GESCAL MODEL FOR WATER QUALITY SIMULATION IN WATER RESOURCE SYSTEMS

User Manual
Version 2.0

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1. INTRODUCTION.

The GESCAL program is a tool for water quality modelling at river basin scale. It has been implemented on AQUATOOL Decision Support System (Andreu et al., 1996) and in its new AquaToolDMA version (Solera et al., 2007) for water resources planning and management. In this way the joint application will allow modelling water management and quality in water resource systems with a single tool.

This module does not attempt to represent the evolution of water quality against specific events, but rather to reflect the temporal evolution of water quality in the modelled systems, resulting from different alternatives of management, purification, pollution and use of the resource.

The program allows the modelling of conventional pollutants with a double objective: on the one hand, simplicity is sought when modelling in a consistent way with the work scale and on the other hand, we try not to lose representativeness or modelling capacity.

This document aims to serve as a technical manual for users of the GESCAL program. Some of the data for the program are obtained from the water resource management simulation model SIMGES (Andreu et al., 2007). Because of this, it is necessary to know the basic management of the SIMGES program prior to the use of GESCAL.

Although the program allows the modelling of water quality, in complex water resource systems, it is very interesting to apply it on a small scale, such as specific river sections or single reservoir analysis. This is due to the complete consideration of processes that is carried out in its formulation.

This document is structured as follows:

- First, a brief description of the SIMGES program (Andreu et al., 2007) and the available elements for the creation of water resources systems management models.
- Secondly, the formulation of the GESCAL model is developed for the different elements and the different pollutants considered.
- The fourth chapter contains the description of the data files
- The following chapter contains the description of the results files.
- The sixth chapter explains possible error messages.
- Finally the last chapter contains specifications on the installation of the model.

2. DESCRIPTION OF THE SIMGES MODULE AND ITS ELEMENTS.

The SIMGES model is a general model for the Simulation of River Basin Management within the AQUATOOL Decision Support System (SSD). AQUATOOL has been developed for more than a decade by the Water Resources Engineering Group of the Technical University of Valencia. This SSD is composed by a series of tools that allow the modelling of water resource systems at all levels such as optimization, simulation, modelling of water quality, economic aspects, groundwater and hydrology, among others.

The SIMGES model allows the modelling of complex hydraulic resource systems, in which elements related to surface and underground regulation, storage, collection, transport, use and/or consumption and artificial recharge devices are available.

The model supports any configuration within the limits imposed only by hardware capabilities, and therefore it is usable for any hydraulic resource scheme.

The simulation is performed monthly and it reproduces the flow of water through the system at the spatial scale detailed by the user. For surface subsystems flow is simply calculated by continuity or balance, while for underground subsystems or aquifers flow is simulated by cell, single or multicellular models, as appropriate, or even by distributed models of linear flow. Evaporation and filtration losses in reservoirs and channels, as well as the relationships between surface water and groundwater, are also taken into account in the simulation.

The management of the hydraulic resources is carried out by means of operation rules tending to maintain a similar level of filling in the reservoirs from a zoned reservoir curves. These curves are the exploitation rules itself and they are supplied by the user of the model. The definition of minimum ecological flows, as well as different user priorities for water use, is allowed.

The simulation and management of the surface system are done by the use of a conservative flow network optimization algorithm. This algorithm is responsible for determining the flow in the system, trying to satisfy the multiple goals of minimization of deficits and of maximum adaptation to the reservoir target volumes curves and hydropower production targets.

The definition of type elements, which are combined by the user in different ways, allows the adaptation of the model to any scheme. The elements considered are:

- **Reservoirs** (surface). They are defined by their physical parameters, their management parameters (maximum volumes, target volumes, and storage priority in relation to other reservoirs).

- **Intermediate streamflows**. They are considered as inflows to the system.

- **Channels**. It is contemplated under the same denomination to the river reaches, channels, and any other connection that is convenient to establish. They are defined by their physical parameters (including maximum capacities), and by their possible minimum (usually ecological) flows. In this group of waterworks there are five types:

    - **Type 1**: They basically respond to the definition of the previous paragraph.

    - **Type 2**: They consider losses by filtration in the riverbed.

    - **Type 3**: They contemplate a hydraulic connection between the river and an underlying aquifer, and therefore the flow from the aquifer to the river and vice versa, depending on the state of the aquifer.

    - **Type 4**: They correspond to the definition of type 1 with instantaneous maximum flow rate, depending on the difference in height between the input and the output of the channel. If there is a reservoir is at its origin or end, the variation in height is considered in order to determine the maximum that can circulate throughout the month.

    - **Type 5**: These are hydraulic connections between nodes and/or reservoirs, for which the flow rate is a function of the difference in height between their ends. The circulation of water can take place in both directions and it is considered the variation in height that can be had in the reservoirs throughout the month.

- **Consumptive demands**. They are those elements that use water and in which part of it is consumed and therefore it is lost to the system. This includes both irrigated areas as well as urban and industrial demands. They are defined by their demand curve, their consumption parameters, their intakes and their connection with some return element. Supplying the same demand from different sources is supported.

- **Return elements**. They are simply definitions of points of reinstatement of water to the system coming from consumptive demands.

- **Non-consumptive demands** (hydroelectric plants). They are those elements that use water without consuming it. They are defined by their physical and production data and by their target monthly flow to be used.

- **Artificial recharge**. They are elements whose flow is going to recharge aquifers, using for that purpose the overhangs. They are defined by their physical features.

- **Additional pumping facilities**. They are elements of abstraction of water from aquifers that is incorporated into the surface system for use in a different place than the area where the pumping takes place.

- **Aquifers**. They are defined by their physical parameters and by means of operating parameters, which, once exceeded, cancel the extractions. The model allows contemplating several types of aquifers:

  - Reservoir type.

  - Single-celled aquifer.

  - Aquifer with discharge through a spring.

  - Aquifer connected to a surface stream and with distributed modelling by the eigenvalues method.

  - Rectangular, homogeneous aquifer connected to a fully penetrating river on one of its sides.

  - Rectangular, homogeneous aquifer connected to two fully penetrating rivers, one perpendicular to the other.

  - Aquifer with drainage at three different levels: it is a simplified model that allows considering the connection with two different levels of surface streams and the variable evapotranspiration throughout the year.

For a more detailed description of these elements or the operation of the program, the reader is referred to the technical manual of the SIMGES model.

3. MODEL FORMULATION.

The GESCAL tool allows the development of water quality models on simulation models of water resource systems previously developed with the SIMGES module. Although water quality has been considered in all possible elements of simulation modelling, the modelling of physicochemical and biological processes affecting quality is considered exclusively in the elements of river reaches (or channels) and reservoirs (or lakes). The main feature of this tool is the possibility of modelling both reservoirs and river reaches in the same application and in an integrated way with the rest of the elements of the system. Thus, quality in a river reach or in a reservoir not only depends on the processes that are produced but also on the management of the system and the quality of the different elements linked to the element in question. The constituents that can be modelled are the following:

- - Temperature.

- - Arbitrary pollutants.

- - Dissolved Oxygen and Carbonaceous Organic Matter (COM).

- - Nitrogen cycle: organic nitrogen, ammonium and nitrates. And its effects on dissolved oxygen.

- - Eutrophication: nitrogen cycle, phytoplankton (such as chlorophyll-organic and inorganic phosphorus, and its effect on dissolved oxygen).

Next chapter is structured in two parts according to the elements and processes. The first one explains how the quality modelling has been considered in the different elements of the river basin. There are three sections: river reaches, reservoirs and other elements. The second part describes the processes that are taken into account for each of the constituents that can be modelled.

3.1. CHANNEL MODELLING.

The channel element conceived in the SIMGES simulation model is used to model any watercourse, either a river reach, a canal or any other type of conduction. In the GESCAL program, the river reach is modelled as follows:

- It is considered unidimensional with homogeneity of concentrations on both the vertical and transverse axis.

