



ASSIMILATION FACTOR ANALYSIS OF RIVERS FOR WATER QUALITY SIMULATION (AFAR-WQS)

User manual for MATLAB

Jonathan Nogales P & Carlos A. Rogéliz P.



TABLE OF CONTENTS

1	Introduction	4
2	Assimilation Factor	4
3	AFAR-WQS Inputs	8
4	Operation de AFAR-WQS	10
5	AFAR-WQS Model.....	13
5.1	Temperature Model (T)	13
5.2	Total Suspended Solids Model (SST)	15
5.3	Pathogenic Organisms Model (X)	17
5.4	Organic Nitrogen Model (NO)	20
5.5	Ammoniacal Nitrogen Model (NH ₄)	22
5.6	Nitrates Model (NO ₃)	26
5.7	Organic Phosphorus Model (Po)	29
5.8	Inorganic Phosphorus Model (Pi)	31
5.9	Organic Matter Model (OM)	34
5.10	Dissolved Oxygen Model – Dissolved Oxygen Deficiency (DOD)	37
5.11	Elemental Mercury Model (Hg ₀)	40
5.12	Divalent Mercury Model	44
5.13	Methyl Mercury Model	47
5.14	Summary of Assimilation Factors for AFAR-WQS Water Quality Determinants	50
6	Referencias	57

List of variables

Parameter	Description	Unit
ReachID	Unique positive integer numeric identifier of each reach in the topological network	-
FromNode	Positive integer numeric identifier of the initial node of a reach of the topological network.	-
ToNode	Positive integer numerical identifier of the end node of a reach of the topological network.	-
ReachType	Identifies whether the reach represents a mountain or plain river. If false is specified, the tool will assume that the reach represents a plain river.	-
RiverMouth	Identifies the river reach that corresponds to the basin closure point. If the value is false, it is considered not to be a closure point reach.	-
A	Drainage area of the river	m ²
Q	Flow in the river	m ³ /s
H	River depth	m
W	River width	m
U	Flow velocity in the river	m/s
TR	Residence time	day
τ	Advection time	day
\bar{t}	Average travel time	day
DF	Dispersive fraction	dimensionless
S	Slope river	m/m
L	River length	m
Z	River elevation	m.a.s.l
v_{sst}	Sedimentation velocity	m/day
k_{dX}	Constant decay of pathogenic organisms (mortality)	dimensionless
F_{px}	Fraction of pathogenic organisms adsorbed on solid particles	dimensionless
v_x	Sedimentation rate of the adsorbed fraction of pathogens on solid particles	m/day
k_{NO}	Decay rate by hydrolysis of organic nitrogen	1/day
v_{NO}	Sedimentation velocity of organic nitrogen	m/day
k_{NH4}	Nitrification decay rate	1/day
k_{dNO3}	Denitrification rate	1/day
F_{oxdNO3}	Factor considering the effect of low oxygen on denitrification	dimensionless
k_{Po}	Organic phosphorus hydrolysis decay rate	1/day
v_{Po}	Organic phosphorus sedimentation velocity	m/day
v_{Pi}	Inorganic phosphorus sedimentation velocity	m/day
k_{dOM}	Organic matter oxidation decay rate	1/day
F_{oxdOM}	Factor considering the effect of low oxygen on organic matter	dimensionless
k_a	Reaeration rate	1/day
v_v	Volatilization velocity of elemental mercury	m/day
k_{ox}	Elemental mercury oxidation reaction rate	1/day
k_{rx}	Oxidation decay rate of mercury	1/day
F_{pHg2}	Fraction of divalent mercury adsorbed onto solid particles	dimensionless
F_{pMeHg}	Fraction of methyl mercury adsorbed on solid particles	dimensionless
$k_{me,a}$	Adsorbed divalent mercury methylation rate	1/day
$k_{me,d}$	Dissolved divalent mercury methylation rate	1/day
g	acceleration of gravity	m/s ²
ν	kinematic viscosity of water	m ² /s
T	Temperature	°C
SST	Suspended solids concentration	mg/l
X	Pathogenic organisms concentration	NMP/l
NO	Organic nitrogen concentration	mg/l
NH4	Ammoniacal nitrogen concentration	mg/l
NO3	Nitrates concentration	mg/l
Po	Organic phosphorus concentration	mg/l
Pi	Inorganic phosphorus concentration	mg/l
OM	Organic matter concentration	mg/l
O	Dissolved oxygen concentration	mg/l
D	Oxygen deficit concentration	mg/l
O_s	Saturation oxygen concentration	mg/l
Hg0	Elemental mercury concentration	mg/l
Hg2	Divalent mercury concentration	mg/l
MeHg	Methyl mercury concentration	mg/l

1 Introduction

AFAR-WQS (Assimilation Factor Analysis of Rivers for Water Quality Simulation) is a mathematical modeling tool designed to facilitate rapid water quality analyzes at the macrobasin scale. This tool is based on the concept of assimilation factors (Chapra, 1997, 2008) and uses the equations formulated by Nogales et al. (2023) to simulate 13 key water quality parameters. These parameters include temperature (T), organic nitrogen (NO), ammoniacal nitrogen (NH_4^+), nitrates (NO_3^-), organic phosphorus (Po), inorganic phosphorus (Pi), organic matter (OM), dissolved oxygen (DO), total suspended solids (SS), pathogenic organisms (X), elemental mercury (Hg^0), divalent mercury (Hg^2) and methylmercury (MeHg).

AFAR-WQS operates on a graph representation of the drainage network of the watershed and uses a Depth-First Search (DFS) algorithm (Hopcroft & Tarjan, 1973). This algorithm explores the network from an initial node, following each path to its terminus before backtracking and exploring alternative paths, iteratively completing the entire network. During this process, the tool accumulates the loadings of the water quality determinants and applies the assimilation factor equations to evaluate the water quality conditions in each river reach. The modeling scheme assumes homogeneity in the physicochemical conditions within each reach of the river, which is defined as the minimum modeling unit.

AFAR-WQS represents a first approach to address water quality problems at the macro-basin scale. Its main objective is to provide an initial framework that encourages discussion on the need for specific tools to model large-scale water quality. While the tool is useful for preliminary decision making, it is not designed for detailed analysis of specific conditions. In such cases, additional efforts are necessary to acquire detailed data to enable calibration and validation of mathematical models adjusted to local conditions. Instead, the purpose of AFAR-WQS is to provide an overview of water quality in water systems at the macro-basin level, allowing comparisons between different scenarios and preliminary assessments of possible impacts.

Requirements

AFAR-WQS requires MATLAB™ R2019b or higher, equipped with Mapping Toolbox™ for correct operation.

2 Assimilation Factor

Conceptually, the assimilation factor can be understood as the capacity of the stream to assimilate a pollution event. According to Chapra (1997), this concept is related to the physical, chemical and biological effects that act on the polluting substance in the receiving stream. In this sense, assimilation factors allow the vulnerability of currents to be directly evaluated with respect to possible loads (Rojas, 2011).

Rivers or water streams can assimilate polluting load through three mechanisms: dilution, transport and decay. Below, these 3 elements are conceptualized theoretically:

- **Dilution:** It is associated with the magnitude of the flow of the receiving body. A river with a high flow and a low pollutant load upstream of a discharge will have the capacity to dilute the concentration of pollutant coming from an inflow, to generate a lower concentration downstream of it.

- **Transport:** The transport of the contaminant will be defined by two basic mechanisms, differential advection and turbulent diffusion, which together generate the phenomenon of longitudinal dispersion.
- **Decay:** It is related to physical (e.g. sedimentation), chemical (e.g. hydrolysis) and biological processes (e.g. oxidation, nitrification and death) that will depend on both the contaminating species and the characteristics of the receiving body.

Based on these three mechanisms, the concept of assimilation factor is defined (Chapra, 1997, 2008).

$$a = \frac{W_u}{C}$$

Where a is the assimilation factor (dependent on the characteristics of the receiving body and the contaminating species), W_u is the polluting load upstream of the section (the subscript u represents the concentration of the determinant upstream of the reach) and C is the downstream concentration.

The assimilation factors can be estimated using the equations of the ADZ-QUASAR water quality model (Lees et al., 1998), which integrates transport and transformation processes of contaminants under dynamic hydraulic conditions.

The Quality Simulation Among River Systems (QUASAR) model (Whitehead et al., 1998)), considers a series of well-mixed reactors, whose mass balance can be expressed for a non-conservative substance as:

$$\frac{dC(t)}{dt} = \frac{1}{\bar{t} - \tau} (C_u(t - \tau) - C(t)) + \sum sources - \sum sinks$$

In this case, t denotes time. When considering transportation phenomena (parameters t and TR of the ADZ model) and the effects of non-conservative substances through a decay term k , it is possible to develop a coupled ADZ-QUASAR model (Lees et al., 1998).

$$\frac{dC(t)}{dt} = \frac{1}{\bar{t} - \tau} ((C_u(t - \tau) * e^{-\tau*k}) - C(t)) + \sum sources - \sum sinks$$

To delve into its meaning and application, the general deduction of the equation that defines its mathematical expression is presented below, based on the foundations of the ADZ-QUASAR model. This deduction seeks to highlight the importance of assimilation factors as a key tool to model the capacity of water bodies to process and dilute contaminants in specific scenarios.

Consider the general equation of the ADZ-QUASAR model for steady state:

$$0 = \frac{1}{\bar{t} - \tau} [C_u e^{-k\tau} - C] - kC$$

Clearing concentration C from the previous equation:

$$kC = \frac{[C_u e^{-k\tau} - C]}{\bar{t} - \tau}$$

$$kC(\bar{t} - \tau) = C_u e^{-k\tau} - C$$

$$C + kC(\bar{t} - \tau) = C_u e^{-k\tau}$$

$$C(1 + k(\bar{t} - \tau)) = C_u e^{-k\tau}$$

$$C = \frac{C_u e^{-k\tau}}{(1 + k(\bar{t} - \tau))}$$

On the other hand, from the relationship of the Aggregate Dead Zone (ADZ) model it is known that:

$$DF = 1 - \frac{\tau}{\bar{t}}$$

That is to say that:

$$t = (1 - DF)\bar{t}$$

Substituting τ you get:

$$C = \frac{C_u e^{-k(1-DF)\bar{t}}}{(1 + k(\bar{t} - (1 - DF)\bar{t}))}$$

$$C = \frac{C_u e^{-k(1-DF)\bar{t}}}{1 + k[\bar{t}(1 - 1 + DF)]}$$

$$C = \frac{C_u e^{-k(1-DF)\bar{t}}}{1 + k\bar{t}DF}$$

Now, multiplying the numerator and denominator on the right side of the previous equation by the flow Q . You get:

$$C = \frac{QC_u e^{-k(1-DF)\bar{t}}}{Q(1 + k\bar{t}DF)}$$

Remembering the definition of load as the flow rate per concentration:

$$W = Q * C$$

It is obtained that:

$$C = \frac{\overbrace{QC_u}^{W_u} e^{-k(1-DF)\bar{t}}}{Q(1 + k\bar{t}DF)}$$

$$C = \frac{W_u e^{-k(1-DF)\bar{t}}}{Q(1 + k\bar{t}DF)}$$

$$\frac{C}{W_u} = \frac{e^{-k(1-DF)\bar{t}}}{Q(1 + k\bar{t}DF)}$$

Returning to the definition of Assimilation Factor, the previous equation can be written as:

$$a = \frac{W_u}{C}$$

$$\frac{1}{a} = \frac{C}{W_u}$$

$$\frac{1}{a} = \frac{e^{-k(1-DF)\bar{t}}}{Q(1 + k\bar{t}DF)}$$

Finally, the Assimilation Factor, based on the equations of the ADZ-R model, is defined as:

$$a = Q * \frac{(1 + k\bar{t}DF)}{e^{-k(1-DF)\bar{t}}}$$

The defined general expression constitutes a fundamental element in the analysis of water quality, since it establishes the theoretical basis for the deduction of the specific assimilation factors of each of the determinants considered in AFAR-WQS.

According to the general equation, the assimilation factor depends on three main components:

- The flow rate, which influences through the dilution assimilation effect.
- The dispersive fraction, associated with the longitudinal dispersion process, which contributes to the transport of the determinants.
- The decay rate (k), which represents assimilation through physicochemical and biological reactions or transformations.

Additionally, the assimilation factor is conditioned by the average travel time of the determinant through the section, a variable that in turn depends on the length of the analyzed section. This approach allows physical and chemical processes to be integrated into a coherent framework, highlighting the relevance of the assimilation factor concept to understand and model the dynamics of contaminants in river systems.

3 AFAR-WQS Inputs

To run AFAR-WQS, it is necessary to provide a structure called ReachData with dimensions [N×1], which represents the river network as a directed and interconnected graph. This structure organizes the information of the N sections of the network, defining the specific characteristics necessary for the modeling of water quality determinants within the AFAR-WQS framework.

Each row of the ReachData matrix contains the relevant data for a particular reach, such as geomorphological characteristics, hydraulic parameters, initial quality conditions and other factors that influence the behavior of the system. The **Figure 1** illustrates the structure and content of a fully defined ReachData array, making it easy to interpret and configure.

Figure 1. Example of an ReachData struct

Fields	Geometry	BoundingBox	X	Y	ReachID	FromNode	ToNode	RiverType	RiverMouth	Z	A	L	Qr	W	H	U	S	T	Qwqd
1	Line	[5.009e+06,2.16...	[5.009e+06...	[2.1651e+06...	867	906	907	0	0	3.1239e+03	52447854	588.5697	1.0025	21.8384	0.2416	0.1900	0.0109	10.6526	0.0501
2	Line	[5.0073e+06,2.16...	[5.0073e+06...	[2.1651e+06...	868	908	907	1	0	3.2579e+03	144029367	6.9235e+03	3.4183	31.1627	0.3945	0.2781	0.0379	9.8952	0.1709
3	Line	[4.9635e+06,2.15...	[4.9635e+06...	[2.1528e+06...	920	970	971	1	0	2.8514e+03	48221728	4.4599e+03	0.5633	21.2087	0.1919	0.1384	0.0968	12.1928	0.0282
4	Line	[4.9635e+06,2.15...	[4.9635e+06...	[2.1528e+06...	921	972	971	1	0	2.8190e+03	81422205	4.6350e+03	1.8842	25.4742	0.3109	0.2379	0.1118	12.3758	0.0942
5	Line	[4.9453e+06,2.15...	[4.9453e+06...	[2.1528e+06...	929	980	981	1	0	2.9003e+03	191382028	2.4743e+04	3.3008	34.3538	0.3890	0.2470	0.0702	11.9162	0.1650
6	Line	[4.9613e+06,2.15...	[4.9613e+06...	[2.1528e+06...	931	971	981	1	0	2.4225e+03	10413277	2.5096e+03	2.6500	30.7971	0.3563	0.2415	0.0737	14.6165	0.1325
7	Line	[5.0073e+06,2.15...	[5.0073e+06...	[2.1528e+06...	945	907	996	1	0	3.3159e+03	105115488	1.4223e+04	6.8650	40.3119	0.5213	0.3267	0.1154	9.5676	0.3433
8	Line	[5.0119e+06,2.15...	[5.0119e+06...	[2.1528e+06...	947	997	996	1	0	3.2502e+03	85766098	2.6266e+03	3.0508	25.9370	0.3770	0.3120	0.1871	9.9388	0.1525
9	Line	[4.9878e+06,2.15...	[4.9878e+06...	[2.1528e+06...	962	1015	1016	1	0	2.9457e+03	53935962	4.6006e+03	1.0008	22.0544	0.2415	0.1879	0.0903	11.6598	0.0500
10	Line	[4.9892e+06,2.15...	[4.9892e+06...	[2.1528e+06...	963	1017	1016	1	0	3.1946e+03	60610400	7.6595e+03	1.3142	22.9727	0.2692	0.2125	0.1300	10.2531	0.0657
11	Line	[5.0084e+06,2.15...	[5.0084e+06...	[2.1528e+06...	964	1018	1019	1	0	3.2369e+03	60231804	2.7899e+03	1.6292	22.9215	0.2994	0.2423	0.1268	10.0140	0.0815
12	Line	[5.0106e+06,2.15...	[5.0106e+06...	[2.1528e+06...	965	996	1019	1	0	2.5822e+03	10974563	3.4034e+03	10.3408	44.4212	0.6116	0.3769	0.1247	13.7142	0.5120
13	Line	[4.9494e+06,2.14...	[4.9494e+06...	[2.1427e+06...	991	1045	1046	1	0	2.8253e+03	70484959	3.6717e+03	1.1850	24.2228	0.2583	0.1894	0.0797	12.3399	0.0593
14	Line	[4.9783e+06,2.14...	[4.9783e+06...	[2.1427e+06...	992	1049	1048	1	0	2.6919e+03	138954204	9.3519e+03	3.6958	30.7108	0.4070	0.2957	0.1307	12.0939	0.1848
15	Line	[4.9381e+06,2.14...	[4.9381e+06...	[2.1427e+06...	994	1072	1046	1	0	2.8668e+03	134604103	1.0237e+04	2.0767	30.3754	0.3233	0.2115	0.0793	12.1059	0.1038
16	Line	[4.9759e+06,2.14...	[4.9759e+06...	[2.1427e+06...	995	1047	1048	1	0	2.4746e+03	56714485	3.0567e+03	1.8067	22.4467	0.3058	0.2632	0.1442	14.3209	0.0903
17	Line	[4.9460e+06,2.14...	[4.9460e+06...	[2.1427e+06...	1012	1046	1064	1	0	2.6049e+03	72908372	9.2889e+03	4.5583	39.1480	0.4426	0.2631	0.0890	13.5859	0.2279
18	Line	[4.9513e+06,2.14...	[4.9513e+06...	[2.1427e+06...	1017	1075	1064	1	0	2.8038e+03	45501282	1.6120e+03	0.9367	20.7838	0.2352	0.1916	0.1359	12.4619	0.0468
19	Line	[4.9524e+06,2.14...	[4.9524e+06...	[2.1427e+06...	1027	1064	1077	1	0	2.3381e+03	20559379	5.0032e+03	5.8942	42.1793	0.4905	0.2849	0.0981	15.0937	0.2947
20	Line	[4.9557e+06,2.14...	[4.9557e+06...	[2.1427e+06...	1028	981	1077	1	0	2.4978e+03	153730712	1.6942e+04	9.5975	47.5658	0.5959	0.3386	0.0735	14.1913	0.4799
21	Line	[5.0049e+06,2.14...	[5.0049e+06...	[2.1427e+06...	1032	1019	1084	1	0	2.3832e+03	72312511	1.4197e+04	14.8025	49.1076	0.7086	0.4254	0.2345	14.8388	0.7401
22	Line	[5.0020e+06,2.14...	[5.0020e+06...	[2.1427e+06...	1034	1085	1084	1	0	2.5884e+03	103951752	3.6120e+03	5.1650	27.7437	0.4652	0.4002	0.1333	13.6788	0.2583
23	Line	[4.9784e+06,2.14...	[4.9784e+06...	[2.1427e+06...	1036	1048	1090	1	0	1.9948e+03	54529664	9.7780e+03	7.5300	37.7265	0.5409	0.3690	0.1198	17.0339	0.3765
24	Line	[4.9824e+06,2.14...	[4.9824e+06...	[2.1427e+06...	1038	1016	1090	1	0	2.5994e+03	138951752	1.6530e+04	7.4617	37.8981	0.5389	0.3653	0.1196	13.6167	0.3731
25	Line	[4.9770e+06,2.13...	[4.9770e+06...	[2.1327e+06...	1060	1115	1110	1	0	1.8113e+03	24404054	5.6446e+03	4.6442	29.3273	0.4459	0.3551	0.1122	18.0710	0.2322
26	Line	[4.9816e+06,2.13...	[4.9816e+06...	[2.1327e+06...	1061	1090	1110	1	0	1.6716e+03	19034863	4.3659e+03	15.7475	48.8183	0.7263	0.4441	0.0762	18.8603	0.7814
27	Line	[4.9761e+06,2.13...	[4.9761e+06...	[2.1327e+06...	1066	1114	1115	1	0	2.5672e+03	46299858	1.2199e+03	1.6217	20.9088	0.2928	0.2648	0.3100	13.7969	0.0811

