

# MIKE HYDRO Basin Water Quality Model

MIKE ECO Lab Template Documentation

Scientific Documentation



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## 1 Introduction

This document describes the water quality templates generated for MIKE HYDRO Basin. The current MIKE HYDRO Basin module uses DHI's generic MIKE ECO Lab module to implement water quality simulations. MIKE ECO Lab is a generic ordinary differential equation solver. Instead of a fixed set of hardcoded water quality calculations, MIKE ECO Lab offers the possibility to load various water quality models from so called MIKE ECO Lab templates. Generally the user can generate or modify their own templates or use pre-defined water quality models.

DHI provides the following two MIKE ECO Lab templates for MIKE HYDRO:

- MikeHydroWQ\_DO.ecolab            Water quality model with oxygen
- MikeHydroWQ\_noDO.ecolab        Water quality model without oxygen

The difference between the two modules is that the first one supports dissolved oxygen whereas the second one does not include dissolved oxygen.

## 2 Process Description

### 2.1 General formulations

#### First order equations

Most of the active processes are modelled as temperature dependent first order process according to

$$process = rate * temp\_factor * [Concentration] \quad (2.1)$$

#### General temperature dependency

Most simulated processes are temperature depended. This temperature dependency is modelled as simple exponential Arrhenius temperature dependency with a reference temperature of 20°C according to

$$temp\_factor = k * e^{T-20} \quad (2.2)$$

Where  $k$  is the applied temperature coefficient. The default value  $k=1.07177$  corresponds to a doubled reaction speed with a temperature increase of 10°C, with  $k=1$  no temperature dependency is present ( $k = \sqrt[10]{reaction\ speed\ increase\ per\ 10^\circ C}$ ).

#### 2.1.1 BOD, Biogeochemical Oxygen Demand

BOD is a common characterisation of the pollution load by organic (and inorganic) substances that consume oxygen during their breakdown.

BOD is often measured as the amount of oxygen (in mg O<sub>2</sub>/l) consumed within 5 days, the so called BOD<sub>5</sub>. You can use the equation below to convert between the BOD<sub>5</sub> and the ultimate BOD. Actually the BOD<sub>5</sub> value is available as extended output in the current model.

$$BOD_5 = BOD * (1 - e^{-kd3*5}) \quad (2.3)$$

Where  $kd3$  is the decay constant in d<sup>-1</sup>.

$$\frac{dBOD}{dt} = -BOD\_Degradation \quad (2.4)$$

#### BOD decay

BOD decay in the current MIKE HYDRO Basin WQ model is simulated as temperature compensated simple 1<sup>st</sup> order decay with the process rate  $kd3$ .

$$BOD\_Degradation = kd3 * temp\_corr * BOD \quad (2.5)$$

## 2.1.2 DO, Dissolved Oxygen

This state variable and the associate process and in-/outputs are only present in the template "MikeHydroWQ\_DO"

This state variable characterises the dissolved oxygen concentration. It is influenced by the exchange with the atmosphere (reaeration), consumption by BOD decay and nitrification process and various other process (bulk flux due photosynthetic O<sub>2</sub> production, respiration etc.).

$$\frac{dDO}{dt} = (\text{Reaeration} - \text{BOD\_Degradation} - \text{NOD} - \text{BPR\_Flux}) \quad (2.6)$$

### Reaeration

Reaeration is the (oxygen) gas exchange with the atmosphere. In the model two different reaeration processes are considered, normal reaeration and reaeration on weirs.

$$\text{Reaeration} = (\text{NormalReaeration} + \text{WeirReaerationRate}) \quad (2.7)$$

### Oxygen saturation concentration

For the reaeration, the oxygen saturation concentration DO<sub>sat</sub> at a given temperature *temp* [°C] is calculated as

$$\text{DO}_{\text{sat}} = 14.65 + \text{temp} * (-0.41022 + \text{temp} * (0.007991 - 0.000077774 * \text{temp})) \quad (2.8)$$

### Normal reaeration

Normal reaeration is based on a temperature corrected O'Connor-Dobbins formulation, taking the gradient to the saturation concentration, the horizontal flow speed *Hspd* [m/s] and the water depth *Depth* [m] into account.

$$\text{NormalReaeration} = k2 * \text{temp\_corr} * (\text{DO}_{\text{sat}} - \text{DO}) \quad (2.9)$$

$$k2 = 3.9 * \text{Hspd}^{0.5} * \text{Depth}^{-1.5} \quad (2.10)$$

### Weir reaeration

When water flows over weirs along a branch, the accumulated reaeration is based on the height difference *WeirHeight* (accumulated value along the branch) and the coefficient *WeirCoef*, dependent on weir geometry. The model calculates the oxygen concentration after the weir using a Holler equation approach and transforms this into a change rate used in a process equation.

