Ecoadvisor model formulas

Institut Català de Recerca de l'Aigua (ICRA)

Compilation command (bash)

groff -e -t -ms formulas.ms -T pdf -K utf-8

1. State Variables

1.1. Inputs

$$Q$$
 (ML/d)

$$S_{VFA,}S_{FBSO,}X_{BPO,}X_{UPO,}S_{USO,}X_{iSS,}S_{FSA,}S_{OP,}S_{NOx,}X_{OHO}$$
 (mg/L)

1.2. Total chemical oxygen demand (COD = S_t)

$$S_t = S_{VFA} + S_{FBSO} + X_{BPO} + X_{UPO} + S_{USO} + X_{OHO}$$
 (mgCOD/L)

and:

$$\begin{split} S_{bs} &= S_{VFA} + S_{FBSO} \\ S_{bp} &= X_{BPO} \\ S_{up} &= X_{UPO} \\ S_{us} &= S_{USO} \\ S_{active} &= X_{OHO} \\ S_t &= S_{bs} + S_{bp} + S_{up} + S_{us} + S_{active} \end{split}$$

The components can be grouped as follows:

$$\begin{array}{ccc} S_s & S_p \\ S_b & S_{bs} & S_{bp} \\ S_u & S_{us} & S_{up} \end{array}$$

So,

$$S_t = S_b + S_u + S_{active}$$

$$S_t = S_s + S_p + S_{active}$$

1.3. Mass ratios for COD, N, P and C

State Variable	COD (f_{cv})	$\mathbf{N}(f_N)$	$\mathbf{P}(f_P)$	$\mathbf{C}(f_C)$
S_{VFA}	1.0667	0.0000	0.0000	0.400
S_{FBSO}	1.4200	0.0464	0.0118	0.471
X_{BPO}	1.5230	0.0323	0.0072	0.498
X_{UPO}	1.4810	0.1000	0.0250	0.518
S_{USO}	1.4930	0.0366	0.0000	0.498
X_{OHO}	1.4810	0.1000	0.0250	0.518
ANO	1.4810	0.1000	0.0250	0.518
PAO	1.4810	0.1000	0.0250	0.518

1.4. Total Kjeldahl Nitrogen (TKN = N_t)

$$N_t = N_o + S_{FSA} + N_{active}$$
 (mgN/L)

where:

$$\begin{split} N_{o} &= N_{obs} + N_{obp} + N_{ous} + N_{oup} \\ N_{obs} &= S_{VFA} \frac{f_{N_{VFA}}}{f_{cv_{VFA}}} + S_{FBSO} \frac{f_{N_{FBSO}}}{f_{cv_{FBSO}}} \\ N_{obp} &= X_{BPO} \frac{f_{N_{BPO}}}{f_{cv_{BPO}}} \\ N_{ous} &= S_{USO} \frac{f_{N_{USO}}}{f_{cv_{USO}}} \\ N_{oup} &= X_{UPO} \frac{f_{N_{UPO}}}{f_{cv_{UPO}}} \\ N_{active} &= X_{OHO} \frac{f_{N_{OHO}}}{f_{cv_{OHO}}} \end{split}$$

1.5. Total Phosphorus (TP = P_t)

$$P_t = P_o + S_{OP} + P_{active}$$
 (mgP/L)

where:

$$\begin{split} P_{o} &= P_{obs} + P_{obp} + P_{ous} + P_{oup} \\ P_{obs} &= S_{VFA} \frac{f_{P_{VFA}}}{f_{cv_{VFA}}} + S_{FBSO} \frac{f_{P_{FBSO}}}{f_{cv_{FBSO}}} \\ P_{obp} &= X_{BPO} \frac{f_{P_{BPO}}}{f_{cv_{BPO}}} \\ P_{ous} &= S_{USO} \frac{f_{P_{USO}}}{f_{cv_{USO}}} \\ P_{oup} &= X_{UPO} \frac{f_{P_{UPO}}}{f_{cv_{UPO}}} \\ P_{active} &= X_{OHO} \frac{f_{P_{OHO}}}{f_{cv_{OHO}}} \end{split}$$

1.6. Total Organic Carbon (TOC = C_t)

$$C_t = C_{obs} + C_{obp} + C_{ous} + C_{oup} + C_{active}$$
 (mgC/L)

where:

$$\begin{split} C_{obs} &= S_{VFA} \frac{f_{C_{VFA}}}{f_{C_{VVFA}}} + S_{FBSO} \frac{f_{C_{FBSO}}}{f_{cv_{FBSO}}} \\ C_{obp} &= X_{BPO} \frac{f_{C_{BPO}}}{f_{cv_{BPO}}} \\ C_{ous} &= S_{USO} \frac{f_{C_{USO}}}{f_{cv_{USO}}} \\ C_{oup} &= X_{UPO} \frac{f_{C_{UPO}}}{f_{cv_{UPO}}} \\ C_{active} &= X_{OHO} \frac{f_{C_{OHO}}}{f_{cv_{OHO}}} \end{split}$$