The description of each of the attributes that the ReachData structure must include is detailed in the variable list.

Table 1. Attributes that are assigned to each topological network reach.

Attributes	Unit	Description
ReachID	-	Unique positive integer numeric identifier of each reach in the topological network
FromNode	-	Positive integer numeric identifier of the initial node of a reach of the topological network.
ToNode	-	Positive integer numerical identifier of the end node of a reach of the topological network.
ReachType	-	Identifies whether the reach represents a plain or mountain river. If false is specified, the tool will assume that the reach represents a plain river. To define whether a river is a plain or a mountain river, a first criterion may be to assume that the former is limited by capacity (slope ≤ 0.025 m/m) and the latter by supply (slope > 0.025 m/m), this, following the slope thresholds defined by Flores et al. (2006) .A second criterion may be to use the slope threshold defined by Wohl & Merritt (2005) to define whether a river is mountain (slope > 0.002 m/m) or plain (slope < 0.002 m/m).
RiverMouth	-	Identifies the river reach that corresponds to the basin closure point. If the value is false, it is considered not to be a closure point reach.
DF^{**}	dimensionless	The tool estimates the dispersive fraction following the criteria of (González, 2008). For the sections of the topological network representing mountain rivers, an overall value of 0.27 is considered, while for plain rivers it is 0.40.
\bar{t}	day	The tool estimates the average travel time as: <div> $U_s = \frac{U}{1 + \beta}$ $\bar{t} = \left(\frac{L}{U_s} \right) * \left(\frac{1}{3600 * 24} \right)$ </div>

		Where U_s is solute velocity (m/s); β is the effective delay coefficient. According to (González, 2008) the effective delay coefficient for mountain rivers has an overall magnitude of 1.10 while for plain rivers it is 2.0.
τ^{**}	day	The tool estimates the advection time as: $\tau = \bar{\tau} * (1 - DF)$
TR^{**}	day	The tool estimates the residence time as: $TR = \bar{\tau} * DF$
L	m	River length representing the reach in the topological network
Z	m.a.s.l	Average elevation of the river representing the reach in the topological network
A	m ²	Drainage area of the river representing the reach in the topological network, accumulated up to the ToNode of the reach
Qr	m ³ /s	Average discharge of the river representing the reach in the topological network, for a selected discharge scenario
Qwwd	m ³ /s	Wastewater discharge
Q	m ³ /s	$Q = Qr + Qwwd$
W	m	Average width of the river's cross-section representing the reach in the topological network, for the selected discharge scenario. The width can be estimated from the DEM, satellite imagery (Schmitt et al., 2016; Tangi et al., 2019), physically-based relationships (Parker et al., 2007; Wilkerson & Parker, 2011), field studies, or global datasets.
H	m	Average depth of the water column in the river representing the reach in the topological network, for the selected discharge scenario. The depth can be estimated from physically-based relationships (Parker et al., 2007; Wilkerson & Parker, 2011), field studies, or global datasets.
U	m/s	Average velocity of the water column in the river representing the reach in the topological network, for the selected discharge scenario. The velocity can be derived by continuity or through physically-based relationships (Parker et al., 2007; Wilkerson & Parker, 2011) as well as from field studies or global datasets.
S	m/m	Slope of the river representing the reach in the topological network. The slope can be estimated from the DEM, field studies, or global datasets.
T	°C	Average river water temperature representing the reach of the topological network.
Load_T	°C	Average temperature of the wastewater discharges entering the river representing the reach of the topological network.
Load_SS*	mg/d	The load of solids entering the river reach.
Load_X*	MPN/day	Total coliform load entering the river reach.
Load_NO*	mg/day	Organic nitrogen load entering the river reach.
Load_NH4*	mg/day	Ammonia nitrogen load entering the river reach.
Load_NO3*	mg/day	Nitrates load entering the river reach.
Load_PO*	mg/day	Organic phosphorus load entering the river reach.
Load_PI*	mg/day	Inorganic phosphorus load entering the river reach.
Load_OM*	mg/day	Organic matter load entering the river reach.
Load_DO*	mg/day	The load of dissolved oxygen entering the river reach.
Load_Hg0*	mg/day	Elemental mercury load entering the river reach.
Load_Hg2*	mg/day	Divalent mercury load entering the river reach.
Load_MeHg*	mg/day	Methylmercury load entering the river reach.

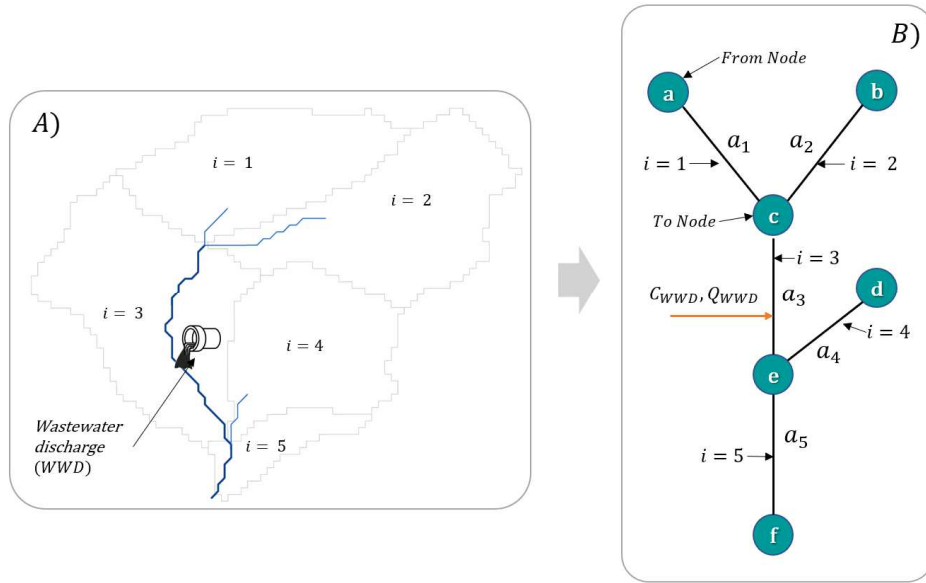
* The loads of various water quality determinants entering the river, represented by a reach in the topological network, are estimated as the sum of diffuse loads (contributions from land covers, livestock, fertilization, etc.) within the sub-basin draining into the river reach, along with the loads contributed by point-source wastewater discharges within the same reach.

** The user can assign a unique value for reach section of the topological network.

4 Operation de AFAR-WQS

As mentioned above, AFAR-WQS operates on a graph-shaped representation of the drainage network of the watershed. In this scheme, each microbasin is represented by two nodes and an arc, as shown in the **Figure 2**. This approach allows for the determination of connections between microwatersheds and facilitates the cumulative calculation of downstream variables, which is crucial for water quality modeling.

Figure 2. Representation of micro-basins in a graph scheme



Source: Nogales et al. (2023)

To illustrate the operation of the model, let's consider the headwater micro-basin $i = 1$ with an from node a and (a) to node (c) (Figure). The concentration of a water quality determinant j ($j = T, SST, NO, NH4, NO3, Po, Pi, OM, O, X, Hg0, Hg2, MeHg$) would be given by the ratio of the product of the concentration at node a ($C_{a1,j}$) and the flow of the micro-basin Q_1 , and the assimilation factor $a_{1,j}$:

$$C_{1,j} = \frac{C_{a1,j} Q_1}{a_{1,j}}$$

In the case of an intermediate micro-basin $i = 3$, where the confluence of micro-basins 1 and 2 occurs, and there is also a discharge with a concentration C_{WWDj} and a flow Q_{WWD} ; the concentration in this micro-basin for the water quality determinant j would be given by:

$$C_{3,j} = \frac{C_{1,j} Q_1 + C_{2,j} Q_2 + C_{WWDj} Q_{WWD}}{a_{3,j}}$$

The general equations for estimating the concentration of a water quality determinant j in intermediate and headwater watersheds are given by:

$$if \begin{cases} \text{Headwater} \\ \text{micro-basins} \end{cases} C_{i,j} = \frac{1}{a_{i,j}} \left[C_{n_{i,j}} Q_i + \sum_{k=1}^K Q_{WWD_{k,i}} C_{WWD_{k,i,j}} \right]$$

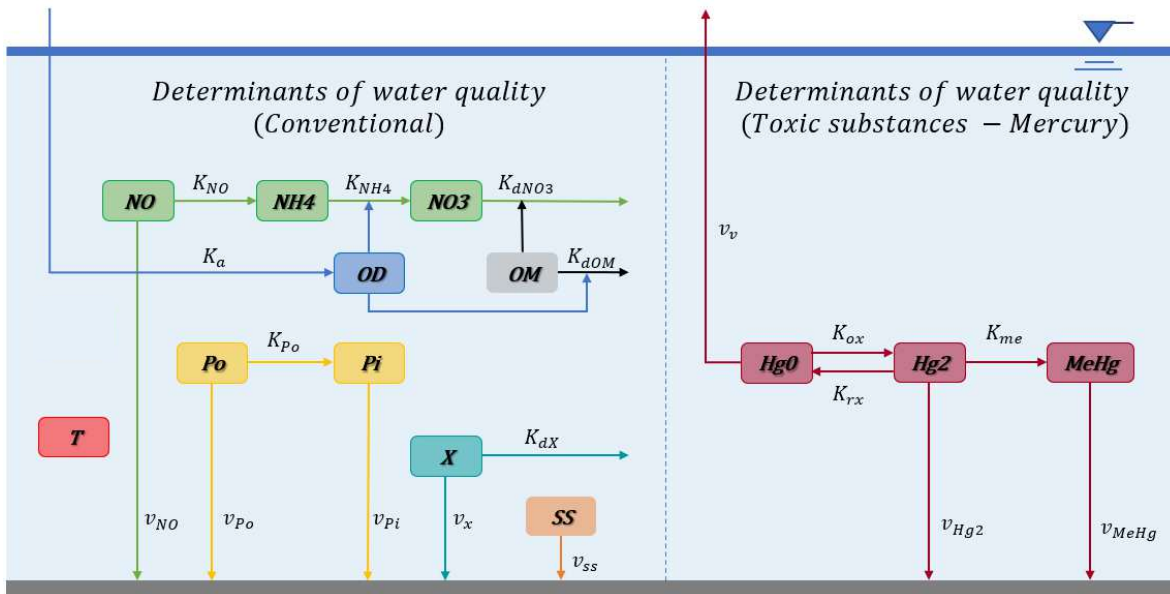
$$if \begin{cases} \text{Intermediate} \\ \text{micro-basins} \end{cases} C_{i,j} = \frac{1}{a_{i,j}} \left[\sum_{i=1}^I C_{i,j} Q_i + \sum_{k=1}^K Q_{WWD_{k,i}} C_{WWD_{k,i,j}} \right]$$

Where:

i	Micro-basin
j	Determinant of water quality
k	Wastewater discharge
I	Number of micro-basins upstream of micro-basin i
K	Number of WWD of determinate j in micro-basin i
Q_i	Flow of micro-basin i
$a_{i,j}$	Assimilation factor of micro-basin i of determinant j
$C_{i,j}$	Concentration of micro-basin i of determinant j
$C_{n_{i,j}}$	Concentration at the from node in micro-basin i of determinant j
$C_{WWD_{k,i,j}}$	Concentration of WWD in micro-basin i of determinant j
$Q_{WWD_{k,i}}$	Flow of WWD k in micro-basin i

The previous equation constitutes the first major equation of the proposed mathematical model. **Figure 3** conceptually summarizes the water quality quality determinants that can be modeled with AFAR-WQS.

Figure 3. AFAR-WQS conceptual model based on Assimilation Factors



Source: Nogales et al. (2023)

As mentioned above, AFAR-WQS uses a Depth-First Search (DFS) algorithm (Hopcroft & Tarjan, 1973)) to solve the drainage topological network. The function that performs this analysis is described below:

AnalysisNetwork_Obj(Network)

Description:

This function performs the cumulative and propagation processes in a topological drainage network using a Depth-First Search (DFS) scheme.

Input:

Network [Structure]

- .ReachID (mandatory): ID of the River Sections (Ad)
- .FromNode (mandatory): Initial Node of the River Sections (Ad)
- .ToNode (mandatory): End Node of the River Sections (Ad)
- .ReachID_RM (mandatory): ReachID of the River Sections corresponding to the River Mouth (Ad)
- .ProVar (optional): Variables to Propagate
- .AccumVar (optional): Variables to Accumulate
- .AccumClipVar (optional): Variables to Accumulate with Clipping
- .AccumLossVar (optional): Variables to Accumulate with Losses
- .AccumClipLossVar (optional): Variables to Accumulate with Losses and Clipping
- .ArcBarrier (optional): ReachID of the River Sections with Barriers (Ad)
- .CurrID (optional): ID of the Functional obj
- .LossRate (optional): Loss Rate (%)

Output:

- FuncNetwork: ID of the Functional Network by Barrier.
- ProVarOut: Propagated Variables
- AccumVarOut: Cumulative Variables
- AccumClipVarOut: Cumulative Variables With Clipping
- AccumLossVarOut: Cumulative Variables With Losses
- AccumClipLossVarOut: Cumulative Variables With Losses and Clipping
- PoNet: Position of the Network in one River Sections Special

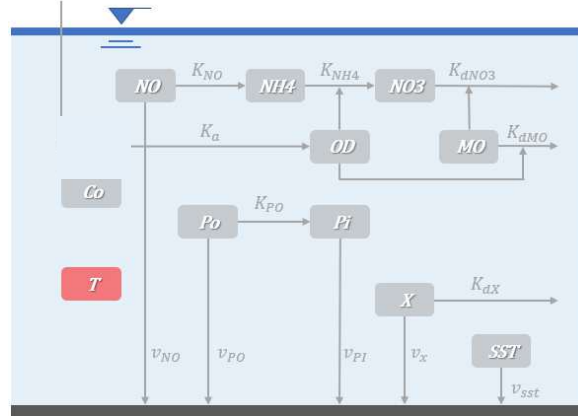
5 AFAR-WQS Model

Below, the models of water quality determinants that can be simulated using AFAR-WQS are described.

5.1 Temperature Model (T)

Temperature can be defined as a conventional determinant by the ADZ-QUASAR equation for conservative solutes (see **Figure 4**).

