WAQTEL

User Manual

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Contents

1. Introduction

WAQTEL (WAter Quality for TELemac) is a component of the Telemac-Mascaret system (TMS) which focuses on the water quality aspects. It was developped to allow the TMS's users to tackle water quality problems together with hydrodynamics.
Up to release V7P0, TELEMAC-2D and TELEMAC-3D were coupled with DELWAQ, the Deltares water quality code. This coupling, though working well for simple and medium sized models, was not suitable and cumbersome for big models. The main issue related to the use of TELEMAC– DELWAQ was the uncompatible parallelization of both codes.
To overcome this issue and in order to fully benefit from the parallelization efficiency of the TMS, the development team introduced a first version of WAQTEL in the V7P1 release.
WAQTEL is developed by the LNHE (Laboratoire National d'Hydraulique et Environnement) of the Research and Development Division of EDF (EDF-R&D). As for previous versions, the 7.1 release of the code complies with the Quality Assurance procedures of scientific and technical softwares of EDF-R&D. It is a process of construction and verification of the product quality in the different phases of his life. In particular, a software following the Quality Assurance procedures comes with a Validation Folder that describes the intended use of the software and a set of test cases. This document allows you to judge the performance and limitations of the software, situating the field of application. These tests are also used in the development of the software and are checked at every new release.

1.1 Position of the WAQTEL code within the telemac modelling system

The WAQTEL software is part of the TELEMAC modelling system developed by the LNHE of EDF R&D. TELEMAC is a set of modelling tools allowing to treat every aspects of natural free surface hydraulics: currents, waves, transport of tracers and sedimentology.
WAQTEL, unlike other compnents of the TMS, can not be run in a stand-alone mode. To run a WAQTEL model, it is necessary to run TELEMAC-2D or TELEMAC-3D coupled with WAQTEL using the keyword `COUPLING WITH` = 'WAQTEL' (in French: `COUPLAGE AVEC` ='WAQTEL').
The pre-processing and post-processing of simulations can be done either directly within the TELEMAC system or with different software that present an interface of communication with the system. We can particularly mention the following tools:

- the FUDAA-PREPRO software, developed from the FUDAA platform by the CEREMA's Recherche, Informatique et Modélisation Department, covers all the pre-processing tasks

involved by the achievement of a numerical hydraulic study, as well as a graphical post-processing tool,

- the Blue Kenue software, developed the Hydraulic Canadian Center, proposes a powerful mesh generation tool and a user-friendly post-processing tool,
- the Janet software, developed by Smile Consult GmbH, which offers among others, a mesh generation tool,
- the ParaView software, developed by Sandia National Laboratories, Los Alamos National Laboratory and Kitware, which enables to visualise 3D results, big data in particular and is open source,
- the SALOME-HYDRO software based on the SALOME platform, developed by EDF, CEA and OPENCASCADE which enables to handle raw data (bathymetry, maps, pictures, LIDAR...) until the mesh generation. The post-processing tool ParaViS available in the SALOME platform is based on the ParaView software and can visualise 1D, 2D or 3D results. A first version of SALOME-HYDRO has been available since Spring 2016,
- the QGIS software, which is an open source Geographic Information System.

1.2 Software environment

All the simulation modules are written in FORTRAN 90, with no use of the specific language extensions in a given machine. They can be run on all the PCs (or PC "clusters") under Windows and Linux operating systems as well as on the workstations under the Unix operating system.

1.3 User programming

When using a simulation module from the TELEMAC system, the user may have to program specific subroutines which are not in the code's standard release. In particular, that is made through a number of so-called « user » subroutines. These subroutines are written so that they can be modified, provided that the user has a basic knowledge in FORTRAN language, with the help of the « Guide for programming in the Telemac system » [9].
The procedure to be carried out in that case comprises the steps of:

- recovering the standard version of the user subroutine(s) as supplied in the distribution and copying it into the current directory,
- amending the subroutine(s) according to the model to be constructed,
- concatenating the whole set of subroutines into a single FORTRAN file which will be compiled during the TELEMAC-2D or TELEMAC-3D launching process.

During that programming stage, the user can gain access to the various variables of the software through the FORTRAN 90 structures.
All the data structures are gathered within FORTRAN files, which are known as modules. For WAQTEL, the file name is **DECLARATION_WAQTEL.f**. To gain access to the WAQTEL data, just insert the command **USE DECLARATIONS_WAQTEL** into the beginning of the subroutine. Adding the command **USE BIEF** may also be necessary in order to reach the structure in the BIEF library.
Nearly all the arrays which are used by WAQTEL are declared in the form of a structure. For example, the access to the water depth array will be in the form **H%R**, **%R** meaning it is a

real-typed pointer. In case of an integer-typed pointer, the **%R** is replaced by a **%I**. However, in order to avoid having to handle too many **%R** and **%I**, a number of aliases are defined, such as, the **NPOIN3**, **NELEM3** and **NPTFR2** variables. For further details, the user can refer to the programming guide in TELEMAC [9].

2. Theoretical aspects

WAQTEL offers the use of 7 water quality (WAQ) processes. These processes generate source terms that are added to the advection-diffusion equation resolved in TELEMAC-2D or TELEMAC-3D. These processes are the following:

- O_2 module: which gives the evolution of oxygen O_2 in the flow and accounts for the interaction with the organic load and ammoniacal load. This module is simple since it does not take into consideration all the complexity of biological phenomena linked to the production, the elimination and the transport of oxygen. For more details about this process, the reader is invited to the following manual and references therein ([6]) or the WAQTEL technical manual,
- BIOMASS module: it allows the computation of the algal biomass. It estimates the vegetal colonization as a function of several parameters such as sunshine, water temperature, ratio of renewing of water etc. This module introduces and uses 5 tracers:
  1. phytoplanktonic biomass (PHY),
  2. dissolved mineral phosphorus (PO_4),
  3. degradable phosphorus assimilated by phytoplankton (POR),
  4. dissolved mineral nitrogen assimilated by phytoplankton (NO_3),
  5. degradable nitrogen assimilated by phytoplankton (NOR),
- EUTRO module: this module describes the oxygenation of a river. It is much more complex than the O_2 module since it takes into account vegetal photosynthesis and nutrients and their interactions with phytoplankton. This module introduces 8 tracers:
  1. phosphorus assimilated by phytoplankton (POR),
  2. dissolved oxygen (O_2),
  3. phytoplanktonic biomass (PHY),
  4. dissolved mineral phosphorus (PO_4),
  5. dissolved mineral nitrogen assimilated by phytoplankton (NO_3),
  6. degradable nitrogen assimilated by phytoplankton (NOR),
  7. ammoniacal load (NH_4),

8. organic load (L).

These tracers are in mg/l, except biomass which is given in μg.

- MICROPOL module: this module gives the evolution of micro-pollutants (radio-elements or heavy metals) in the main locations in river flows i.e. water, suspended load and bed sediments. This module introduces 5 tracers:

  1. suspended sediments (SS),
  2. bed sediments (BS), which are considered fix (not advected neither dispersed),
  3. micro-pollutant species in dissolved form,
  4. part adsorbed by suspended sediments,
  5. part adsorbed by bed sediments,

- THERMIC module: this module computes the evolution of water temperature as a function of heat exchange balance with atmosphere. Only the exchanges with atmosphere are considered, those with lateral boundaries and with the bed are neglected or have to be given in the boundary conditions file,

- the Aquatic Ecodynamics library (AED2): this library is fully developed by an Australian consortium, see website for more information http://aed.see.uwa.edu.au/research/models/AED/

- degradation law: it enables to model the evolution of one or several tracer(s) over time from an initial condition according to a degradation law that is assumed to be 1st order (i.e. a tracer decrease).

