WAQTEL

Technical manual

Contents

Abstract

This technical manual is mainly based on the translation of the TRACER principle note "Outil de simulation 1-D MASCARET V7.1. Module de qualité d'eau TRACER. Note de principe" written by Kamal El Kadi Abderrezzak and Marilyne Luck in 2012 [6] (ref: EDF R&D-LNHE H-P73-2011-01786-FR). It also includes the heat atmosphere exchange subsection of the TELEMAC-3D theory guide.

TRACER is the transport and water quality module of the 1D free surface code MASCARET. TRACER simulates the evolution of several coupled tracers without retroaction on the flow with respect to hydraulic conditions, boundary conditions, external sources and biochemical interactions between tracers.

This note contains an explanation of the method retained for solving the advection-dispersion equation, and its application to water quality modeling.

All the processes existing in TRACER were implemented in TELEMAC-2D and TELEMAC-3D through a new module called WAQTEL between v7.0 and v7.2. The following water quality modules are described:

- O_2 (dissolved oxygen, organic and ammonia loads),

- BIOMASS (phytoplankton biomass and nutrients),

- EUTRO (dissolved oxygen, phytoplankton biomass, nutrients, organic and ammonia loads),

- MICROPOL (micropollutants and suspended matter),

- THERMIC (water temperature),

- degradation law.

A reference to the library documentation of the water quality and aquatic ecology model AED2 is also given.

1. Water quality models

For the sake of simplicity, the following operator $F(C)$ is defined:

$$F(C) = \frac{\partial C}{\partial t} + \boldsymbol{U} \cdot \boldsymbol{\nabla} C - \nabla \cdot (k\boldsymbol{\nabla} C), \tag{1.1}$$

with $C(x, y, z, t)$ is the tracer concentration, t is time, (x, y, z) the coordinates, k the diffusion coefficient (m^2/s), $\boldsymbol{U}$ the velocity vector (m/s).

The studied substances are advected and dispersed in the water mass. The dispersion is due to the flow transport and to the flow turbulence.
The concentration of a substance (e.g. pollutant, oxygen) is also influenced by:

- punctual contributions, caused by releases (industrial, sewage treatment plants, etc.) called *external sources*,

- the presence of other substances in the water mass, with which the tracer may react through biochemical transformations or the existence of forcings linked to its own concentration (e.g. the reaeration phenomenon for oxygen). These source terms for one tracer are called *internal sources* (because internal to the water mass) and they characterize the water quality module (description of the interactions between the tracers).

Solving a water quality problem consists in solving a system of N (number of tracers) advection-dispersion equations (one equation per tracer) considering the presence of external (e.g. releases) and internal sources.
A water quality model is characterized in WAQTEL by the coupled treatment of different tracers and the description of the *internal* source terms.

The internal source term for a given tracer i can be written through the following form:

$$S_{intern_i} = \lambda_i^0 + \sum_{j=1}^{N} \lambda_i^j C_j + \frac{\mu_i^0}{h} + \frac{\sum_{j=1}^{N} \mu_i^j C_j}{h} \tag{1.2}$$

with λ_i^0 and μ_i^0 are terms not depending on the tracer concentration i and h is the water depth. The 1st term represents the volumic internal sources (e.g. chemical reactions) whereas the 2nd term represents the surface internal sources (e.g. deposition, re-suspension, evaporation).

Depending on the water quality module, matrices $[\lambda]$ and $[\mu]$ containing the coefficients λ_i^j and μ_i^j are written differently. The internal source terms are treated in an explicit way in the advection-diffusion equation, because they depend on the concentration of other tracers that remain unknown at the time step $n+1$.

If there are interactions between tracers or specific evolution laws of tracers, a water quality module can be used to determine the internal sources of tracers that can be involved in the transport equation.

Internal sources of tracers are computed in the water quality module WAQTEL at each time step, with respect to physical parameters and the concentrations of different tracers. Then they are given to TELEMAC-2D or TELEMAC-3D for computing the tracer evolution (by advection and diffusion+dispersion) taking the external source terms into account.

Several water quality modules are available in the WAQTEL library:

- O_2 module: simplified model of dissolved oxygen,

- BIOMASS module: phytoplankton biomass model,

- EUTRO module: eutrophication model (dissolved oxygen and algal biomass),

- MICROPOL module: evolution of heavy metals or radioelements, taking into account interactions with fine sediments (suspended matter). However, no changes of the bed geometry is considered,

- THERMIC module: evolution of water temperature under the influence of atmospheric fluxes,

- AED2 model: the water quality and aquatic ecology model,

- degradation law.

The different modules and their features are described in the following chapters in which the internal source terms are also detailed.

Note that the structure chosen for WAQTEL enables to easily add new water quality modules, by implementing terms relating to internal sources.

2. O$_2$ Module

The O$_2$ module is a simple oxygen evolution module, intermediate between the Streeter and Phelps [24] model, which is restricted to modeling reaeration and the global oxidizable load, and a more complete module, such as EUTRO, simulating several oxidation processes and explicitly computes the phytoplankton evolution and its influence on oxygen. The O$_2$ model advantage is its simplicity (eight parameters to calibrate, excluding parameterization of weirs). Some important parameters are assumed constant, such as benthic demand or plant respiration. The use of the model is consequently limited to phenomena of a few days duration, such as reservoir emptying. Three tracers are involved:

- dissolved oxygen O$_2$ (mgO$_2$/l),

- the organic load L (mgO$_2$/l),

- the ammonia load NH4 (mgH$_4$/l).

These variables are advected and dispersed in the water mass accordingly to the advection-dispersion equation, with external and internal sources. Six factors influencing the concentration of dissolved oxygen are considered:

- four factors consuming oxygen: organic load, ammonia load, benthic demand and plant respiration,

- two processes creating oxygen: photosynthesis and reaeration.

The terms dealing with internal sources of each considered tracer are explained in the following sections.

2.1 Dissolved oxygen

2.1.1 Benthic demand

The benthic demand BEN is provided by the user in gO$_2$/m^2/d. It is adjusted according to the temperature T as:

$$BEN_T = BEN_{20°C}(1.065)^{T-20}. \tag{2.1}$$

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

2.1.2 Plant respiration

The plant respiration R (in mgO$_2$/d/l) is provided by the user.

2.1.3 Photosynthesis

The photosynthesis P (in mgO$_2$/d/l) depends on algae, water depth and light, with order of magnitude between 0.3 mgO$_2$/l/d and 9 mgO$_2$/l/d depending on the flow discharge [24]. In the O$_2$ model, P is provided by the user.

2.1.4 Reaeration

Natural reaeration

Reaeration is an oxygen supply through the free surface. At macroscopic scale, it can be modeled as linearly proportional to (C_s - [O$_2$]), where C_s is the oxygen concentration at saturation in the water (in mgO$_2$/l) (Reminder: C_s = 9 mg/l at 20°C). Therefore:

$$Reaeration = k_2\left(C_s - [\mathrm{O_2}]\right). \tag{2.2}$$

The coefficient k_2 (d^{-1}) is a parameter with orders of magnitude indicated in the Table below (from [26]).

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 flow velocity	0.35-0.46
Large streams of normal flow velocity	0.46-0.69
Swift streams	0.69-1.15
Rapids and waterfalls	> 1.15

There are plenty of formulae calculating k_2, which indicates the low level of our understanding of this process. We can distinguish conceptual formulae, valid only within limited conditions, and semi-empirical and empirical formulae that are valid where conditions are not too far from those of calibration. Actually, there is little difference between the formulae when the water depth is between 0.3 m and 3 m. The O$_2$ model allows using four formulae cited in [17]:

$$k_2 = 5.23 U h^{-1.67} \quad \text{(Tennessee Valley Authority)}, \tag{2.3}$$

$$k_2 = 5.33 U^{0.67} h^{-1.85} \quad \text{(Owens et al.)}, \tag{2.4}$$

$$k_2 = 0.746 U^{2.695} h^{-3.085} J^{-0.823} \quad \text{(Churchill et al.)}, \tag{2.5}$$

$$k_2 = 3.9 U^{0.5} h^{-1.5} \quad (\text{O'Connor and Dobbins}), \tag{2.6}$$

with U is the magnitude of velocity (in m/s) and J is the energy slope (in m).
The O'Connor and Dobbins formula provides the best results for shallow rivers. For deep and rapid rivers, Churchill et al.'s formula is preferable. Figure 2.1 shows the areas of application for selected formulae [17]:
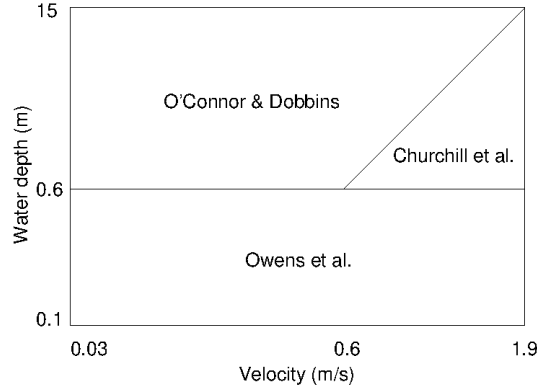

Figure 2.1: Application areas of Owens et al., Churchill et al. and O'Connor and Dobbins formulae [17].