Figure 4. AFAR-WQS conceptual model – Temperature



In this way, the partial temperature equation of the ADZ-QUASAR model can be written as:

$$\frac{dT}{dt} = \frac{1}{TR} [T_u(t - \tau) - T(t)]$$

In stable state:

$$0 = \frac{1}{TR} [T_u - T]$$

In this way, it is concluded that:

$$T = T_u$$

Multiplying the right side by Q/Q , you get:

$$T = \frac{QT_u}{Q}$$

From the definition of load as flow times concentration:

$$W = Q * C$$

It is obtained that:

$$T = \frac{W_{T_u}}{\widehat{QT_u}}$$

$$T = \frac{W_{T_u}}{Q}$$

Therefore:

$$\frac{T}{W_{T_u}} = \frac{1}{Q}$$

Returning to the definition of Assimilation Factor, the previous expression can be written as:

$$a = \frac{W}{C}$$

$$\frac{1}{a} = \frac{C}{W}$$

$$\frac{1}{a_T} = \frac{1}{Q}$$

Finally, the assimilation factor for this water quality determinant is defined as follows:

$$a_T = Q$$

The function in AFAR-WQS that allows modeling this water quality determinant is described below.:

AFAR_Obj.WQS_T(Load_T)

Input:

Load_T (mandatory): Average temperature of the wastewater discharges entering the river representing the reach of the topological network [°C].

Output:

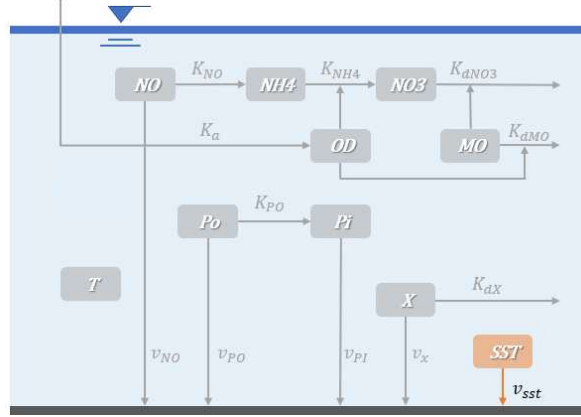
AF_T: Temperature assimilation factor [liters]

C_T: Temperature [°C]

5.2 Total Suspended Solids Model (SST)

AFAR-WQS considers that total suspended solids decay only by sedimentation, associated with a sedimentation velocity v_{ss} (see **Figure 5**). By default, AFAR-WQS considers $v_{ss} = 0.1 \text{ m/d}$ which is the default value that Qual2Kw uses.

Figure 5. Conceptual model of AFAR-WQS – Total Suspended Solids



With the aim of simplifying the mathematical handling in deduction, it is defined k_{sst} as:

$$k_{sst} = \frac{v_{sst}}{H}$$

Under these considerations, the formulation for the ADZ-QUASAR model for total suspended solids corresponds to:

$$\frac{dSST}{dt} = \frac{1}{TR} \left((SST_u(t - \tau) * e^{-\tau * k_{sst}}) - SST(t) \right) - \underbrace{k_{sst} * SST}_{\text{Sedimentation}}$$

Under the steady state assumption we have:

$$0 = \frac{1}{TR} \left((SST_u * e^{-\tau * k_{sst}}) - SST \right) - k_{sst} * SST$$

$$k_{sst} * SST = \frac{1}{TR} \left((SST_u * e^{-\tau * k_{sst}}) - SST \right)$$

$$k_{sst} * SST * TR = (SST_u * e^{-\tau * k_{sst}}) - SST$$

$$k_{sst} * SST * TR + SST = (SST_u * e^{-\tau * k_{sst}})$$

$$SST * (k_{sst} * TR + 1) = (SST_u * e^{-\tau * k_{sst}})$$

$$SST = SST_u * \left(\frac{e^{-\tau * k_{sst}}}{(k_{sst} * TR) + 1} \right)$$

Considering the definition of load as the flow rate per concentration:

$$W = Q * C$$

It is possible to multiply on the right side of the equation by Q/Q , obtaining:

$$SST = \frac{W_{SST_u}}{Q * SST_u} * \left(\frac{e^{-\tau * k_{sst}}}{(k_{sst} * TR) + 1} \right)$$

$$SST = \frac{W_{SST_u}}{Q} * \left(\frac{e^{-\tau * k_{sst}}}{(k_{sst} * TR) + 1} \right)$$

$$\frac{SST}{W_{SST_u}} = \frac{1}{Q} * \left(\frac{e^{-\tau * k_{sst}}}{(k_{sst} * TR) + 1} \right)$$

Returning to the definition of Assimilation Factor, the previous expression can be written as:

$$a = \frac{W_u}{C}$$

$$\frac{1}{a} = \frac{C}{W_u}$$

$$\frac{1}{a_{sst}} = \frac{1}{Q} * \left(\frac{e^{-\tau * k_{sst}}}{(k_{sst} * TR) + 1} \right)$$

Finally, the assimilation factor for this water quality determinant is defined as follows:

$$a_{sst} = Q * \left(\frac{(TR * k_{sst}) + 1}{e^{-\tau * k_{sst}}} \right)$$

From the relationship of the Aggregate Dead Zone (ADZ) model it is known that:

$$DF = 1 - \frac{\tau}{\bar{t}}$$

That is to say that:

$$\tau = \bar{t} * (1 - DF)$$

$$TR = \bar{t} * DF$$

Therefore, the concentration relationships and assimilation factor for suspended solids can be written as follows:

$$SST = SST_u * \left(\frac{e^{-\bar{t} * (1 - DF) * k_{sst}}}{(\bar{t} * DF * k_{sst}) + 1} \right)$$

$$a_{sst} = Q * \left(\frac{(\bar{t} * DF * k_{sst}) + 1}{e^{-\bar{t} * (1 - DF) * k_{sst}}} \right)$$

The function in AFAR-WQS that allows modeling this water quality determinant is described below.:

AFAR_Obj.WQS_SS('Load_SS','Vss')

Input:

Load_SS (mandatory): The load of solids entering the river, which represents the reach in the topological network [mg/d].

Vss (optional): Sedimentation velocity [m/d].

Output:

AF_SS: Suspended solids assimilation factor [liters].

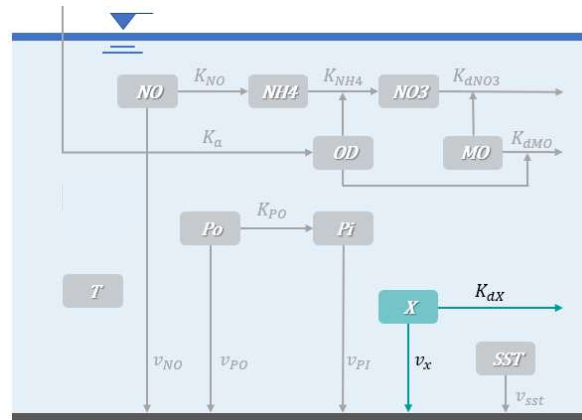
C_SS: Suspended solids concentration [mg/l].

W_SS: Solids suspended load [mg]

5.3 Pathogenic Organisms Model (X)

AFAR-WQS considers that pathogenic organisms decay due to mortality following a thermodependent rate, k_{dX} and by sedimentation associated with a sedimentation velocity v_X of the adsorbed fraction of pathogens to solid particles (F_p) (see **Figure 6**).

Figure 6. AFAR-WQS conceptual model – Pathogenic organisms



By default AFAR-WQS $k_{dX} = 0.8$ (Rojas, 2011). However, this value corresponds to the mortality rate for a temperature of 20°C, so it is corrected for the temperature of the network section, using the Arrhenius equation (Chapra, 2008):

$$k_{dX} = 0.8 * \theta^{T-20}$$

Where $\theta = 1.07$ according to Navas (2016)

AFAR-WQS considers by default $v_X = 1$ m/d which is the default value that Qual2Kw uses.

With regards to F_p , AFAR-WQS takes a default value of 0.7 which is a typical value according to (Rojas, 2011).

With the aim of simplifying the mathematical handling in deduction, it is defined k_X as:

$$k_X = k_{dX} + F_p * \frac{v_X}{H}$$

Under these considerations, the formulation for the ADZ-QUASAR model of Pathogenic Organisms (X) corresponds to:

$$\frac{dX}{dt} = \frac{1}{TR} \left((X_u(t - \tau) * e^{-\tau * k_X}) - X(t) \right) - \overbrace{\frac{k_{dX} * X}{\text{Mortality}}}^{-k_X * X} - \underbrace{F_p * \frac{v_X}{H} * X}_{\text{Sedimentation}}$$

In stable state:

$$0 = \frac{1}{TR} \left((X_u * e^{-\tau * k_X}) - X \right) - k_X * X$$

$$k_X * X = \frac{1}{TR} \left((X_u * e^{-\tau * k_X}) - X \right)$$

$$k_X * X * \frac{1}{TR} = (X_u * e^{-\tau * k_X}) - X$$

$$k_X * X * TR + X = X_u * e^{-\tau * k_X}$$

$$X * ((k_X * TR) + 1) = X_u * e^{-\tau * k_X}$$

$$X = X_u * \left(\frac{e^{-\tau * k_X}}{(k_X * TR) + 1} \right)$$

Considering the definition of load as the flow rate per concentration:

$$W = Q * C$$

It is possible to multiply on the right side of the equation by Q/Q, obtaining:

$$X = \frac{\overbrace{Q * X_u}^{W_{X_u}}}{Q} * \left(\frac{e^{-\tau * k_X}}{(k_X * TR) + 1} \right)$$

$$X = \frac{W_{X_u}}{Q} * \left(\frac{e^{-\tau * k_X}}{(k_X * TR) + 1} \right)$$

$$\frac{X}{W_{X_u}} = Q * \left(\frac{e^{-\tau * k_X}}{(k_X * TR) + 1} \right)$$

Returning to the definition of Assimilation Factor, the previous expression can be written as:

$$a = \frac{W_u}{C}$$

$$\frac{1}{a} = \frac{C}{W_u}$$

$$\frac{1}{a_X} = Q * \left(\frac{e^{-\tau * k_X}}{(k_X * TR) + 1} \right)$$

Finally, the assimilation factor for this water quality determinant is defined as follows:

$$a_X = Q * \left(\frac{(TR * k_X) + 1}{e^{-\tau * k_X}} \right)$$

From the relationship of the Aggregate Dead Zone (ADZ) model it is known that:

$$DF = 1 - \frac{\tau}{\bar{t}}$$

That is to say that:

$$\tau = \bar{t} * (1 - DF)$$

$$TR = \bar{t} * DF$$

Therefore, the concentration and assimilation factor relationships for pathogenic organisms can be written as follows:

$$X = X_u * \left(\frac{e^{-\bar{t} * (1 - DF) * k_X}}{(\bar{t} * DF * k_X) + 1} \right)$$

$$a_X = Q * \left(\frac{(\bar{t} * DF * k_X) + 1}{e^{-\bar{t} * (1 - DF) * k_X}} \right)$$

The function in AFAR-WQS that allows modeling this water quality determinant is described below.:

AFAR_Obj.WQS_X('Load_X','Vx','Fpx','Kdx')

Input:

- Load_X (mandatory):** The load of Pathogenic organisms entering the river, which represents the reach in the topological network [mg/d].
- Vx (optional):** Sedimentation velocity of the adsorbed fraction of pathogens on solid particles [m/d].
- Fpx (optional):** Fraction of pathogenic organisms adsorbed on solid particles [dimensionless].
- Kdx (optional):** Constant decay of pathogenic organisms (mortality) [dimensionless].

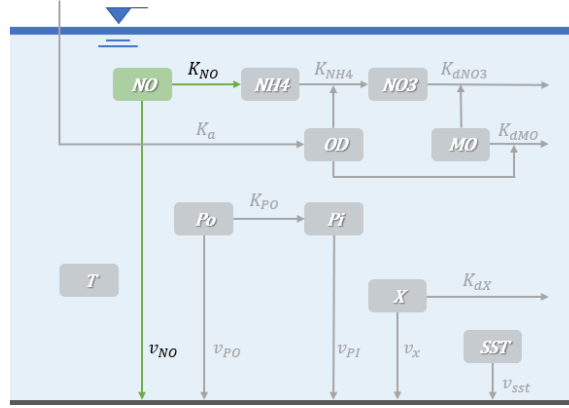
Output:

- AF_X:** Assimilation factor of Pathogenic organisms [liters].
- C_X:** Concentration of Pathogenic organisms [NMP/l].
- W_X:** Pathogenic organisms load [NMP]

5.4 Organic Nitrogen Model (NO)

AFAR-WQS considers that organic nitrogen decays by hydrolysis at a thermodependent rate k_{NO} and by sedimentation defined by a sedimentation velocity v_{NO} (see **Figure 7**).

Figure 7. AFAR-WQS conceptual model – Organic Nitrogen



By default AFAR-WQS considers $k_{NO} = 0.02$ (Bowie et al., 1985) However, this value corresponds to the hydrolysis rate for a temperature of 20°C, so it is corrected for the temperature of the network section, using the Arrhenius equation (Chapra, 2008):

$$k_{NO} = 0.02 * \theta^{T-20}$$

Where $\theta = 1.047$ according to Navas (2016).

AFAR-WQS considers by default $v_{NO} = 0.0005 \text{ m/d}$ which is the default value that Qual2Kw uses.

With the aim of simplifying the mathematical handling in deduction, it is defined k_{N1} as:

$$k_{N1} = k_{NO} + \frac{v_{NO}}{H}$$

Under these considerations, the formulation for the ADZ-QUASAR model of Organic Nitrogen (NO) corresponds to:

$$\frac{dNO}{dt} = \frac{1}{TR} \left((NO_u(t - \tau) * e^{-\tau * k_{N1}}) - NO(t) \right) - \overbrace{\frac{k_{NO} * NO}{Hydrolysis}}^{k_{N1} * NO} - \underbrace{\frac{v_{NO}}{H} * NO}_{Sedimentation}$$

Under the steady state assumption:

$$0 = \frac{1}{TR} \left((NO_u * e^{-\tau * k_{N1}}) - NO \right) - k_{N1} * NO$$

$$k_{N1} * NO = \frac{1}{TR} \left((NO_u * e^{-\tau * k_{N1}}) - NO \right)$$

$$TR * k_{N1} * NO = (NO_u * e^{-\tau * k_{N1}}) - NO$$

$$TR * k_{N1} * NO + NO = NO_u * e^{-\tau * k_{N1}}$$

$$(TR * k_{N1} + 1) * NO = NO_u * e^{-\tau * k_{N1}}$$

$$NO = NO_u * \left(\frac{e^{-\tau * k_{N1}}}{(TR * k_{N1}) + 1} \right)$$

Considering the definition of load as the flow rate per concentration:

$$W = Q * C$$

It is possible to multiply on the right side of the equation by Q/Q , obtaining:

$$NO = \frac{\overbrace{Q * NO_u}^{W_{NO_u}}}{Q} * \left(\frac{e^{-\tau * k_{N1}}}{(TR * k_{N1}) + 1} \right)$$

$$NO = \frac{W_{NO_u}}{Q} * \left(\frac{e^{-\tau * k_{N1}}}{(TR * k_{N1}) + 1} \right)$$

$$\frac{NO}{W_{NO_u}} = \frac{1}{Q} * \left(\frac{e^{-\tau * k_{N1}}}{(TR * k_{N1}) + 1} \right)$$

Returning to the definition of Assimilation Factor:

$$a = \frac{W_u}{C}$$

$$\frac{1}{a} = \frac{C}{W_u}$$

$$\frac{1}{a_{NO}} = \frac{1}{Q} * \left(\frac{e^{-\tau * k_{N1}}}{(TR * k_{N1}) + 1} \right)$$

Finally, the assimilation factor for this water quality determinant is defined as follows:

$$a_{NO} = Q * \left(\frac{(TR * k_{N1}) + 1}{e^{-\tau * k_{N1}}} \right)$$

From the relationship of the Aggregate Dead Zone (ADZ) model it is known that:

$$DF = 1 - \frac{\tau}{\bar{t}}$$

That is to say that:

$$\tau = \bar{t} * (1 - DF)$$

$$TR = \bar{t} * DF$$

Therefore, the concentration and assimilation factor relationships for organic nitrogen can be written as follows:

$$NO = NO_u * \left(\frac{e^{-\bar{t} * (1 - DF) * k_{N1}}}{(\bar{t} * DF * k_{N1}) + 1} \right)$$

$$a_{NO} = Q * \left(\frac{(\bar{t} * DF * k_{N1}) + 1}{e^{-\bar{t} * (1 - DF) * k_{N1}}} \right)$$

The function in AFAR-WQS that allows modeling this water quality determinant is described below.:

AFAR_Obj.WQS_NO('Load_NO','vno','kno')

Input:

Load_NO (mandatory): The load of organic nitrogen entering the river, which represents the reach in the topological network [mg/d].
vno (optional): Sedimentation velocity of organic nitrogen [m/d].
kno (optional): Decay rate by hydrolysis of organic nitrogen [1/d]

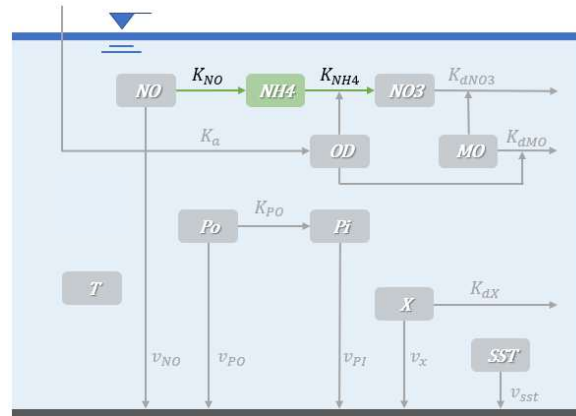
Output:

AF_NO: Assimilation factor of organic nitrogen [liters].
C_NO: Concentration of organic nitrogen [mg/l].
W_NO: Organic nitrogen load [mg].