3. Practical aspects

To activate the water quality module WAQTEL, the integer keyword `WATER QUALITY PROCESS` must be set to a value different from 1 (default = 1) in the TELEMAC-2D or TELEMAC-3D `STEERING FILE`. The possible choices are:

- 0: all available processes,
- 1: nothing (default value),
- 2: O_2 module,
- 3: BIOMASS module,
- 5: EUTRO module,
- 7: MICROPOL module,
- 11: THERMIC module,
- 13: AED2 model,
- 17: degradation law.

Several modules can be combined by giving the multiplication of the process choices, e.g. $55 = 5 \times 11$ activates EUTRO and THERMIC modules. It is noted that AED2 should be used on its own, for the time being, without possible combination with other processes.

In WAQTEL, a new dictionary is created and fully dedicated to water quality applications. The description of this new dictionary will be the subject of a separate manual (see the WAQTEL reference manual). To introduce WAQ parameters, a separate steering file is necessary. It is read with the use of the keyword `STEERING FILE` and its name has to be declared in the TELEMAC-2D or TELEMAC-3D `STEERING FILE`. In the next sections which are dedicated to water quality, all the keywords to be introduced to the water quality steering file will be written in `THIS FONT`.
Depending on the WAQTEL module, TELEMAC-2D or TELEMAC-3D automatically increase the number of tracers of the model. In fact, the total number of tracers (variable **NTRAC**) is increased by 3 (for O_2 process), by 5 (for BIOMASS and MICROPOL processes) or by 8 (for EUTRO process).

Some general parameters can also be chosen for any water quality process. For instance, user can give a title for the study by using `WAQ CASE TITLE`. He/she can introduce water density (`WATER DENSITY`).

3.1 The meteo file or ASCII ATMOSPHERIC DATA FILE

Most of the water quality processes are tightly linked to meteorological data on the domain. Besides the specific treatment for wind, atmospheric pressure and rainfall described in the section 6.3 of the TELEMAC-2D User Manual or in the section 5.5 of the TELEMAC-3D User Manual, water quality needs different meteorological data such as nebulosity, air temperature, evaporation pressure etc.

Since release 8.2 and the creation of the new **METEO_TELEMAC** module based on the already existing **METEO_KHIONE** module, it is possible to manage meteo data in the `ASCII ATMOSPHERIC DATA FILE`. Moreover, this module enables to use flexible format for this file as long as the names of the meteo data are included in a specific list. Therefore, the order of columns is flexible.

Here is a list of the available variables for this module and the shortnames to be used in the headline of the `ASCII ATMOSPHERIC DATA FILE`:

- WINDS and WINDD: wind speed + wind direction (in m/s) or,
- WINDX and WINDY: wind velocity components along x and y (in m/s),
- TAIR: air temperature (in °C),
- PATM: atmospheric pressure (in mbar or hPa),
- CLDC: cloud cover or nebulosity (in octas for WAQTEL or tenths for KHIONE),
- RAINI or RAINC: rainfall (last letter I or C depending on if it is an interpolated variable as other usual variables or if it is given as cumulated variable),
- RAY3: solar radiation (in W/m^2),
- HREL: relative humidity (in %),
- PVAP: saturated vapor pressure (in hPa),
- TDEW: dewpoint temperature (in °C),
- VISBI: visibility (in m),
- SNOW: snow (in m),

Hereafter we give examples of `ASCII ATMOSPHERIC DATA FILE` when coupling with TELEMAC-2D (see Table 3.1) or with TELEMAC-3D (see Table 3.2).

The user can change the order of columns. If additional parameters are needed, it can be done by changing the **METEO_TELEMAC** available in the sources/utils/bief folder.

Since release 8.2, a time reference can be given: If a #REFDATE with a date + hour in YYYY-MM-DD HH:MM:SS in year, month, day, hour, minute, second format is written in ASCII

files related to time, the date+hour will be added to the times in these ASCII files when using TELEMAC-2D and TELEMAC-3D. For SERAFIN or MED binary files, the date in these files will be used.
Such feature is used in the `ASCII ATMOSPHERIC DATA FILE` of the heat_exchange example of WAQTEL (see Table 3.2).

T	TAIR	PVAP	WINDS	WINDD	CLDC	RAY3	PATM	RAINI
s	degC	hPa	m/s	degree	octa	W/m2	mbar	mm
0	20	10	0.5	70	5	160	1012.7	0
3600	20	10	0.5	70	5	160	1012.7	0
7200	20	10	0.5	70	5	160	1012.7	0

Table 3.1: Example of meteo data file for THERMIC module in 2D

#REFDATE 2006-10-01 00:00:00

T	WINDS	WINDD	TAIR	PATM	HREL	CLDC	RAINI
sec	m/s	deg	degC	mbar	%	octa	mm3/s/mm2
0	6	140	22.1	1012.5	84	7	0.000E+00
10800	5	140	22	1011.8	83	7	0.000E+00
21600	5	130	21.6	1012.2	80	7	0.000E+00

Table 3.2: Example of meteo data file for heat exchange module in 3D

4. O2 module

The O_2 module is a simple model that describes the oxygen density evolution in the water. It is activated by setting `WATER QUALITY PROCESS` = 2. It offers the advantage of being simple and then easy to calibrate. Indeed, since some important parameters are kept constant (such as vegetal respiration `VEGETAL RESPIRATION R`, benthic demand `BENTHIC DEMAND`), only 8 parameters have to be introduced (and, if necessary calibrated). The use of this module is, consequently, recommended for short time periods (several days).
O_2 module uses 3 tracers:

1. dissolved oxygen O_2 (mgO_2/l),
2. organic load L (mgO_2/l),
3. ammoniacal load NH_4 ($mgNH_4/l$).

These tracers are hence, advected and dispersed in the whole water mass and their evolution obeys the advection-diffusion equation linked to external and internal source terms.
For more details about the theory of the O_2 module, the reader can refer to the WAQTEL technical manual.

4.1 The dissolved oxygen

The dissolved oxygen density is influenced by the following factors:

- 4 factors consuming oxygen:
    1. organic load L,
    2. ammoniacal load,
    3. benthic demand,
    4. vegetal respiration,
- 2 factors producing oxygen
    1. photosynthesis,
    2. reaeration.

We will introduce briefly how the source terms linked to these six factors are estimated.

4.1.1 The benthic demand

The benthic demand *BEN* is provided by using the keyword `BENTHIC DEMAND` (default = 0.1 $gO_2/m^2/d$). It is then corrected with water temperature T like:

$$BEN_T = BEN_{20°C}(1.065)^{T-20}$$

Where T is given in °C using the keyword `WATER TEMPERATURE` (default = 7°C). This value of temperature is useful when the temperature is not considered as a tracer in the model. Otherwise, the real temperature is taken into account.
The following Table gives some typical values of benthic demand at T = 20°C (i.e. $BEN_{20°C}$).