- Stationary state: For each month, the steady-state conditions of water quality that would reach the river reach are estimated considering that the conditions remain constant within that time interval.

- The processes of advection and dispersion are considered.

- The modelling of the river reaches also takes into account the possible hydraulic relation with the aquifers, either by loses to or gains from the aquifer.

- The introduction of elements of diffuse pollution is allowed.

- Hydraulic parameters are estimated either by power relations or Manning equations assuming trapezoidal section.

- Point loads are considered at nodes.
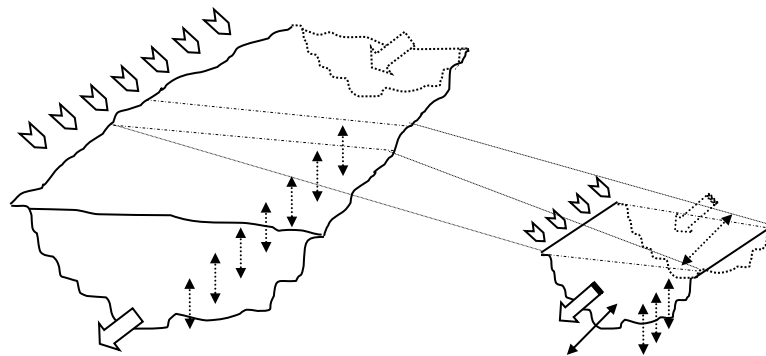
Figure 1. Modelling scheme for channels.

3.1.1. General formulation for channels.

Independently of the constituent that is being modelled the differential equation that is solved to simulate the evolution of the quality of the water in the river reach is the same and it is defined by the following mass balance:

$$0 = \frac{d}{dx}\left(E\frac{dC}{dx}\right) - \frac{d(uC)}{dx} + \frac{S_d + C_e q_e - C q_s + \sum W_i}{V} \qquad (1)$$

Where: E represents the dispersion (m^{2}day^{-1}); C the concentration of the constituent (mg/l); C_e the concentration of the constituent in the aquifer to which the river is connected (mg/l); x the distance along the length of the river reach (m); u speed (m day^{-1}); V the volume of the mass of water (m^3); q_e is the flow that the aquifer brings (m^{3}day^{-1}); q_s the possible flow filtered to the aquifer (m^{3}day^{-1}); S_d the amount of

mass diffusely contributed to the river reach (g/day). ΣWi (M) represents the set of processes that eliminate or contribute matter to the element. This term depends on the constituent that is being modelled and it is explained for each case later.

3.1.2. River hydraulics.

Under the hypothesis of unidimensionality in rivers it is required to establish a hydraulic model that relates the flow rates with the speed, depth and width of the river. Two methods are available for the establishment of this relationship. The first, developed by Leopold and Maddock (1953), establishes power relation between the different hydraulic variables and flow:

$$u = \alpha_1 Q^{\beta_1} \qquad (2)$$

$$h = \alpha_2 Q^{\beta_2} \qquad (3)$$

$$b = \alpha_3 Q^{\beta_3} \qquad (4)$$

Where u represents the velocity (ms^{-1}); Q is the flow rate (m^{3}s^{-1}); h is the depth (m); b the width of the river (m). The coefficients α_1, β_1, α_2, β_2, α_3 and β_3 are parameters that are established empirically and that they must comply by continuity:

$$\beta_1 + \beta_2 + \beta_3 = 1 \qquad (5) \qquad \text{and} \qquad \alpha_1 \cdot \alpha_2 \cdot \alpha_3 = 1 \qquad (6)$$

The following table shows typical values in the literature.

Exponent	Typical Value	Range
β_1	0.43	0.4-0.6
β_2	0.45	0.3-0.5

Table 1. Typical values for hydraulic coefficients.

The second method implemented in the program is the hydraulic calculation by Manning's formula:

$$u = \frac{R_h^{2/3} I^{1/2}}{n} \qquad (7)$$

Where: R_h (m) represents the hydraulic radius obtained as the quotient between the wet area and the wet perimeter. I (m/m) represents the slope of the channel and n is the Manning or roughness number. The velocity is obtained in ms-1.

When considering a trapezoidal section, the previous equation is the following:

$$u = \frac{\left(\dfrac{b_o y + s y^2}{b_o + 2y\sqrt{s^2+1}} \right)^{2/3} I^{1/2}}{n} \quad (8)$$

Where: bo represents the bottom width of the river (m). "s" is the lateral slope (m/m). "y" represents the flow depth (m); "n" is the Manning coefficient.

The resolution of the Manning equation goes by applying a numerical resolution method by successive iteration. Due to the possible relations of the river reaches with the aquifers, the flow does not have to be the same along the reach. Therefore, assuming that the flow losses or gains are uniform along the stretch, the hydraulic ratios are solved for each of the "segments" or differentials in which the section is divided for the calculation.

On the other hand, it is possible to emphasize that the choice of one method or another is not global for all the river reaches allowing applying a method or another of discretionary.

3.1.3. Longitudinal dispersion.

The longitudinal dispersion values for each river section can be entered directly by the user or calculated through the expression established by Fischer et. al. (1979):

$$E = 0.011 \frac{u^2 b^2}{h u^*} \quad (9)$$

Where u^* is the gravitational velocity (ms^{-1}) calculated as:

$$u^* = \sqrt{ghs} \quad (10)$$

Where g is the gravitational acceleration (ms^{-2}) and s is the slope of the channel.

This option can only be used if the river section is modelled by the Manning method.

Another option included in the program is the estuaries dispersion calculation, a formula to obtain approximated values is defined by Thomman (1987):

$$E = \frac{uL}{\ln\left(s_2/s_1\right)} \quad (11)$$

Where: L is the length of the reach (m), s_2 and s_1 the salinity at the end and at the beginning of the reach.

3.1.4. Particular cases.

In this section we collect some situations where the concentrations of the different constituents modelled are not estimated by solving the developed differential equations. These situations are as follows:

- Null initial and final flow in a river reach. This is the case of a dry river, where it is assumed that concentrations along the entire reach of river are zero.

- Not null initial flow and null final flow. This is the case of a river that due to leaks in it is dried along its length. In this case, like the previous one, zero concentrations are considered in the whole reach.

- Null initial flow and not null final flow. This is the case where the river stretch does not reach resource from upstream elements but, by being connected with the aquifer, it gains volume of water along its length. For this case it is considered that the concentrations of the river are equal to those of the contributing aquifer.

3.2. RESERVOIR MODELLING.

The GESCAL program allows the modelling of water quality in reservoirs with the following features:

- It has been conceived the possibility of modelling them in two layers representing the epilimnion and the hypolimnion or as a single element of complete mixture. This consideration can be variable depending on the month of simulation.

- In the reservoirs, the quota of the thermocline and the distribution of inflows and outflows between the two layers are established, on a monthly variable basis. In addition, the program automatically estimates if the volume is not enough for the thermal stratification to occur and then it eliminates it.

- When modelling stratified, diffusion between the two layers is considered.

- Due to the variability of the volume of the reservoirs over time, a dynamic estimation of the quality is made.