5.5 Ammoniacal Nitrogen Model (NH4)

In the case of Ammoniacal Nitrogen (NH₄), AFAR-WQS considers contributions resulting from the hydrolysis of Organic Nitrogen (which must be carried out previously) and decay associated with the nitrification process, with a thermodependent rate. k_{NH4} (see **Figure 8**).

Figure 8. AFAR-WQS conceptual model – Ammoniacal Nitrogen



Various researchers have estimated the decay associated with the nitrification process considering the classification of the river as plain or mountainous. In this context, AFAR-WQS calculates the ammonium decay coefficient k_{NH4} according to this distinction.

A similar approach is presented by Nogales et al. (2023), who classify plain and mountain rivers based on limiting processes: plain rivers are limited by transportation, while mountain rivers are limited by supply. This classification uses a slope threshold (slope ≤ 0.025 m/m) based on the methodology of Flores et al. (2006). However, in AFAR-WQS, this classification is a configurable parameter that must be entered by the user, allowing the adaptation of the model to the specific conditions of the study basin.

For plain rivers, AFAR-WQS applies the equation proposed by Bansal, while for mountain rivers it uses the formulations developed by Couchaine following the recommendation of Robles & Camacho (2005).

$$\begin{aligned} \text{Plain rivers} \quad k_{NH40} &= \frac{10 \left(-3.421 + \log \left(\frac{\sqrt{gH^3}}{v} \right)^{1.36} \right) v}{H^2} \\ \text{Mountain rivers} \quad k_{NH40} &= 0.4381 \frac{U}{H} + 0.5394 \end{aligned}$$

It should be noted that the value of k_{NH4} calculated corresponds to a reference temperature of 20°C. To adjust this value to the specific temperature of each section of the river network, AFAR-WQS applies the Arrhenius equation (Chapra, 2008), whose use guarantees adequate correction according to thermal variation. The equation is expressed as:

$$k_{NH4} = k_{NH40} \theta^{T-20}$$

Where $\theta = 1.047$ according to Navas (2016).

With the aim of simplifying the mathematical handling in deduction, it is defined k_{N2} as:

$$k_{N2} = k_{NO} * \frac{NO}{NH4_u} - k_{NH4}$$

The formulation for the ADZ-QUASAR model of Ammoniacal Nitrogen (NH4) corresponds to:

$$\frac{dNH4}{dt} = \frac{1}{TR} \left((NH4_u(t - \tau) * e^{\tau * k_{N2}}) - NH4(t) \right) + \underbrace{\frac{k_{NO} * NO}{Hydrolysis}} - \underbrace{\frac{k_{NH4} * NH4}{Nitrification}}$$

Where k_{NH4} corresponds to the temperature-corrected nitrification rate.

Under the steady state assumption:

$$\begin{aligned} 0 &= \frac{1}{TR} \left((NH4_u * e^{\tau * k_{N2}}) - NH4 \right) + k_{NO} * NO - k_{NH4} * NH4 \\ k_{NH4} * NH4 - k_{NO} * NO &= \frac{1}{TR} \left((NH4_u * e^{\tau * k_{N2}}) - NH4 \right) \\ k_{NH4} * NH4 * TR - k_{NO} * NO * TR &= (NH4_u * e^{\tau * k_{N2}}) - NH4 \\ k_{NH4} * NH4 * TR + NH4 - k_{NO} * NO * TR &= NH4_u * e^{\tau * k_{N2}} \\ NH4 * (k_{NH4} * TR + 1) - k_{NO} * NO * TR &= NH4_u * e^{\tau * k_{N2}} \\ NH4 * (k_{NH4} * TR + 1) &= NH4_u * e^{\tau * k_{N2}} + k_{NO} * NO * TR \\ NH4 &= \frac{NH4_u * e^{\tau * k_{N2}} + k_{NO} * NO * TR}{(k_{NH4} * TR) + 1} \end{aligned}$$

Knowing that:

$$k_{N2} = k_{NO} \frac{NO}{NH4_u} - k_{NH4}$$

You have to:

$$NO = NH4_u \left(\frac{k_{N2} + k_{NH4}}{k_{NO}} \right)$$

Substituting into the equation we have:

$$NH4 = \frac{NH4_u * e^{\tau * k_{N2}} + k_{NO} * NH4_u * \left(\frac{k_{N2} + k_{NH4}}{k_{NO}} \right) * TR}{(k_{NH4} * TR) + 1}$$

$$NH4 = \frac{NH4_u * e^{\tau * k_{N2}} + NH4_u * (k_{N2} + k_{NH4}) * TR}{(k_{NH4} * TR + 1)}$$

$$NH4 = NH4_u * \left(\frac{e^{\tau * k_{N2}} + (TR * (k_{N2} + k_{NH4}))}{(k_{NH4} * TR) + 1} \right)$$

Considering the definition of load as the flow rate per concentration:

$$W = Q * C$$

It is possible to multiply on the right side of the equation by Q/Q , obtaining:

$$NH4 = \frac{\overbrace{Q * NH4_u}^{W_{NH4_u}}}{Q} * \left(\frac{e^{\tau * k_{N2}} + (TR * (k_{N2} + k_{NH4}))}{(k_{NH4} * TR) + 1} \right)$$

$$NH4 = \frac{W_{NH4_u}}{Q} * \left(\frac{e^{\tau * k_{N2}} + (TR * (k_{N2} + k_{NH4}))}{(k_{NH4} * TR) + 1} \right)$$

$$\frac{NH4}{W_{NH4_u}} = \frac{1}{Q} * \left(\frac{e^{\tau * k_{N2}} + (TR * (k_{N2} + k_{NH4}))}{(k_{NH4} * TR) + 1} \right)$$

Returning to the definition of Assimilation Factor:

$$a = \frac{W_u}{C}$$

$$\frac{1}{a} = \frac{C}{W_u}$$

$$\frac{1}{a_{NH4}} = \frac{1}{Q} * \left(\frac{e^{\tau * k_{N2}} + (TR * (k_{N2} + k_{NH4}))}{(k_{NH4} * TR) + 1} \right)$$

Finally, the assimilation factor for this water quality determinant is defined as follows:

$$a_{NH4} = Q * \left(\frac{(k_{NH4} * TR) + 1}{e^{\tau * k_{N2}} + (TR * (k_{N2} + k_{NH4}))} \right)$$

From the relationship of the Aggregate Dead Zone (ADZ) model it is known that:

$$DF = 1 - \frac{\tau}{\bar{t}}$$

That is to say that:

$$\tau = \bar{t} * (1 - DF)$$

$$TR = \bar{t} * DF$$

Therefore, the concentration and assimilation factor relationships for ammoniacal nitrogen can be written as follows:

$$NH4 = NH4_u * \left(\frac{e^{\bar{t} * (1 - DF) * k_{N2}} + (\bar{t} * DF * (k_{N2} + k_{NH4}))}{(k_{NH4} * \bar{t} * DF) + 1} \right)$$

$$a_{NH4} = Q * \left(\frac{(k_{NH4} * \bar{t} * DF) + 1}{e^{\bar{t} * (1 - DF) * k_{N2}} + (\bar{t} * DF * (k_{N2} + k_{NH4}))} \right)$$

The function in AFAR-WQS that allows modeling this water quality determinant is described below.:

AFAR_Obj.WQS_NH4('Load_NH4','C_NO','knh4','kno')

Input:

- Load_NH4 (mandatory):** The load of Ammoniacal nitrogen entering the river, which represents the reach in the topological network [mg/d].
- C_NO (optional):** Concentration of organic nitrogen [mg/l]. This parameter is optional as long as the organic nitrogen model has been run.
- knh4 (optional):** Nitrification decay rate [1/d].
- kno (optional):** Decay rate by hydrolysis of organic nitrogen [1/d]. This parameter is optional as long as the organic nitrogen model has been run.

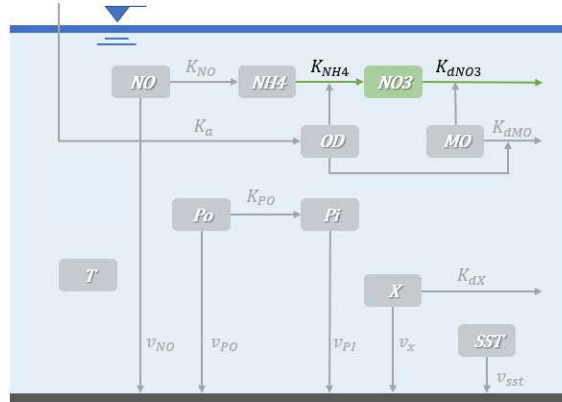
Output:

- AF_NH4:** Assimilation factor of ammoniacal nitrogen [liters].
- C_NH4:** Concentration of ammoniacal nitrogen [mg/l]
- W_NH4:** Ammoniacal nitrogen load [mg]

5.6 Nitrates Model (NO3)

AFAR.WQS considers that nitrates are generated as a result of the nitrification process and decay by denitrification (a process that occurs only under anaerobic conditions), with a thermodependent rate, k_{dNO3} . Inhibition in the presence of oxygen is considered by AFAR-WQS through the exponential model (see **Figure 9**).

Figure 9. AFAR-WQS conceptual model – Nitrates



By default AFAR-WQS considers $k_{dNO3} = 0.1$ (indicated in Qual2Kw as default value). However, this value corresponds to a temperature of 20°C, so it is corrected for the temperature of the network section, using the Arrhenius equation (Chapra, 2008):

$$k_{dNO3} = 0.1 * \theta^{T-20}$$

Where $\theta = 1.0698$ according to Navas (2016).

With the aim of simplifying the mathematical handling in deduction, it is defined k_{N3} and k_{NO3} as:

$$k_{NO3} = F_{oxdNO3} * k_{dNO3}$$

$$k_{N3} = k_{NH4} * \frac{NH4}{NO3_u} - k_{NO3}$$

Where F_{oxdNO3} It is the factor that considers the effect of low oxygen on denitrification. It is usually used $F_{oxdNO3} = \text{and}^{-0.60}$.

The formulation of Nitrates (NO3) corresponds to:

$$\frac{dNO3}{dt} = \frac{1}{TR} \left((NO3_u(t - \tau) * e^{\tau * k_{N3}}) - NO3(t) \right) + \underbrace{k_{NH4} * NH4}_{\text{Nitrification}} - \underbrace{k_{NO3} * NO3}_{\text{Desnitrification}}$$

Under the steady state assumption:

$$0 = \frac{1}{TR} \left((NO3_u * e^{\tau * k_{N3}}) - NO3 \right) + k_{NH4} * NH4 - k_{NO3} * NO3$$

$$k_{NO3} * NO3 - k_{NH4} * NH4 = \frac{1}{TR} \left((NO3_u * e^{\tau * k_{N3}}) - NO3 \right)$$

$$k_{NO3} * NO3 * TR - k_{NH4} * NH4 * TR = (NO3_u * e^{\tau * k_{N3}}) - NO3$$

$$\begin{aligned}
 k_{NO3} * NO3 * TR + NO3 - k_{NH4} * NH4 * TR &= NO3_u * e^{\tau * k_{N3}} \\
 NO3 * ((k_{NO3} * TR) + 1) - k_{NH4} * NH4 * TR &= NO3_u * e^{\tau * k_{N3}} \\
 NO3 * ((k_{NO3} * TR) + 1) &= NO3_u * e^{\tau * k_{N3}} + k_{NH4} * NH4 * TR \\
 NO3 &= \frac{NO3_u * e^{\tau * k_{N3}} + k_{NH4} * NH4 * TR}{(k_{NO3} * TR) + 1}
 \end{aligned}$$

Knowing that:

$$k_{N3} = k_{NH4} * \frac{NH4}{NO3_u} - k_{NO3}$$

You have to:

$$NH4 = NO3_u * \left(\frac{k_{N3} + k_{NO3}}{k_{NH4}} \right)$$

Substituting into the equation we have:

$$\begin{aligned}
 NO3 &= \frac{NO3_u * e^{\tau * k_{N3}} + k_{NH4} * NO3_u * \left(\frac{k_{N3} + k_{NO3}}{k_{NH4}} \right) * TR}{(k_{NO3} * TR) + 1} \\
 NO3 &= \frac{NO3_u * e^{\tau * k_{N3}} + NO3_u * (k_{N3} + k_{NO3}) * TR}{(k_{NO3} * TR) + 1} \\
 \mathbf{NO3} &= \mathbf{NO3_u * \left(\frac{e^{\tau * k_{N3}} + (TR * (k_{N3} + k_{NO3}))}{(k_{NO3} * TR) + 1} \right)}
 \end{aligned}$$

Considering the definition of load as the flow rate per concentration:

$$W = QC$$

It is possible to multiply on the right side of the equation by Q/Q , obtaining:

$$\begin{aligned}
 NO3 &= \frac{\overbrace{Q * NO3_u}^{W_{NO3u}}}{Q} * \left(\frac{e^{\tau * k_{N3}} + (TR * (k_{N3} + k_{NO3}))}{(k_{NO3} * TR) + 1} \right) \\
 NO3 &= \frac{W_{NO3u}}{Q} * \left(\frac{e^{\tau * k_{N3}} + (TR * (k_{N3} + k_{NO3}))}{(k_{NO3} * TR) + 1} \right) \\
 \frac{NO3}{W_{NO3u}} &= \frac{1}{Q} * \left(\frac{e^{\tau * k_{N3}} + (TR * (k_{N3} + k_{NO3}))}{(k_{NO3} * TR) + 1} \right)
 \end{aligned}$$

Returning to the definition of Assimilation Factor:

$$a = \frac{W_u}{C}$$

$$\frac{1}{a} = \frac{C}{W_u}$$

$$\frac{1}{a_{NO3}} = \frac{1}{Q} * \left(\frac{e^{\tau * k_{N3}} + (TR * (k_{N3} + k_{NO3}))}{(k_{NO3} * TR) + 1} \right)$$

Finally, the assimilation factor for this water quality determinant is defined as follows:

$$a_{NO3} = Q * \left(\frac{(k_{NO3} * TR) + 1}{e^{\tau * k_{N3}} + (TR * (k_{N3} + k_{NO3}))} \right)$$

From the relationship of the Aggregate Dead Zone (ADZ) model it is known that:

$$DF = 1 - \frac{\tau}{\bar{t}}$$

That is to say that:

$$\tau = \bar{t} * (1 - DF)$$

$$TR = \bar{t} * DF$$

Therefore, the concentration and assimilation factor relationships for nitrates can be written as follows:

$$NO3 = NO3_u * \left(\frac{e^{\bar{t} * (1 - DF) * k_{N3}} + (\bar{t} * DF * (k_{N3} + k_{NO3}))}{(\bar{t} * DF * k_{NO3}) + 1} \right)$$

$$a_{NO3} = Q * \left(\frac{(\bar{t} * DF * k_{NO3}) + 1}{e^{\bar{t} * (1 - DF) * k_{N3}} + (\bar{t} * DF * (k_{N3} + k_{NO3}))} \right)$$

The function in AFAR-WQS that allows modeling this water quality determinant is described below.:

AFAR_Obj.WQS_NO3('Load_NO3','C_NH4','knh4','kno')

Input:

Load_NO3 (mandatory): The load of nitrates entering the river, which represents the reach in the topological network [mg/d].

C_NH4 (optional): Concentration of ammoniacal nitrogen [mg/l]. This parameter is optional as long as the ammoniacal nitrogen model has been run.

knh4 (optional): Nitrification decay rate [1/d]. This parameter is optional as long as the ammoniacal nitrogen model has been run.

FoxdNO3 (optional): Factor considering the effect of low oxygen on denitrification [dimensionless].

kdNO3 (optional): Denitrification rate [1/d].

Output:

AF_NO3: Assimilation factor of nitrates [liters].

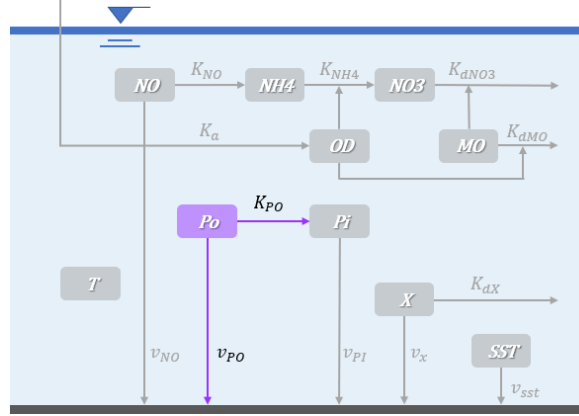
C_NO3: Concentration of nitrates [mg/l]

W_NO3: Nitrates load [mg]

5.7 Organic Phosphorus Model (Po)

AFAR-WQS considers that Organic Phosphorus (Po) decays by hydrolysis with a thermodependent rate k_{After} , and by sedimentation with a sedimentation velocity v_{Po} (see **Figure 10**).