Bottom type	Typical value of *BEN* ($gO_2/m^2/d$) at 20°C
Filamentous bacteria (10 g/m^2)	7
Mud from waste water, near to release	4
Mud from waste water, far from release	1.5
Estuarine silt	1.5
Sand	0.5
Mineral soil	0.007

4.1.2 Vegetal respiration

It is given directly by the user with keyword `VEGETAL RESPIRATION R` (default = 0.06 $mgO_2/d/l$).

4.1.3 Photosynthesis P

The photosynthesis P depends on algae density, water depth and sunlight, with order of magnitude between 0.3 and 9 $mgO_2/d/l$. For O_2 module, P is given by the user with the keyword `PHOTOSYNTHESIS P` (default = 1 $mgO_2/d/l$).

4.1.4 Reaeration

It is the gain oxygen through the free surface of water. It is due to 2 main reasons:

- the natural reaeration,
- the weir reaeration.

Natural reaeration

It can be seen at a macroscopic level as a term which is linearly dependent on $(C_s - [O_2])$, where C_s is O_2 saturation density of water (given through keyword `O2 SATURATION DENSITY OF WATER (CS)`, default = 11 mgO_2/l) and $[O_2]$ is the O_2 density. For instance C_s = 9 mgO_2/l at 20°C. We get finally:

$$Natural\ reaeration = k_2(C_s - [O_2]),$$

where k_2 (given in d^{-1}) is an empirical parameter which can be computed using 4 empirical laws.
Its orders of magnitude are indicated in the Table below (from [12]).

Type of watercourse	Interval of k_2 (d^{-1}) at 20°C
Small ponds and backwaters	0.10-0.23
Sluggish streams and large lakes	0.23-0.35
Large streams of low velocity flow	0.35-0.46
Large streams of normal velocity flow	0.46-0.69
Swift streams	0.69-1.15
Rapids and waterfalls	> 1.15

The choice of the law is given by the keyword `FORMULA FOR COMPUTING K2` which can have the following values:

- 0: k_2 constant (default formula), its value is given by keyword `K2 REAERATION COEFFICIENT` (default = 0.9 d^{-1}),
- 1: formula of the Tenessee Valley Authority,
- 2: formula of Owens et al.,
- 3: formula of Churchill et al.,
- 4: formula of O'Connor & Dobbins,
- 5: formula mixing the last 3 formulae.

Since these formulae are valid for a temperature of 20°C, the value of k_2 is corrected like:

$$k_2 = (k_2)_{20°C} \ (1.0241)^{T-20}.$$

The oxygen density at saturation C_s can be estimated using the temperature of water (at 20°C, C_s = 9 mgO_2/l). Hence if the temperature in the model is varying with time (for example when THERMIC module is activated), C_s can be estimated with different ways using the keyword `FORMULA FOR COMPUTING CS` (default = 0) which can have the following values:

- 0: constant value (default) given by `O2 SATURATION DENSITY OF WATER (CS)` (default = 11 mgO_2/l),
- 1: Elmore & Hayes formula,
- 2: Montgomery formula,
- 3: Benson and Krause formula (1984) [2] with dependence on both temperature and salinity (available since release 8.5). Warning: this 3rd formula is only valid for 0°C < T < 40°C and 0 g/l < S < 40 g/l.

Since release 8.5, oxygen saturation concentration C_s can be written in the TELEMAC-2D `RESULTS FILE`, the TELEMAC-3D `2D RESULT FILE` or the TELEMAC-3D `3D RESULT FILE`. CSO2 is to be written in the list of `VARIABLES FOR GRAPHIC PRINTOUTS` in the TELEMAC-2D steering file. It is to be written in the list of `VARIABLES FOR 2D GRAPHIC PRINTOUTS` (with values averaged along the vertical) and/or `VARIABLES FOR 3D GRAPHIC PRINTOUTS` (with values computed at every 3D node) in the TELEMAC-3D steering file.
In addition to the concentration of oxygen saturation in water C_s, the percentage of oxygen saturation defined as the ratio concentration of oxygen over concentration of oxygen saturation can be written in the previous result file: O2SAT is to be written in the list of variables of the dedicated TELEMAC steering file. It is expressed in %.

Reaeration at weirs (not used at the moment in WAQTEL)

For the O_2 process, a reaeration of the water due to the existence of weirs is implemented. The water oxygen concentration is increased when crossing from one side of a weir to the other side. The raise of the concentration is managed through the keywords `WEIR REAERATION COEFFICIENT RS` and `FORMULA FOR COMPUTING RS` which can have 5 options (see [6] for theoretical details):

- 0: *RS* is constant, in this case *RS* is given by `WEIR REAERATION COEFFICIENT RS` (default 1.),
- 1: formula of Gameson 1,
- 2: formula of Gameson 2,
- 3: formula of Water Research Laboratory 1,
- 4: formula of Water Research Laboratory 2.

4.2 Organic load L

The evolution of the organic load density [L] in time is assumed to be with a 1st order law:

$$F([L]) = -k_1[L],$$

where k_1 is a constant that describes the kinetic degradation of the organic load. It is given using the keyword `CONSTANT OF DEGRADATION OF ORGANIC LOAD K1` (default 0.25 d^{-1}). The organic load is in mgO_2/l.

4.3 Ammoniacal load

The ammoniacal load NH_4, which is also consuming oxygen, has a density varying in time with a 1st order law given by:

$$F([NH_4]) = -k_4[NH_4],$$

where k_4 is a nitrification kinetic constant. It is given by `CONSTANT OF NITRIFICATION KINETIC K4` (default 0.35 d^{-1}). In this module, k_4 is assumed to be constant and independent of remaining variables.

5. The THERMIC module

For a majority of water quality processes, the interaction with atmosphere is a key parameter. The THERMIC module is activated by setting `WATER QUALITY PROCESS = 11`. The neighboring conditions are taken into account through a meteorological file like the one described in section 3.1. It is important to underline that the data contained in this file can vary depending on the considered case. The subroutine **meteo.f** can be edited by the user to customize it to his specific model.
Before version 7.0, heat exchange between water and atmosphere could have been done with a linearised formula of the balance of heat exchange fluxes at the free surface in TELEMAC-3D. An example of an exchange with a constant atmosphere temperature and a constant sea salinity was given as standard (as comments) through a direct programming in the **BORD3D** subroutine.

A much more elaborated model has been introduced in WAQTEL for 2D and 3D.
The evolution of temperature of water is tightly linked to heat fluxes through the free surface. These fluxes (in W/m^2) are of 5 natures:

- solar radiation or sun ray flux RS,
- atmospheric radiation flux RA,
- water radiation or free surface radiation flux RE,
- latent heat or heat flux due to advection CV,
- sensitive heat of conductive origin or heat flux due to evaporation CE.

The final balance of (surface) source terms is given by:

$$S_{surf} = RS + RA - RE - CV - CE$$

We will give a brief description for each of these terms, for more details see [6]. This surface source term is treated explicitly in TELEMAC-2D, the following term is added in the explicit source term of advection-diffusion equation of tracer $\frac{S_{surf}}{\rho C_p H}$.

There is a distinction done in 3D compared to 2D: whereas the long wave radiation (atmospheric radiation RA) is absorbed in the first centimetres of the water column, the short wave radiation (solar radiation RS) penetrates the water column. Evaporation is calculated in 3D.