- It also includes, for all pollutants, the possibility of introducing flows of constituents from the sediment. This allows modelling the demands of dissolved oxygen from the sediment and nutrient supply, among others.
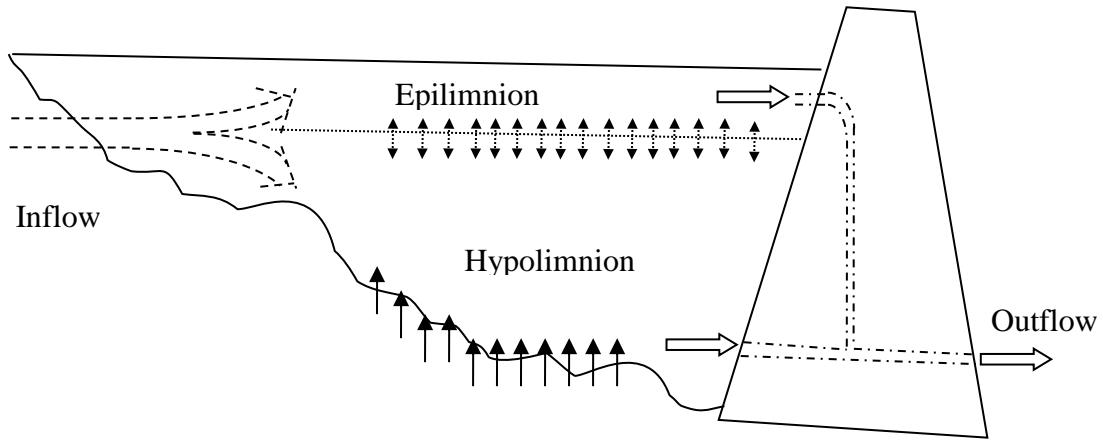
Figure 2. Modelling scheme for reservoirs.

3.2.1. General formulation for reservoirs.

The estimation of the concentrations of each constituent passes through the resolution of a system of differential equations that is common to all constituents except a summing. This system of differential equations is as follows:

$$V_1 \frac{dC_1}{dt} + C_1 \frac{dV_1}{dt} + C_{1/2} \frac{dV}{dt} = Q_{1e}C_e - Q_{1s}C_1 + E'_{12}(C_2 - C_1) + \sum W_i \qquad (12)$$

$$V_2 \frac{dC_2}{dt} + C_2 \frac{dV_2}{dt} - C_{1/2} \frac{dV}{dt} = Q_{2e}C_e - Q_{2s}C_2 + E'_{12}(C_1 - C_2) + Sed + \sum W_{i2} \qquad (13)$$

Where: The subscript "1" represents the epilimnion or upper layer; the subindex "2" the hypolimnion or lower layer; V_1 and V_2 are the volumes of the layers (m^3); V is the volume gained or lost (if negative) of the epilimnion over the hypolimnion due to heating or cooling over the month (m^3); C_1 and C_2 are concentrations of each layer (M/V); $C_{1/2}$ is the hypolimnion concentration if the volume increase is negative and the epilimnion if it is positive (mgl^{-1}); C_e is the concentration of the inflows (mgl^{-1}); t represents the time variable; Q_{1e} and Q_{2e} are the inflows in the time interval (m^3t^{-1}); Q_{1s} and Q_{2s} are the outflows in the time interval (m^3t^{-1}); Sed is the flow of constituent from the sediment (M/T); W_{i1} and W_{i2} are the set of processes of degradation or contribution of constituent in the mass of water. E'_{12} represents the dispersion coefficient between the two layers (m^3t^{-1}), which is estimated as follows:

$$E'_{12} = \frac{E_{12}A_{12}}{Z_{12}} \qquad (14)$$

Where: E_{12} represents vertical diffusion (m^2t^{-1}); A_{12} is the area between the two layers (m^2); Z_{12} is the height of the thermocline (m).

For the case of a modelling as a single fully mixed cell the equation to be solved is the following:

$$V_1 \frac{dC_1}{dt} + C_1 \frac{dV_1}{dt} = Q_{1e}C_e - Q_{1s}C_1 + \sum W_i \qquad (15)$$

3.3 WATER QUALITY IN THE REST OF ELEMETS OF THE SYSTEM.

For the rest of elements considered the water quality has been taken into account as follows:

- In the nodes the hypothesis made is that an instantaneous mixing of the water of all the elements that converge to that node takes place: streamflows, channels, returns, hydroelectric plants, punctual loads, among others. Therefore, a mass balance of all the inflows is done, obtaining the outflow concentration according to the following expression:

$$C_s = \frac{\sum_{i=1}^{n} C_i \cdot Q_i}{\sum_{i=1}^{n} Q_i} \qquad (16)$$

Where Qi is the inflow of each element "i", which arrives at the node; Ci is the constituent concentration at the end of the input element "i"; "n" is the number of elements whose final destination is that node.

- The quality of the different streamflows is an input to the model. A series of concentrations are introduced per constituent to be modelled and with the same length as the series of streamflows modelled in the management.

- The quality of the water that reaches each demand is estimated by mixing the quality of the water from all the intakes that supply the demand.

- The quality of the water entering to an intake corresponds to the water quality of the node where the intake is connected. The outflow quality can be the same or a constant outflow quality that can be defined by some processes of treatment or contamination that takes place in it.

- The same possibility is offered for the returns. The quality of the returned water can be estimated by mass balance between the different intakes that return to that element or a defined concentration that represents some processes of variation of the quality in the return.

- It is assumed that hydroelectric plants do not make any changes in the water quality.

-Finally it is assumed that the water quality of aquifers remains constant and it is defined as an input data for the model.

Below there is a summary table with the processes that are considered according to the different elements.

Element	Processes
River reaches	Physics: Advection and longitudinal dispersion Chemical and biological: Depending on the constituent modelled.
Reservoirs	Physical: Complete mixture or stratification in two layers. Chemical and biological: Depending on the constituent modelled.
Streamflows	The time series of inflow concentration of each of the constituents modelled are entered as input data.
Nodes	A complete mixture is assumed in the node. The outflow concentration of the node is estimated by mass balance.
Demands	It is assumed that the quality of the water that arrives at a demand is a product of the mixture of the quality of the water at the exit of each one of its takes.
Intakes	Outflow concentrations of an intake are the same as those of the origin of the intake or they can be entered as input data.
Returns	Outflow concentrations of a return are obtained by balance between the different intakes related to that return or they can be entered as input data.
Hydropower Plants	Outflow concentrations are equal to those at the entry point
Aquifers	Constant concentrations provided as input data.
Additional pumping facilities	Outflow concentrations are equal to those of the aquifer from which it is pumped

Element	Processes
Artificial Recharge	They have no effect.

Table 2. Processes considered in the different elements.

3.4. CONSTITUENTS AND PROCESSES MODELLED.

As previously mentioned the constituents that can be modelled are the following: Temperature, Arbitrary Constituents, Carbonaceous Organic Matter, Dissolved Oxygen, Organic Nitrogen, Ammonia, Nitrates, Phytoplankton, Organic Phosphorus and Phosphates. As can be seen the tool has focused on the modelling of the most common constituents of surface waters including eutrophication processes.

Each of the processes for each of the constituents and their relations with the rest are explained below.

3.4.1. Temperature.

There are two widely used methods for modelling water temperature in natural systems. The first is the balance method in which a thermal balance between the atmosphere and the mass of the water is proposed. The second method is to assume a linear behaviour of the mass of water towards a state of balance.

3.4.1.1. Thermal balance approach.

Although initially the Gescal program did not include this method, the updates after the month of December 2008 include this possibility. The equations on which this method is based are the same as the matter balances but substituting concentrations (mg/l) for heat (cal/m^3). For a natural system the net energy flow can be estimated as follows:

$$\phi_{net} = J_{sw} + J_{alw} - J_{wlw} - J_e + J_c \ (17)$$

Where: ϕ_{net} is the net heat flux; J_{sw} is the short-wave radiation; J_{alw} is the long-wave atmospheric radiation; J_{wlw} is the long-wave radiation emitted by the mass of water; J_e represents the energy consumed in evaporation; J_c is the energy transmitted by convection from or to the volume of water.

All variables are expressed in Wm^{-2}. The model enables to estimate all the previous terms from the data of: air temperature, humidity, solar radiation, wind speed and cloudiness. All, with the exception of the solar radiation that is introduced as one more piece of data. Different studies develop the estimation of the previous terms, being one of the most well-known and used the one developed by Wunderlich

(TVA, 1972). The method used for the estimation of each component of the heat balance is explained below.