One option allows the user fixing a value for k_2. Another option allows choosing one of the four formulae described above. The value of k_2, valid at 20°C, is adjusted according to the temperature as:

$$k_2 = (k_2)_{20°\text{C}} (1.0241)^{T-20}. \tag{2.7}$$

The oxygen concentration at saturation in the water C_s can be determined according to the water temperature (at 20°C, $C_s = 9$ mgO$_2$/l). This is a parameter that must be known and can be calculated if connected to a temperature module such as THERMIC. Elmore and Hayes (cited in [17]) proposed the following formula (with T in °C) for calculating C_s:

$$C_s = 14.652 - 0.41022 T + 0.007991 T^2 - 7.7774.10^{-5} T^3. \tag{2.8}$$

More recent models include a correction for atmospheric pressure and, in estuaries, for salinity. However, we consider that we are far from estuarial conditions and the variations in pressure entail insignificant variations in dissolved oxygen compared to those that we need. Montgomery et al.'s equation (cited in [17]) only deviates from standard formulae by ± 0.02 mgO$_2$/l between 0 and 50°C when there is negligible salinity.

$$C_s = \frac{468}{31.6 + T}. \tag{2.9}$$

The model allows choosing either a fixed C_s value given by the user or by one of the two formulae described above.

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

A weir can provide between 1 and 3 mg/l of dissolved oxygen [17]. The ratio r is defined by the relationship

$$r = \frac{C_s - C_u}{C_s - C_d},$$

with C_u = oxygen concentration upstream of weir, C_d = oxygen concentration downstream of weir. The knowledge of C_u and r enables calculating C_d. C_d is directly applied. This term therefore is not treated as a source. The rate r can be determined empirically [17]: e.g.,

$$r = 1 + 0.5ab\Delta h \quad \text{(Gameson)}, \tag{2.10}$$

$$r = 1 + 0.36ab(1 + 0.046T)\Delta h \quad \text{(Gameson et al.)}, \tag{2.11}$$

$$r = 1 + 0.69\Delta h(1 - 0.11\Delta h)(1 + 0.046T) \quad \text{(Water Research Laboratory)}, \tag{2.12}$$

$$r = 1 + 0.38ab\Delta h(1 - 0.11\Delta h)(1 + 0.046T), \quad \text{(Water Research Laboratory)} \tag{2.13}$$

with a = measure of water quality (= 0.65 for highly polluted streams, = 1.8 for clear streams), b = characteristic parameter of the weir, Δh = water level difference between upstream and downstream of the weir. The following Table gives b values for different weirs [17]:

Type of weir	b
flat broad-crested regular step	0.7
flat broad-crested irregular step	0.8
flat broad-crested vertical face	0.8
flat broad-crested straight slope face	0.9
flat broad-crested curved face	0.75
round broad-crested curved face	0.6
sharp-crested straight slope face	1.05
sharp-crested vertical face	0.8
sluice gates with submerged discharge	0.05

In the model, r can be either a fixed value given by the user or calculated by one of the 4 formulae previously described.

2.2 Organic load

The organic load L (in mgO$_2$/l) is a variable evolving over time from an initial condition according to a 1st order law:

$$F([L]) = -k_1[L], \tag{2.14}$$

where k_1 is the kinetic degradation constant of the organic load (d^{-1}). It is a parameter of the model. In the O$_2$ model, the organic load L is considered to be an independent variable.

2.3 Ammonia load

Also consuming oxygen, the variable ammonia load NH$_4$ (in mgH$_4$/l) follows a 1st order decay law

$$F([NH_4]) = -k_4[NH_4], \tag{2.15}$$

where k_4 the kinetic constant of nitrification (d^{-1}), a parameter of the model. In the O_2 model, the ammonia load is considered to be an independent variable.

2.4   Solved equation in 2D

The concentration of dissolved oxygen $[O_2]$ (in mgO_2/l) changes according to the effect of sources:

$$F([O_2]) = k_2(C_s - [O_2]) - k_1[L] - k_4[NH_4] + P - R - \frac{BEN_T}{h}. \tag{2.16}$$

Using the terminology and notations of section 1 and setting $C_1 = [O_2]$, $C_2 = [L]$ and $C_3 = [NH_4]$, the matrices $[\lambda]$ and $[\mu]$ are written as:

$$[\lambda] = \frac{1}{86400} \begin{pmatrix} -k_2 & -k_1 & -k_4 \\ 0 & -k_1 & 0 \\ 0 & 0 & -k_4 \end{pmatrix}$$

$$[\mu] = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

(Note: Division by 86,400 scales down the time to one second).

The only non-zeros terms λ_1^0 and μ_1^0 are:

$$\lambda_1^0 = \frac{k_2 C_s + P - R}{86400}, \tag{2.17}$$

$$\mu_1^0 = -\frac{BEN_T}{86400}. \tag{2.18}$$

2.5   Solved equation in 3D

The concentration of dissolved oxygen $[O_2]$ (in mgO_2/l) changes according to the effect of sources:

$$F([O_2]) = k_2(C_s - [O_2]) - k_1[L] - k_4[NH_4] + P - R - \frac{BEN_T}{\Delta z}. \tag{2.19}$$

with Δz half height of the bottom layer cells.
Using the terminology and notations of section 1 and setting $C_1 = [O_2]$, $C_2 = [L]$ and $C_3 = [NH_4]$, the matrices $[\lambda]$ and $[\mu]$ are written as:

$$[\lambda] = \frac{1}{86400} \begin{pmatrix} -k_2 & -k_1 & -k_4 \\ 0 & -k_1 & 0 \\ 0 & 0 & -k_4 \end{pmatrix}$$

$$[\mu] = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

(Note: Division by 86,400 scales down the time to one second).

The only non-zeros terms λ_1^0 and μ_1^0 are:

$$\lambda_1^0 = \frac{k_2 C_s + P - R - \frac{BEN_T}{\Delta z}}{86400}, \tag{2.20}$$

$$\mu_1^0 = 0. \tag{2.21}$$

3. 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 [9]. The BIOMASS module 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.

We assume these substances acting as tracers, i.e. they are carried and dispersed in the water mass. In addition, they react with each other through biochemical processes.

The following sections explain the internal source terms.

3.1 Phytoplankton

3.1.1 Algal growth

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

$$CP = C_{max}RAY\,g_1\,LNUT\,\alpha_1, \tag{3.1}$$

with C_{max} = algal growth maximum rate at 20°C; one can take C_{max} = 2. RAY represents the effect of sunlight on algal growth; this dimensionless parameter ranges between 0 and 1; g_1 represents the effect of temperature on algal growth; $g_1 = T/20$, where T is the water temperature (°C) (valid for 5°C $< T <$ 25°C). $LNUT$ 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).

