WaterStrategyMan
EVK1-CT-2001-00098

MANUAL OF THE INTEGRATED DECISION SUPPORT SYSTEM

Chapter Five

Water Quality

Chapter 5: Water Quality

The idea behind the inclusion of a simple water quality algorithm within the WSM DSS is to provide the Decision Makers with an estimation of how the concentration of selected quality parameters evolve during a simulated period of time, under specific water demands, climatic conditions and allocation rules (priorities). In particular the key concentrations addressed are those at the water resource nodes of the network: groundwater, river reaches, artificial and natural lakes. Being the source nodes connected to the demand nodes they supply water to, their water quality directly influences the one at every location of the case study region: the assumption is that water flowing in the pipelines, computed at each time step by the Water Allocation Model, has the same concentration as the water sources (supply nodes) it comes from, and it does not change during the transfer towards the demand sites. The strict connection between the water quantity and quality is evident: by distributing water volumes through out the system, the kernel of the DSS also distributes the levels of quality parameters based on the paths traced by the network links.

The set of quality variables simulated comprises of: salinity, chlorophyll alpha, ammonia nitrogen, nitrate nitrogen, coliform bacteria, total phosphorus, heavy metals in general, Biochemical Oxygen Demand and Dissolved Oxygen. New parameters are currently being added, such as suspended and inhibiting matters and adsorbable organic halogens. Their concentrations are updated at each time step and for each supply node using two different algorithms, according to the quality parameter. For some of them, the continuity equation on the loads is applied: the variation of load in the water volume stored in the generic supply node (where load is concentration multiplied by the water volume) equals the difference between the incoming load and the outgoing load. The incoming load comes from the links carrying water to the supply node, while the outgoing load is made explicit as function of current concentration at the supply node, that is what each equation calculates at each time step. In these equations, additional terms are accounted, relating the generation or decay of load, due to the presence of algae and to the nitrogen cycle for instance. Moreover, some of these water quality variables, such as Chlorophyll alpha, ammonia nitrogen and nitrate nitrogen are strictly inter-related and their equations are solved following a sequence of computation (first Chlorophyll, then ammonia nitrogen and then nitrate nitrogen) or some iterations. This approach requests the user to specify initial concentrations of the quality variables, that are referred to the first month in the simulation horizon. Then, from the second month on, the quality equations use the concentrations updated by them at the previous time step.

The differential continuity equation can be written for each quality variable as follows:

$$\frac{di}{dt} = -A \cdot i + B$$

which has an analytical solution of type:

$$i = i_0 \cdot e^{-A \cdot t} + \frac{B}{A} \cdot (1 - e^{-A \cdot t})$$

Hereunder, the specific equations for the variables are presented:

- Volume V of the water body:

$$\frac{dV}{dt} = I - O$$

where:

I = water flow entering the water body
O = water flow exiting the water body

- Salinity S :

$$\frac{d(S \cdot V)}{dt} = Load(S)_{in} - O \cdot S$$

where:

S = salinity (amount of salt per cubic metre)
O = water flow exiting the water body
$Load(S)in$ = salinity load entering water body
V = water volume (for the river reach it is the water volume flowing in it)

- Chlorophyll alpha:

Chlorophyll alpha is directly proportional to the concentration of algal biomass through the α_0 conversion factor.

$$Chl\alpha = \alpha_0 A$$

Hereunder is the equation used to model the behaviour of algal biomass in time:

$$\frac{d(A \cdot V)}{dt} = Load(A)_{in} - O \cdot A + V \cdot [(\mu - \rho - \sigma 1) \cdot A]$$

where:

$Load(A)_{in}$ = algal biomass load entering the water body;
O = water outflow
A = concentration of algal biomass
V = water volume
μ = algal growth rate
ρ = algal respiration rate
σ_1= algal settling rate
- Ammonia N_1:

$$\frac{d(N_1 \cdot V)}{dt} = Load(N_1)_{in} - O \cdot N_1 + V \cdot \left[- \beta_1 N_1 - F_1 \, \alpha_1 \mu A \right]$$

with

$$F_1 = \frac{P_N N_1}{P_N N_1 + (1 - P_N) \cdot N_3}$$

where:

$Load(N_1)_{in}$ = ammonia nitrogen load entering the water body;
O = water outflow
N_1 = concentration of ammonia nitrogen
V = water volume
F_1 = fraction of algal nitrogen uptake from ammonia pool
α_1= fraction of algal biomass that is nitrogen
A = concentration of algal biomass
β_3= rate constant for hydrolysis of organic nitrogen to ammonia nitrogen
β_1= rate constant for the biological oxidation of ammonia nitrogen
μ = algal growth rate
P_N = preference factor for ammonia nitrogen

- Nitrates:

$$\frac{d(N_3 \cdot V)}{dt} = Load(N_3)_{in} - O \cdot N_3 + V \cdot \left[\beta_1 N_1 - (1 - F_1) \alpha_1 \mu A \right]$$

with

$$F_1 = \frac{P_N \cdot N_1}{P_N \cdot N_1 + (1 - P_N) \cdot N_3}$$

where:

$Load(N_3)_{in}$ = nitrate nitrogen load entering the water body;
O = water outflow
N_3 = concentration of nitrate nitrogen
N_1 = concentration of ammonia nitrogen
V = water volume
F_1 = fraction of algal nitrogen uptake from ammonia pool
α_1= fraction of algal biomass that is nitrogen
A = concentration of algal biomass

β_1= rate constant for the biological oxidation of ammonia nitrogen
μ = algal growth rate
P_N = preference factor for ammonia nitrogen

- Coliform bacteria:

$$\frac{d(E \cdot V)}{dt} = Load(E)_{in} - O \cdot E + V \cdot [- k_5 \cdot E]$$

where:

$Load(E)_{in}$ = coliform load entering the water body;
O = water outflow
E = concentration of coliform bacteria
V = water volume
k_5 = coliform die-off rate

- BOD:

$$\frac{d(BOD \cdot V)}{dt} = Load(BOD)_{in} - O \cdot BOD + V \cdot [- (k_1 + k_3) \cdot BOD]$$

where:

$Load(BOD)_{in}$ = Biochemical Oxygen Demand load entering the water body;
O = water outflow
BOD = concentration of Biochemical Oxygen Demand
V = water volume
k_1 = deoxigenation rate coefficient
k_3 = rate of BOD loss due to settling

- DO:

$$\frac{d(DO \cdot V)}{dt} = Load(DO)_{in} - O \cdot DO +$$

$$+ V \cdot \left[k_2 \left(DO^* - DO\right) + (\alpha_3 \mu - \alpha_4 \rho) \cdot A - k_1 \cdot BOD - \alpha_5 \beta_1 \cdot N_1\right]$$

where:

$Load(DO)_{in}$ = Dissolved Oxygen load entering the water body

DO = concentration of Dissolved Oxygen
DO^* = saturation concentration of Dissolved Oxygen
O = water outflow
BOD = concentration of Biochemical Oxygen Demand
V = water volume
N_1 = concentration of ammonia nitrogen
A = concentration of algal biomass
k_1 = deoxigenation rate coefficient
k_2 = reareation rate
μ = algal growth rate
ρ = algal respiration rate
α_3= rate of oxygen production per unit of algal photo-synthesis
α_4= rate of oxygen uptake per unit of algae respired
α_5= rate of oxygen uptake per unit of ammonia nitrogen oxidation

Definition	Notation Used in the Equations	Range of values	Units
Algal growth rate	μ	1.0 - 3.0	day^{-1}
Algal respiration rate	ρ	0.05 - 0.5	day^{-1}
Algal settling rate	σ_1	0.5 - 6.0	day^{-1}
Fraction of algal biomass that is nitrogen	α_1	0.07 - 0.09	dimensionless
Preference factor for ammonia nitrogen	P_N	0.0 - 1.0	dimensionless
Rate constant for the biological oxidation of ammonia nitrogen	β_1	0.1 - 1.0	day^{-1}
Coliform die-off rate	k_5	0.05 - 4	day^{-1}
Deoxigenation rate coefficient	k_1	0.02 - 3.4	day^{-1}
Rate of BOD loss due to settling	k_3	-0.36 - 0.36	day^{-1}
Reareation rate	k_2	0.0 - 100	day^{-1}
Rate of oxygen production per unit of algal photo-synthesis	α_3	1.4 - 1.8	dimensionless
Rate of oxygen uptake per unit of algae respired	α_4	1.6 - 2.3	dimensionless
Rate of oxygen uptake per unit of ammonia nitrogen oxidation	α_5	3.0 - 4.0	dimensionless
Ratio of chlorophyll alpha to algal biomass	α_0	10 - 100	μg-Chla/mg-A
Saturation concentration of Dissolved Oxygen	DO^*	-	mg/l

Table 1 Summary Table of water quality parameter involved in the differential continuity equations

Within the formulation as above, these assumption have been made:

- For dissolved oxygen: rate of oxygen involved in oxidation of ammonia to nitrite has been disregarded as nitrification-oxidation of ammonia to nitrate in one-stage process has been considered. Benthic oxygen uptake has not been considered.

- For ammonia nitrogen: benthos source rates have been disregarded

- For nitrate nitrogen: nitrification-oxidation of ammonia to nitrate has been considered a one-stage process. Contribution of organic nitrogen has not been considered.

The continuity equation algorithm is applied to river reach nodes and reservoirs nodes (lakes, storage reservoirs and small reservoirs).

For quality variables such as heavy metals, total phosphorus, suspended and inhibiting matters and adsorbable organic halogens, the DSS applies a heuristic proportionality approach, which updates the concentration as a function of incoming load and of reference concentrations and loads. Water quality is assumed to keep constant if the corresponding load keeps the same value as the reference, it worsens if the load increases, and it improves in the opposite case. In other words, the behaviour of the quality parameter at the generic supply node is in this case simulated according to the load received, by making the very rough estimation that it behaves in the same way as when reference concentrations and loads were measured. The reference concentrations and loads may be the ones at time zero, equal to the initial concentrations, and should be the *Most Recently Measured* (MRM) values. The models uses twelve reference values, one per month so as to consider the different monitored conditions over the period of one year. The equation used is the following:

$$X_{t+1} = X^0_{t+1} \cdot (Load(X)_t \, / \, Load(X)^0_t)$$

where:

X = Concentration of the generic pollutant
X0 = Reference concentration of the generic pollutant
Load(X) = Load of the generic pollutant
Load(X)0 = Reference Load of the generic pollutant

In case of groundwater, this heuristic proportionality approach is used for all the quality variables.

Water quality at supply nodes changes at each time step due to incoming loads carried by return flows from demand nodes and treatment plants. The loads at the exit of each waste water treatment plant are computed based on removal rates the DSS user has to assign to each quality variable before running the simulation. Analogously is for drinking treatment plant, but instead of removal rates, concentrations after process are here set. The loads generated from demand nodes are user-defined as well: a rate per unit of activity level is specified for each quality variable (see table below).

Demand Node	Generated Load Rate
Animal Breeding	Kg/(m^3 of return flow)
Industry	Kg/(unit production)
Irrigation	Kg/(m^2 irrigated area)
Settlement	g/capita*day
Tourist	g/capita*day

Table 2 Summary Table of Generated Load Rates for each demand category