The long-wave radiation flow that descends from the atmosphere can be calculated using Stefan-Boltzmann's Law.

$$J_{alw} = \sigma(T_a + 273)^4 \varepsilon_{sky}(1 - R_L) \quad (18)$$

Where: J_{awl} is the long-wave atmospheric radiation and σ is the Stefan-Boltzmann constant.

$$\sigma = 11,702 \times 10^{-8} \frac{cal}{cm^2 \cdot d \cdot K^4}$$

T_a is the air temperature (°C) and RL is the long-wave refractive coefficient (dimensionless with a value of 0.03).

ε_{sky} represents the effective emissivity of the atmosphere.

$$\boldsymbol{\varepsilon_{sky} = \varepsilon_{clear}(1 + 0.17 C_L^2)} \qquad \textbf{(19)}$$

Where C_L is the fraction of the sky covered by clouds.

ε_{clear} represents the emissivity of the cloudless atmosphere. It can be estimated by the expression of Brunt (1932).

$$\boldsymbol{\varepsilon_{clear} = 0.6 + 0.031\sqrt{e_a}} \quad \textbf{(20)}$$

Finally, e_a is the vapour pressure of the air (mmHg). The vapour pressure of the air can be calculated with the following expression:

$$\boldsymbol{e_{air} = \frac{H_r e_{sat}}{100}} \quad \textbf{(21)}$$

It can also be estimated from the dew temperature.

$$\boldsymbol{e_{air}(mmHg) = 4.596 * exp\left(\frac{17.27 * T_d}{T_d + 237.3}\right)} \quad \textbf{(22)}$$

Where H_r (%) is the relative air humidity, T_d is the dew temperature and e_{sat} (mmHg) is the saturation vapour pressure of the air estimated as follows:

$$\boldsymbol{e_{sat}(mmHg) = 4.596 * exp\left(\frac{17.27 * T_a}{T_a + 237.3}\right)} \quad \textbf{(23)}$$

Where T_a is the air temperature.

The long-wave radiation emitted by the surface of water is represented by Stefan-Boltzmann's Law.

$$\boldsymbol{J_{wlw} = \sigma \epsilon (T_w + 273)^4} \quad \textbf{(24)}$$

Where: ε is the emissivity of water (0.97) since it is not a perfect emitter. And T_w is the temperature of the mass of water (ºC).

For natural conditions the heat lost by evaporation can be represented by Dalton's Law. Among the different factors that affect evaporation the wind is one of the main. In general, it is a not very understood process.

$$\mathbf{J_e} = \mathbf{f(u_w)} * (\mathbf{e_s(T_w)} - \mathbf{e_{air}}) \qquad \textbf{(25)}$$

Where $f(u_w)$ is a wind-dependent function defined as

$$f(u_w) = a + bu_w^c \qquad (26)$$

Where a, b and c can be adjusted. A very common value is: a = 19, b = 0.95 and c = 2. And u_w is the value of the measured wind speed at 2 meters in height (m/s).

$e_s(T_w)$ is the saturation vapour pressure estimated for the water temperature.

e_{air} is the measured vapour pressure of the air.

Conduction is the process of heat transfer from molecule to molecule when materials at different temperatures are brought into contact. Convection is the heat transfer process that occurs due to the mass movement in the fluids. Both can occur in the air-water interface and it is possible to describe them with the expression:

$$\mathbf{J_c} = \mathbf{c_1} * \mathbf{f(u_w)} * (\mathbf{T_w} - \mathbf{T_a}) \textbf{ (27)}$$

Where c_1 is the Bowen coefficient (0.47 mmHg/°C). $f(u_w)$ is the same function as for evaporation. T_w is the temperature of the surface of water.

Once all the components of the heat balance between the atmosphere and the mass of water have been estimated, the sump term of equations (1), (12) and (13) is replaced by the following expression:

$$\sum W_i = \frac{\emptyset_{net} * A_s}{\rho * C_{esp}} \qquad \textbf{(28)}$$

In this way it is assumed that the density of the water and the specific heat are constant and in equations (1), (12) and (13) which are representative of the mass balance in rivers and reservoirs, the concentrations become temperature.

A process of convergence is carried out for the case of the river reaches since the term of heat between the atmosphere and the mass of water depends on the temperature of the mass of water.

When reservoirs are modelled with two layers, the radiation that reaches the hypolimnion is estimated assuming that only 45% of the short-wave radiation

penetrates. The remaining types of radiation are absorbed in the first few centimetres of depth. From 55% of the short-wave penetrating it is assumed that the water is absorbing the heat according to Beer-Lambert law. In this way the amount of heat that reaches the hypolimnion is as follows:

$$H_{swh} = 0.55 H_{sw} A_s (1 - \beta) * e^{-KH_1} \qquad \textbf{(29)}$$

Where H_{swh} is the short-wave radiation incident on the hypolimnion, A_s is the surface area of the reservoir sheet of water. β is the proportion of short-wave that is absorbed in the most superficial layer of water (assuming 0.45). K is the light attenuation constant. H_1 is the height of the epilimnion.

3.4.1.2. Linearization approach

The second method that can be used in the program for temperature estimation is based on the work of Edinger and Geyer (1965) who proposed the net heat flow as a function of the total heat exchange and the equilibrium temperature, as follows:

$$\sum W_i = \emptyset_{net} = K_{eq} * A_s * (T_{eq} - T) \qquad \text{(30)}$$

Where: K_{eq} is the rate of heat exchange (Wm^{-2}ºC^{-1}); T_{eq} is the equilibrium temperature (°C), T is the water temperature and A_s is the surface area of the sheet of water.

The equilibrium temperature is defined as the temperature that would reach the mass of water if the weather conditions were constant. It can be obtained by iterative methods by making zero the net energy flow in equation 18. This approximation is usually used, as it has validity for medium and long term time scales.

For reservoirs that are modelled in two layers the formulation changes as follows. For the epilimnion:

$$\sum W_{i\_ep} = \emptyset_{net} = K_{eq} * A_s * (T_{eq} - T) - (1 - \beta) * I_o * e^{-KH_1} * A_s \qquad \textbf{(31)}$$

And for the hypolimnion:

$$\sum W_{i\_hip} = (1 - \beta) * I_o * e^{-KH_1} * A_s \qquad \textbf{(32)}$$

Where: β is the short-wave ratio that is absorbed in the most superficial layer of water. I_o is the net shortwave solar radiation incident on the mass of water, K is the light attenuation constant of the reservoir, H_1 is the height of the epilimnion and A_s is the surface of the water.

This formulation discounts the short-wave radiation that does not contribute heat to the epilimnion because it crosses it. It is assumed that the attenuation of light follows Beer-Lambert's law. In the program the whole second term is introduced as a single data called "short-wave radiation in the hypolimnion".

3.4.1.3. Temperature as input data.

Due to the difficulty of having meteorological data throughout the river basin but taking into account the importance of the temperature in the different processes, the possibility of introducing the evolution of the temperature within the year as input data for each element (river reach or reservoir) is provided. In this way, without modelling the temperature it is allowed to be considered for the rest of processes.

3.4.2 Arbitrary pollutants.

For arbitrary pollutants, the decomposition process is modelled by a first-order kinetic process and a sedimentation process of the particulate part.

$$\sum W_i = -K\left(\theta^{T-20}\right)C - \frac{VS}{h}C \quad (33)$$

Where: K represents the degradation rate at 20 °C (day^{-1}); θ is the temperature correction coefficient; sedimentation is considered by a parameter VS that represents the sedimentation rate of the constituent (m day^{-1}); H is the depth of the river (m); C represents the pollutant concentration in the river (mgl^{-1}).

