DO}}{DO+HS\_nitr}$

denitrification = $K_6 \cdot \underline{NO_3} \cdot \theta_6^{(T-20)}$

3.5.3 Explanation to nitrate expressions

K_6= denitrification rate (1/day)
θ_6= Arrhenius temperature coefficient

The nitrification term is the same as that described under nitrite processes.

3.6 Phosphorus, PO_4

3.6.1 Phosphorus balance

BOD contain phosphorus. When BOD is degraded this phosphorus is released as orthophosphate.

Taking into account the uptake of orthophosphate in the production of algae the equation governing the orthophosphate concentration reads:

$$\frac{dPO_4}{dt} = \begin{array}{l} +phosphorus\ yield\ from\ BOD\ decay \\ -phosphorus\ uptake\ by\ plants \\ -phosphorus\ uptake\ by\ bacteria \\ -heterotrophic\ respiration \end{array}$$

3.6.2 Phosphorus processes

Phosphorus yield from BOD decay

One fraction of BOD

Phosphorus yield from BOD decay = $K_3 \cdot \underline{BOD} \cdot Y_2 \cdot \theta_3^{(T-20)} \cdot \frac{\underline{PO_4}}{PO_4+HS\_PO_4}$

Three fractions of BOD

Phosphorus yield from BOD decay =

$+K_{b3} \cdot \underline{BOD_b} \cdot Y_{b2} \cdot \theta_{b3}^{(T-20)} \cdot \frac{\underline{PO_4}}{PO_4+HS\_PO_4}$ (degradation of BOD_b)

$+K_{d3} \cdot \underline{BOD_d} \cdot Y_{d2} \cdot \theta_{d3}^{(T-20)} \cdot \frac{\underline{PO_4}}{PO_4+HS\_PO_4}$ (degradation of BOD_d)

$+K_{s3} \cdot \left(\underline{BOD_s} \cdot Y_{s2} \cdot \theta_{s3}^{(T-20)}\right)\Big/_{dz} \cdot \frac{\underline{PO_4}}{PO_4+HS\_PO_4}$ (degradation of BOD_s)

Uptake by plants

phosphorus uptake by plants = *(template #5)*

$$
\begin{aligned}
& if\ (P - R_1) > \ 0.8 * \left(\frac{P_{max}}{H} - R_1\right)\ then \\
& \qquad UP_P * (P - R_1) * \frac{\underline{PO_4}}{PO_4 + HS\_PO4} \\
& else \\
& \qquad UP_P * 0.8 * \left(\frac{P_{max}}{H} - R_1\right) * \frac{\underline{PO_4}}{PO_4 + HS\_PO4}
\end{aligned}
$$

phosphorus uptake by plants = *(template #6)*

$$
\begin{aligned}
& if\ (P - R_1) > \ 0.8 * \left(\frac{P_{max}}{H} - R_1\right)\ then \\
& \qquad UP_P * (P - R_1) * fnp \\
& else \\
& \qquad UP_P * 0.8 * \left(\frac{P_{max}}{H} - R_1\right) * fnp
\end{aligned}
$$

Uptake by bacteria

One fraction of BOD

phosphorus uptake by bacteria = $UP_b \cdot K_3 \cdot \underline{BOD} \cdot \theta_3^{(T-20)} \cdot \frac{\underline{PO_4}}{PO_4 + HS\_PO_4}$

Three fractions of BOD

phosphorus uptake by bacteria =

$$
\begin{aligned}
& + UP_b \cdot K_{b3} \cdot \underline{BOD_b} \cdot \theta_{b3}^{(T-20)} \cdot \frac{\underline{PO_4}}{PO_4 + HS\_PO_4} \\
& + UP_b \cdot K_{d3} \cdot BOD_d \cdot \theta_{d3}^{(T-20)} \cdot \frac{\underline{PO_4}}{PO_4 + HS_{PO_4}} \\
& + UP_b \cdot \left(K_{s3} \cdot \underline{BOD_s} \cdot \theta_{s3}^{(T-20)}\right) \Big/ dz \cdot \frac{\underline{PO_4}}{PO_4 + HS\_PO_4}
\end{aligned}
$$