In 2D, *RAY* is calculated by the Smith formula averaged over the vertical:

$$RAY = \frac{1}{k_e h} \log \left(\frac{I_0 + \sqrt{IK^2 + I_0^2}}{I_h + \sqrt{IK^2 + I_h^2}} \right), \tag{3.2}$$

where k_e is the extinction coefficient of solar rays in water (m^{-1}). It is calculated either by the Secchi depth Z_s using the Atkins formula: $k_e = 1.7/Z_s$, or, if Z_s is unknown, by the Moss relation: $k_e = k_{pe} + \beta$ [PHY], where k_{pe} is the coefficient of vegetal turbidity without phytoplankton (m^{-1}) and β the Moss coefficient ($\beta \approx 0.015$). *IK* is a calibrating parameter (W/m^2), of an order of magnitude 100. I_0 is the flux density of solar radiation on the surface (W/m^2) and I_h is the flux density of solar radiation at the bed bottom (W/m^2), calculated as:

$$I_h = I_0 \exp(-k_e h). \tag{3.3}$$

In 3D, *RAY* is calculated by a generalisation of the Smith formula over the vertical:

$$RAY = \frac{1}{k_e \Delta z} \log \left(\frac{I_0 + \sqrt{IK^2 + I_0^2}}{I_{\Delta z} + \sqrt{IK^2 + I_{\Delta z}^2}} \right), \tag{3.4}$$

with everything like in 2D except Δz the height of the prism in 3D and $I_{\Delta z}$ is the flux density of solar radiation at the considered depth (W/m^2), calculated as:

$$I_{\Delta z} = I_0 \exp(-k_e \Delta z), \tag{3.5}$$

LNUT is calculated by the formula:

$$LNUT = \min \left(\frac{[PO_4]}{KP + [PO_4]}, \frac{[NO_3]}{KN + [NO_3]} \right), \tag{3.6}$$

with *KP* = phosphate half-saturation constant (mg/l) (about 0.005 mgP/l), and *KN* = nitrate half-saturation constant (mg/l) (about 0.03 mgN/l).

Note: Nutrients affect phytoplankton growth PHY only by limiting the factor *LNUT*. When [PO$_4$] and [NO$_3$] are high enough, *LNUT* is close to 1 and phytoplankton evolution no longer depends on nutrients. In this case, there is no need to model the cycles of phosphorus and nitrogen for simulating the evolution of phytoplankton.

3.1.2 Algal disappearance

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

$$DP = (RP + MP)g_2, \tag{3.7}$$

with *RP* = algal biomass respiration rate at 20°C (d^{-1}), *MP* = algal biomass disappearance rate at 20°C (d^{-1}). g_2 represents the effect of temperature on algal disappearance. $g_2 = T/20$ (valid for 5°C < *T* < 25°C). *MP* is given by the following relation:

$$MP = M_1 + M_2[PHY] + \alpha_2, \tag{3.8}$$

with M_1 and M_2 = algal mortality coefficients at 20°C, α_2 = water toxicity coefficient for algae.

3.2 Nitric and phosphoric nutrients

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

- fp: average proportion of phosphorus in the cells of living phytoplankton (mgP/μgChlA),

- dtp: proportion of directly assimilable phosphorus in dead phytoplankton (%),

- k_1: transformation rate of POR into PO_4 through bacterial mineralization (d^{-1}),

- k_2: transformation rate of NOR into NO_3 through heterotrophic and autotrophic bacterial mineralization (d^{-1}),

- fn: average proportion of directly assimilable nitrogen in living phytoplankton (mgN/μgChlA),

- dtn: proportion of directly assimilable nitrogen in dead phytoplankton (%),

- 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 (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 (m/s).

Note: sediment transport and resulting bed changes 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.

3.3 Solved equations in 2D

The BIOMASS model equations are described below, detailing the internal source terms S_{intern_i}.

Tracer #1: phytoplankton biomass

$$F([PHY]) = (CP - DP)[PHY].$$
(3.9)

Tracer #2: assimilable mineral phosphorus

$$F([PO_4]) = fp(dtpDP - CP)[PHY] + k_1g_2[POR].$$
(3.10)

Tracer #3: non-assimilable phosphorus

$$F([POR]) = fp(1 - dtp)DP[PHY] - k_1g_2[POR] - \frac{F_{POR}}{h}.$$
(3.11)

Tracer #4: assimilable mineral nitrogen

$$F([NO_3]) = fn(dtnDP - CP)[PHY] + k_2g_2[NOR].$$
(3.12)

Tracer #5: non-assimilable nitrogen

$$F([NOR]) = fn(1 - dtn)DP[PHY] - k_2g_2[NOR] - \frac{F_{NOR}}{h},$$
(3.13)

with $C_1 = [PHY]$, $C_2 = [PO_4]$, $C_3 = [POR]$, $C_4 = [NO_3]$ and $C_5 = [NOR]$, the matrices (5×5) $[\lambda]$ and $[\mu]$ are written as (only non-zero terms are included):

$$\lambda_i^j = \frac{1}{86400} \begin{pmatrix} CP - DP & 0 & 0 & 0 & 0 \\ fp(dtpDP - CP) & 0 & k_1g_2 & 0 & 0 \\ fp(1 - dtp)DP & 0 & -k_1g_2 & 0 & 0 \\ fn(dtnDP - CP) & 0 & 0 & 0 & k_2g_2 \\ fn(1 - dtn)DP & 0 & 0 & 0 & -k_2g_2 \end{pmatrix} \tag{3.14}$$

$$\mu_i^j = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -W_{POR} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -W_{NOR} \end{pmatrix}$$

The terms λ_i^0 and μ_i^0 are zero for every i.

Divisions by 86,400 are performed to scale down time to one second.

3.4   Solved equations in 3D

The BIOMASS model equations are described below, detailing the internal source terms S_{intern_i}.

Tracer #1: phytoplankton biomass

$$F([PHY]) = (CP - DP)[PHY]. \tag{3.15}$$

Tracer #2: assimilable mineral phosphorus

$$F([PO_4]) = fp(dtpDP - CP)[PHY] + k_1g_2[POR]. \tag{3.16}$$

Tracer #3: non-assimilable phosphorus

$$F([POR]) = fp(1 - dtp)DP[PHY] - k_1g_2[POR]. \tag{3.17}$$

Tracer #4: assimilable mineral nitrogen

$$F([NO_3]) = fn(dtnDP - CP)[PHY] + k_2g_2[NOR]. \tag{3.18}$$

Tracer #5: non-assimilable nitrogen

$$F([NOR]) = fn(1 - dtn)DP[PHY] - k_2g_2[NOR], \tag{3.19}$$

with $C_1 = [PHY]$, $C_2 = [PO_4]$, $C_3 = [POR]$, $C_4 = [NO_3]$ and $C_5 = [NOR]$, the matrices (5×5) $[\lambda]$ and $[\mu]$ are written as (only non-zero terms are included):

$$\lambda_i^j = \frac{1}{86400} \begin{pmatrix} CP - DP & 0 & 0 & 0 & 0 \\ fp(dtpDP - CP) & 0 & k_1g_2 & 0 & 0 \\ fp(1 - dtp)DP & 0 & -k_1g_2 & 0 & 0 \\ fn(dtnDP - CP) & 0 & 0 & 0 & k_2g_2 \\ fn(1 - dtn)DP & 0 & 0 & 0 & -k_2g_2 \end{pmatrix} \tag{3.20}$$

$$\mu_i^j = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

The terms λ_i^0 and μ_i^0 are zero for every i.

Divisions by 86,400 are performed to scale down time to one second.

> **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*.

4. 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 ([10] and [8]).

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.

These substances act as tracers, i.e. they are carried and dispersed in the water mass. In addition, they react with each other through biochemical processes.

4.1 Processes represented

Figure 4.1 presents the various phenomena modeled by the EUTRO model.