In order to consider a pollutant as conservative, it is enough to consider the degradation constant and the sedimentation velocity as null. On the other hand in reservoirs modelled with two layers the sedimentation term of the epilimnion appears as an adding for the hypolimnion.

3.4.3. Organic matter, dissolved oxygen and eutrophication processes.

For the dissolved oxygen modelling, three possible incremental levels of complexity are considered. The simplest option considers the modelling of COM and dissolved oxygen. The second degree of complexity considers further the nitrogen cycle. The different forms considered are organic nitrogen, ammonia and nitrates. Finally, the last level of complexity allows the modelling of COM, nitrogen cycle, phytoplankton, phosphorus (organic and soluble reactive), their relationships and their affections on dissolved oxygen.

In this way the modelling of the carbonaceous organic matter is included within the modelling of the eutrophication process. The different forms of approach can be seen in the following schemes.

The following figure shows the processes considered in the basic modelling option in terms of dissolved oxygen (DO) and carbonaceous organic matter (COM). Note DOS: Demand for Oxygen from the Sediment.
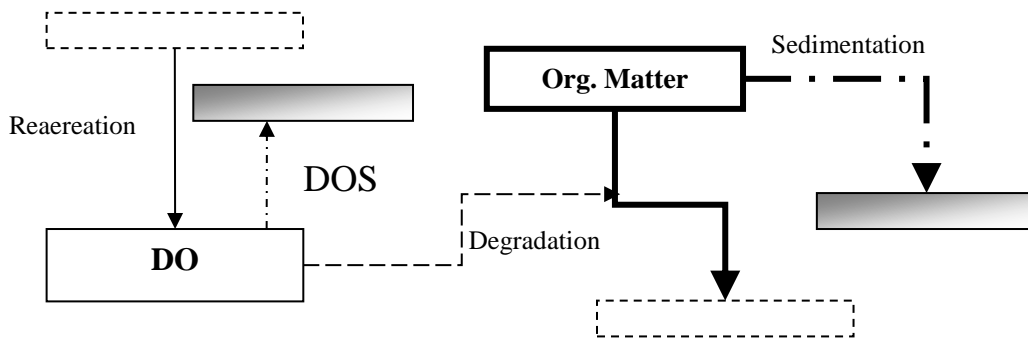
Figure 3. Processes considered in the basic hypothesis for dissolved oxygen modelling.

The following figure shows the processes and constituents included in the second option of dissolved oxygen, COM and nitrogen cycle modelling.
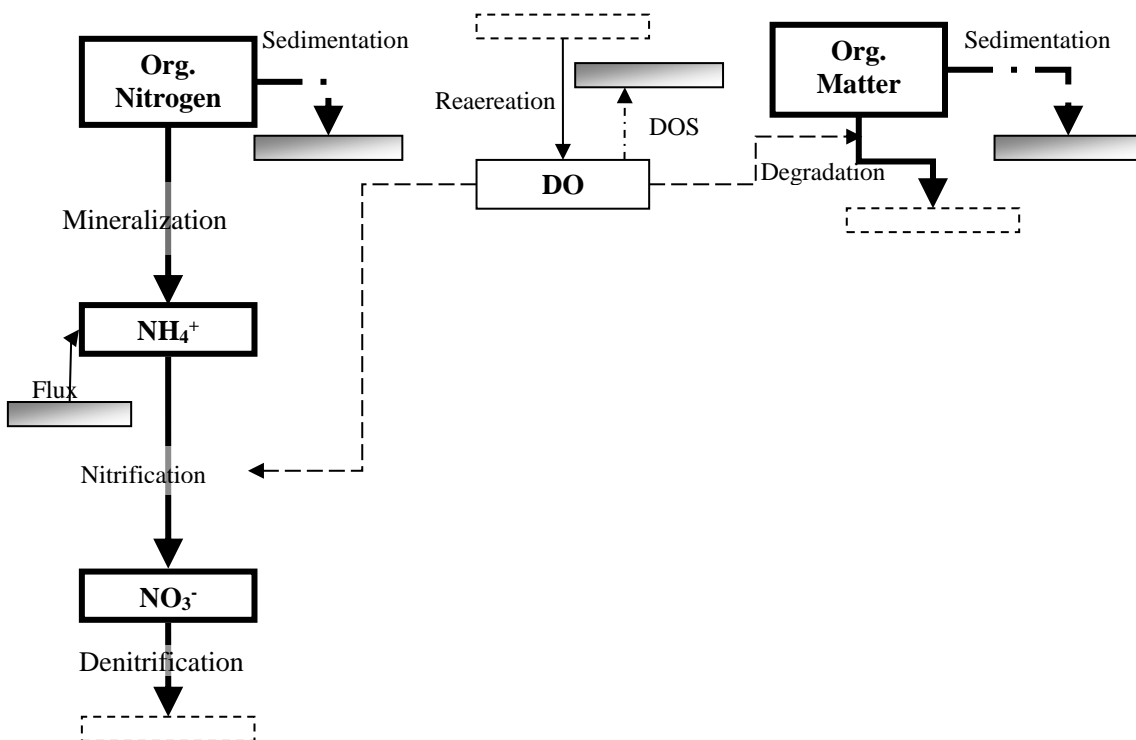

Figure 4. Processes considered in the joint modelling of dissolved oxygen and nitrogen cycle

Finally Figure 6 shows all the processes that are taken into account with the modelling of a problem of eutrophication.
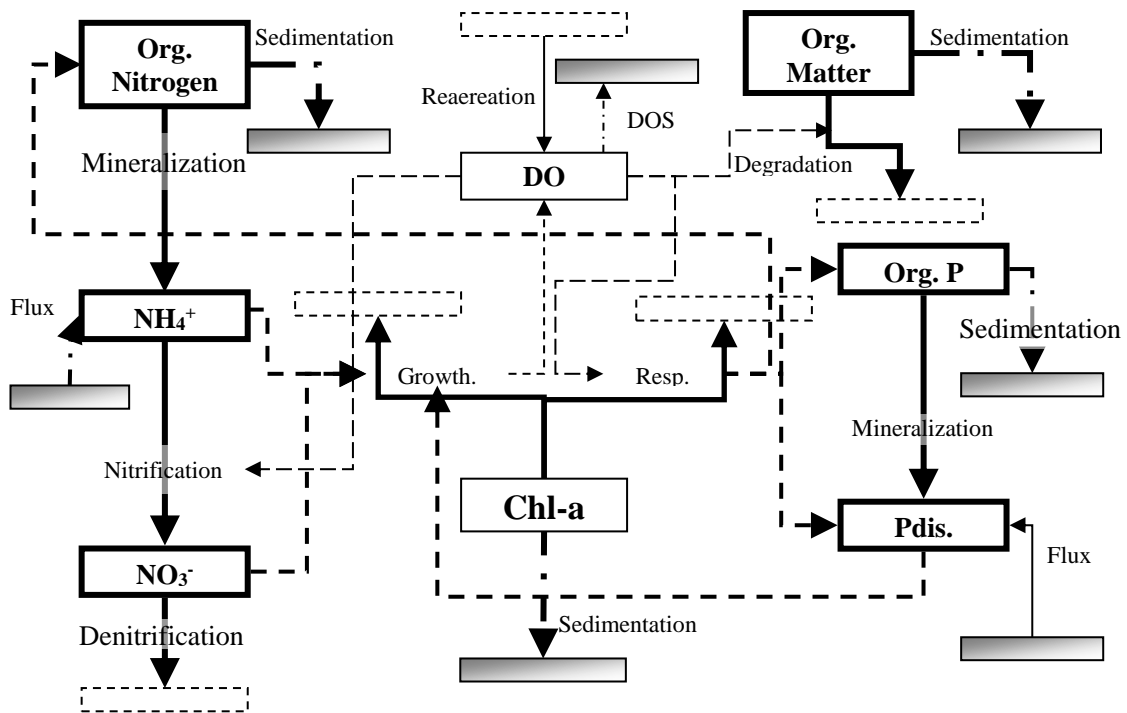
Figure 5. Processes considered in an eutrophication problem modelling

3.4.3.1. Carbonaceous Organic Matter.

For the modelling of the COM, the degradation by heterotrophic aerobic microorganisms and the sedimentation of the particulate part are considered.

$$\sum W_i = -K_d \theta_d^{T-20} \frac{O}{O + K_{d\frac{1}{2}}} L - \frac{VS_L}{h} L \qquad (34)$$

Where: L is the concentration of COM in the river (M/V); K_d is the degradation rate (T^{-1}); θ_d is the temperature correction coefficient of the constant K_d; VS_L is the sedimentation rate (mdía^{-1}); H is the depth of the mass of water; T is the temperature of the mass of water.