3.6.3 Explanation to phosphorus processes

UP_p=	phosphorus uptake by plants (mg P/mg O_2)
UP_b=	phosphorus uptake by bacteria (mg P/mg BOD)
Y_{b2}=	phosphorus content in sedimented organic matter (mg P/mg O_2)
Y_{d2}=	phosphorus content in dissolved organic matter (mg P/mg O_2)
Y_{s2}=	phosphorus content in suspended organic matter (mg P/mg O_2)
F(N,P)=	nutrient limitation on the photosynthesis
HS_PO_4=	halfsaturation concentration for phosphorus uptake by bacteria (mg P/l)

3.7 Chlorophyll-a, CHL

3.7.1 Chlorophyll-a balance (Template #6)

The production of chlorophyll-a is assumed proportional to the carbon production and hereby also to the oxygen production.

A constant chlorophyll-a to carbon ratio is assumed. Furthermore, death and sedimentation of chlorophyll are included.

$\frac{dCHL}{dt} =$

+ production of chlorophyll

- respiration of chlorophyll
- death of chlorophyll
- sedimentation of chlorophyll

production of chlorophyll = $photosynthesis \cdot K_{10} \cdot K_{11} \cdot F(N,P)$

respiration of chlorophyll = $respiration \cdot K_{10} \cdot K_{11} \cdot F(N,P)$

death of chlorophyll = $-K_8 \cdot \underline{CHL}$

sedimentation of chlorophyll = $-K_9/H \cdot \underline{CHL}$

where

CHL= the chlorophyll-a concentration (mg/l)
K_8= death rate of chlorophyll-a (1/day)
K_9= settling rate of chlorophyll-a (m/day)
K_{10}= chlorophyll-a to carbon ratio (mg CHL/mg carbon)
K_{11}= carbon to oxygen ratio at primary production (mg carbon/mg oxygen)

3.8 Temperature processes, T

Details about the temperature model for MIKE 3 can be seen in the Scientific Documentation of the Advection-Dispersion Module.

In the templates #3 and #4 the heat balance calculation incorporates an exchange rate to account for the net surface heat transfer at the interface with the air.:

$$dT/dt = -(E(T-A))/(STC \cdot H)$$

where

E= surface heat exchange coefficient (Watts/m^2 K)
T= water temperature (°C)
A= ambient air temperature (°C)
STC= specific thermal capacity of sea water (Mega-joules/ m^3 K)
H= water depth (m)

The user defines the ambient air and water temperature for the simulation. The water depth is input from the HD-module.

3.9 Bacterial processes, C_F, C_T

The WQ templates can describe the spreading and fate of total coliforms and faecal coliforms.

The die-off of bacteria is described by:

$$\frac{d\ C_{F/T}}{dt} = -K_{dF/T} \cdot CorSTL \cdot C_{F/T}$$

where

$C_{F/T}$= concentration of faecal/total coliforms (1/100 ml)
$K_{dF/T}$= decay coefficient for faecal/total coliforms at 20°C (1/day)
CorSTL= temperature, salinity and light dependency function

The decay coefficient is dependent on the light conditions as well as the salinity and water temperature.

$$\text{CorSTL} = \cdot\ \theta_T^{(T-20)} \cdot \theta_S^{(S)} \cdot \theta_L^{(IL)}$$

θ_T= temperature coefficient for bacteria decay (1.09)
θ_S= salinity coefficient for bacteria decay function (1.006)
θ_L= light coefficient for bacteria decay function (7.4)
T= water temperature (°C)
S= salinity (PSU)
IL= light intensity (kW/m³)

4 Data Requirements

- Basic Model Parameters
  - Model Grid size and extent
  - Time step and length of simulation
  - Type of output required and its frequency

- Bathymetry and Hydrodynamic Input

- Combined Advection-Dispersion Model
  - Dispersion coefficients

- Initial Conditions
  - Concentration of parameters

- Boundary Conditions
  - Concentration of parameters

- Pollution Sources
  - Discharge magnitudes and concentration of parameters

- Process rates
  - Size of coefficients governing the process rates. Only some of these coefficients can be determined by calibration. Others will be based on literature values or found from actual measurements and laboratory tests.

5 List of Literature

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