Figure 10. AFAR-WQS conceptual model – Organic Phosphorus



By default AFAR-WQS considers $k_{Po} = 0.03$ (1/d) (default value uses Qual2Kw). However, this value corresponds to the hydrolysis rate for a temperature of 20°C, so it is corrected for the temperature of the network section, using the Arrhenius equation (Chapra, 2008):

$$k_{Po} = 0.03 * \theta^{T-20}$$

Where $\theta = 1.07$ according to Navas (2016).

AFAR-WQS considers by default $v_{Po} = 0.001$ (m/d) which is the default value that Qual2Kw uses.

With the aim of simplifying the mathematical handling in deduction, it is defined k_{Po1} as:

$$k_{Po1} = k_{Po} + \frac{v_{Po}}{H}$$

The formulation of the equation of the ADZ-QUASAR model of Organic Phosphorus (Po) corresponds to:

$$\frac{dPo}{dt} = \frac{1}{TR} \left((Po_u(t - \tau) * e^{-\tau * k_{Po1}}) - Po(t) \right) - \underbrace{\frac{-k_{Po1} * Po}{k_{Po1} * Po}}_{Hydrolysis} - \underbrace{\frac{v_{Po}}{H} Po}_{Sedimentation}$$

Under the steady state assumption:

$$0 = \frac{1}{TR} \left((Po_u * e^{-\tau * k_{Po1}}) - Po \right) - k_{Po1} * Po$$

$$k_{Po1} * Po = \frac{1}{TR} \left((Po_u * e^{-\tau * k_{Po1}}) - Po \right)$$

$$k_{Po1} * Po * TR = (Po_u * e^{-\tau * k_{Po1}}) - Po$$

$$k_{Po1} * Po * TR + Po = Po_u * e^{-\tau * k_{Po1}}$$

$$Po * ((TR * k_{Po1}) + 1) = Po_u * e^{-\tau * k_{Po1}}$$

$$Po = Po_u * \left(\frac{e^{-\tau * k_{Po1}}}{(TR * k_{Po1}) + 1} \right)$$

Considering the definition of load as the flow rate per concentration:

$$W = Q * C$$

It is possible to multiply on the right side of the equation by Q/Q , obtaining:

$$Po = \frac{\overbrace{Q * Po_u}^{W_{Po_u}}}{Q} * \left(\frac{e^{-\tau * k_{Po1}}}{TR * k_{Po1} + 1} \right)$$

$$Po = \frac{W_{Po_u}}{Q} * \left(\frac{e^{-\tau * k_{Po1}}}{TR * k_{Po1} + 1} \right)$$

$$\frac{Po}{W_{Po_u}} = \frac{1}{Q} * \left(\frac{e^{-\tau * k_{Po1}}}{TR * k_{Po1} + 1} \right)$$

Returning to the definition of Assimilation Factor:

$$a = \frac{W_u}{C}$$

$$\frac{1}{a} = \frac{C}{W_u}$$

$$\frac{1}{a_{Po}} = \frac{1}{Q} * \left(\frac{e^{-\tau * k_{Po1}}}{TR * k_{Po1} + 1} \right)$$

Finally, the assimilation factor for this water quality determinant is defined as follows:

$$a_{Po} = Q * \left(\frac{(TR * k_{Po1}) + 1}{e^{-\tau * k_{Po1}}} \right)$$

From the relationship of the Aggregate Dead Zone (ADZ) model it is known that:

$$DF = 1 - \frac{\tau}{\bar{t}}$$

That is to say that:

$$\tau = \bar{t} * (1 - DF)$$

$$TR = \bar{t} * DF$$

Therefore, the concentration and assimilation factor relationships for organic phosphorus can be written as follows:

$$Po = Po_u * \left(\frac{e^{-\bar{t} * (1 - DF) * k_{Po1}}}{(\bar{t} * DF * k_{Po1}) + 1} \right)$$

$$a_{Po} = Q * \left(\frac{(\bar{t} * DF * k_{Po1}) + 1}{e^{-\bar{t} * (1-DF) * k_{Po1}}} \right)$$

The function in AFAR-WQS that allows modeling this water quality determinant is described below.:

AFAR_Obj.WQS_PO('Load_PO','vpo','kpo')

Input:

Load_PO (mandatory): The load of organic phosphorus entering the river, which represents the reach in the topological network [mg/d].
vpo (optional): Organic phosphorus sedimentation velocity [m/d].
kpo (optional): Organic phosphorus hydrolysis decay rate [1/d]

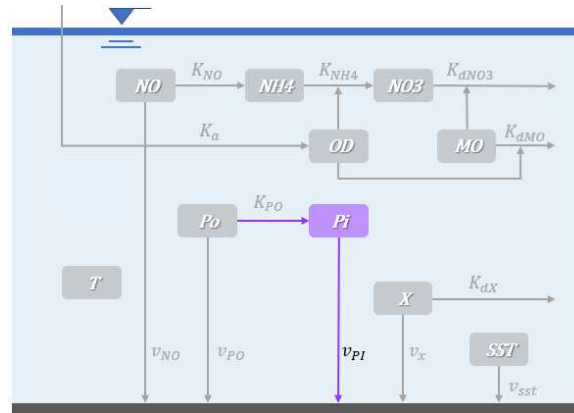
Output:

AF_PO: Assimilation factor of organic phosphorus [liters].
C_PO: Concentration of organic phosphorus [mg/l].
W_PO: Organic phosphorus load [mg].

5.8 Inorganic Phosphorus Model (Pi)

For the AFAR-WQS inorganic phosphorus model, it considers contributions resulting from the hydrolysis of organic phosphorus and losses only through sedimentation, associated with a sedimentation velocity v_{Pi} (**Figure 11** By default, AFAR-WQS considers $v_{Pi} = 0.8$ (m/d) which is the default value that Qual2Kw uses.

Figure 11. AFAR-WQS conceptual model – Inorganic Phosphorus



With the aim of simplifying the mathematical handling in deduction, it is defined k_{Pi2} and k_{Pi} as:

$$k_{Pi} = \frac{v_{Pi}}{H}$$

$$k_{Pi2} = k_{Po} * \frac{Po}{Pi_u} - k_{Pi}$$

The formulation for the ADZ-QUASAR model corresponds to:

$$\frac{dPi}{dt} = \frac{1}{TR} \left((Pi_u(t - \tau) e^{\tau * k_{Pi2}}) - Pi(t) \right) + \underbrace{\frac{k_{HPO} * Po}{Hydrolysis}} - \underbrace{\frac{k_{Pi} * Pi}{Sedimentation}}$$

Under the steady state assumption:

$$\begin{aligned}
 0 &= \frac{1}{TR} \left((Pi_u e^{\tau * k_{Pi2}}) - Pi \right) + k_{HPo} * Po - k_{Pi} * Pi \\
 k_{Pi} * Pi - k_{HPo} * Po &= \frac{1}{TR} \left((Pi_u e^{\tau * k_{Pi2}}) - Pi \right) \\
 k_{Pi} * Pi * TR - k_{HPo} * Po * TR &= (Pi_u e^{\tau * k_{Pi2}}) - Pi \\
 k_{Pi} * Pi * TR + Pi - k_{HPo} * Po * TR &= (Pi_u e^{\tau * k_{Pi2}}) \\
 Pi * ((TR * k_{Pi}) + 1) - k_{HPo} * Po * TR &= (Pi_u e^{\tau * k_{Pi2}}) \\
 Pi * ((TR * k_{Pi}) + 1) &= Pi_u e^{\tau * k_{Pi2}} + k_{HPo} * Po * TR \\
 Pi &= \frac{Pi_u e^{\tau * k_{Pi2}} + k_{HPo} * Po * TR}{((TR * k_{Pi}) + 1)}
 \end{aligned}$$

Knowing that:

$$k_{P2} = k_{Po} * \frac{Po}{Pi_u} - k_{Pi}$$

You have to:

$$Po = Pi_u * \left(\frac{k_{P2} + k_{Pi}}{k_{Po}} \right)$$

Substituting into the equation we have:

$$\begin{aligned}
 Pi &= \frac{Pi_u e^{\tau * k_{Pi2}} + k_{Po} * Pi_u * \left(\frac{k_{P2} + k_{Pi}}{k_{Po}} \right) * TR}{((TR * k_{Pi}) + 1)} \\
 Pi &= \frac{Pi_u e^{\tau * k_{Pi2}} + Pi_u * (k_{P2} + k_{Pi}) * TR}{((TR * k_{Pi}) + 1)} \\
 \mathbf{Pi} &= \mathbf{Pi_u * \left(\frac{e^{\tau * k_{Pi2}} + (TR * (k_{P2} + k_{Pi}))}{(TR * k_{Pi}) + 1} \right)}
 \end{aligned}$$

Considering the definition of load as the flow rate per concentration:

$$W = Q * C$$

It is possible to multiply on the right side of the equation by Q/Q , obtaining:

$$\begin{aligned}
 Pi &= \frac{\overbrace{Q * Pi_u}^{W_{Pi_u}}}{Q} * \left(\frac{e^{\tau * k_{Pi2}} + (TR * (k_{P2} + k_{Pi}))}{(TR * k_{Pi}) + 1} \right) \\
 Pi &= \frac{W_{Pi_u}}{Q} * \left(\frac{e^{\tau * k_{Pi2}} + (TR * (k_{P2} + k_{Pi}))}{(TR * k_{Pi}) + 1} \right)
 \end{aligned}$$

$$\frac{Pi}{W_{Pi_u}} = \frac{1}{Q} * \left(\frac{e^{\tau * k_{Pi2}} + (TR * (k_{P2} + k_{Pi}))}{(TR * k_{Pi}) + 1} \right)$$

Returning to the definition of Assimilation Factor:

$$a = \frac{W_u}{C}$$

$$\frac{1}{a} = \frac{C}{W_u}$$

$$\frac{1}{a_{Pi}} = \frac{1}{Q} * \left(\frac{e^{\tau * k_{Pi2}} + (TR * (k_{P2} + k_{Pi}))}{(TR * k_{Pi}) + 1} \right)$$

Finally, the assimilation factor for this water quality determinant is defined as follows:

$$a_{Pi} = Q * \left(\frac{(TR * k_{Pi}) + 1}{e^{\tau * k_{Pi2}} + (TR * (k_{P2} + k_{Pi}))} \right)$$

From the relationship of the Aggregate Dead Zone (ADZ) model it is known that:

$$DF = 1 - \frac{\tau}{\bar{t}}$$

That is to say that:

$$\tau = \bar{t} * (1 - DF)$$

$$TR = \bar{t} * DF$$

Therefore, the concentration and assimilation factor relationships for inorganic phosphorus can be written as follows:

$$Pi = Pi_u * \left(\frac{e^{\bar{t} * (1 - DF) * k_{Pi2}} + (\bar{t} * DF * (k_{P2} + k_{Pi}))}{(\bar{t} * DF * k_{Pi}) + 1} \right)$$

$$a_{Pi} = Q * \left(\frac{(\bar{t} * DF * k_{Pi}) + 1}{e^{\bar{t} * (1 - DF) * k_{Pi2}} + (\bar{t} * DF * (k_{P2} + k_{Pi}))} \right)$$

The function in AFAR-WQS that allows modeling this water quality determinant is described below.:

AFAR_Obj.WQS_PI('Load_PI','C_PO','vpi','kpo')

Input:

- Load_PI (mandatory):** The load of inorganic phosphorus entering the river, which represents the reach in the topological network [mg/d].
- C_PO:** Concentration of organic phosphorus [mg/l].
- vpi (optional):** Inorganic phosphorus sedimentation velocity [m/d].
- kpo (optional):** Organic phosphorus hydrolysis decay rate [1/d].

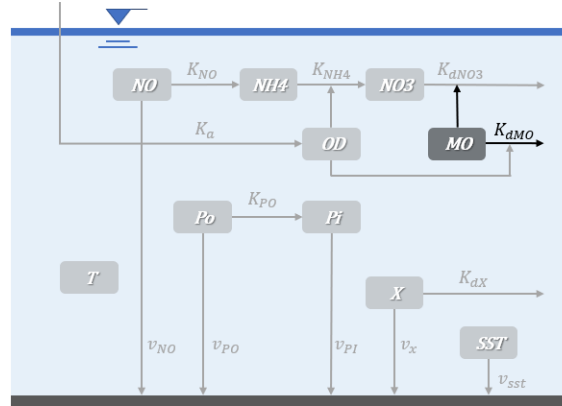
Output:

- AF_PI:** Assimilation factor of inorganic phosphorus [liters].
- C_PI:** Concentration of inorganic phosphorus [mg/l].
- W_PI:** Inorganic phosphorus load [mg].

5.9 Organic Matter Model (OM)

AFAR-WQS considers that Organic Matter decays by oxidation under aerobic conditions, determined by a thermodependent rate, k_{dMO} and by denitrification under anaerobic conditions, following an exponential inhibition model (see **Figure 12**).

Figure 12. AFAR-WQS conceptual model – Organic Matter



With the aim of simplifying the mathematical handling in deduction, it is defined σ_{MO} , θ_{MO} , and k_{MO2} as:

$$\begin{aligned}\sigma_{MO} &= F_{oxdMO} * k_{dMO} \\ \theta_{MO} &= 0.00286 * (1 - F_{oxdNO3}) * k_{dNO3} \\ k_{MO2} &= -\theta_{MO} * \frac{NO3}{MO_u} - \sigma_{MO}\end{aligned}$$

Where F_{oxdMO} It is the factor that considers the effect of oxygen. It is usually used $F_{oxdMO} = 1 - e^{-0.60}$.

Default AFAR-WQS estimates k_{dMO} as a function of flow following the expression proposed by Wright y McDonnell (1979).

$$\begin{aligned}\text{if } Q \leq 23 \text{ m}^3/\text{s} \quad & k_{dMO} = 1.796Q^{-0.49} \\ \text{if } Q > 23 \text{ m}^3/\text{s} \quad & k_{dMO} = 3.5\end{aligned}$$

However, this value corresponds to the oxidation rate for a temperature of 20°C, so it is corrected for the temperature of the network section, using the Arrhenius equation (Chapra, 2008):

$$k_{dMO} = k_{dMO} * \theta^{T-20}$$

Where $\theta = 1.047$ according to Navas (2016).

The formulation for the ADZ-QUASAR model for Organic Matter corresponds to:

$$\frac{dMO}{dt} = \frac{1}{TR} \left((MO_u(t - \tau) * e^{\tau * k_{MO2}}) - MO(t) \right) - \underbrace{\frac{\theta_{MO} * NO3}{\text{Nitrification}}}_{\text{Nitrification}} - \underbrace{\frac{\sigma_{MO} * MO}{\text{Oxidation}}}_{\text{Oxidation}}$$

Under the steady state assumption:

$$\begin{aligned}
 0 &= \frac{1}{TR} \left((MO_u * e^{\tau * k_{MO2}}) - MO \right) - \theta_{OD} * NO3 - \sigma_{OD} * MO \\
 \theta_{OD} * NO3 + \sigma_{OD} * MO &= \frac{1}{TR} \left((MO_u * e^{\tau * k_{MO2}}) - MO \right) \\
 TR * \theta_{OD} * NO3 + TR * \sigma_{OD} * MO &= (MO_u * e^{\tau * k_{MO2}}) - MO \\
 TR * \theta_{OD} * NO3 + TR * \sigma_{OD} * MO + MO &= MO_u * e^{\tau * k_{MO2}} \\
 TR * \theta_{OD} * NO3 + MO * (TR * \sigma_{OD} + 1) &= MO_u * e^{\tau * k_{MO2}} \\
 MO * (TR * \sigma_{OD} + 1) &= MO_u * e^{\tau * k_{MO2}} - TR * \theta_{OD} * NO3 \\
 MO &= \frac{MO_u * e^{\tau * k_{MO2}} - TR * \theta_{OD} * NO3}{(TR * \sigma_{OD}) + 1}
 \end{aligned}$$

Knowing that:

$$k_{MO2} = -\theta_{MO} * \frac{NO3}{MO_u} - \sigma_{MO}$$

You have to:

$$NO3 = MO_u * \left(\frac{-\sigma_{OD} - k_{MO2}}{\theta_{OD}} \right)$$

Substituting into the equation we have:

$$\begin{aligned}
 MO &= \frac{MO_u * e^{\tau * k_{MO2}} - TR * \theta_{OD} * MO_u * \left(\frac{-\sigma_{OD} - k_{MO2}}{\theta_{OD}} \right)}{(TR * \sigma_{OD}) + 1} \\
 MO &= \frac{MO_u * e^{\tau * k_{MO2}} - TR * MO_u * (-\sigma_{OD} - k_{MO2})}{(TR * \sigma_{OD}) + 1} \\
 MO &= MO_u * \left(\frac{e^{\tau * k_{MO2}} - (TR * (-\sigma_{OD} - k_{MO2}))}{(TR * \sigma_{OD}) + 1} \right) \\
 \mathbf{MO} &= \mathbf{MO_u * \left(\frac{e^{\tau * k_{MO2}} + (TR * (k_{MO2} + \sigma_{MO}))}{(TR * \sigma_{OD}) + 1} \right)}
 \end{aligned}$$

Considering the definition of load as the flow rate per concentration:

$$W = QC$$

It is possible to multiply on the right side of the equation by Q/Q , obtaining:

$$MO = \frac{\overbrace{Q * MO_u}^{W_{MO_u}}}{Q} * \left(\frac{e^{\tau * k_{MO2}} + (TR * (k_{MO2} + \sigma_{MO}))}{(TR * \sigma_{OD}) + 1} \right)$$

$$MO = \frac{W_{MO_u}}{Q} * \left(\frac{e^{\tau * k_{MO2}} + (TR * (k_{MO2} + \sigma_{MO}))}{(TR * \sigma_{OD}) + 1} \right)$$

$$\frac{MO}{W_{MO_u}} = \frac{1}{Q} * \left(\frac{e^{\tau * k_{MO2}} + (TR * (k_{MO2} + \sigma_{MO}))}{(TR * \sigma_{OD}) + 1} \right)$$

Returning to the definition of Assimilation Factor:

$$a = \frac{W_u}{C}$$

$$\frac{1}{a} = \frac{C}{W_u}$$

$$\frac{1}{a_{MO}} = \frac{1}{Q} * \left(\frac{e^{\tau * k_{MO2}} + (TR * (k_{MO2} + \sigma_{MO}))}{(TR * \sigma_{OD}) + 1} \right)$$

Finally, the assimilation factor for this water quality determinant is defined as follows:

$$a_{MO} = Q * \left(\frac{(\sigma_{MO} * TR) + 1}{e^{\tau * k_{MO2}} + (TR * (k_{MO2} + \sigma_{MO}))} \right)$$

From the relationship of the Aggregate Dead Zone (ADZ) model it is known that:

$$DF = 1 - \frac{\tau}{\bar{t}}$$

That is to say that:

$$\tau = \bar{t} * (1 - DF)$$

$$TR = \bar{t} * DF$$

Therefore, the concentration and assimilation factor relationships for organic matter can be written as follows:

$$MO = MO_u * \left(\frac{e^{\bar{t} * (1 - DF) * k_{MO2}} + (\bar{t} * DF * (k_{MO2} + \sigma_{MO}))}{(\bar{t} * DF * \sigma_{OD}) + 1} \right)$$

$$a_{MO} = Q * \left(\frac{(\bar{t} * DF * \sigma_{MO}) + 1}{e^{\bar{t} * (1 - DF) * k_{MO2}} + (\bar{t} * DF * (k_{MO2} + \sigma_{MO}))} \right)$$

The function in AFAR-WQS that allows modeling this water quality determinant is described below:

AFAR_Obj.WQS_OM('Load_OM','C_NO3','kdOM','FoxdNO3','kdNO3')

Input:

Load_OM (mandatory): The load of organic matter entering the river, which represents the reach in the topological network [mg/d].