3.4.3.2. Organic Nitrogen.

For the organic nitrogen the processes of ammonification and sedimentation are considered:

$$\sum W_i = -K_{Noa} \theta_{noa}^{T-20} N_o - \frac{VS_{No}}{h} N_o + r_{na} K_{resp} \theta_{resp}^{T-20} A \qquad (35)$$

Where: K_{noa} represents the ammonification constant (day^{-1}); θ_{noa} represents the temperature correction coefficient of the previous constant; N_o is the concentration of organic nitrogen in the river (MT^{-1}); VS_{NO} is the sedimentation rate of

organic nitrogen (mday^{-1}); r_{na} represents the nitrogen content in the algae (mgN/mgA). The last term is only considered when phytoplankton is modelled, representing the contribution due to the respiration thereof.

3.4.3.3. Ammonia.

The processes considered on the ammonia have been the increase of concentration by the ammonification of the organic nitrogen and the decrease of concentration by nitrification. The nitrification has been considered in its entirety including the passage of ammonia to nitrites and from these to nitrates.

$$\sum W_i = +K_{Noa}\theta_{Knoa}^{T-20}N_o - \left(K_{Nai}\theta_{nai}^{T-20}\frac{O}{O+K_{n1/2}}\right)N_a + -r_{na}F_n K_g^{'}A \qquad (36)$$

Where: N_a represents the concentration of ammonia (NH_4^+) in the river (mgl^{-1}); K_{Nai} is the nitrification constant (day^{-1}); θ_{nai} is the temperature correction coefficient of the nitrification constant; $K_{n1/2}$ is the nitrogen half-saturation constant (mgl^{-1}); O is the concentration of dissolved oxygen. F_n represents the preference factor for ammonia versus nitrates; r_{na} is the stoichiometric coefficient (mgN/mgA); $K_g^{''}$ is the phytoplankton growth constant considering the temperature correcting factor, nutrient limitation and light attenuation (day^{-1}); A is the concentration of chlorophyll-a (mgl^{-1}). The last term is only considered when the global set is modelled. The effect of the reduction of nitrification by anoxic conditions has been considered correcting the constant with a factor dependent on dissolved oxygen concentration and a half-saturation constant.

3.4.3.4. Nitrites y Nitrates.

Due to the rapid oxidation of nitrates to nitrites, both nitrates and nitrites are modelled together. The nitrate modelling process considers the effect of the increase of concentration by the ammonia transformation and the decrease of the nitrates by possible processes of denitrification and phytoplankton growth.

$$\sum W_i = \left(K_{Nai}\theta_{nai}^{T-20}\frac{O}{O+K_{nai1/2}}\right)N_a - \left(K_{no3}\theta_{no3}^{T-20}\frac{K_{no31/2}}{O+K_{no31/2}}\right)N_{o3} - r_{na}(1-F_n)K_g^{'}A \qquad (37)$$

Where: N_{o3} is the concentration of nitrates (mgl^{-1} -N); K_{no3} represents the denitrification constant (day^{-1}); θ_{no3} is the temperature correction factor for the previous constant; $K_{No31/2}$ represents the half-saturation constant to take into account that denitrification only occurs in cases of anoxia.

3.4.3.5. Phytoplankton.

Phytoplankton modelling includes the growth, respiration and sedimentation processes. The growth of the algae is conditioned by the temperature, the light factor and the availability of nutrients:

$$\sum W_i = + \left[K_g^{'} - K_{resp} \theta_{resp}^{T-20} \right] A - \frac{VS_A}{h} A \qquad (38)$$

Obtaining the corrected growth constant, $K_g^{''}$, as follows:

$$K_g^{'} = K_{g\max} \cdot \theta_g^{T-20} \cdot F_l \cdot F_N \qquad (39)$$

Where: K_{gmax} is the phytoplankton maximum growth constant at 20 °C (day^{-1}); θ_g is the temperature correction factor of phytoplankton growth; F_l is the attenuation light factor with monthly variation; F_N is the nutrient limit factor; K_{resp} represents the coefficient for phytoplankton death and respiration (day^{-1}); θ_{resp} is the temperature correction factor; VS_A is the sedimentation rate of chlorophyll-a (mday^{-1}).

Nutrient limitation is considered as the minimum of the limitation terms for nitrogen and phosphorus. The expression of Michaelis-Menten is used to estimate each of them.

$$Min \left(\frac{N_{aio3}}{N_{aio3} + K_{NF1/2}} ; \frac{P}{P + K_{P1/2}} \right) \qquad (40)$$

N_{aio3} represents the concentration of inorganic nitrogen (mgl^{-1}); $K_{NF1/2}$ is the nitrogen half-saturation constant; P is the concentration of phosphates in the river reach (mgl^{-1}); $K_{p1/2}$ is the half-saturation constant for phosphorus (mgl^{-1}).

The factor introduced to include the light limitation for phytoplankton growth is determined from the light attenuation with depth by Beer - Lambert law and the effect of luminosity level on growth.

The Beer - Lambert equation enables to obtain the luminous intensity in a certain depth:

$$I_z = I_0 \cdot e^{-Ke \cdot z} \quad (41)$$

Where: I_0 is the luminous intensity on the surface (langleys/day), of which the visible light range corresponding to approximately 50% of incident solar radiation is used; K_e is the coefficient of light extinction. This coefficient, K_e, introduces the effect of self-enlightenment by the expression:

$$Ke = Ke_0 + \alpha_{at} \cdot A \quad (42)$$

Where: Ke_0 represents the water light extinction coefficient (m^{-1}); α_{at} is the specific light extinction coefficient of phytoplankton ($Lmg^{-1}m^{-1}$) and A is the concentration of chlorophyll-a (mgL^{-1}).

The effect of the luminosity level on growth can be introduced by saturation or photo-inhibition curves. The formulation used in this study is that photo-inhibition, which follows Steele's law:

$$FL = \frac{I}{I_s} \cdot e^{\left(1 - \frac{I}{I_s}\right)} \quad (43)$$

Where I (langleys) is the luminous intensity and Is (langleys) the luminous intensity of saturation.