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 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).
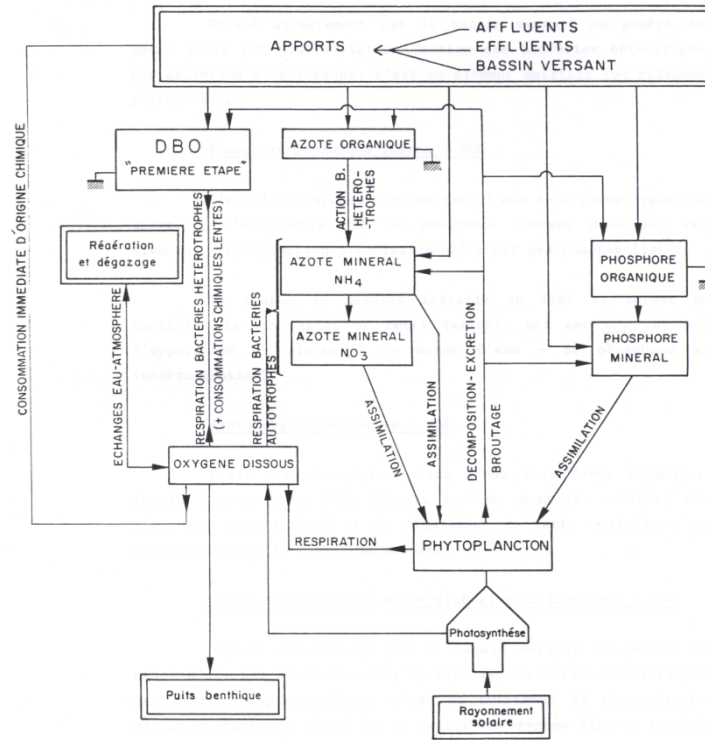
Figure 4.1: Schematic representation of the ecosystem modeled by the EUTRO module [10]. Figure taken from [6].

4.2 Phytoplankton

4.2.1 Algal growth

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

$$CP = C_{max}RAY\,g_1LNUT\,\alpha_1. \tag{4.1}$$

The parameters C_{max}, RAY, g_1 and α_1 are defined in the same way as in the BIOMASS module.

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:

$$LNUT = \min\left(\frac{[PO_4]}{KP + [PO_4]}, \frac{[NO_3] + [NH_4]}{KN + [NO_3] + [NH_4]}\right), \tag{4.2}$$

with KP half-saturation constant in phosphate (mg/l) (about 0.005 mgP/l), and KN half-saturation constant in nitrates (mg/l) (about 0.03 mgN/l).

Note: The influence of nutrients on phytoplankton growth PHY is only an intermediate limiting factor $LNUT$. When $[PO_4]$ and $[NO_3]$ are high enough, $LNUT$ is close to 1 and phytoplankton evolution no longer depends on nutrients. In this case, there is no need to model the cycles of phosphorus and nitrogen for simulating the evolution of phytoplankton.

4.2.2 Algal disappearance

The algal disappearance rate DP (d^{-1}) is given by the equation:

$$DP = (RP + MP)g_2, \tag{4.3}$$

where RP and MP are defined in the BIOMASS module. The effect of temperature on algal disappearance is represented by the function $g_2 = (1,050)^{T-20}$, where T is the water temperature (°C) (valid for $5°C < T < 25°C$).

4.3 Nitric and phosphoric nutrients

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

- fp: average proportion of phosphorus in the cells of living phytoplankton (mgP/μgChlA),

- dtp: proportion of directly assimilable phosphorus in dead phytoplankton (%),

- k_{320}: transformation rate of POR into PO$_4$ through bacterial mineralization at 20°C (d^{-1}),

- k_{620}: transformation rate of NOR into NO$_3$ through heterotrophic and autotrophic bacterial mineralization at 20°C (d^{-1}),

- fn: average proportion of nitrogen in the cells of living phytoplankton (mgN/μgChlA),

- dtn: proportion of directly assimilable nitrogen in dead phytoplankton (%),

- n: quantity of oxygen consumed by nitrification (mgO$_2$/mgNH$_4$),

- k_{520}: kinetics of nitrification at 20°C (d^{-1}),

- F_{POR}: deposition flux of non-algal organic phosphorus (g/m^2/s) = W$_{POR}$.[POR], with W$_{POR}$ the sedimentation velocity of non-algal organic phosphorus (m/s),

- F_{NOR}: deposition flux of non-algal organic nitrogen (g/m^2/s) = W$_{NOR}$.[NOR], with W$_{NOR}$ the sedimentation velocity of non-algal organic nitrogen (m/s),

- Rn: proportion of nitrogen assimilated in the form of NH$_4$ = $\frac{[NH_4]}{[NH_4] + [NO_3]}$.

4.4 Organic load

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

- k_{120}: kinetic degradation constant for the organic load at 20°C (d^{-1}),

- g_3: effect of temperature on the degradation of organic load = $(1.047)^{T-20}$, where T is the water temperature (°C) (valid for 5°C $< T <$ 25°C),

- F_{LOR}: deposition flux of the organic load (g/m²/s) = $W_{LOR}.[L]$, with W_{LOR} the sedimentation velocity of the organic load (m/s).

4.5 Dissolved oxygen

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

- f: oxygen quantity produced by photosynthesis (mgO$_2$/μgChlA),

- BEN: benthic oxygen demand (gO$_2$/m²/d) (cf. O$_2$ model),

- k_2: coefficient of water-atmosphere gaseous exchange, also called reaeration coefficient, at 20°C (d^{-1}). It can be provided by the user or calculated using formulae in the literature (cf. O$_2$ module),

- g_4: effect of temperature on natural reaeration = $(1.025)^{T-20}$, where T is the water temperature (°C) (valid for 5°C $< T <$ 25°C),

- C_s: concentration of oxygen saturation in water (mgO$_2$/l). It can be determined from the water temperature (cf. O$_2$ module).

4.6 Solved equations in 2D

The EUTRO model equations are described below:

Tracer #1: phytoplankton biomass

$$F([PHY]) = (CP - DP)[PHY]. \tag{4.4}$$

Tracer #2: assimilable mineral phosphorus

$$F([PO_4]) = fp(dtpDP - CP)[PHY] + k_{320}g_2[POR]. \tag{4.5}$$

Tracer #3: non-assimilable phosphorus

$$F([POR]) = fp(1 - dtp)DP[PHY] - k_{320}g_2[POR] - \frac{F_{POR}}{h}. \tag{4.6}$$

Tracer #4: assimilable mineral nitrogen

$$F([NO_3]) = -fn(1 - Rn)CP[PHY] + k_{520}g_2[NH_4]. \tag{4.7}$$

Tracer #5: non-assimilable nitrogen

$$F([NOR]) = fn(1 - dtn)DP[PHY] - k_{620}g_2[NOR] - \frac{F_{NOR}}{h}. \tag{4.8}$$

Tracer #6: ammonia load

$$F([NH_4]) = fn(dtnDP - RnCP)[PHY] + k_{620}g_2[NOR] - k_{520}g_2[NH_4]. \qquad (4.9)$$

Tracer #7: organic load

$$F([L]) = f.MP[PHY] - k_{120}g_3[L] - \frac{F_{LOR}}{h}. \qquad (4.10)$$

Tracer #8: dissolved oxygen

$$F([O_2]) = f(CP - RP.g_1)[PHY] - nk_{520}g_2[NH_4] - k_{120}g_3[L] + k_2g_4(C_s - [O_2]) - \frac{BEN}{h}. \qquad (4.11)$$

Using the terminology and notations of section 1 and setting C_1 = [PHY], C_2 = [PO$_4$], C_3 = [POR], C_4 = [NO$_3$], C_5 = [NOR], C_6 = [NH$_4$], C_7 = [L], and C_8 = [O$_2$], matrices (8 × 8) $[\lambda]$ and $[\mu]$ are written as (only non-zero terms are mentioned):

$$\lambda_i^j = \frac{1}{86400} \begin{pmatrix} CP - DP & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ fp(dtpDP - CP) & 0 & k_{320}g_2 & 0 & 0 & 0 & 0 & 0 \\ fp(1 - dtp)DP & 0 & -k_{320}g_2 & 0 & 0 & 0 & 0 & 0 \\ -fn(1 - Rn)CP & 0 & 0 & 0 & 0 & k_{520}g_2 & 0 & 0 \\ fn(1 - dtn)DP & 0 & 0 & 0 & -k_{620}g_2 & 0 & 0 & 0 \\ fn(dtnDP - RnCP) & 0 & 0 & 0 & k_{620}g_2 & -k_{520}g_2 & 0 & 0 \\ f.MP & 0 & 0 & 0 & 0 & 0 & -k_{120}g_3 & 0 \\ f(CP - RP.g_1) & 0 & 0 & 0 & 0 & -n.k_{520}g_2 & -k_{120}g_3 & -k_2g_4 \end{pmatrix}$$

$$\mu_i^j = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -W_{POR} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -W_{NOR} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -W_{LOR} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

The only non-zero terms λ_i^0 and μ_i^0 are:

$\lambda_8^0 = \frac{k_2g_4C_s}{86400}$; $\mu_8^0 = -\frac{BEN}{86400}$.
Divisions by 86,400 are performed to scale down time to one second.