C_NO3 (optional): Nitrates concentration [mg/l]. This parameter is optional as long as the nitrates model has been run.

kdOM (optional): Organic matter oxidation decay rate [1/d].

FoxdNO3 (optional): Factor considering the effect of low oxygen on denitrification [dimensionless]. This parameter is optional as long as the nitrates model has been run.

kdNO3 (optional): Denitrification rate [1/d]. This parameter is optional as long as the nitrates model has been run.

Output:

AF_OM: Organic matter assimilation factor [liters].

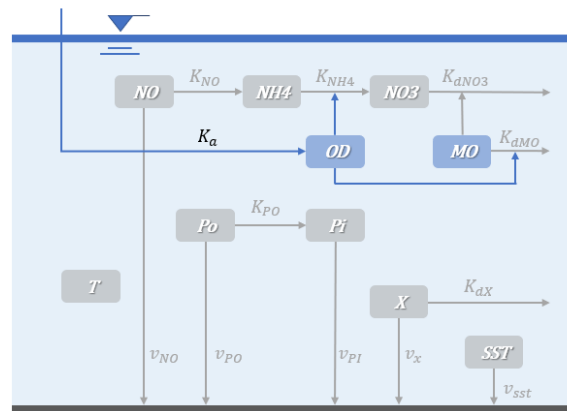
C_OM: Organic matter concentration [mg/l]

W_OM: Organic matter load [mg]

5.10 Dissolved Oxygen Model – Dissolved Oxygen Deficiency (DOD)

AFAR-WQS uses assimilation factors for determinants that represent a pollution load for the river. Since dissolved oxygen cannot be defined as a contaminant load, instead of oxygen AFAR-WQS uses the Oxygen Deficit Assimilation Factor with respect to saturation oxygen. For this, AFAR-WQS considers that the oxygen deficit will increase due to the contributions of the oxidation of organic matter and the nitrification process and will decrease or increase depending on the re-aeration processes associated with the thermodependent rate. k_a (see **Figure 13**).

Figure 13. AFAR-WQS conceptual model – Dissolved Oxygen Deficiency



The difference between Oxygen Saturation (O_s) and the concentration of Dissolved Oxygen (O), is called oxygen deficiency and is represented by the letter D .

$$O = O_s - D$$

AFAR-WQS uses the equation proposed by Zison et al. (1978) to estimate oxygen saturation, using temperature and elevation.

$$O_s = (1 - (0.0001148 * Z)) * e^{(-139.34411 + \frac{(1.575701E5)}{(T+273.15)} - \frac{(6.642308E7)}{(T+273.15)^2} + \frac{(1.243800E10)}{(T+273.15)^3} - \frac{(8.621949E11)}{(T+273.15)^4})}$$

AFAR-WQS estimates the reaeration rate using the equations presented in the **Table 2**.

Table 2. Reaeration rate equations

Parameters	Mountain Rivers			plain rivers	
Range	O'Connor – Dubbins $0.3 \leq H < 9.14$ $0.15 \leq U < 0.49$	Churchill $0.31 \leq H$ < 3.35 $0.55 \leq U$ < 1.42	Owens – Gibbs $0.12 \leq H$ < 0.73 $0.03 \leq U$ < 0.55	Tsivoglou y Neal $0.0283 \leq Q < 0.4247$	Tsivoglou y Neal $0.4247 \leq Q < 84.938$
Equation	$k_a = 3.93 \frac{U^{0.5}}{H^{1.5}}$	$k_a = 5.026 \frac{U}{H^{1.67}}$	$k_a = 5.32 \frac{U^{0.67}}{H^{1.85}}$	$k_a = 31.183(U)(S)$	$k_a = 15.308(U)(S)$
Fountain	Chapra (2008)	Chapra (2008)	Chapra (2008)	Holguín & Camacho (2003)	Holguín & Camacho (2003)

With the aim of simplifying the mathematical handling in deduction, it is defined k_{pi2} as:

$$k_o = \left(k_{dMO} * \frac{MO}{O_u} \right) + \left(4.57 * k_{NH4} * \frac{NH4}{O_u} \right) - k_a$$

The mathematical formulation for the dissolved oxygen deficit corresponds to:

$$\frac{dD}{dt} = \frac{1}{TR} \left((D_u(t - \tau) * e^{\tau * k_o}) - D(t) \right) + \underbrace{k_{dMO} * MO}_{Oxidation} + \underbrace{4.57 * k_{NH4} * NH4}_{Nitrification} - \underbrace{k_a * D(t)}_{Reaeration}$$

Under the steady state assumption:

$$\begin{aligned} 0 &= \frac{1}{TR} \left((D_u * e^{\tau * k_o}) - D \right) + k_{dMO} * MO + 4.57 * k_{NH4} * NH4 - k_a * D \\ k_a * D - k_{dMO} * MO - 4.57 * k_{NH4} * NH4 &= \frac{1}{TR} \left((D_u * e^{\tau * k_o}) - D \right) \\ TR * k_a * D - TR * k_{dMO} * MO - TR * 4.57 * k_{NH4} * NH4 &= (D_u * e^{\tau * k_o}) - D \\ TR * k_a * D + D - TR * k_{dMO} * MO - TR * 4.57 * k_{NH4} * NH4 &= D_u * e^{\tau * k_o} \\ D * ((TR * k_a) + 1) - TR * k_{dMO} * MO - TR * 4.57 * k_{NH4} * NH4 &= D_u * e^{\tau * k_o} \\ D * ((TR * k_a) + 1) &= D_u * e^{\tau * k_o} + TR * k_{dMO} * MO + TR * 4.57 * k_{NH4} * NH4 \\ D * ((TR * k_a) + 1) &= D_u * e^{\tau * k_o} + TR * (k_{dMO} * MO + 4.57 * k_{NH4} * NH4) \\ D &= \frac{D_u * e^{\tau * k_o} + TR * (k_{dMO} * MO + 4.57 * k_{NH4} * NH4)}{(TR * k_a) + 1} \end{aligned}$$

Knowing that:

$$k_o = \left(k_{dMO} * \frac{MO}{O_u} \right) + \left(4.57 * k_{NH4} * \frac{NH4}{O_u} \right) - k_a$$

You have to:

$$O_u * (k_a + k_o) = k_{dMO} * MO + 4.57 * k_{NH4} * NH4$$

Substituting into the equation we have:

$$D = \frac{D_u * e^{\tau * k_o} + TR * (O_u * (k_a + k_o))}{(TR * k_a) + 1}$$

Considering the definition of load as the flow rate per concentration:

$$W = QC$$

It is possible to multiply on the right side of the equation by Q/Q , obtaining:

$$\begin{aligned} D &= \frac{W_{D_u}}{D_u * Q} * \left(\frac{D_u * e^{\tau * k_o} + TR * (O_u * (k_a + k_o))}{(TR * k_a) + 1} \right) \\ D &= \frac{W_{D_u}}{D_u * Q} * \left(\frac{D_u * e^{\tau * k_o} + TR * (O_u * (k_a + k_o))}{(TR * k_a) + 1} \right) \\ \frac{D}{W_{D_u}} &= \frac{1}{D_u * Q} * \left(\frac{D_u * e^{\tau * k_o} + TR * (O_u * (k_a + k_o))}{(TR * k_a) + 1} \right) \end{aligned}$$

Returning to the definition of Assimilation Factor:

$$\begin{aligned} a &= \frac{W_u}{C} \\ \frac{1}{a} &= \frac{C}{W_u} \\ \frac{1}{a_D} &= \frac{1}{D_u * Q} * \left(\frac{D_u * e^{\tau * k_o} + TR * (O_u * (k_a + k_o))}{(TR * k_a) + 1} \right) \end{aligned}$$

Finally, the assimilation factor for this water quality determinant is defined as follows:

$$a_D = D_u * Q * \left(\frac{(TR * k_a) + 1}{D_u * e^{\tau * k_o} + TR * (O_u * (k_a + k_o))} \right)$$

From the relationship of the Aggregate Dead Zone (ADZ) model it is known that:

$$DF = 1 - \frac{\tau}{\bar{t}}$$

That is to say that:

$$\tau = \bar{t} * (1 - DF)$$

$$TR = \bar{t} * DF$$

Therefore, the concentration and assimilation factor relationships for organic matter can be written as follows:

$$D = \frac{D_u * e^{\bar{t} * (1-DF) * k_o} + \bar{t} * DF * O_s * (k_a - k_o)}{((\bar{t} * DF * k_a) + 1) + \bar{t} * DF * (k_a - k_o)}$$

$$a_D = D_u * Q \left(\frac{((\bar{t} * DF * k_a) + 1) + \bar{t} * DF * (k_a - k_o)}{D_u * e^{\bar{t} * (1-DF) * k_o} + \bar{t} * DF * O_s * (k_a - k_o)} \right)$$

The function in AFAR-WQS that allows modeling this water quality determinant is described below.:

AFAR_Obj.WQS_DOD('Load_DO','C_NH4','C_OM','ka','knh4','kdOM')

Input:

Load_OM (mandatory): The load of dissolved oxygen entering the river, which represents the reach in the topological network [mg/d].

C_NH4 (optional): Nitrates concentration [mg/l]. This parameter is optional as long as the ammoniacal nitrogen model has been run.

C_OM (optional): Organic matter concentration [mg/l]. This parameter is optional as long as the organic matter model has been run.

ka (optional): Reaeration rate [1/d].

knh4 (optional): Nitrification decay rate [1/d]. This parameter is optional as long as the ammoniacal nitrogen model has been run.

kdOM (optional): Organic matter oxidation decay rate [1/d]. This parameter is optional as long as the organic matter model has been run.

Output:

AF_DO: Dissolved oxygen assimilation factor [liters].

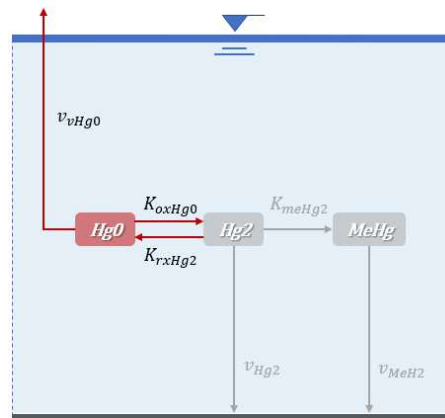
C_DO: Dissolved oxygen concentration [mg/l]

W_DO: Dissolved oxygen load [mg]

5.11 Elemental Mercury Model (Hg0)

AFAR-WQS considers that Elemental Mercury ($Hg0$) presents decay due to oxidation, determined by a rate k_{ox} and a decay due to volatilization, determined by a velocity v_v . Also consider that there are gains from the reduction of Divalent Mercury ($Hg2$), determined by a rate k_{rx} (see **Figure 14**).

Figure 14. AFAR-WQS conceptual model – Elemental Mercury



According to Correa-Caselles (2022), the default values that AFAR-WQS takes for these variables are $v_v = 10$ (m/d), $k_{ox} = 0.01$ (1/d) and $k_{rx} = 0.01$ (1/d).

For the case of F_d the equation described by Allison & Allison (2005). It is used $k_d = 0$.

$$F_d = \frac{1}{1 + 10^{k_d} \left(\frac{SST}{1E6} \right)}$$

With the aim of simplifying the mathematical handling in deduction, it is defined K_{Hg0} and K_{dHg0} as:

$$K_{Hg0} = F_d * \frac{v_v}{H} + k_{ox}$$

$$K_{dHg0} = k_{rx} * \frac{Hg2}{Hg0_u} - K_{Hg0}$$

The formulation for the ADZ-QUASAR model corresponds to:

$$\frac{dHg0}{dt} = \frac{1}{TR} * (Hg0_u(t - \tau) * e^{\tau * K_{dHg0}} - Hg0(t)) + \underbrace{k_{rx} * Hg2}_{Reduction} - \overbrace{F_d * \frac{v_v}{H} * Hg0 - k_{ox} * Hg0}^{-K_{Hg0} * Hg0}$$

$\underbrace{\hspace{10em}}_{Volatilization}$
 $\underbrace{\hspace{10em}}_{Oxidation}$

Under the steady state assumption:

$$0 = \frac{1}{TR} * (e^{\tau * K_{dHg0}} * Hg0_u - Hg0) - K_{Hg0} * Hg0 + k_{rx} * Hg2$$

$$K_{Hg0} * Hg0 - k_{rx} * Hg2 = \frac{1}{TR} * (e^{K_{dHg0} * \tau} * Hg0_u - Hg0)$$

$$TR * K_{Hg0} * Hg0 - TR * k_{rx} * Hg2 = e^{K_{dHg0} * \tau} * Hg0_u - Hg0$$

$$TR * K_{Hg0} * Hg0 + Hg0 - TR * k_{rx} * Hg2 = e^{K_{dHg0} * \tau} * Hg0_u$$

$$Hg0 * (TR * K_{Hg0} + 1) - TR * k_{rx} * Hg2 = e^{K_{dHg0} * \tau} * Hg0_u$$

$$Hg0 * (TR * K_{Hg0} + 1) = e^{K_{dHg0} * \tau} * Hg0_{(u)} + TR * k_{rx} * Hg2$$

$$Hg0 = \frac{e^{\tau * K_{dHg0}} * Hg0_u + TR * k_{rx} * Hg2}{(TR * K_{Hg0} + 1)}$$

Knowing that:

$$K_{dHg0} = k_{rx} * \frac{Hg2}{Hg0_u} - K_{Hg0}$$

You have to:

$$Hg2 = \left(\frac{K_{dHg0} + K_{Hg0}}{k_{rx}} \right) Hg0_{(u)}$$

Substituting into the equation we have:

$$Hg0 = \frac{e^{\tau * K_{dHg0}} * Hg0_u + TR * k_{rx} * \left(\frac{K_{dHg0} + K_{Hg0}}{k_{rx}} \right) Hg0_{(u)}}{(TR * K_{Hg0} + 1)}$$

$$Hg0 = \frac{e^{\tau * K_{dHg0}} * Hg0_u + TR * (K_{dHg0} + K_{Hg0}) * Hg0_{(u)}}{(TR * K_{Hg0} + 1)}$$

$$Hg0 = Hg0_u * \left(\frac{\left(e^{\tau * K_{dHg0}} * + TR * (K_{dHg0} + K_{Hg0}) \right)}{(TR * K_{Hg0} + 1)} \right)$$

Considering the definition of load as the flow rate per concentration:

$$W = QC$$

It is possible to multiply on the right side of the equation by Q/Q , obtaining:

$$Hg0 = \frac{\frac{W_{Hg0_u}}{Q * Hg0_u} \left(e^{\tau * K_{dHg0}} * + TR * (K_{dHg0} + K_{Hg0}) \right)}{Q (TR * K_{Hg0} + 1)}$$

$$Hg0 = \frac{W_{Hg0_u} \left(e^{\tau * K_{dHg0}} * + TR * (K_{dHg0} + K_{Hg0}) \right)}{Q (TR * K_{Hg0} + 1)}$$

$$\frac{Hg0}{W_{Hg0_u}} = \frac{1}{Q} \frac{\left(e^{\tau * K_{dHg0}} * + TR * (K_{dHg0} + K_{Hg0}) \right)}{(TR * K_{Hg0} + 1)}$$

Returning to the definition of Assimilation Factor:

$$a = \frac{W_u}{C}$$

$$\frac{1}{a} = \frac{C}{W_u}$$

$$\frac{1}{a_{Hg0}} = \frac{1}{Q} * \frac{\left(e^{\tau * K_{dHg0}} * + \left(TR * (K_{dHg0} + K_{Hg0}) \right) \right)}{(TR * K_{Hg0} + 1)}$$

Finally, the assimilation factor for this water quality determinant is defined as follows:

$$a_{Hg0} = Q * \left(\frac{(TR * K_{Hg0} + 1)}{\left(e^{\tau * K_{dHg0}} * + \left(TR * (K_{dHg0} + K_{Hg0}) \right) \right)} \right)$$

From the relationship of the Aggregate Dead Zone (ADZ) model it is known that:

$$DF = 1 - \frac{\tau}{\bar{t}}$$

That is to say that:

$$\tau = \bar{t} * (1 - DF)$$

$$TR = \bar{t} * DF$$

Therefore, the concentration and assimilation factor relationships for inorganic phosphorus can be written as follows:

$$Hg0 = Hg0_u \left(\frac{\left(e^{\tau * K_{dHg0}} * \bar{t} * DF * (K_{dHg0} + K_{Hg0}) \right)}{(\bar{t} * DF * K_{Hg0} + 1)} \right)$$

$$a_{Hg0} = Q * \left(\frac{(\bar{t} * DF * K_{Hg0} + 1)}{\left(e^{\bar{t} * (1 - DF) * K_{dHg0}} * \bar{t} * DF * (K_{dHg0} + K_{Hg0}) \right)} \right)$$

The function in AFAR-WQS that allows modeling this water quality determinant is described below.:

AFAR_Obj.WQS_Hg0('Load_Hg0','C_Hg2','Vv','kox','krx','Fd')

Input:

- Load_Hg0 (mandatory):** The load of elemental mercury entering the river, which represents the reach in the topological network [mg/d].
- C_Hg2 (optional):** Divalent mercury concentration [mg/l].
- Vv (optional):** Volatilization velocity of elemental mercury [m/d].
- kox (optional):** Elemental mercury oxidation reaction rate [1/d].
- krx (optional):** Oxidation decay rate of mercury [1/d].