Integrating both equations together with a function that introduces the variation of light throughout the day, called photoperiod (f) and taking into account that the model works with two layers, it is possible to calculate the luminance factor for each of the layers according to the following expressions:

$$FL_1 = \frac{e \cdot f}{Ke \cdot H_1} \cdot \left(e^{-I_0 \cdot \frac{AtI_o}{I_{sat}} \cdot e^{-Ke \cdot H_1}} - e^{-I_0 \cdot \frac{AtI_o}{I_{sat}} \cdot e^{-Ke \cdot 0}} \right) \quad (44)$$

$$FL_2 = \frac{e \cdot f}{Ke \cdot H_2} \cdot \left(e^{-I_0 \cdot \frac{AtI_o}{I_{sat}} \cdot e^{-Ke \cdot H_2}} - e^{-I_0 \cdot \frac{AtI_o}{I_{sat}} \cdot e^{-Ke \cdot H_1}} \right) \quad (45)$$

3.4.3.6. Organic phosphorous.

For the modelling of the organic phosphorus it is considered the effect of the phytoplankton respiration, the mineralization of the phytoplankton to the inorganic form and the sedimentation. With these considerations the equation is as follows:

$$\sum W_i = -K_{mp}\theta_{mp}^{T-20}P_{or} + f_p r_{pa} K_{resp}\theta_{resp}^{T-20}A - \frac{VS_{or}}{h}P_{or} \quad (46)$$

Where: P_{or} is the concentration of organic phosphorus (mgl^{-1}). K_{mp} represents the mineralization constant of organic phosphorus (day^{-1}); θ_{mp} is the temperature correction coefficient of the mineralization constant; r_{pa} is the stoichiometric coefficient (mgP/mgA); VS_{or} is the sedimentation rate of organic phosphorus ($mday^{-1}$); f_p is the fraction of organic phosphorus that is generated during the phytoplankton respiration.

3.4.3.7. Phosphates.

The effect of mineralization of the organic form and the growth of phytoplankton is considered for the modelling of phosphates:

$$\sum W_i = +K_{mp}\theta_{mp}^{T-20}P_{or} - r_{pa}K_g'A + +(1-f_p)r_{pa}K_{resp}\theta_{resp}^{T-20}A \qquad (47)$$

Where: P represents the concentration of inorganic phosphorus in the river (mgl^{-1}).

3.4.3.8. Dissolved Oxygen.

For the modelling of dissolved oxygen, the following processes are considered:

- Dissolved oxygen consumption during the process of carbonaceous organic matter degradation.

- Dissolved oxygen consumption during the nitrification process

- Oxygen consumption during the phytoplankton respiration.

- Production of dissolved oxygen during the process of growth through photosynthesis.

$$\sum W_i = +K_a\theta_{Ka}^{T-20}(O_{sat} - O) - K_d\theta_d^{T-20}L -$$

$$- r_a\left(K_{Nai}\theta_{nai}^{T-20}\frac{O}{O + K_{n1/2}}\right)N_a +$$

$$+ r_{ocrec}\left(K_{g\max}\theta_g^{T-20}F_l Min(\frac{N_{aio3}}{N_{aio3} + K_{NF1/2}};\frac{P}{P + K_{P1/2}})\right)A - r_{oresp}K_{resp}\theta_{resp}^{T-20}A \qquad (48)$$

Where: O is the dissolved oxygen concentration in the river (mgl^{-1}); Osat is the concentration of dissolved oxygen saturation (mgl^{-1}); K$_a$ is the reaeration constant (day^{-1}); θ_a is the temperature correction factor; r$_a$ represents the oxygen consumption by ammonium oxidation (mgO/mgN); r$_{ocrec}$ and r$_{oresp}$ represent the oxygen produced and consumed by the growth of algae and respiration.

Each of the lines of the formula represents the terms that are added according to the modelling considerations: simple mode (only dissolved oxygen and organic matter), second mode where nitrogen cycle is included and complete mode where the effect of phytoplankton and phosphorus is included.

The saturation of dissolved oxygen is estimated from the temperature of the river reach using the equation proposed in APHA (1992).

$$\ln O_{satpo} = -139.34411 + \frac{1.575701 \cdot 10^{5}}{T_a} - \frac{6.642308 \cdot 10^{7}}{T_a^{2}} + \frac{1.2438 \cdot 10^{10}}{T_a^{3}} - \frac{8.621949 \cdot 10^{11}}{T_a^{4}}$$

(49)

Where: T_a is the water temperature in degrees Kelvin.

The reaeration constant can be introduced as a data or obtained by the Covar method:

If H (depth) <0.61 (m) then the Owens-Gibbs formula is employed:

$$K_a = 5.32 \frac{u^{0.67}}{H^{1.85}}$$ (50)

Where u is the velocity in m/s. If H>0.61 (m) and H>3.44*u^2.5 then the O'Connor-Dobbins formula is employed:

$$K_a = 3.93 \frac{u^{0.5}}{H^{1.5}}$$ (51)

In any other case the formula of Churchill is used:

$$K_a = 5.026 \frac{u}{H^{1.67}}$$ (52)

The following table lists ranges for the parameters used in the model found in the literature.

Par.	U.	Range	Temp Corr Factor	Parameter
Ka	1/d	0-100	1.024	Coefficient of reaeration
Kd	1/d	0.02-3.4	1.047	Coefficient of CBOD breakdown
VsL	m/d	0.01-0.36	1.024	Sedimentation rate of CBOD
KNoa	1/d	0.02-0.4	1.047	Coefficient for ammonification
VSNo	m/d	0.001-0.1	1.024	Sedimentation rate of organic nitrogen
KNai	1/d	0.01-1	1.083	Half saturation for nitrification
Kno3	1/d	0.001-0.1	1.045	Coefficient for denitrification
Kg	1/d	1-3	1.047	Coefficient for phytoplankton growth
Kresp	1/d	0.05-0.5	1.047	Coefficient for phytoplankton death and respiration
VSA	m/d	0.15-1.83	1.024	Sedimentation rate of chlorophyll-a
Kmp	1/d	0.01-0.7	1.047	Organic phosphorous mineralization parameter

Vsor	m/d	0.001-0.1	1.024	Sedimentation rate of organic phosphorous

Table 3. Typical values of the parameters employed in the model.

3.4.4. General considerations.

The following table summarizes the processes considered that affect each of the constituents:

PARAMETER	PROCESSES
Temperature	(±)Exchange with the atmosphere
Arbitrary pollutant	(-)Sedimentation.
	(-)Degradation.
Organic matter	(-)Sedimentation.
	(-)Degradation.
Dissolved oxygen	(+)Reaeration.
	(-)Organic matter degradation.
	(-)Demand of the sediment.
	(-)Nitrification.
	(+)Phytoplankton growth and (-) Phytoplankton respiration
Organic nitrogen	(-)Mineralization.
	(-)Sedimentation.
	(+)Phytoplankton respiration.
Ammonia	(+)Mineralization.
	(-)Nitrification.
	(-)Phytoplankton growth.
Nitrates	(+)Nitrification.
	(-)Denitrification.
	(-)Phytoplankton growth.
Phytoplankton (Chlorophyll-a)	(+)Growth.
	(-)Respiration.

PARAMETER	PROCESSES
	(-)Sedimentation.
Organic phosphorous	(-)Mineralization.
	(-)Sedimentation.
	(+)Phytoplankton respiration.
Inorganic phosphorous	(+)Mineralization.
	(-)Sedimentation-Adsorption.
	(-)Phytoplankton growth.
	(+)Phytoplankton respiration.

Table 4. Processes considered in the different constituents

The signs (+) and (-) mean that the process contributes or decreases constituents respectively. In addition, each of them can be influenced by processes of diffuse contamination in river reaches and sediment flows in reservoirs.

3.4.4.1. Temperature influence.

The velocity of the reactions that are considered in the model increases with the temperature, according to the Arrhenius equation:

$$K(T) = K(20) \cdot \theta^{T-20} \tag{53}$$

Where K(T) is the value of the constant at temperature T, K(20) is the value of the constant at 20°C and θ is the temperature correction factor and depends on the process.

3.4.4.2. Dissolved oxygen concentration influence.

The velocity of processes that depend on the available oxygen (organic matter degradation, nitrification, denitrification) is corrected by the concentration of oxygen generally according to the expression:

$$K = K \cdot \frac{OD}{OD + K_{1/2}} \tag{54}$$

Where OD is the oxygen concentration and $K_{1/2}$ is a half-saturation constant different for each process.