4.7 Solved equations in 3D

The EUTRO model equations are described below:

Tracer #1: phytoplankton biomass

$$F([PHY]) = (CP - DP)[PHY]. \qquad (4.12)$$

Tracer #2: assimilable mineral phosphorus

$$F([PO_4]) = fp(dtpDP - CP)[PHY] + k_{320}g_2[POR]. \quad (4.13)$$

Tracer #3: non-assimilable phosphorus

$$F([POR]) = fp(1 - dtp)DP[PHY] - k_{320}g_2[POR]. \quad (4.14)$$

Tracer #4: assimilable mineral nitrogen

$$F([NO_3]) = -fn(1 - Rn)CP[PHY] + k_{520}g_2[NH_4]. \quad (4.15)$$

Tracer #5: non-assimilable nitrogen

$$F([NOR]) = fn(1 - dtn)DP[PHY] - k_{620}g_2[NOR]. \quad (4.16)$$

Tracer #6: ammonia load

$$F([NH_4]) = fn(dtnDP - RnCP)[PHY] + k_{620}g_2[NOR] - k_{520}g_2[NH_4]. \quad (4.17)$$

Tracer #7: organic load

$$F([L]) = f.MP[PHY] - k_{120}g_3[L]. \quad (4.18)$$

Tracer #8: dissolved oxygen

$$F([O_2]) = f(CP - RP.g_1)[PHY] - nk_{520}g_2[NH_4] - k_{120}g_3[L] + k_2g_4(C_s - [O_2]) - \frac{BEN_T}{\Delta z}. \quad (4.19)$$

with Δz half height of the bottom layer cells.

Using the terminology and notations of section 1 and setting $C_1 = [PHY]$, $C_2 = [PO_4]$, $C_3 = [POR]$, $C_4 = [NO_3]$, $C_5 = [NOR]$, $C_6 = [NH_4]$, $C_7 = [L]$, and $C_8 = [O_2]$, matrices (8×8) $[\lambda]$ and $[\mu]$ are written as (only non-zero terms are mentioned):

$$\lambda_i^j = \frac{\begin{pmatrix} CP - DP & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ fp(dtpDP - CP) & 0 & k_{320}g_2 & 0 & 0 & 0 & 0 & 0 \\ fp(1 - dtp)DP & 0 & -k_{320}g_2 & 0 & 0 & 0 & 0 & 0 \\ -fn(1 - Rn)CP & 0 & 0 & 0 & 0 & k_{520}g_2 & 0 & 0 \\ fn(1 - dtn)DP & 0 & 0 & 0 & -k_{620}g_2 & 0 & 0 & 0 \\ fn(dtnDP - RnCP) & 0 & 0 & 0 & k_{620}g_2 & -k_{520}g_2 & 0 & 0 \\ f.MP & 0 & 0 & 0 & 0 & 0 & -k_{120}g_3 & 0 \\ f(CP - RP.g_1) & 0 & 0 & 0 & 0 & -n.k_{520}g_2 & -k_{120}g_3 & -k_2g_4 \end{pmatrix}}{86400}$$

$$\mu_i^j = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

The only non-zero terms λ_i^0 and μ_i^0 are:

$\lambda_8^0 = \frac{k_2 g_4 C_s - BEN/\Delta z}{86400}$; $\mu_8^0 = 0$.

Divisions by 86,400 are performed to scale down time to one second.

> **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*.

5. 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. 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.

5.1 Suspended matter

5.1.1 Description of phenomena

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 [16] and Partheniades [18].

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. It is then assumed that the SPM settles at a constant velocity w (known as the settling velocity or velocity of sedimentation),

- re-suspension occurs when a threshold τ_r, known as the critical shear stress for re-suspension, is exceeded. Its importance is weighted by a constant e, the rate of erosion characteristic of deposited SPM (also known as the Partheniades constant).

5.1.2 Equations

These phenomena translate into the following expressions of deposition flux (*SED*) and erosion (*RS*), in kg/m^2/s:

$$SED = \begin{cases} wSS\left(1 - \frac{\tau_b}{\tau_s}\right) & \text{if} \quad \tau_b < \tau_s \\ 0 & \text{if} \quad \tau_b \geq \tau_s \end{cases} \tag{5.1}$$

$$RS = \begin{cases} e\left(\frac{\tau_b}{\tau_r} - 1\right) & \text{if} \quad \tau_b > \tau_r \\ 0 & \text{if} \quad \tau_b \leq \tau_r \end{cases} \tag{5.2}$$

The bottom shear stress τ_b (in Pa) is given by $\tau_b = \frac{1}{2}\rho C_f U^2$, with C_f = the friction coefficient and U^2 the square of the velocity.

The equations of the evolution of SPM tracers (variable *SS*) and bottom sediments (variable *SF*) are as follows:

Tracer #1: suspended particulate matter

$$F(SS) = \frac{RS - SED}{h}. \tag{5.3}$$

Tracer #2: bottom sediments (tracer neither advected nor diffused)

$$\frac{\partial(SF)}{\partial t} = SED - RS. \tag{5.4}$$

The model relating to SPM has four parameters: the velocity of sedimentation w, the erosion rate e, the critical shear stress for deposition τ_s and the critical shear stress for erosion τ_r.

5.2 Micropollutants

5.2.1 Description of phenomena

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 [4]. In the case of direct adsorption, the reaction can be represented in the form of the following formula:

$$R^* + \cdot - S \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} R - S^*$$
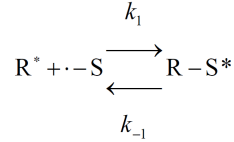
with R* = micropollutant in dissolved form, − S = surface site associated with SPM, R–S* = adsorbed micropollutant.

It is a reversible reaction, controlled by adsorption (k_1 in l/g/s) and desorption velocities (k_{-1} in 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 (in l/g):

$$K_d = \frac{[R - S^*]}{[R^*]} = \frac{k_1}{k_{-1}}, \tag{5.5}$$

where [R*] is the activity (or concentration of micropollutant) in dissolved phase (in Bq/m^3 or kg/m^3), [R-S*] is the activity (or concentration of micropollutant) associated to SPM (in Bq/kg or kg/kg).

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 (expressed in s^{-1}).

5.2.2 Two-step reversible model

One option allows the user to consider a two successive-step reversible model. In this case, a second reaction of 2nd order introducing a slowly reversible site is considered [5].

This new reaction can be represented by the following formula:

$$R - S^* + \cdot - S_2 \underset{k_{-2}}{\overset{k_2}{\rightleftharpoons}} R - S_2 + \cdot - S$$
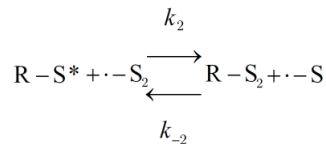
with R–S$_2$ = adsorbed micropollutant bound to slowly reversible sites −S$_2$ of the suspended particle.

It is a reversible reaction, controlled by adsorption (k_2 in s^{-1}) and desorption velocities (k_{-2} in s^{-1}). It leads to an equilibrium state, and then a distribution of micropollutants between the "non specific" and "specific" sites described by the distribution coefficient K_{d2}:

$$K_{d2} = \frac{[R-S_2]}{[R-S^*]} = \frac{k_2}{k_{-2}}, \tag{5.6}$$

where [R-S_2] is the activity (or concentration of micropollutant) in the internal "specific" sites (in Bq/kg or kg/kg), [R-S^*] is the activity (or concentration of micropollutant) associated to SPM surfacic "non specific" sites (in Bq/kg or kg/kg).

5.2.3 Equations

The system includes an equation for each micropollutant phase, namely 3 tracers:

- C: concentration of micropollutants in water (Bq/m^3),

- C_s: concentration of micropollutants adsorbed by SPM (Bq/kg) (dry weight),

- C_f: concentration of micropollutants adsorbed by bottom sediments (Bq/kg).