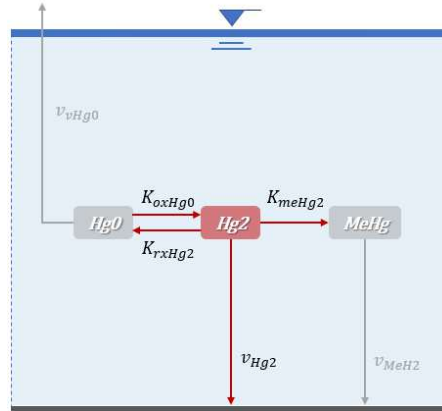
Output:

- AF_Hg0:** Elemental mercury assimilation factor [liters].
- C_Hg0:** Elemental mercury concentration [mg/l]
- W_Hg0:** Elemental mercury load [mg]

5.12 Divalent Mercury Model

AFAR-WQS considers that Divalent Mercury ($Hg2$) presents decay due to reduction, determined by a rate k_{rx} , decay due to methylation, determined by a rate k_{me} (which is subdivided into the adsorbed part $k_{me,a}$ and dissolved $k_{me,d}$) and decay by sedimentation, determined by a velocity $v_{s,1}$. Also consider that there are gains from the oxidation of Elemental Mercury ($Hg0$), determined by a rate k_{ox} (see **Figure 15**).

Figure 15. AFAR-WQS conceptual model – Divalent Mercury



According to Correa-Caselles (2022), the default values that AFAR-WQS takes for these variables are:

$$k_{me,a} = 0.001 \text{ (1/d)}$$

$$k_{me,d} = 0.01 \text{ (1/d)}$$

For the case of F_{pHg2} the equation described Allison & Allison (2005).). It is used $k_d = 3.6$.

$$F_{pHg2} = \frac{10^{k_d} * \left(\frac{SST}{1E6}\right)}{1 - \left(10^{k_d} * \left(\frac{SST}{1E6}\right)\right)}$$

$$v_{s,1} = 0.6 \text{ (m/d)}$$

With the aim of simplifying the mathematical handling in deduction, it is defined K_{Hg2} and K_{dHg2} as:

$$K_{Hg2} = F_{pHg2} * \frac{v_{s,1}}{H} + k_{rx} + k_{me}$$

$$k_{me} = F_{pHg2} * k_{me,a} + (1 - F_{pHg2}) * k_{me,d}$$

$$K_{dHg2} = k_{ox} * \frac{Hg0}{Hg2_u} - K_{Hg2}$$

The formulation for the ADZ-QUASAR model corresponds to:

$$\frac{dHg2}{dt} = \frac{1}{TR} * \left((Hg2_u(t - \tau) * e^{\tau * K_{dHg2}}) - Hg2(t) \right) - K_{Hg2} * Hg2$$

$$+ \underbrace{k_{ox} * Hg0}_{\text{Oxidation}} - \underbrace{F_p * \frac{v_{s,1}}{H} * Hg2}_{\text{Sedimentation}} - \underbrace{k_{rx} * Hg2}_{\text{Reduction}} - \underbrace{k_{me} * Hg2}_{\text{Methylation}}$$

Under the steady state assumption:

$$0 = \frac{1}{TR} * (e^{\tau * K_{dHg2}} * Hg2_u - Hg2) + k_{ox} * Hg0 - K_{Hg2} * Hg2$$

$$K_{Hg2} * Hg2 - k_{ox} * Hg0 = \frac{1}{TR} * (e^{\tau * K_{dHg2}} * Hg2_u - Hg2)$$

$$TR * K_{Hg2} * Hg2 - TR * k_{ox} * Hg0 = e^{\tau * K_{dHg2}} * Hg2_u - Hg2$$

$$TR * K_{Hg2} * Hg2 + Hg2 - TR * k_{ox} * Hg0 = e^{\tau * K_{dHg2}} * Hg2_{(u)}$$

$$Hg2 * (TR * K_{Hg2} + 1) - TR * k_{ox} * Hg0 = e^{\tau * K_{dHg2}} * Hg2_u$$

$$Hg2 * (TR * K_1 + 1) = e^{\tau * K_{dHg2}} * Hg0 + TR * k_{ox} * Hg0$$

$$Hg2 = \frac{e^{\tau * K_{dHg2}} * Hg2_u + TR * k_{ox} * Hg0}{(TR * K_{Hg2} + 1)}$$

Knowing that:

$$Hg0 = \left(\frac{K_{dHg2} + K_{Hg2}}{k_{ox}} \right) * Hg2_u$$

Substituting into the equation we have:

$$Hg2 = \frac{e^{\tau * K_{dHg2}} * Hg2_u + TR * k_{ox} * \left(\frac{K_{dHg2} + K_{Hg2}}{k_{ox}} \right) * Hg2_{(u)}}{(TR * K_{Hg2} + 1)}$$

$$Hg2 = \frac{e^{\tau * K_{dHg2}} * Hg2_u + TR * (K_{dHg2} + K_{Hg2}) * Hg2_{(u)}}{(TR * K_{Hg2} + 1)}$$

$$Hg2 = Hg2_u * \left(\frac{(e^{\tau * K_{dHg2}} + TR * (K_{dHg2} + K_{Hg2}))}{(TR * K_{Hg2} + 1)} \right)$$

Considering the definition of load as the flow rate per concentration:

$$W = QC$$

It is possible to multiply on the right side of the equation by Q/Q , obtaining:

$$Hg2 = \frac{\overbrace{Q * Hg2_u}^{W_{Hg2_u}}}{Q} * \frac{(e^{\tau * K_{dHg2}} + TR * (K_{dHg2} + K_{Hg2}))}{(TR * K_{Hg2} + 1)}$$

$$Hg2 = \frac{W_{Hg2u}}{Q} * \frac{(e^{\tau * K_{dHg2}} + TR * (K_{dHg2} + K_{Hg2}))}{(TR * K_{Hg2} + 1)}$$

$$\frac{Hg2}{W_{Hg2u}} = \frac{1}{Q} * \frac{(e^{\tau * K_{dHg2}} + TR * (K_{dHg2} + K_{Hg2}))}{(TR * K_{Hg2} + 1)}$$

Returning to the definition of Assimilation Factor:

$$a = \frac{W_u}{C}$$

$$\frac{1}{a} = \frac{C}{W_u}$$

$$\frac{1}{a_{Hg2}} = \frac{1}{Q} * \frac{(e^{\tau * K_{dHg2}} + TR * (K_{dHg2} + K_{Hg2}))}{(TR * K_{Hg2} + 1)}$$

Finally, the assimilation factor for this water quality determinant is defined as follows:

$$a_{Hg2} = Q * \left(\frac{(TR * K_{Hg2} + 1)}{(e^{\tau * K_{dHg2}} + TR * (K_{dHg2} + K_{Hg2}))} \right)$$

From the relationship of the Aggregate Dead Zone (ADZ) model it is known that:

$$DF = 1 - \frac{\tau}{\bar{\tau}}$$

That is to say that:

$$\tau = \bar{\tau} * (1 - DF)$$

$$TR = \bar{\tau} * DF$$

Therefore, the concentration and assimilation factor relationships for inorganic phosphorus can be written as follows:

$$Hg2 = Hg2_u \left(\frac{(e^{\bar{\tau} * (1-DF) * K_{dHg2}} + \bar{\tau} * DF * (K_{dHg2} + K_{Hg2}))}{(\bar{\tau} * DF * K_{Hg2} + 1)} \right)$$

$$a_{Hg2} = Q * \left(\frac{(TR * K_{Hg2} + 1)}{(e^{\bar{\tau} * (1-DF) * K_{dHg2}} + \bar{\tau} * DF * (K_{dHg2} + K_{Hg2}))} \right)$$

The function in AFAR-WQS that allows modeling this water quality determinant is described below:

AFAR_Obj.WQS_Hg2('Load_Hg0','C_Hg2','Kme_d','Kme_p','kox','krx','Fp')

Input:

Load_Hg2 (mandatory): The load of divalent mercury entering the river, which represents the reach in the topological network [mg/d].
C_Hg0 (optional): Elemental mercury concentration [mg/l].
Kme_d (optional): Dissolved divalent mercury methylation rate [1/d].
Kme_p (optional): Adsorbed divalent mercury methylation rate [1/d].
kox (optional): Elemental mercury oxidation reaction rate [1/d].
krx (optional): Oxidation decay rate of mercury [1/d].
Fp (optional): Fraction of divalent mercury found in particulate matter [dimensionless].

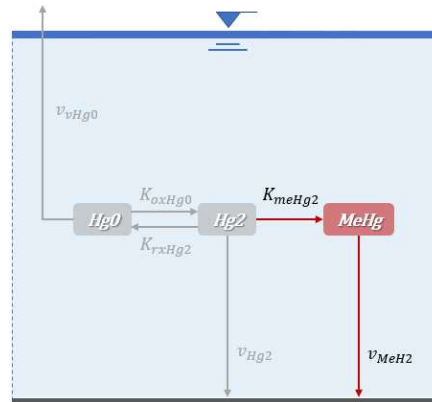
Output:

AF_Hg2: Divalent mercury assimilation factor [liters].
C_Hg2: Divalent mercury concentration [mg/l]
W_Hg2: Divalent mercury load [mg]

5.13 Methyl Mercury Model

AFAR-WQS considers that Methyl Mercury (*MeHg*) presents decay due to bioaccumulation, determined by a rate k_{in} and decay by sedimentation, determined by a velocity $v_{in,2}$. Also consider that there are gains from the melization of Divalent Mercury (*Hg2*), determined by a rate k_{me} (see **Figure 16**).

Figure 16. AFAR-WQS conceptual model – Methyl Mercury



According to Correa-Caselles (2022), the default values that AFAR-WQS takes for these variables are:

$$v_{s,2} = 0.5 \text{ (m/d)}$$

For the case of F_{pMeHg} the equation described by Allison & Allison (2005). It is used $k_d = 2.7$.

$$F_{pMeHg} = \frac{10^{k_d} * \left(\frac{SST}{1E6}\right)}{1 - \left(10^{k_d} * \left(\frac{SST}{1E6}\right)\right)}$$

AFAR-WQS considers $k_{in} = 0$, since this is particular to the species being analyzed.

With the aim of simplifying the mathematical handling in deduction, it is defined K_{Hg2} and K_{dHg2} as:

$$K_{MeHg} = F_{pMeHg} * \frac{v_{s,2}}{H} + k_u$$

$$K_{dMeHg} = k_{me} * \frac{Hg2}{MeHg_u} - K_{MeHg}$$

The formulation for the ADZ-QUASAR model corresponds to:

$$\frac{dMeHg}{dt} = \frac{1}{TR} * \left((MeHg_u(t - \tau) * e^{\tau * K_{dMeHg}}) - MeHg(t) \right) - K_{MeHg} * MeHg + \underbrace{k_{me} * Hg2}_{\text{Methylation}} - \underbrace{F_p \frac{v_{s,2}}{H} MeHg}_{\text{Sedimentation}} - \underbrace{k_u MeHg}_{\text{Bioaccumulation}}$$

Under the steady state assumption:

$$0 = \frac{1}{TR} * (e^{\tau * K_{dMeHg}} * MeHg_u - MeHg) - K_{MeHg} * MeHg + k_{me} * Hg2$$

$$K_{MeHg} * MeHg - k_{me} * Hg2 = \frac{1}{TR} * (e^{\tau * K_{dMeHg}} * MeHg_u - MeHg)$$

$$TR * K_{MeHg} * MeHg - TR * k_{me} * Hg2 = e^{\tau * K_{dMeHg}} * MeHg_u - MeHg$$

$$TR * K_{MeHg} * MeHg + MeHg - TR * k_{me} * Hg2 = e^{\tau * K_{dMeHg}} * MeHg_u$$

$$MeHg * (K_{MeHg} * TR + 1) - TR * k_{me} * Hg2 = e^{\tau * K_{dMeHg}} * MeHg_u$$

$$MeHg * (TR * K_{MeHg} + 1) = e^{-K_2 * \tau} * MeHg_u + TR * k_{me} * Hg2$$

$$MeHg = \frac{e^{\tau * K_{dMeHg}} * MeHg_u + TR * k_{me} * Hg2}{(TR * K_{MeHg} + 1)}$$

Knowing that:

$$Hg2 = \left(\frac{K_{dMeHg} + K_{MeHg}}{k_{me}} \right) * MeHg_u$$

Substituting into the equation we have:

$$MeHg = \frac{e^{\tau * K_{dMeHg}} * MeHg_u + TR * k_{me} * \left(\frac{K_{dMeHg} + K_{MeHg}}{k_{me}} \right) * MeHg_u}{(TR * K_{MeHg} + 1)}$$

$$MeHg = \frac{e^{\tau * K_{dMeHg}} * MeHg_u + TR * (K_{dMeHg} + K_{MeHg}) * MeHg_u}{(TR * K_{MeHg} + 1)}$$

$$\mathbf{MeHg = MeHg_u * \left(\frac{(e^{\tau * K_{dMeHg}} + (K_{dMeHg} + K_{MeHg}) * TR)}{(TR * K_{MeHg} + 1)} \right)}$$

Considering the definition of load as the flow rate per concentration:

$$W = QC$$

It is possible to multiply on the right side of the equation by Q/Q , obtaining:

$$MeHg = \frac{\overbrace{Q * MeHg_u}^{W_{MeHg_u}}}{Q} * \frac{(e^{\tau * K_{dMeHg}} + TR * (K_{dMeHg} + K_{MeHg}))}{(TR * K_{MeHg} + 1)}$$

$$\frac{MeHg}{W_{MeHg_u}} = \frac{1}{Q} * \frac{(e^{\tau * K_{dMeHg}} + (K_{dMeHg} + K_{MeHg}) * TR)}{(TR * K_{MeHg} + 1)}$$

Returning to the definition of Assimilation Factor:

$$a = \frac{W_u}{C}$$

$$\frac{1}{a} = \frac{C}{W_u}$$

$$\frac{1}{a_{MeHg}} = \frac{1}{Q} * \frac{(e^{\tau * K_{dMeHg}} + (K_{dMeHg} + K_{MeHg}) * TR)}{(TR * K_{MeHg} + 1)}$$

Finally, the assimilation factor for this water quality determinant is defined as follows:

$$a_{MeHg} = Q * \left(\frac{(TR * K_{MeHg} + 1)}{(e^{\tau * K_{dMeHg}} + TR * (K_{dMeHg} + K_{MeHg}))} \right)$$

From the relationship of the Aggregate Dead Zone (ADZ) model it is known that:

$$DF = 1 - \frac{\tau}{\bar{t}}$$

That is to say that:

$$\tau = \bar{t} * (1 - DF)$$

$$TR = \bar{t} * DF$$

Por tanto, las relaciones de concentración y factor de asimilación para fósforo inorgánico pueden escribirse de la siguiente manera:

$$MeHg = \frac{MeHg_u * (e^{\bar{t} * (1-DF) * K_{dMeHg}} + (\bar{t} * DF * (K_{dMeHg} + K_{MeHg})))}{(\bar{t} * DF * K_{MeHg} + 1)}$$

$$a_{MeHg} = Q * \frac{(\bar{t} * DF * K_{MeHg} + 1)}{(e^{\bar{t} * (1-DF) * K_{dMeHg}} + (\bar{t} * DF * (K_{dMeHg} + K_{MeHg})))}$$

Therefore, the concentration and assimilation factor relationships for inorganic phosphorus can be written as follows:

AFAR_Obj.WQS_MeHg('Load_MeHg','C_Hg2','Kme_d','Kme_p','vs','ku','Fp')

Input:

Load_MeHg (mandatory): The load of methyl mercury entering the river, which represents the reach in the topological network [mg/d].
C_Hg2 (optional): Dissolved divalent concentration [mg/l].
Kme_d (optional): Dissolved divalent mercury methylation rate [1/d].
Kme_p (optional): Adsorbed divalent mercury methylation rate [1/d].
vs (optional): Methyl mercury sedimentation rate [m/d].
ku (optional): Methyl mercury bioaccumulation rate [1/d].
Fp (optional): Fraction of methyl mercury found in particulate matter [dimensionless].