The choice of the heat exchange model can be done with the keyword ATMOSPHERE-WATER EXCHANGE MODEL in the WAQTEL steering file (default value = 0: no exchange model). Value 1 will use with the linearised formula at the free surface, whereas value 2 will use with the model with complete balance.

These calculations require additional meteo data which may vary in time in an expected format, rather defined in the ASCII ATMOSPHERIC DATA FILE of the TELEMAC-3D steering file, see the example "heat_exchange".

Since release v8.2 the format of the ASCII ATMOSPHERIC DATA FILE is flexible with respect to the order of columns (but with the mandatory convention for data names with the shortnames listed in 3.1).

If not filling the necessary variables (in 3D: wind velocities, air temperature, atmospheric pressure, cloud cover, rainfall, relative humidity; in 2D: wind velocities, air temperature, atmospheric pressure, cloud cover, rainfall, solar radiation, saturated vapour pressure), the missing variables are considered constant along the whole computation and their values are set by associated keywords values (WIND VELOCITY ALONG X, WIND VELOCITY ALONG Y, or SPEED AND DIRECTION OF WIND for wind velocity, VALUE OF ATMOSPHERIC PRESSURE for atmospheric pressure, RAIN OR EVAPORATION IN MM PER DAY for rainfall, AIR TEMPERATURE, CLOUD COVER, RELATIVE HUMIDITY, SOLAR RADIATION, VAPOROUS PRESSURE).

When using the complete module, evaporation is calculated by TELEMAC-3D, but the user has to provide rainfall data with units homogeneous with length over time.

The main developments of this module are implemented in the module **EXCHANGE_WITH_ATMOSPHERE** in 3D and in the **CALCS2D_THERMIC** in 2D.

5.1 Sun ray flux RS

Sun ray flux is simply provided in the ASCII ATMOSPHERIC DATA FILE in 2D. In a majority of cases, when no measurements are available, this flux is estimated using the method of Perrin & Brichambaut ([6]), which uses the cloud cover of the sky that varies during the day (function of time). So far, this flux is considered constant in space.

Since release 8.2, solar radiation or sun ray can be either read in the ASCII ATMOSPHERIC DATA FILE or computed by WAQTEL in 3D. To read it in the meteo file, the keyword SOLAR RADIATION READ IN METEO FILE is to be activated (default = NO, i.e. it is computed by WAQTEL in 3D). Moreover, an additional column is to be written with the shortname RAY3 as headline of the column.

For more real cases, the user is invited to use the “heat exchange” module (in folder sources/telemac3d). A sun ray flux varying in space, common between TELEMAC-2D and TELEMAC-3D will be implemented in next releases.

In 3D, examples of solar radiation penetration in the water *RS* are given in the **CALCS3D_THERMICV** subroutine. Two laws are suggested: the first one uses the *in situ* measurements of Secchi length and is recommended if available; the second one uses two exponential laws that may be difficult to calibrate and require an estimation of the type of water from turbidity. An example of the a double exponential law is commented. A similar law as Atkins formula with Secchi length (see BIOMASS module) can also be used with light extinction coefficient directly given with the keyword LIGHT EXTINCTION COEFFICIENT as soon as METHOD OF COMPUTATION OF RAY EXTINCTION COEFFICIENT is set to 3.

The type of sky related to the luminosity of the site has to be chosen with respect to the considered area, with the WAQTEL keyword LIGHTNESS OF THE SKY (1: very pure sky, 2: mean pure sky which is default or 3: industrial zone sky) in 3D.

Type of cloud	k
Cirrus	0.04
Cirro-stratus	0.08
Altocumulus	0.17
Altostratus	0.2
Cumulus	0.2
Stratus	0.24

Table 5.1: Values of k depending on cloud type

5.2 Atmospheric radiation RA

The atmospheric radiation *RA* is estimated with meteorological data collected at the ground level. It takes into account energy exchanges with the ground, water (and energy) exchanges with the underground, etc.

In 2D, *RA* is estimated mainly by the air temperature, like:

$$RA = e_{air}\sigma\,(T_{air}+273.15)^4\left(1+k\left(\frac{c}{8}\right)^2\right),$$

where:

- e_{air} is a calibrating coefficient given by the keyword `COEFFICIENTS FOR CALIBRATING ATMOSPHERIC RADIATION` (default = 0.97),
- σ is the constant of Stefan-Boltzmann (= $5.67.10^{-8}$ $\mathrm{Wm^{-2}K^{-4}}$),
- T_{air} is air temperature given in the `ASCII ATMOSPHERIC DATA FILE`,
- c = cloudiness (octas), given in the atmospheric data file (WARNING: in KHIONE, it is given in tenths),
- k is the coefficient that represents the nature and elevation of clouds, it has a mean value of 0.2 and can be changed with the keyword `COEFFICIENT OF CLOUDING RATE`. To simplify calculations, an average value of k = 0.2 is usually taken in 2D (but default value = 0.17 like in 3D since release 8.2, old default value was 0.2 until release 8.1). However, it varies like indicated in Table 5.1.

In 3D, clouds and albedo at the free surface determine the atmospheric radiation *RA* penetrating the water:

$$RA = (1-alb_{lw})e_{air}\sigma(T_{air}+273.15)^4(1+k.\left(\frac{C}{8}\right)^2),$$

where:

- alb_{lw} = 0.03 is the water albedo for long radiative waves (common value used in the literature [8], [7]), (1-alb_{lw}) is equal to the calibrating coefficient given by the keyword `COEFFICIENTS FOR CALIBRATING ATMOSPHERIC RADIATION` (default = 0.97, hence alb_{lw} = 0.03 as default value),
- e_{air} is the air emissivity (= $0.937.10^{-5}(T_{air}+273.15)^2$ if using Swinbank formula, default option),
- $\sigma = 5.67.10^{-8}$ $\mathrm{W.m^{-2}.K^{-4}}$ is Stefan-Boltzmann's constant,

- C is the nebulosity (octas). Some meteorological services such as Météo France provide this data in octas, it needs to be converted into tenths, hence the division by 8 in the formula, (WARNING: in KHIONE, it is given in tenths),
- k (dimensionless) is a parameter characterising the type of cloud. In practise, it is difficult to know the type of cloud during the period of simulation and a mean value of 0.17 is often used [1], [8]. This is the new default value for the keyword `COEFFICIENT OF CLOUDING RATE` since release 8.2. Other choices are possible (see the table 5.1).

When coupling WAQTEL with TELEMAC-3D, the `FORMULA OF ATMOSPHERIC RADIATION` can be changed:

- 1: Idso and Jackson (1969),
- 2: Swinbank (1963) which is the default formula,
- 3: Brutsaert (1975),
- 4: Yajima Tono Dam (2014).

The formulae in 2D and 3D are almost the same with few differences.

5.3 Free surface radiation RE

The available water is assumed to behave like a grey body. Radiation generated by this grey body through the free surface is given by:

$$RE = e_{water}\sigma\left(T_{water} + 273.15\right)^4,$$

where:

- T_{water} is the mean water temperature in °C. T_{water} is given by the keyword `WATER TEMPERATURE` (default 7°C),
- e_{water} can be seen as a calibration coefficient which depends on the nature of the site and obstacles around it. This coefficient is given with `COEFFICIENTS FOR CALIBRATING SURFACE WATER RADIATION` (default 0.97). For instance, for a narrow river with lots of trees on its banks, e_{water} is around 0.97, for large rivers or lakes it is about 0.92.