For the case of the channels where the steady-state is sought, an iterative process of calculation between the different constituents related in the dissolved oxygen modelling is performed. The value of the sum of the concentrations of dissolved oxygen in the segments in which the river reach is divided is used as the convergence criterion. The convergence limit is defined as a difference of 0.5 mg/l between two iterations. In order to ensure convergence, the organic matter degradation constant is estimated as the average value between the obtained for the previous simulation and the one obtained for the oxygen levels of this simulation.

In particular, for the denitrification process, which takes place in the absence of oxygen, the oxygen correction is introduced as follows:

$$K = K \cdot \frac{K_{1/2}}{OD + K_{1/2}} \quad (55)$$

3.4.4.3. Sediment flux in reservoirs.

Sediment fluxes can be defined for any pollutant by adding to the concentrations of hypolimnion in the case of two-layer modelling or to the single layer in the case of a single layer. For the case of ammonia, nitrates and inorganic phosphorus it is assumed that only sediment flow occurs when the hypolimnion (or the entire reservoir) is in anoxic conditions. Although some of these constituents may have fluxes at times where oxygen concentrations are high, the higher fluxes occur in conditions of anoxia. The situation of anoxia with dissolved oxygen concentrations below 1mg/l has been considered.

3.4.4.3. Coefficients and stoichiometry.

There are a set of constants or parameters fairly fixed that have not been considered for calibration so they are located in a file which has been called "constant file". This file is explained later but in this section we want to mention a set of parameters that are related to the processes explained. The selected values have been obtained from the scientific literature but they can be modified if, by some specific case, other values are required. Among these values we can find:

- Half-saturation constants. To take into account the effect of anoxic conditions on the degradation of organic matter and nitrification. Two other half-saturation constants, one for nitrogen and one for phosphorus, are considered in the limitation of nutrients for phytoplankton growth.

- Coefficients of consumption and production of oxygen. Equivalences of oxygen produced or consumed in different processes, such as nitrification of ammonia and respiration and death of phytoplankton.

- Nutrient content in phytoplankton. These values are the most variable depending on the type of algae prevalent in the system. Nitrogen and phosphorus ratios are defined with chlorophyll-a.

- Phytoplankton preference factor for ammonia.

- Proportion of organic phosphorus produced during the growth of phytoplankton.

The following table shows the values adopted for the model constants.

Name	Units	Adopted Value	Description
Kd1/2	mgO	0.5	Half-saturation constant to correct Kd due to low concentrations of DO
KN1/2	mgO	0.5	Half-saturation constant to correct KNai due to low concentrations of DO
KNF1/2	mgN	0.03	Half-saturation constant to correct Kgrow due to nutrients limitation. Nitrogen
KP1/2	mgP	0.02	Half-saturation constant to correct Kgrow due to nutrients limitation. Phosphorous
Ra	mgO/mgN	4.57	Oxygen consumption for each mgN oxidized in the nitrification of ammonia
Roresp	mgO/mgA	100	Oxygen consumption for each mgChla during the respiration and growth of phytoplankton
Rocrec	mgO/mgA	130	Oxygen produced for each mgChla during the growth of phytoplankton
Rna	mgN/mgA	15	Stoichiometric coefficient that establishes the relationship between mgChla and mgN
Rpa	mgP/mgA	1	Stoichiometric coefficient that establishes the relationship between mgChla and mgP
Fn	Parts per unit	0.9	Preference factor of algae for ammonia against nitrates
Fp	Parts per unit	0.5	Part of the organic phosphorous produced

Table 5. Adopted values for the constants in the model.

These values can be changed according to the study river basin.

3.4.5. Processing units.

The use of the input and output units to the model is, mostly, configurable in the file of constants and coefficients. We have tried to be consistent with the input units used in the networks of quality monitoring. This is a fundamental difference compared to most quality models and it may mislead users accustomed to handling other quality models. The treatment details of the units are specified below:

- The variables that are obtained from the output files or data from AQUATOOL DSS are, mostly, volume and flow variables. The first are expressed in hm^3 and the latter in hm^3/month. The program internally transforms these units to m^3 and m^3/day. In the file of constants and coefficients, the change of units of input volume to m^3 (1E6) and the coefficient of temporal change (30.5 days/month) is provided.

- Concentrations of the arbitrary pollutants can be introduced in any unit of concentration, but always maintaining coherence with what is defined in the rest of elements: streamflows, returns, intakes and initial conditions.

- Dissolved oxygen concentrations should be defined in mg/l.

- The COM is introduced as mgO/l of BOD5. The program internally estimates the boundary BOD (L) by the following expression:

$$L = \frac{DBO_5}{1 - e^{-k5}} \quad (56)$$

Where "k" is defined in the coefficient and constant file. The output is presented in BOD5. This is a difference with traditional models where the input to the model is usually done in limit BOD. If this option is required the user simply must consider "0" the constant in the coefficient file and obviate the labelling of the results.

- The organic nitrogen data is entered as mg/l of nitrogen. The ammonia and nitrate forms are introduced as mg/l of constituent. The program internally, using the values of the coefficient file, transforms all values to mg/l of nitrogen. This is due to the fact that mass balances of the different forms are made in mg/l of nitrogen. The results are converted to mg/l of the constituent before being written in the different files. This is another point where traditional quality models differ with GESCAL. In general it is common to introduce the ammonia and nitrate data in mg of nitrogen and not in mg of ammonia or

nitrates. As in the case of organic matter, in order to use this option user must vary the coefficients of the file of constants and coefficients.

- Phytoplankton must be introduced in mg/m^3 of chlorophyll-a. In the coefficient file, there is the factor by which it is multiplied in order to obtain mg/l internally.

- Organic phosphorus is introduced in mg/l of phosphorus while the inorganic phosphorus is considered to have been measured as PO_4. Internally it is transformed to mg of phosphorus. The coefficient of change of unit is in the file of constants and coefficients, which is configurable.

- Diffuse pollution values should be included in gr/day since no change is made to it. They are total grams in the whole reach. In the program it is divided by the length in order to take into account how many grams enter each segment.

- All degradation constants must be entered on $days^{-1}$.

- Reservoir sediment flux should be entered in $gr/m^2/day$.

All changes of units that are made internally are undone when writing the results so that the outputs have the same units as the inputs.

The internal change coefficients of units for: BOD_5, NH_4, NO_3, PO_4, Chl-a are in the coefficients and constants file being configurable for each case.

For the river reaches:

- Dispersion: in m^2/s.

- The length and length step meters.

- The hydraulic coefficients must be adjusted to obtain the velocity in m/s and the depth in meters using the flow in m^3/s.

- The width must be in meters and the cross slopes and longitudinal slope in m/m.

For the reservoirs:

- The dispersion between layers has as input units cm^2/s.

- The ratio of the initial volume which is epilimnion must be introduced in parts per unit.

- The calculation differential refers to the number of time intervals in which the month is fragmented. A differential of 30 represents approximately a daily time scale.

- The proportions of entrance to and exit to the epilimnion must be introduced in parts per unit.

- The height of the thermocline must be entered in meters.

In relation with temperature:

- If temperature is not modelled, then the input data must be done in ºC.

- If the equilibrium temperature is modelled, then it must be entered in ºC.

- The temperature constant units are W/m^2.

- The radiation absorbed by the hypolimnion must be introduced in W/m^2.

- The density of the water is considered constant and equal to 1000 kg/m^3 and it is defined in the file of coefficients. It is advised not to change this parameter because it would lead to unit errors in temperature modelling.

- The specific heat of water is entered in the coefficient file in J/(ºCKg) and, as in the case of density, it is advisable not to change this variable.

- If temperature is modelled by balance, the short-wave radiation is introduced in W/m^2; air temperature in °C; Relative humidity in percent; dew temperature in °C; the cloudiness in parts per unit and the speed of the wind in m/s.

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