Output:

AF_MeHg: Methyl mercury assimilation factor [liters].
C_MeHg: Methyl mercury concentration [mg/l]
W_MeHg: D Methyl mercury load [mg]

5.14 Summary of Assimilation Factors for AFAR-WQS Water Quality Determinants

Table 3 summarizes the assimilation factors for the determinants and processes considered by AFAR-WQS. **Table 4** summarizes the default values considered by AFAR-WQS for the parameters of the water quality determinants.

Table 3. Assimilation Factors for conventional determinants included in AFAR-WQS

Water quality determinants	Processes considered	ADZ-QUASAR equation	Assimilation factors
Temperature	No processes (Conservative determinant)	$\frac{dT}{dt} = \frac{1}{TR} [T_u(t - \tau) - T(t)]$	$a_T = Q$
Suspended Solids	Sedimentation	$k_{sst} = \frac{v_{sst}}{H}$ $\frac{dSST}{dt} = \frac{1}{TR} ((SST_u(t - \tau) * e^{-\tau * k_{sst}}) - SST(t)) - \underbrace{k_{sst} * SST}_{Sedimentation}$	$a_{sst} = Q * \left(\frac{(\bar{t} * DF * k_{sst}) + 1}{e^{-\bar{t} * (1 - DF) * k_{sst}}} \right)$
Pathogenic Organisms	Decay (mortality) Sedimentation	$k_X = k_{dX} + F_{px} * \frac{v_X}{H}$ $\frac{dX}{dt} = \frac{1}{TR} ((X_u(t - \tau) * e^{-\tau * k_X}) - X(t)) - \overbrace{\underbrace{k_{dX} * X}_{Decay (mortality)} - \underbrace{F_{px} * \frac{v_X}{H} * X}_{Sedimentation}}^{-k_X * X}$	$a_X = Q * \left(\frac{(\bar{t} * DF * k_X) + 1}{e^{-\bar{t} * (1 - DF) * k_X}} \right)$

Organic Nitrogen	Hydrolysis Sedimentation	$k_{N1} = k_{NO} + \frac{v_{NO}}{H}$ $\frac{dNO}{dt} = \frac{1}{TR} \left((NO_u(t - \tau) * e^{-\tau * k_{N1}}) - NO(t) \right) - \overbrace{\frac{k_{HNO} * NO}{Hydrolysis}}^{k_{N1} * NO} - \underbrace{\frac{v_{NO}}{H} * NO}_{Sedimentation}$	$a_{NO} = Q * \left(\frac{(\bar{t} * DF * k_{N1}) + 1}{e^{-\bar{t} * (1 - DF) * k_{N1}}} \right)$
Ammoniacal Nitrogen	Hydrolysis Nitrification	$k_{N2} = k_{NO} * \frac{NO}{NH4_u} - k_{NH4}$ $\frac{dNH4}{dt} = \frac{1}{TR} \left((NH4_u(t - \tau) * e^{\tau * k_{N2}}) - NH4(t) \right) + \underbrace{\frac{k_{NO} * NO}{Hydrolysis}} - \underbrace{\frac{k_{NH4} * NH4}{Nitrification}}$	$a_{NH4} = Q * \left(\frac{(k_{NH4} * \bar{t} * DF) + 1}{e^{\bar{t} * (1 - DF) * k_{N2}} + (\bar{t} * DF * (k_{N2} + k_{NH4}))} \right)$
Nitrates	Nitrification Denitrification	$k_{NO3} = F_{oxdNO3} * k_{dNO3}$ $k_{N3} = k_{NH4} * \frac{NH4}{NO3_u} - k_{NO3}$ $\frac{dNO3}{dt} = \frac{1}{TR} \left((NO3_u(t - \tau) * e^{\tau * k_{N3}}) - NO3(t) \right) + \underbrace{\frac{k_{NH4} * NH4}{Nitrification}} - \underbrace{\frac{k_{NO3} * NO3}{Desnitrification}}$	$a_{NO3} = Q * \left(\frac{(\bar{t} * DF * k_{NO3}) + 1}{e^{\bar{t} * (1 - DF) * k_{N3}} + (\bar{t} * DF * (k_{N3} + k_{NO3}))} \right)$
Organic Phosphorus	Hydrolysis Sedimentation	$\frac{dPo}{dt} = \frac{1}{TR} \left((Po_u(t - \tau) * e^{-\tau * k_{Po1}}) - Po(t) \right) - \overbrace{\frac{k_{Po} Po}{Hydrolysis}}^{-k_{Po1} * Po} - \underbrace{\frac{v_{Po}}{H} Po}_{Sedimentation}$	$a_{Po} = Q * \left(\frac{(\bar{t} * DF * k_{Po1}) + 1}{e^{-\bar{t} * (1 - DF) * k_{Po1}}} \right)$

Inorganic Phosphorus	Hydrolysis Sedimentation	$k_{Pi} = \frac{v_{Pi}}{H}$ $k_{Pi2} = k_{Po} * \frac{Po}{Pi_u} - k_{Pi}$ $\frac{dPi}{dt} = \frac{1}{TR} ((Pi_u(t - \tau) e^{\tau * k_{Pi2}}) - Pi(t)) + \underbrace{\frac{k_{Po} * Po}{Hydrolysis}} - \underbrace{\frac{k_{Pi} * Pi}{Sedimentation}}$	$a_{Pi} = Q * \left(\frac{(\bar{t} * DF * k_{Pi}) + 1}{e^{\bar{t} * (1 - DF) * k_{Pi2}} + (\bar{t} * DF * (k_{P2} + k_{Pi}))} \right)$
Organic Matter	Oxidation Nitrification	$\sigma_{OM} = F_{oxDOM} * k_{dOM}$ $\theta_{OM} = 0.00286 * (1 - F_{oxdNO3}) * k_{dNO3}$ $k_{OM2} = -\theta_{OM} * \frac{NO3}{OM_u} - \sigma_{OM}$ $\frac{dOM}{dt} = \frac{1}{TR} ((MO_u(t - \tau) * e^{\tau * k_{MO2}}) - MO(t)) - \underbrace{\theta_{OM} * NO3}_{Nitrification} - \underbrace{\sigma_{MO} * OM}_{Oxidation}$	$a_{OM} = Q * \left(\frac{(\bar{t} * DF * \sigma_{OM}) + 1}{e^{\bar{t} * (1 - DF) * k_{OM2}} + (\bar{t} * DF * (k_{OM2} + \sigma_{OM}))} \right)$
Oxygen Deficit	Oxidation Nitrification Reaeration	$O = O_s - D$ $k_O = \left(k_{dOM} * \frac{OM}{O_u} \right) + \left(4.57 * k_{NH4} * \frac{NH4}{O_u} \right) - k_a$ $\frac{dD}{dt} = \frac{1}{TR} ((D_u(t - \tau) * e^{\tau * k_O}) - D(t)) + \underbrace{\frac{k_{dOM} * OM}{Oxidation}} + \underbrace{\frac{4.57 * k_{NH4} * NH4}{Nitrification}} - \underbrace{k_a * D(t)}_{Reaeration}$	$a_D = D_u * Q * \left(\frac{((\bar{t} * DF * k_a) + 1) + \bar{t} * DF * (k_a - k_O)}{D_u * e^{\bar{t} * (1 - DF) * k_O} + \bar{t} * DF * O_s * (k_a - k_O)} \right)$
Elemental Mercury	Reduction Volatilization Oxidation	$K_{Hg0} = F_d * \frac{v_v}{H} + k_{ox}$ $K_{dHg0} = k_{rx} * \frac{Hg2}{Hg0_u} - k_1$ $\frac{dHg0}{dt} = \frac{1}{TR} * (Hg0_u(t - \tau) * e^{\tau * K_{dHg0}} - Hg0(t)) + \underbrace{k_{rx} * Hg2}_{Reduction} - \underbrace{F_d * \frac{v_v}{H} * Hg0}_{Volatilization} - \underbrace{k_{ox} * Hg0}_{Oxidation}$	$a_{Hg0} = Q * \left(\frac{(\bar{t} * DF * K_{Hg0}) + 1}{e^{\bar{t} * (1 - DF) * K_{dHg0}} + (\bar{t} * DF * (K_{dHg0} + K_{Hg0}))} \right)$

Divalent Mercury	Oxidation Reduction Sedimentation Methylation	$K_{Hg2} = F_{pHg2} * \frac{v_{s,1}}{H} + k_{rx} + k_{me}$ $k_{me} = F_{pHg2} * k_{me,a} + (1 - F_{pHg2}) * k_{me,d}$ $K_{dHg2} = k_{ox} * \frac{Hg_o}{Hg2_u} - K_{Hg2}$ $\frac{dHg2}{dt} = \frac{1}{TR} * ((Hg2_u(t - \tau) * e^{\tau * K_{dHg2}}) - Hg2(t)) + \underbrace{k_{ox} * Hg_o}_{Oxidation} - \underbrace{F_p * \frac{v_{Hg2}}{H} * Hg2}_{Sedimentation} - \underbrace{k_{rx} * Hg2}_{Reduction} - \underbrace{k_{me} * Hg2}_{Methylation}$	$a_{Hg2} = Q * \left(\frac{(\bar{t} * DF * K_{Hg2}) + 1}{e^{\bar{t} * (1 - DF) * K_{dHg2}} + (\bar{t} * DF * (K_{dHg2} + K_{Hg2}))} \right)$
Methyl mercury	Methylation Sedimentation Bioaccumulation	$K_{MeHg} = F_{pMeHg} * \frac{v_{s,2}}{H} + k_u$ $K_{dMeHg} = k_{me} * \frac{Hg2}{MeHg_u} - K_{MeHg}$ $\frac{dMeHg}{dt} = \frac{1}{TR} * ((MeHg_u(t - \tau) * e^{\tau * K_{dMeHg}}) - MeHg(t)) + \underbrace{k_{me} * Hg2}_{Methylation} - \underbrace{F_p * \frac{v_{s,2}}{H} MeHg}_{Sedimentation} - \underbrace{k_u MeHg}_{Bioacumulation}$	$a_{MeHg} = Q * \left(\frac{(K_{MeHg} * \bar{t} * DF) + 1}{e^{\bar{t} * (1 - DF) * K_{dMeHg}} + ((K_{dMeHg} + K_{MeHg}) * \bar{t} * DF)} \right)$

Table 4. Summary of parameters required for the modeling of conventional determinants and toxic substances (mercury)

Water quality determinants	Parameters	Description	Units	Value/Equation	Fuente
Conductivity	-	Conductivity is modeled as a ratio of suspended solids [mg/l].	μS/cm	$C_o = (SST/0.65)$	Rusydi (2018)
Suspended solids	v_{sst}	Sedimentation velocity	m/day	0.1	Chapra (2008)
Pathogenic organisms	k_{dX}	Constant decomposition of pathogenic organisms (mortality)	Dimensionless	$k_{dX} = 0.8 * ((1.07)^{T-20})$	Chapra (2008)
	F_{pX}	Fraction of pathogenic organisms adsorbed on solid particles	Dimensionless	0.7	Rojas (2011)
	v_X	Sedimentation velocity of the adsorbed fraction of pathogens on solid particles	m/day	1	Chapra et al. (2003)
Organic nitrogen	k_{NO}	Hydrolysis decomposition rate of organic nitrogen	1/day	$k_{dX} = 0.02 * ((1.047)^{T-20})$	Bowie et al. (1985)
	v_{NO}	Sedimentation velocity of organic nitrogen	m/day	0.0005	Chapra et al. (2003)
Ammoniacal nitrogen	k_{NH4}	Nitrification decay rate	1/day	<div><div><div><div><div>$Plain\ rivers$</div><div>$k_{NH4o} = \frac{10 \left(-3.421 + Log \left(\frac{\sqrt{gH^3}}{v} \right)^{1.36} \right) v}{H^2}$</div></div><div><div>$Mountain\ rivers$</div><div>$k_{NH4o} = 0.4381 \frac{U}{H} + 0.5394$</div></div></div><div>$k_{dX} = k_{NH4o} * ((1.047)^{T-20})$</div></div></div>	Robles & Camacho (2005)
Nitrates	k_{dNO3}	Denitrification rate	1/day	$k_{dNO3} = 0.1 * 1.0698^{T-20}$	Chapra et al. (2003)
	F_{oxdNO3}	Factor that takes into account the effect of oxygen deficiency on denitrification.	Dimensionless	$F_{oxdNO3} = e^{-0.60}$	Chapra et al. (2003)
Organic phosphorus	k_{Po}	Organic phosphorus hydrolysis decay rate	1/day	$k_{NO} = 0.03 * 1.07^{T-20}$	Chapra et al. (2003)
	v_{Po}	Organic phosphorus sedimentation velocity	m/day	0.001	Chapra et al. (2003)
Inorganic phosphorus	v_{Pi}	Inorganic phosphorus sedimentation velocity	m/day	0.8	Chapra et al. (2003)
Organic matter	k_{dOM}	Oxidation decomposition rate of organic matter	1/day	<div><div>$if\ Q \leq 23\ m^3/s$</div><div>$k_{dMO} = 1.796Q^{-0.49}$</div><div>$if\ Q > 23\ m^3/s$</div><div>$k_{dMO} = 3.5$</div><div>$k_{dMO} = k_{dMO} * 1.047^{T-20}$</div></div>	Bowie et al. (1985)
	F_{oxdOM}	Factor considering the effect of low oxygen on organic matter	Dimensionless	$F_{oxdOM} = 1 - e^{-0.60}$	Chapra et al. (2003)
Oxygen deficit	k_a	Reaction rate	1/day	Table 5	Chapra (2008); Holguín & Camacho (2003)
Elemental mercury	v_v	Volatilization velocity of elemental mercury	m/day	10	Correa-Caselles (2022)

Water quality determinants	Parameters	Description	Units	Value/Equation	Fuente
	k_{ox}	Elemental mercury oxidation reaction rate	1/day	0.01	Correa-Caselles (2022)
	k_{rx}	Oxidation decay rate of elemental mercury	1/day	0.01	Correa-Caselles (2022)
Divalent mercury	$k_{me,a}$	Adsorbed divalent mercury methylation rate	1/day	0.001	Correa-Caselles (2022)
	$k_{me,d}$	Dissolved divalent mercury methylation rate	1/day	0.01	Correa-Caselles (2022)
	F_{pHg2}	Fraction of divalent mercury adsorbed onto solid particles	Dimensionless	$F_{pHg2} = \frac{10^{3.6} * \left(\frac{SST}{1E6}\right)}{1 - \left(10^{3.6} * \left(\frac{SST}{1E6}\right)\right)}$	Allison & Allison (2005)
	$v_{s,1}$	Sedimentation velocity of divalent mercury	m/day	0.6	Correa-Caselles (2022)
Methylmercury	F_{pMeHg}	Fraction of methyl mercury adsorbed on solid particles	Dimensionless	$F_{pMeHg} = \frac{10^{2.7} * \left(\frac{SST}{1E6}\right)}{1 - \left(10^{2.7} * \left(\frac{SST}{1E6}\right)\right)}$	Allison & Allison (2005)
	$v_{s,2}$	Methyl mercury sedimentation velocity	m/day	0.5	Correa-Caselles (2022)

Table 5. Reaeration rate equations

Parameters	Mountain river (limited by supply)			Plain rivers (limited by transport)	
Range	O’Connor – Dubbins $0.3 \leq H < 9.14$ $0.15 \leq U < 0.49$	Churchill $0.31 \leq H < 3.35$ $0.55 \leq U < 1.42$	Owens – Gibbs $0.12 \leq H < 0.73$ $0.03 \leq U < 0.55$	Tsivoglou y Neal $0.0283 \leq Q < 0.4247$	Tsivoglou y Neal $0.4247 \leq Q < 84.938$
Equation	$k_a = 3.93 \frac{U^{0.5}}{H^{1.5}}$	$k_a = 5.026 \frac{U}{H^{1.67}}$	$k_a = 5.32 \frac{U^{0.67}}{H^{1.85}}$	$k_a = 31.183(U)(S)$	$k_a = 15.308(U)(S)$
Source	Chapra (2008)	Chapra (2008)	Chapra (2008)	Holguín & Camacho (2003)	Holguín & Camacho (2003)

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