Note: The unit of concentration chosen for the demonstration is Bq/m^3, but it could also be written in kg/m^3 (for example, in the case of a metal).

The internal sources of each of these tracers correspond to the phenomena of adsorption/desorption, deposition/re-suspension and exponential decay. Taking these phenomena into account leads to the following equations in each of the three compartments, water, SPM and bottom sediments (with section 1 notations):

- dissolution phase

$$F(C) = -k_{-1}.SS(K_d.C - C_s) - L.C, \tag{5.7}$$

- adsorption by suspended particulate matter phase

$$F(SS.C_s) = k_{-1}.SS(K_d.C - C_s) + \frac{RS.C_f - SED.C_s}{h} - L.SS.C_s, \tag{5.8}$$

- adsorption by bottom sediments (tracer neither advected nor diffused)

$$\frac{\partial(SF.C_f)}{\partial t} = SED.C_s - RS.C_f - L.SF.C_f. \tag{5.9}$$

Setting the new variables as: $C_{ss} = SS.C_s$, in Bq/m^3 of water, $C_{ff} = SF.C_f$, in Bq/m^2 of bottom sediments, and $SEDP = \frac{SED}{SS} = w\left(1 - \frac{\tau_b}{\tau_s}\right)$ if $\tau_b < \tau_s$ or 0 otherwise, the equations become:

Tracer #3: dissolution phase

$$F(C) = -k_{-1}.SS.K_d.C + k_{-1}.C_{SS} - L.C. \tag{5.10}$$

Tracer #4: phase of adsorption by suspended particulate matter

$$F(C_{SS}) = k_{-1}.K_d.SS.C - k_{-1}.C_{SS} + \frac{\frac{RS}{SF}C_{ff} - SEDP.C_{SS}}{h} - L.C_{SS}. \tag{5.11}$$

Tracer #5: phase of adsorption by bottom sediments

$$\frac{\partial C_{ff}}{\partial t} = SEDP.C_{SS} - \frac{RS}{SF}C_{ff} - L.C_{ff}. \tag{5.12}$$

Terms with SF as denominator are nullified when SF is equal to 0.

Therefore, there are three parameters of the micropollutant model: the distribution coefficient at equilibrium K_d, the kinetic constant of desorption k_{-1}, and the exponential decay constant L (radioactive decay, for example). In total, the MICROPOL model includes 7 physical parameters.

5.3 Two-step reversible model equations

The system includes an equation for each micropollutant phase, namely 5 tracers:

- C: concentration of micropollutants in water (Bq/m^3),

- C_{ss1}: concentration of micropollutants adsorbed by SPM "non specific sites" (Bq/m^3),

- C_{ff1}: concentration of micropollutants adsorbed by bottom sediments "non specific sites" (Bq/m^2),

- C_{ss2}: concentration of micropollutants adsorbed by SPM "specific sites" (Bq/m^3),

- C_{ff2}: concentration of micropollutants adsorbed by bottom sediments "specific sites" (Bq/m^2).

Note: The unit of concentration chosen for the demonstration is Bq/m^3, but it could also be written in kg/m^3 (for example, in the case of a metal).

The internal sources for sediment tracers SS and SF are the same as in the previous section. Taking the two-step reversible model into account leads to the following equations for each micropollutant phases:

Tracer #3: dissolution phase

$$F(C) = -k_{-1}.SS.K_d.C + k_{-1}.C_{SS1} - L.C. \qquad (5.13)$$

Tracer #4: phase of adsorption by suspended particulate matter "non specific" sites

$$F(C_{SS1}) = k_{-1}.K_d.SS.C - k_{-1}.C_{SS1} + \frac{\frac{RS}{SF}C_{ff1} - SEDP.C_{SS1}}{h} - k_{-2}.K_{d2}.C_{SS1} + k_{-2}.C_{SS2} - L.C_{SS1}. \qquad (5.14)$$

Tracer #5: phase of adsorption by bottom sediments "non specific" sites

$$\frac{\partial C_{ff1}}{\partial t} = SEDP.C_{SS1} - \frac{RS}{SF}C_{ff1} - k_{-2}.K_{d2}.C_{ff1} + k_{-2}.C_{ff2} - L.C_{ff1}. \qquad (5.15)$$

Tracer #6: phase of adsorption by suspended particulate matter "specific" sites

$$F(C_{SS2}) = \frac{\frac{RS}{SF}C_{ff2} - SEDP.C_{SS2}}{h} + k_{-2}.K_{d2}.C_{SS1} - k_{-2}.C_{SS2} - L.C_{SS2}. \qquad (5.16)$$

Tracer #7: phase of adsorption by bottom sediments "specific" sites

$$\frac{\partial C_{ff2}}{\partial t} = SEDP.C_{SS2} - \frac{RS}{SF}C_{ff2} + k_{-2}.K_{d2}.C_{ff1} - k_{-2}.C_{ff2} - L.C_{ff2}. \qquad (5.17)$$

Terms with SF as denominator are nullified when SF is equal to 0.

Therefore, there are five parameters of the micropollutant model: the distribution coefficient at equilibrium K_d between the dissolved and particulate phase, the kinetic constant of desorption k_{-1} between the dissolved and particulate phase, the distribution coefficient at equilibrium K_{d2} between the "non specific" and "specific" sites, the kinetic constant of desorption k_{-2}, and the exponential decay constant L (radioactive decay, for example).

5.4   Solved equations

Noting $C_1 = SS$, $C_2 = SF$, $C_3 = C$, $C_4 = C_{ss}$, $C_5 = C_{ff}$, the matrices (5×5) $[\lambda]$ and $[\mu]$ are written as:

$$\lambda = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ SED - RS & 0 & 0 & 0 & 0 \\ 0 & 0 & -L - k_{-1}.SS.K_d & k_{-1} & 0 \\ 0 & 0 & k_{-1}.K_d.SS & -k_{-1} - L & 0 \\ 0 & 0 & 0 & SEDP & -\frac{RS}{SF} - L \end{pmatrix}$$

$$\mu = \begin{pmatrix} RS - SED & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -SEDP & \frac{RS}{SF} \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

Note the case where $SF = 0$: $C_{ff} = 0$, $\lambda_5^5 = -L$ and $\mu_4^5 = 0$. The only non-zero terms λ_i^0 and μ_i^0 are $\lambda_2^0 = -RS$ and $\mu_1^0 = RS$.

5.5   Solved equations (two-step reversible model)

Noting $C_1 = SS$, $C_2 = SF$, $C_3 = C$, $C_4 = C_{SS1}$, $C_5 = C_{ff1}$, $C_6 = C_{SS2}$, $C_7 = C_{ff2}$, the matrices (7×7) $[\lambda]$ and $[\mu]$ are written as:

$$\lambda = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ SED - RS & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -L - k_{-1}.SS.K_d & k_{-1} & 0 & 0 & 0 \\ 0 & 0 & k_{-1}.K_d.SS & -k_{-1} - k_{-2}.K_{d2} - L & 0 & k_{-2} & 0 \\ 0 & 0 & 0 & SEDP & -\frac{RS}{SF} - k_{-2}.K_{d2} - L & 0 & k_{-2} \\ 0 & 0 & 0 & k_{-2}.K_{d2} & 0 & -k_{-2} - L & 0 \\ 0 & 0 & 0 & 0 & k_{-2}.K_{d2} & SEDP & -\frac{RS}{SF} - k_{-2} - L \end{pmatrix}$$

$$\mu = \begin{pmatrix} RS - SED & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -SEDP & \frac{RS}{SF} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -SEDP & \frac{RS}{SF} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

6. THERMIC Module

The THERMIC module computes the water mass temperature through the conservation of energy. Only atmospheric exchanges through the free surface are taken into account, the heat exchanges with banks or bottom are neglected.

6.1 Origin of the tracer formulation: the equation of conservation of energy

The energy conservation equation is written as:

$$\frac{\partial E}{\partial t} + \boldsymbol{U} \cdot \boldsymbol{\nabla} E - \nabla \cdot (\lambda \boldsymbol{\nabla} T), = S_{vol} + \frac{S_{surf}}{h}, \tag{6.1}$$

with E = internal energy (J), λ = thermal conductivity (W.m^{-1}.$^\circ$C^{-1}), T = water temperature.