5.4 Advection heat flux CV

This flux (also called sensitive heat flux) is estimated empirically:

$$CV = \rho_{air} C_{p_{air}} f(V)\left(T_{water} - T_{air}\right),$$

where:

- ρ_{air} is the air density given by $\rho_{air} = \frac{100\ P_{atm}}{(T_{air}+273.15)287}$ where P_{atm} is the atmospheric pressure, introduced in the `ASCII ATMOSPHERIC DATA FILE` or using the keyword `VALUE OF ATMOSPHERIC PRESSURE` (default 100,000 Pa), this is a keyword of TELEMAC-2D and TELEMAC-3D,
- $C_{p_{air}}$ is the air specific heat (J/kg°C) given by `AIR SPECIFIC HEAT` (default 1,005),
- $f(V)$ is a function of the wind velocity V:

  - in 2D: $f(V) = a + bV$,
  - in 3D: $f(V) = b(1+V)$ for wind velocity at 2 m high or $f(V) = a + bV$ for wind velocity at 10 m high, depending on user's choice,

- V is the wind velocity (m/s),

- a, b are empirical coefficients to be calibrated in 2D and in 3D (only a if one single calibrating coefficient). Their values are very close to 0.0025, but they can be changed using `COEFFICIENTS OF AERATION FORMULA` (default = (0.002, 0.0012)).

Because the site of a study may not be equipped with local wind measurements and these kinds of data are available at a different location, possibly far from the studied site, a wind function is used. In 3D, this can be a linear function with a single coefficient of calibration $b : f(U_2) = b(1+U_2)$ where U_2 is the wind velocity at 2 m high.
To get the wind velocity at 2 m high from classical wind data at 10 m high, a roughness length of $z_0 = 0.0002$ m has been chosen in the code, that leads to $U_2 \approx 0.85 U_{10}$. This value of 0.85 (or the roughness length) may be changed by the user if needed.

In 3D, except for the coefficient to model the penetration of solar radiation in the water column, and if there is only one single calibrating coefficient, the parameter b that appears in the wind function is the single calibration parameter of this module. Its value is given by the keyword `COEFFICIENT TO CALIBRATE THE ATMOSPHERE-WATER EXCHANGE MODEL` in the WAQTEL steering file (default value = 0.0025 but recommended values are between 0.0017 and 0.0035). This keyword is both used for the linearised formula at the free surface and the model with complete balance (values 1 and 2 for the keyword `ATMOSPHERE-WATER EXCHANGE MODEL` in the WAQTEL steering file).
Since release 8.2, the user can define a wind function depending on 2 coefficients by filling in the `COEFFICIENTS OF AERATION FORMULA` (not letting the default values). These 2 coefficients are then taken into account rather the 1 single coefficient if using `ATMOSPHERE-WATER EXCHANGE MODEL` = 2. Contrary to the wind function with one single coefficient to calibrate where wind velocity is taken at 2 m high, the wind function with 2 coefficients uses wind velocity taken at 10 m high.

5.5 Evaporation heat flux CE

The evaporative heat flux CE (also called latent heat flux) is given by the following empirical formula:

$$CE = L(T_{water})\rho_{air} f(V)\left(H^{sat} - H\right)$$

where:

- $L(T_{water})$ = 2,500,900 - 2,365.T_{water} is the vaporization latent heat (J/Kg),

- $f(V)$ is a function of the wind velocity V:

  - in 2D: $f(V) = a + bV$,
  - in 3D: $f(V) = b(1+V)$ for wind velocity at 2 m high or $f(V) = a + bV$ for wind velocity at 10 m high, depending on user's choice,

- V is the wind velocity (m/s),

- $H^{sat} = \frac{0.622 P_{vap}^{sat}}{P_{atm} - 0.378 P_{vap}^{sat}}$ is the air specific moisture (humidity) at saturation (kg/kg),

- $H = \frac{0.622 P_{vap}}{P_{atm} - 0.378 P_{vap}}$ is the air specific humidity (kg/kg),
- P_{vap} is the partial pressure of water vapour in the air (hPa) which is given in the `ASCII ATMOSPHERIC DATA FILE`,
- P_{vap}^{sat} is the partial pressure of water vapour at saturation (hPa) which is estimated with:

$$P_{vap}^{sat} = 6.11 \exp\left(\frac{17.27 T_{water}}{T_{water} + 237.3}\right).$$

When $H^{sat} < H$, the atmospheric radiation RA is corrected by multiplying it with 1.8.

6. BIOMASS Module

The BIOMASS module is a water quality module which allows the calculation of algal biomass. It estimates the extent of vegetal colonization in terms of various parameters: sunlight, water temperature, fertilization degree, water renewal ratio, water turbidity and toxicity [4]. The BIOMASS module is activated by setting `WATER QUALITY PROCESS` = 3.
It takes into account five tracers:

- phytoplankton biomass PHY,
- the principal nutrients influencing its production (phosphorus, nitrogen) as well as the associated mineral forms, namely:
  - dissolved mineral phosphorus assimilable by phytoplankton PO_4,
  - degradable phosphorus not assimilable by phytoplankton POR,
  - dissolved mineral nitrogen assimilable by phytoplankton NO_3,
  - degradable nitrogen not assimilable by phytoplankton NOR.

These variables are all expressed in mg/l except biomass that is expressed in μg(Chlorophyl a)/l.

The following sections explain the internal source terms.
For more details about the theory of the O2 module, the reader can refer to the WAQTEL technical manual.

6.1 Processes represented

The bottom and the processes that occur there are not modeled in the BIOMASS model. Deposition is only represented by the deposition flux and, once organic matter is deposited, it no longer appears in the equations and can no longer be resuspended. These deposition fluxes therefore correspond to a definitive loss of mass.

6.2 Phytoplankton

6.2.1 Algal growth

The algal growth rate CP (d^{-1}) is given by:

$$CP = C_{max} RAY\, g_1 LNUT\, \alpha_1,$$

with C_{max} = maximum algal growth rate at 20°C; one can set its value with the keyword `MAXIMUM ALGAL GROWTH RATE AT 20C` (default = 2). *RAY* represents the effect of sunlight on algal growth, this dimensionless parameter ranges between 0 and 1. $g_1 = T/20$ represents the effect of temperature on algal growth. *LNUT* represents the effects of phosphoric and nitric nutrients on algal growth. α_1 = water toxicity coefficient for algae (α_1 = 1 in the absence of toxicity), this last value can be chosen with the 1st value of the keyword `ALGAL TOXICITY COEFFICIENTS` (default = 1).
RAY is calculated by the Smith formula averaged over the vertical:

$$RAY = \frac{1}{k_e h} \log \left(\frac{I_0 + \sqrt{IK^2 + I_0^2}}{I_h + \sqrt{IK^2 + I_h^2}} \right),$$

where k_e is the extinction coefficient of solar rays in water. The formula to compute k_e can be chosen with the keyword `METHOD OF COMPUTATION OF RAY EXTINCTION COEFFICIENT` (default = 1):

- 1: Atkins formula, it is calculated either by the Secchi depth Z_s (keyword `SECCHI DEPTH`, default = 0.9 m, if it is a constant value),
- 2: the Moss relation: $k_e = k_{pe} + \beta$ [PHY] if Z_s is unknown, where k_{pe} is the coefficient of vegetal turbidity without phytoplankton provided with the keyword `VEGETAL TURBIDITY COEFFICIENT WITHOUT PHYTO` (default = 0 m^{-1}) and β the Moss coefficient ($\beta \approx 0.015$),
- 3: constant given by the user with the keyword `LIGHT EXTINCTION COEFFICIENT` (default = 0.2 m^{-1}).