Please note that hydrodynamic structures like weirs are not calculated in MIKE HYDRO Basin. The weir height has to be specified by the user as the height difference between the upstream and downstream water level in a branch if weir reaeration need to be taken into account.

$$\text{WeirReaerationRate} = (\text{DO}_{\text{afterWeir}} - \text{DO}) * \frac{86400}{dt} \quad (2.11)$$

$$DO_{\text{afterWeir}} = \text{if}(\text{WeirHeight} > 0) \begin{cases} \text{then} & \text{MIN} \left( DO_{\text{sat}}, \left( DO_{\text{sat}} - \frac{(DO_{\text{sat}} - DO)}{(1 + \text{WeirCoef} * \text{WeirHeight})} \right) \right) \\ \text{else} & 0 \end{cases} \quad (2.12)$$

## BOD decay

During BOD decay oxygen is consumed. See eq. 2.5 for details.

## NOD, Nitrification Oxygen Demand

The oxygen demand of the nitrification is controlled by the nitrification yield factor  $y_1$ , specifying the relative amount of oxygen needed (g O<sub>2</sub> / g NH<sub>4</sub>-N). The default value is  $y_1=4.6$ .

$$\text{NOD} = y_1 * \text{Nitrification} \quad (2.13)$$

## BPR fluxes

Various other oxygen fluxes from general respiration and production (photosynthesis) process can be supplied as additional time series.

### 2.1.3 NH<sub>4</sub>, Ammonia

Actually ammonia reacts in water according to the following equation



This reaction is depended on pH and temperature; under normal conditions and a pH < 8 most of the Ammonia is present as Ammonium (NH<sub>4</sub><sup>+</sup>). Ammonium is considered harmless and is a relevant source of nitrogen for many organisms whereas ammoniacal nitrogen (NH<sub>3</sub>-N) is toxic, especially to fish.

The current MIKE HYDRO Basin Water Quality model does not include pH and assumes that Ammonia is present in its ionised form (Ammonium, NH<sub>4</sub><sup>+</sup>). It is released during BOD decay and consumed by nitrification.

$$\frac{d\text{NH}_4}{dt} = (\text{BOD\_NH}_4\text{\_Release} - \text{Nitrification}) \quad (2.15)$$

#### NH<sub>4</sub>-release during BOD decay

When organic material decays, NH<sub>4</sub> is released proportional to the nitrogen content in the organic matter. The default for the proportional constant is  $Y_d=0.1$  [g O<sub>2</sub> / g NH<sub>4</sub>-N]

$$\text{BOD\_NH}_4\text{\_Release} = Y_d * \text{BOD\_Degradation} \quad (2.16)$$



## 2.1.4 NO<sub>3</sub>, Nitrate

Nitrate is another important source for nitrogen. It is generated by nitrification of NH<sub>4</sub>. It is assumed that denitrification removes nitrogen from the nitrogen cycle as elementary nitrogen N<sub>2</sub> or N<sub>2</sub>O.

$$\frac{dNO_3}{dt} = (\text{Nitrification} - \text{Denitrification}) \quad (2.17)$$

### Nitrification

Nitrification is modelled as 1<sup>st</sup> order process with the process rate  $k_4$ .

$$\text{Nitrification} = k_4 * \text{temp\_corr} * \text{NH}_4 \quad (2.18)$$

### Denitrification

Denitrification removes nitrogen from the nitrogen cycle as elementary nitrogen N<sub>2</sub> or N<sub>2</sub>O. Denitrification is modelled as 1<sup>st</sup> order process with a process rate  $k_6$ .

$$\text{Denitrification} = k_6 * \text{temp\_corr} * \text{NO}_3 \quad (2.19)$$

## 2.1.5 P<sub>tot</sub>, Total Phosphorous

$$\frac{dP_{tot}}{dt} = (-P_{tot\_Degradation} - P_{DepositInSediment}) \quad (2.20)$$

The phosphorus degeneration is modelled as simple 1<sup>st</sup> order decay. In lakes and reservoirs phosphorus sedimentation may deposit larger amounts of phosphorus in the sediments.