The volumic sources S_{vol} (inputs linked to tributaries or load releases, inputs through the Joule effect, etc.) are implemented by the user. The surface sources S_{surf}, which are the exchange fluxes through the free surface, are calculated by the THERMIC module.

The conservation energy is rearranged as a function of temperature T, considering that the internal energy E is:

$$E = \rho C_p T, \tag{6.2}$$

where C_p is water specific heat (J/kg$^\circ$C) and ρ (kg.m^{-3}) is the water density. Omitting S_{vol}, equation 6.1 reads as:

$$\frac{\partial T}{\partial t} + \boldsymbol{U} \cdot \boldsymbol{\nabla} T - \nabla \cdot (\alpha \boldsymbol{\nabla} T) = \frac{S_{surf}}{\rho C_p h}, \tag{6.3}$$

where $\alpha = \frac{\lambda}{\rho C_p}$ is the thermic diffusivity coefficient (m^2/s).

If turbulence is taken into account, the coefficient of turbulent diffusion (or dispersion) k is added to the diffusivity coefficient. However, it can be negected as the value is usually low. The final equation is therefore:

$$F(T) = \frac{\partial T}{\partial t} + \boldsymbol{U} \cdot \boldsymbol{\nabla} T - \nabla \cdot (k\boldsymbol{\nabla} T) = \frac{S_{surf}}{\rho C_p h}. \tag{6.4}$$

Equation 6.4 shows that the calculation of temperature T is carried out in the same way as for all other tracers, and comes down to determining the right-hand side of the equation, i.e. surface source terms.

6.2   A first simplified model of heat exchanges with the atmosphere in 3D

Two models computing water-atmosphere heat exchange are available in 3D: a linearised formula of the balance of heat exchange fluxes at the free surface that firstly described in this section and a model that computes the complete balance of exchange fluxes (which gather common formulae in 2D and 3D).

In the first model, the thermal power liberated into the atmosphere per surface unit, denoted as Φ, is assumed to be proportional to $(T - T_{air})$ where T is the water temperature on the surface and T_{air} that of air. $\Phi = A(T - T_{air})$, where A is the exchange coefficient in W/m^2/$^\circ$C.
The heat flux leaving the liquid domain is written as:

$$\Phi = -\rho C_p k \nabla T.\boldsymbol{n} = -\rho C_p k \frac{\partial T}{\partial z}, \tag{6.5}$$

with $C_p = 4180$ J/kg/$^\circ$C. Recall that k (m^{2}s^{-1}) is the molecular heat diffusion coefficient in water, $\boldsymbol{n}$ the normal vector to the surface.
By equating the two formulations, one deduces the boundary conditions:

$$k\frac{\partial T}{\partial z} = -\frac{A}{\rho C_p}(T - T_{air}). \tag{6.6}$$

The coefficient A should include phenomena such as radiation, air convection in contact with water and latent heat produced by water evaporation. Sweers [25] expresses the coefficient A, in W/m^2/$^\circ$C, according to the water temperature T and wind velocity V measured at the point under consideration (in m/s):

$$A = (4.48 + 0.049T) + 2021.5\,b\,(1 + V)\,(1.12 + 0.018\,T + 0.00158\,T^2) \tag{6.7}$$

The parameter b varies depending on the location. Its average value on the shores of the English Channel and of the Atlantic ocean is 0.0025. It is higher in the Mediterranean sea, where it reaches approximately 0.0035.

A much more elaborated model is also implemented both in 2D and 3D. This module calculates the complete balance of exchanged fluxes involved and is described in the following section.

6.3   Heat fluxes affecting the energy balance

Surface sources are fluxes through the free surface.

There are 5 fluxes, expressed in W/m^2:

- the solar radiation flux RS,

- the atmospheric radiation flux RA,

- the radiation flux from water body RE,

- the heat flux driven by convection CV,

- the heat flux driven by evaporation CE.

Every flux is detailed in [7]. The result in 2D is:

$$S_{surf} = RS + RA - RE - CV - CE. \tag{6.8}$$

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. Heat exchanges with the atmosphere are taken into account at two levels **in 3D**:

- the complete balance of exchange fluxes at the free surface is calculated at the surface boundary conditions for temperature:

$$k \left. \frac{\partial T}{\partial z} \right|_{z=\eta} = \frac{RA - RE - CE - CV}{\rho C_p}, \tag{6.9}$$

- the penetration of solar radiation into the water column is taken into account in the source term of the advection-diffusion equation of the temperature:

$$S = \frac{1}{\rho C_p} \frac{\partial Q(z, RS)}{\partial z}, \tag{6.10}$$

where the function $Q(z, RS)$ is the residual solar radiation at the elevation z.

6.3.1 Solar radiation RS

The solar radiation RS can be provided to the THERMIC module in the atmospheric data file in 2D. If there is no measurement, global solar radiation on a water body can be calculated by Perrin de Brichambaut's method, depending on the cloudiness of the sky, the date and the hour [14].

In 3D, the solar flux penetrating the water RS is calculated with:

- the solar radiation reaching the surface with a clear sky. It depends on time and the location of the site. Perrin de Brichambaut's method [20], [21] is used,

- cloud cover: a corrective term depending on the nebulosity is applied (Berliand's formulae [2], [3]),

- albedo that enables to compute the effective part of solar radiation penetrating the water.

Solar radiation RS is written as:

$$RS = AA.\sin(ang)^{BB}(1 - 0.65C^2)(1 - Alb), \tag{6.11}$$

where:

- AA (W.m^{-2}) and BB (dimensionless) are coefficients related to luminosity and sky colour. They have to be chosen with respect to the considered area. Three possibilities are suggested (see the table 6.1) but mean values are used by default in 3D,

- *ang* is the angular height of the sun (rad), which depends on the latitude and longitude of the location and changes with day and hour,

- *Alb* water albedo for short waves that may vary every month [22].

Table 6.1: Proposed values of the coefficients *AA* and *BB* for the calculation of solar radiation related to luminosity and sky colour

Type of sky	AA (W.m^{-2})	BB
Very pure sky (type 1)	1130	1.15
Mean pure sky (type 2)	1080	1.22
Industrial area (type 3)	995	1.25

The penetration of solar radiation into the water column is taken into account in the advection-diffusion equation of temperature by introducing a source term. It depends on the water turbidity and is linked to dissolved and suspended particles (mineral or organic). Two laws describing the solar radiation penetration are suggested:

- the first one consists of two exponential laws that may be difficult to calibrate and require an estimation of the degree of water turbidity,

- the second one uses the *in situ* measurements of Secchi length and is therefore recommended.

In the first case, the source term reads:

$$Q(z, RS) = RS . \left(R \exp\left(-\frac{z_s - z}{\zeta_1} \right) + (1 - R) \exp\left(-\frac{z_s - z}{\zeta_2} \right) \right), \qquad (6.12)$$

with RS (W.m^{-2}) is the solar radiation penetrating the water, z_s (m) the free surface elevation, ζ_1 and ζ_2 (m) are attenuation lengths and R is a dimensionless coefficient. This equation takes into account a selective absorption of the solar spectrum by water, separating the radiation quickly attenuated in the water column and the one penetrating deeply.