IK is a calibrating parameter associated to the keyword `PARAMETER OF CALIBRATION OF SMITH FORMULA` (default = 120 W/m^2) of an order of magnitude 100. I_0 is the flux density of solar radiation on the surface which can be set with the keyword `SUNSHINE FLUX DENSITY ON WATER SURFACE` (default = 0 W/m^2) and I_h is the flux density of solar radiation at the bed bottom (W/m^2), calculated as:

$$I_h = I_0 \exp(-k_e h).$$

LNUT is calculated by the formula:

$$LNUT = \min \left(\frac{[PO_4]}{KP + [PO_4]}, \frac{[NO_3]}{KN + [NO_3]} \right),$$

with *KP* = phosphate half-saturation constant set with the keyword `CONSTANT OF HALF-SATURATION WITH PHOSPHATE` (default = 0.005 mgP/l), and *KN* = nitrate half-saturation constant set with the keyword `CONSTANT OF HALF-SATURATION WITH NITROGEN` (default = 0.03 mgN/l).

6.2.2 Algal disappearance

The algal disappearance rate *DP* (d^{-1}) is given as:

$$DP = (RP + MP) g_2,$$

with RP = algal biomass respiration rate at 20°C given by the keyword `RESPIRATION RATE OF ALGAL BIOMASS` (default = 0.05 d^{-1}), MP = algal biomass disappearance rate at 20°C (d^{-1}). $g_2 = T/20$ represents the effect of temperature on algal disappearance. MP is given by the following relation:

$$MP = M_1 + M_2[PHY] + \alpha_2,$$

with M_1 and M_2 = algal mortality coefficients at 20°C which can be set with the keyword `COEFFICIENTS OF ALGAL MORTALITY AT 20C` (default = (0.1;0.003)), α_2 = water toxicity coefficient for algae, this last value can be chosen with the 2nd value of the keyword `ALGAL TOXICITY COEFFICIENTS` (default = 0).

6.3 Nitric and phosphoric nutrients

The following physical and biochemical parameters are used to describe the processes influencing the evolution of nitric and phosphoric nutrients:

- `PROPORTION OF PHOSPHORUS WITHIN PHYTO CELLS` for the average proportion of phosphorus in the cells of living phytoplankton fp (0.0025 mgP/μgChlA),
- `PERCENTAGE OF PHOSPHORUS ASSIMILABLE IN DEAD PHYTO` for the proportion of directly assimilable phosphorus in dead phytoplankton dtp (default = 0.5),
- `RATE OF TRANSFORMATION OF POR TO PO4` for transformation rate of POR into PO_4 through bacterial mineralization k_1 (default = 0.03 d^{-1}),
- `RATE OF TRANSFORMATION OF NOR TO NO3` for transformation rate of NOR into NO_3 through heterotrophic and autotrophic bacterial mineralization k_2 (default = 0 d^{-1}),
- `PROPORTION OF NITROGEN WITHIN PHYTO CELLS` for the average proportion of directly assimilable nitrogen in living phytoplankton fn (0.0035 mgN/μgChlA),
- `PERCENTAGE OF NITROGEN ASSIMILABLE IN DEAD PHYTO` for the proportion of directly assimilable nitrogen in dead phytoplankton dtn (default = 0.5),
- F_{POR}: deposition flux of non-algal organic phosphorus (g/m^2/s). $F_{POR} = W_{POR}[POR]$, W_{POR} is the sedimentation velocity of non-algal organic phosphorus given by the keyword `SEDIMENTATION VELOCITY OF ORGANIC PHOSPHORUS` (default = 0 m/s),
- F_{NOR}: deposition flux of non-algal organic nitrogen (g/m^2/s). $F_{NOR} = W_{NOR}[NOR]$, W_{NOR} is the sedimentation velocity of non-algal organic nitrogen given by the keyword `SEDIMENTATION VELOCITY OF NON ALGAL NITROGEN` (default = 0 m/s).

Warning:

Since release 8.5 and as long as no good solution to implement the treatment of sedimentation velocities (N and P) is found, this treatment has been commented in the source code so that it is not possible to take them into account *in 3D*. Thus keywords `SEDIMENTATION VELOCITY OF ORGANIC PHOSPHORUS` and `SEDIMENTATION VELOCITY OF NON ALGAL NITROGEN` are not taken into account. The behaviour is as they would be let to default value = 0 m/s.

7. EUTRO Module

The EUTRO module describes the oxygenation of a river and is not restricted to modeling reaeration and the global oxidizable load. It takes into account the effect of planktonic photosynthesis, models the nitric and phosphoric nutrients and their effect on phytoplankton ([5] and [3]). It is activated by setting `WATER QUALITY PROCESS` = 5.

This module is a combination of the O_2 and BIOMASS modules, except for a more precise treatment of some parameters, taking into account the ammonia load in exchanges between nitrogen and phytoplankton, and of phytoplankton in the calculation of photosynthesis. More sophisticated than the O_2 module, the EUTRO module requires setting the values of 28 parameters (excluding the parameterization of the weirs).

The EUTRO module involves 8 tracers:

- dissolved oxygen O_2,
- phytoplankton biomass (which consumes oxygen through photosynthesis) PHY,
- the main elements influencing their production (phosphorus, nitrogen, ammonia load, organic load) as well as the mineral forms associated with phosphorus and nitrogen:
  - dissolved mineral phosphorus assimilable by phytoplankton PO_4,
  - degradable phosphorus non-assimilable by phytoplankton POR,
  - dissolved mineral nitrogen assimilable by phytoplankton NO_3,
  - ammonia load assimilable by phytoplankton (and consuming oxygen) NH_4,
  - degradable nitrogen non-assimilable by phytoplankton NOR,
  - organic load (consuming oxygen) L.

These variables are expressed in mg/l, except for biomass which is expressed in μg (Chlorophyll a)/l.

For more details about the theory of the EUTRO module, the reader can refer to the WAQTEL technical manual.

7.1 Processes represented

The following parts show the parameters used and detail internal sources for each of the 8 tracers studied.

As with the BIOMASS module, sediment transport and resulting bed geometry changes are not modeled in the EUTRO module (only a deposition flux is taken into account and the quantities deposited no longer appear in the equations).

7.2 Phytoplankton

7.2.1 Algal growth

The algal growth rate CP (d^{-1}) is given by the exactly same equation as in BIOMASS module. The parameters C_{max} (`MAXIMUM ALGAL GROWTH RATE AT 20C`, default = 2), RAY, g_1 and α_1 (this last value can be chosen with the 1st value of the keyword `ALGAL TOXICITY COEFFICIENTS`, default = 1 i.e. absence of toxicity) are defined in the same way as in the BIOMASS module.
The parameters `METHOD OF COMPUTATION OF RAY EXTINCTION COEFFICIENT` (default = 1 i.e. Atkins formula with Secchi depth), `VEGETAL TURBIDITY COEFFICIENT WITHOUT PHYTO` (default = 0 m^{-1}), `PARAMETER OF CALIBRATION OF SMITH FORMULA` (default = 120 W/m^2), `SUNSHINE FLUX DENSITY ON WATER SURFACE` (default = 0 W/m^2) are still to be set as in BIOMASS.