### Phosphorus degradation

Phosphorus degradation is modelled as simple 1<sup>st</sup> order process with the process rate  $k_{Ptot}$ .

$$P_{tot\_Degradation} = k_{Ptot} * \text{temp\_corr} * P_{tot} \quad (2.21)$$

### Phosphorus sedimentation

This sedimentation in lakes or reservoirs is based on a modified Vollenweider equation. In the model, the sedimentation is active if the value *VollenweiderCoef* is different from zero. In this case the sedimentation rate is computed as:

$$P_{SedRate} = \text{IF}(\text{VollenweiderCoef}=0) \left\{ \begin{array}{l} \text{THEN} \\ \text{ELSE} \end{array} \right. \left( 1 - \frac{0}{(1 + \sqrt{\text{ResidenceTime}})} \right) \quad (2.22)$$

The theoretical residence time is calculated as

$$\text{ResidenceTime} = \frac{\text{dt} * \frac{365.25}{12}}{\text{MonthLength}} \quad (2.23)$$

Please note: The phosphorus sedimentation should only be used in lakes and reservoirs. At all other locations the value of the sedimentation should be disabled by  $\text{VollenweiderCoef}=0$ .

### 2.1.6 E.coli, Bacteria concentration

The bacteria concentration is modelled as simple 1<sup>st</sup> order decay with the process rate  $k_{EColi}$  according to:

$$\frac{dE_{Coli}}{dt} = -E_{Coli\_Degradation} \quad (2.24)$$

$$E_{Coli\_Degradation} = k_{E_{Coli}} * \text{temp\_corr} * E_{Coli} \quad (2.25)$$

### 2.1.7 USER, User defined concentration component

The MIKE HYDRO Basin water quality model contains a user defined “wildcard” substance with a potential 1<sup>st</sup> order decay process. If the process rate  $k_{User}$  is set to zero, the substance will act as a conservative tracer.

$$\frac{dUSER}{dt} = -User\_Degradation \quad (2.26)$$

$$User\_Degradation = k_{User} * \text{temp\_corr} * USER \quad (2.27)$$

# APPENDICES

# APPENDIX A

## Model Default Values

## A Model Default Values

Table A. 1 Default values for process rates and other constants and forcings

Variable	Description	Default	Unit
RateCorr	Temperature coefficient	1.07177	-
kd3	Decay rate for BOD (20°C)	0.1	d <sup>-1</sup>
k4	Nitrification rate (20°C)	0.2	d <sup>-1</sup>
k6	Denitrification rate (20°C)	0.2	d <sup>-1</sup>
kPtot	Decay rate for P_tot (20°C)	0	d <sup>-1</sup>
kEColi	Decay rate for E.Coli (20°C)	0	d <sup>-1</sup>
kUser	Decay rate for user defined substance (20°C)	0	d <sup>-1</sup>
Yd	N/BOD ratio	0.1	g NH4-N/ g BOD
y1*	Nitrification yield factor, g O2 / g NH3-N	4.57	g O2/ g NH4-N
VollenweiderCoef	Vollenweider coefficient for P sedimentation in lakes and reservoirs	0	-
WeirCoef *	Weir aeration coefficient in Holler formula	0.21	-
dt	MIKE ECO Lab time step	Built-in	Sec
Temp	Water temperature	10	°C
Hspd*	Current speed	Built-in	m·s <sup>-1</sup>
Depth*	Water depth	Built-in	m·s <sup>-1</sup>
WeirHeight*	Accumulated weir height	0	m
BPR*	Various oxygen flux time series P: production from photosynthesis B: consumption in bottom sediment R: consumption from respiration	0	mg·l <sup>-1</sup> ·d <sup>-1</sup>

(\* only present in the template "MikeHydroWQ\_DO" including oxygen process)