In the second case, the source term is written from Beer-Lambert's law:

$$Q(z, RS) = RS . \exp\left(-\frac{1.7(z_s - z)}{Z_s} \right) \qquad (6.13)$$

with RS (W.m^{-2}) is also the solar radiation penetration the water, z_s (m) the free surface elevation, Z_s (m) is the Secchi length provided by *in situ* measurements.
The coefficients ζ_1, ζ_2 and R are characteristics of optical properties of water adjusted to the studied water body. Examples of combination are suggested in Table 6.2. This classification has been done for coastal and marine flows and is widely used in numerical modelling.
The formulae require additional data (wind magnitude and direction, air temperature, atmospheric pressure, relative humidity, nebulosity and rainfall). The study site may not be equipped for local wind measurements, while data are available at a different location (even far from the studied site). A wind function is then used, which is a linear function with a single coefficient of calibration b:

$$f(V_2) = b(1 + V_2) \qquad (6.14)$$

with V_2 that is the wind velocity at 2 m high. As for the linearised formula (6.7), the parameter b varies depending on the location. Its average value on the shores of the English Channel and

Table 6.2: Selected values of R, ζ_1, ζ_2 according to the water turbidity ([19], [13], [15])

Type of water	R	ζ_1 (m)	ζ_2 (m)
Very clear (Kraus)	0.40	5	40
Type I (Jerlov)	0.58	0.35	23
Type IA (Jerlov)	0.62	0.6	20
Type IB (Jerlov)	0.67	1.0	17
Type II (Jerlov)	0.77	1.5	14
Very turbid - Type III (Jerlov)	0.78	1.4	7.9

of the Atlantic ocean is 0.0025. It is higher in the Mediterranean sea, reaching approximately 0.0035 and can be around 0.0017 [23].

Wind data are often provided at 10 m high whereas latent and sensible fluxes need wind velocities at 2 m high. Velocities at 2 m high need to be calculated from wind velocities at 10 m high V_{10}. A logarithmic wind velocity vertical profile is considered, with a roughness length of $z_0 = 0.0002$ m. This leads to $V_2 = 0.85V_{10}$. This value of 0.85 (or the roughness length) may be changed if needed.

$$V_2 = \frac{V_{10} \log\left(\dfrac{2}{z_0}\right)}{\log\left(\dfrac{10}{z_0}\right)} \tag{6.15}$$

6.3.2 Atmospheric radiation RA

The atmosphere emits a long wave radiation corresponding to the reemission of a part of direct solar energy. It emits like a black body.

In 2D, the atmospheric radiation RA is estimated through meteorological data collected at ground level. Some processes of energy exchange (exchanges of heat with the bottom, and of water with the water table, biodegradation reactions, industrial or urban effluents) are unknown or poorly known. They considerably depend on temperature. In the 2D calculation, they are combined with atmospheric radiation through the calibration coefficient e_{air}. The formula in 2D is:

$$RA = e_{air}\sigma(T_{air} + 273.15)^4\left(1 + k\left(\frac{c}{8}\right)^2\right), \tag{6.16}$$

with:

- e_{air} = calibration coefficient of atmospheric radiation (1st parameter of the model),

- σ = Stefan-Boltzman constant, $\sigma = 5.67.10^{-8}$ Wm^{-2}K^{-4},

- T_{air} = air temperature (°C),

- c = cloudiness (octas), given in the atmospheric data file (WARNING: in KHIONE, it is given in tenths),

- k = coefficient of cloud type, which depends on the type of clouds and their height (see Table 6.3).

To simplify calculations, an average value of $k = 0.2$ is usually taken in 2D.

Table 6.3: Coefficient k for the calculation of atmospheric radiation

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

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

$$RA = (1 - alb_{lw})e_{air}\sigma(T_{air} + 273.15)^4 \left(1 + k.\left(\frac{C}{8}\right)^2\right), \qquad (6.17)$$

where:

- alb_{lw} = 0.03 is the water albedo for long radiative waves (common value used in the literature [12], [11]), (1-alb_{lw}) is a calibrating coefficient of atmospheric radiation,

- e_{air} is the air emissivity ($= 0.937.10^{-5}(T_{air} + 273.15)^2$ if using Swinbank formula, default option),

- $\sigma = 5.67.10^{-8}$ 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], [12] but other choices are possible (see the table 6.3).

When coupling WAQTEL with TELEMAC-3D, the formula to compute air emissivity e_{air} times the factor depending on cloud cover C can be chosen:

- 1: Idso and Jackson (1969),

- 2: Swinbank (1963),

- 3: Brutsaert (1975),

- 4: Yajima Tono Dam (2014).

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

6.3.3 Radiation emitted from a water body RE

One can assume, as a good approximation, that a water body behaves like a grey body. The expression of radiation emitted by the water body RE (also called water radiation) is then:

$$RE = e_{water}\sigma(T_{water} + 273.15)^4, \qquad (6.18)$$

with T_{water} = water temperature (°C) taken at the surface in 3D, e_{water} = water emissivity which can be seen as a calibration coefficient of radiation from a water body, which depends on the

location and obstacles surrounding the water body. For a narrow river bordered by trees, e_{water} could be around 0.97 (which is the default value) and for a widely uncovered area, e_{water} could be close to 0.92.

6.3.4 Convection heat flux CV

This flux (also called sensitive heat flux) is estimated by the following empirical formula:

$$CV = \rho_{air}C_{p_{air}}f(V)(T_{water} - T_{air}), \qquad (6.19)$$

with:

- ρ_{air} = air density (kg/m^3), given by $\rho_{air} = \frac{100P_{atm}}{(T_{air}+273.15).287}$, where P_{atm} is the atmospheric pressure in hPa,

- $C_{p_{air}}$ = air thermic capacity (J/kg°C),

- $f(V)$ 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 = wind velocity (m/s),

- a, b = empirical coefficients to be calibrated (2 in 2D and 3D, only a in 3D if one single calibrating coefficient). Their values are very close, around 0.0025.

6.3.5 Evaporative heat flux CE

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

$$CE = L(T_{water})\rho_{air}f(V)(H^{sat} - H), \qquad (6.20)$$

with:

- $L(T_{water}) = 2500900 - 2365T_{water}$ = latent heat of evaporation (J/kg) taken at the surface in 3D,

- $f(V)$ 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 = wind velocity (m/s),

- $H^{sat} = \frac{0.622P_{vap}^{sat}}{P_{atm}-0.378P_{vap}^{sat}}$ = the saturated air specific humidity (kg/kg), in 3D at the surface temperature,

- $H = \frac{0.622P_{vap}}{P_{atm}-0.378P_{vap}}$ = the air specific humidity (kg/kg),

- P_{vap} the partial pressure of air water vapor (hPa) provided in the atmospheric data file in 2D and calculated with the following formula in 3D: $P_{vap} = \frac{H_{rel}}{100}P_{air}$,

- P_{vap}^{sat} the partial pressure of saturation water vapor (hPa) calculated by Magnus-Tetens's formula:

$$P_{sat}^{vap} = 6.11 \exp\left(\frac{17.27 T_{water}}{T_{water} + 237.3}\right) = \exp\left(2.3026\left(\frac{7.5 T_{water}}{T_{water} + 237.3} + 0.7858\right)\right). \quad (6.21)$$

When $H_{sat} < H$, the atmospheric radiation RA is corrected by multiplying the preceding expression by 1.8 in 2D.

The surface evaporation flow rate is then calculated in 3D by:

$$Deb = \frac{CE}{\rho_{water} L(T_{water})}, \quad (6.22)$$

6.4   Solved equation

The global surface source reads as:

$$S_{surf} = RS + RA - RE - CV - CE. \quad (6.23)$$

In the calculations, the global surface source S_{surf} is treated explicitly and the (λ_i^j, μ_i^j) are all equal to zero.

The following equation is explicitly solved:

$$F(T) = \frac{S_{surf}}{\rho C_p h}. \quad (6.24)$$

7. 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

8. 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 $\frac{2.3}{T_{90}}$:

$$F([C]) = -\frac{2.3}{T_{90}}[C], \qquad (8.1)$$

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):

$$F([C]) = -k_1[C], \qquad (8.2)$$

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}).

9. Conclusion

WAQTEL simulates the transport of several tracers in a river or the sea (by resolution of the advection-diffusion equation) possibly coupled (*via* source terms of the equation). WAQTEL offers a structure that allows programming further water quality modules.

This technical manual first shows the method of resolving the convection-dispersion equation and its application to water quality.

The water quality modules available in the WAQTEL tool library are described, namely:

- O2: a simplified module for dissolved oxygen,

- BIOMASS: a module for phytoplankton biomass,

- EUTRO: a module for river eutrophication (dissolved oxygen and algal biomass),

- MICROPOL: a module for heavy metals or radioelements, taking into account their interaction with fine sediments (suspended particulate matter),

- THERMIC: a module for water temperature evolution under the influence of atmospheric fluxes,

- AED2: the water quality and aquatic ecology model,

- a degradation law.

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