The parameter representing the effects of phosphoric and nitric nutrients on the algal growth $LNUT$ takes into account the ammonia load assimilable by the phytoplankton NH_4 and is therefore defined by:

$$LNUT = \min\left(\frac{[PO_4]}{KP+[PO_4]}, \frac{[NO_3]+[NH_4]}{KN+[NO_3]+[NH_4]}\right), \tag{7.1}$$

with KP half-saturation constant in phosphate set with the keyword `CONSTANT OF HALF-SATURATION WITH PHOSPHATE` (default = 0.005 mgP/l) as in BIOMASS, and KN half-saturation constant in nitrates set with the keyword `CONSTANT OF HALF-SATURATION WITH NITROGEN` (default = 0.03 mgN/l) as in BIOMASS.

7.2.2 Algal disappearance

The algal disappearance rate DP (d^{-1}) is given by the the same equation as in BIOMASS module. `RESPIRATION RATE OF ALGAL BIOMASS` (default = 0.05 d^{-1}) and the keyword `COEFFICIENTS OF ALGAL MORTALITY AT 20C` (default = (0.1;0.003)) and `ALGAL TOXICITY COEFFICIENTS` (default = (1;0)) are still to be set as in BIOMASS.

The effect of temperature on algal disappearance is represented by the function $g_2 = (1,050)^{T-20}$.

7.3 Nitric and phosphoric nutrients

The following physical and biochemical parameters are used to describe processes influencing the evolution of nitric and phosphoric nutrients:

- `PROPORTION OF PHOSPHORUS WITHIN PHYTO CELLS` for the average proportion of phosphorus in the cells of living phytoplankton fp (0.0025 mgP/μgChlA),

- PERCENTAGE OF PHOSPHORUS ASSIMILABLE IN DEAD PHYTO for the proportion of directly assimilable phosphorus in dead phytoplankton dtp (default = 0.5),
- RATE OF TRANSFORMATION OF POR TO PO4 for the transformation rate of POR into PO_4 through bacterial mineralization at 20°C k_{320} (default = 0.03 d^{-1}),
- RATE OF TRANSFORMATION OF NOR TO NO3 for the transformation rate of NOR into NO_3 through heterotrophic and autotrophic bacterial mineralization at 20°C k_{620} (default = 0 d^{-1}),
- PROPORTION OF NITROGEN WITHIN PHYTO CELLS for the average proportion of directly assimilable nitrogen in living phytoplankton fn (0.0035 mgN/μgChlA),
- PERCENTAGE OF NITROGEN ASSIMILABLE IN DEAD PHYTO for the proportion of directly assimilable nitrogen in dead phytoplankton dtn (default = 0.5),
- CONSUMED OXYGEN BY NITRIFICATION for the quantity of oxygen consumed by nitrification n (default = 5.2 $mgO_2/mgNH_4$),
- CONSTANT FOR THE NITRIFICATION KINETIC K520 for the kinetics of nitrification at 20°C k_{520} (default = 0.35 d^{-1}),
- F_{POR}: deposition flux of non-algal organic phosphorus (g/m^2/s). $F_{POR} = W_{POR}[POR]$, W_{POR} is the sedimentation velocity of non-algal organic phosphorus given by the keyword SEDIMENTATION VELOCITY OF ORGANIC PHOSPHORUS (default = 0 m/s),
- F_{NOR}: deposition flux of non-algal organic nitrogen (g/m^2/s). $F_{NOR} = W_{NOR}[NOR]$, W_{NOR} is the sedimentation velocity of non-algal organic nitrogen given by the keyword SEDIMENTATION VELOCITY OF NON ALGAL NITROGEN (default = 0 m/s).
- Rn: proportion of nitrogen assimilated in the form of NH_4 = $\frac{[NH_4]}{[NH_4]+[NO_3]}$.

7.4 Organic load

The following physical and biochemical parameters are used to describe processes influencing the evolution of the organic load (L):

- CONSTANT OF DEGRADATION OF ORGANIC LOAD K120 for kinetic degradation constant for the organic load at 20°C k_{120} (default = 0.35 d^{-1}),
- $g_3 = (1.047)^{T-20}$: effect of temperature on the degradation of organic load,
- F_{LOR}: deposition flux of the organic load (g/m^2/s) = W_{LOR}.[L], with W_{LOR} the sedimentation velocity of the organic load given by the keyword SEDIMENTATION VELOCITY OF ORGANIC LOAD (default = 0 m/s).

7.5 Dissolved oxygen

The following physical and biochemical parameters are used to describe processes influencing the dissolved oxygen balance (O_2):

- OXYGEN PRODUCED BY PHOTOSYNTHESIS for oxygen quantity produced by photosynthesis f (default = 0.15 mgO_2/μgChlA),

- BENTHIC DEMAND (default = 0.1 $gO_2/m^2/d$) for benthic oxygen demand *BEN* (cf. O_2 model),
- k_2: water-atmosphere gaseous exchange coefficient, also called reaeration coefficient, at 20°C (d^{-1}). It can be provided by the user with the keyword K2 REAERATION COEFFICIENT (default = 0.9 d^{-1}) or calculated using formulae in the literature with the keyword FORMULA FOR COMPUTING K2 (cf. O_2 module),
- $g_4 = (1.025)^{T-20}$: effect of temperature on natural reaeration,
- C_s: concentration of oxygen saturation in water (mgO_2/l). It can be determined from the water temperature (and possibly water salinity) with the formula chosen with the keyword FORMULA FOR COMPUTING CS (default = 0 i.e. constant value given by O2 SATURATION DENSITY OF WATER (CS), default = 11 mgO_2/l), cf. O_2 module. Since release 8.5, it can be written in the TELEMAC-2D RESULTS FILE, the TELEMAC-3D 2D RESULT FILE or the TELEMAC-3D 3D RESULT FILE. CSO2 is to be written in the list of VARIABLES FOR GRAPHIC PRINTOUTS in the TELEMAC-2D steering file. It is to be written in the list of VARIABLES FOR 2D GRAPHIC PRINTOUTS (with values averaged along the vertical) and/or VARIABLES FOR 3D GRAPHIC PRINTOUTS (with values computed at every 3D node) in the TELEMAC-3D steering file.

In addition to the concentration of oxygen saturation in water C_s, the percentage of oxygen saturation defined as the ratio concentration of oxygen over concentration of oxygen saturation can be written in the previous result file: O2SAT is to be written in the list of variables of the dedicated TELEMAC steering file. It is expressed in %.

Warning:

Since release 8.5 and as long as no good solution to implement the treatment of sedimentation velocities (N, P and organic load) is found, this treatment has been commented in the source code so that it is not possible to take them into account *in 3D*. Thus keywords SEDIMENTATION VELOCITY OF ORGANIC PHOSPHORUS, SEDIMENTATION VELOCITY OF NON ALGAL NITROGEN and SEDIMENTATION VELOCITY OF ORGANIC LOAD are not taken into account. The behaviour is as they would be let to default value = 0 m/s.

8. MICROPOL Module

The MICROPOL module simulates the evolution of a micropollutant (radioelement or heavy metal) in the three compartments considered to be of major importance in a river ecosystem: water, Suspended Particulate Matter (SPM) and bottom material.
It is activated by setting `WATER QUALITY PROCESS` = 7.

Each of these compartments represents an homogeneous class: SPM and sediments represent the grain-size class of clay and silt (cohesive fine sediments, of diameter about less than 20 to 25 μm), likely to attach the majority of micropollutants.

Due to adsorption and desorption of micropollutants, SPM is one of the first links in the chain of contamination. SPM is carried and dispersed in the water mass as a tracer and is also subject to the laws of sedimentary physics: it settles in calm waters and produces bottom sediments, and can be re-suspended by a high flow. Deposits cannot move. They are treated as tracers that can be neither advected nor dispersed by the water mass, but are likely to be re-suspended.

The model considers 5 tracers:

- suspended matter (SS),
- bottom sediments (SF), neither advected nor dispersed,
- dissolved form of micropollutant,
- the fraction adsorbed by suspended particulate matter,
- the fraction adsorbed by bottom sediments, neither advected nor dispersed.

Notes, and limitations of the MICROPOL module

- whether in suspension or deposited on the bottom, the matter is considered to be a passive tracer: in other words, it does not influence the flow (no feedback). This hypothesis involves that the deposits depth must be negligible compared to the water depth (the bed is assumed to be unmodified).
- there is no direct adsorption/desorption of dissolved micropollutants on the deposited matter, only on the SPM (the model assumes a preponderance of water – SPM exchanges over direct water – bottom sediment exchanges). Bottom sediments only become radioactive by means of polluted SPM deposition.

8.1 Suspended matter

The model describing the evolution of SPM and bottom sediments involved in MICROPOL is a classic representation of the deposition laws and re-suspension of cohesive SPM, that are the laws of Krone [10] and Partheniades [11].

Both processes require the knowledge of characteristic constants:

- deposition occurs when bottom shear stress τ_b, which varies according to the flow conditions, becomes lower than a threshold value τ_s, known as the critical shear stress for sedimentation and which can be set with the keyword `SEDIMENTATION CRITICAL STRESS` (default = 5 Pa) . It is then assumed that the SPM settles at a constant velocity w (known as the settling velocity or velocity of sedimentation) with the keyword `SEDIMENT SETTLING VELOCITY` (default = 6.10^{-6} m/s),
- re-suspension occurs when a threshold τ_r, known as the critical shear stress for re-suspension, is exceeded. It can be set with the keyword `CRITICAL STRESS OF RESUSPENSION` (default = 1,000 Pa). Its importance is weighted by a constant e, the rate of erosion characteristic of deposited SPM (also known as the Partheniades constant), which associated keyword is `EROSION RATE` (default = 0).

8.2 Micropollutants

The model representing the evolution of micropollutants assumes that the transfers of micropollutants (radioelement, metal) between the dissolved and particulate phases correspond to either direct adsorption or ionic exchanges modeled by a reversible reaction, of 1st kinetic order. In the case of direct adsorption, the reaction can be represented in the form of a reversible reaction, controlled by adsorption (k_1 in l/g/s) and desorption velocities (k_{-1} in s^{-1}) which last associated keyword is `CONSTANT OF DESORPTION KINETIC` (default = 2.5 $10^{-7} s^{-1}$). It leads to an equilibrium state, and then a distribution of micropollutants between the dissolved and particulate phase described by the distribution coefficient $K_d = \frac{k_1}{k_{-1}}$ (set with the keyword `COEFFICIENT OF DISTRIBUTION`, default = 1,775 l/g). Once adsorbed, the fixed micropollutants act like SPM (deposition, re-suspension) and can also produce areas of polluted sediment.

The model includes an exponential decay law (radioactive decay type) of micropollutant concentrations in each compartment of the modeled ecosystem, through a constant written L which can be set with the keyword `EXPONENTIAL DESINTEGRATION CONSTANT` (default = 1.13 10^{-7} s^{-1}).

8.2.1 Two-step reversible model

Two successive-step reversible model is activated by setting the keyword `KINETIC EXCHANGE MODEL` = 2.

This allows the model to consider two additional tracers:

- C_{ss2}: concentration of micropollutants adsorbed by SPM “specific sites”,
- C_{ff2}: concentration of micropollutants adsorbed by bottom sediments “specific sites”.

Ionic exchanges are then modelled with one supplementary slower step, associated with keywords `CONSTANT OF DESORPTION KINETIC 2` (default = 2.5 10^{-9} s^{-1}) and `COEFFICIENT OF DISTRIBUTION 2`, default = 1,775 g/g). Because of the slower exchange dynamics in the second reversible step, the default value of `CONSTANT OF DESORPTION KINETIC 2` is significantly smaller than the one of `CONSTANT OF DESORPTION KINETIC`.

9. AED2 Module

See the AED2 model technical manual (water quality and aquatic ecology model) available on the AED2 website:

http://aed.see.uwa.edu.au/research/models/AED/downloads/AED_ScienceManual_v4_draft.pdf

and also the 2 examples available in the following folders:

$HOMETEL/examples/waqtel/waq3d_aed2 and $HOMETEL/examples/waqtel/waq3d_aed2_flume

10. Degradation law

WAQTEL can simulate usual laws for bacterial degradation with T_{90} coefficient(s): time(s) required for 90% of the initial bacterial population to disappear or also described as the time for bacterial or viral concentration to decrease by one log unit (hence the 2.3 coefficient below). It is expressed in hours.
In other words, it simulates the evolution of tracer(s) C over time from initial condition(s) according to a degradation law assumed to be of 1st order (i.e. a tracer decrease) with constant(s) of tracer kinetic degradation equal to $\frac{2.3}{T_{90}}$:

$$F([C]) = -\frac{2.3}{T_{90}}[C], \tag{10.1}$$

with T_{90} coefficient(s) described above, in hours.

WAQTEL can also simulate the evolution of tracer(s) C over time from initial condition(s) according to a degradation law that is assumed to be of 1st order (i.e. a tracer decrease):

$$F([C]) = -k_1[C], \tag{10.2}$$

where k_1 is the constant (or one of the constants) of tracer kinetic degradation C (it can be given in h^{-1} or d^{-1}).

The user can decide whether a tracer follows such laws with the keyword `LAW OF TRACERS DEGRADATION` which is an array containing as many values as the number of tracers. Possible choices are:

- 0: no degradation (default),
- 1: law for bacterial degradation with T_{90} coefficient in hours,
- 2: degradation law of first order, constant of tracer kinetic degradation in h^{-1},
- 3: degradation law of first order, constant of tracer kinetic degradation in d^{-1},
- 4: law implemented by user (with the help of **USER_CALCS2D_DEGRADATION** or **USER_CALCS3D_DEGRADATION** subroutines in 2D or 3D).

The T_{90} or k_1 coefficients can be specified with the keyword `COEFFICIENT 1 FOR LAW OF TRACERS DEGRADATION` (one per tracer, expressed in hours for law 1, in h^{-1} for law 2, in d^{-1} for law 3).

11. API

Information on the WAQTEL API can be found in the telapy user documentation. The WAQTEL API does not exist in stand alone you must use the TELEMAC-2D or TELEMAC-3D API.

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