1.7. Total suspended solids (TSS = X_T)

$$X_T = X_V + X_{iSS}$$
 (mgTSS/L)

where:

$$X_V = \frac{X_{BPO}}{f_{cv_{BPO}}} + \frac{X_{UPO}}{f_{cv_{UPO}}} + \frac{X_{OHO}}{f_{cv_{OHO}}}$$
 (mgVSS/L)

2. Activated sludge

2.1. Inputs

$$T, V_{p}, R_{s}, RAS$$

2.2. Volatile suspended solids (VSS)

$$Y_H = 0.45$$
 (gVSS/gCOD)

$$b_H = 0.24$$
 (1/d)

$$b_{HT} = b_H (1.029)^{T-20} (1/d)$$

$$f_{X_{BH}} = \frac{Y_H \cdot R_s}{1 + b_{HT} \cdot R_s}$$
 (gVSS·d/gCOD)

$$k_{vT} = 0.007 \cdot (1.035)^{T-20}$$
 (L/gVSS·d)

$$S_{nd} = \frac{1}{f_{X_{nu}} k_{vT}}$$
 (mgCOD/L)

$$FdS_{bi} = FS_{bi} - Q \cdot S_{nd}$$
 (kgCOD/d)

$$MX_{BH} = FdS_{bi} \cdot f_{X_{RH}}$$
 (kgVSS)

$$MX_{EH} = f_H \cdot b_{HT} \cdot R_s \cdot MX_{BH}$$
 (kgVSS)

$$MX_I = FX_{Ti} \cdot R_s$$
 (kgVSS)

$$MX_V = MX_{BH} + MX_{EH} + MX_I (kgVSS)$$

$$X_V = \frac{MX_V}{V_p}$$
 (kgVSS/m³)

2.3. Total inert solids (iSS)

$$f_{iOHO} = 0.15$$
 (giSS/gVSS)

$$MX_{IO} = FiSS \cdot R_s + f_{iOHO} \cdot MX_{BH} + F_{iSS_precipitation} \cdot R_s$$
 (kgiSS)

2.4. Total suspended solids (TSS)

$$MX_T = MX_V + MX_{IO} (kgTSS)$$

$$X_T = \frac{MX_T}{V_p}$$
 (kgTSS/m³)

2.5. Nominal hydraulic retention time

$$HRT = \frac{V_p}{O} \tag{d}$$

2.6. Wastage flowrate

$$Q_w = \frac{V_p}{R_s} \tag{ML/d}$$

2.7. Effluent flowrate

$$Q_{e} = Q - Q_{w} \tag{ML/d}$$

2.8. Nitrogen and Phosphorus required for sludge production

$$N_s = \frac{f_{N_{OHO}}(MX_{BH} + MX_{EH}) + f_{N_{UPO}}MX_I}{R_s \cdot Q}$$
 (mgN/L)

$$P_{s} = \frac{f_{P_{OHO}}(MX_{BH} + MX_{EH}) + f_{P_{UPO}}MX_{I}}{R_{c} \cdot O}$$
 (mgP/L)

2.9. Effluent Ammonia (N_{ae}) and effluent Orthophosphate (P_{se}) concentration

$$N_{ae} = N_{ti} - N_s - N_{ouse}$$
 (mgN/L)

$$P_{se} = P_{ti} - P_s - P_{ouse} - P_{precipitation}$$
 (mgP/L)

2.10. Wastage solids concentration

$$BPO_{was} = 0$$
 (mgCOD/L)

$$UPO_{was} = f_{cv_{UPO}} \cdot X_I$$
 (mgCOD/L)

$$OHO_{was} = f_{cv_{OHO}}(X_{BH} + X_{EH})$$
 (mgCOD/L)

$$iSS_{was} = \frac{MX_{IO}}{V_n}$$
 (mgiSS/L)

2.11. Oxygen demand

$$FO_c = Y_H (1 - f_{cv_{OHO}}) + f_{cv_{OHO}} (1 - f_H) \cdot b_{HT} \cdot f_{X_{RH}}$$
 (kgO/d)

$$FO_n = 4.57 \cdot Q \cdot N_{ae} \tag{kgO/d}$$

$$FO_t = FO_c + FO_n \tag{kgO/d}$$

$$OUR = \frac{FO_t}{V_p}$$
 (mgO/L·h)

3. Chemical P removal

3.1. Inputs

$$mass_{FeCl_3}$$

3.2. Molar weights

Sludge component	weight (g/mol)
M_{Fe}	55.845
M_P	30.974
M_{FeCl_3}	162.195
$M_{Fe(OH)_3}$	106.866
$M_{Fe_{1.6}H_2PO_4OH_{3.8}}$	250.9646

3.3. Moles of Fe added

$$moles_{Fe} = \frac{mass_{FeCl_3}}{M_{FeCl_3}} \frac{1mol_{Fe}}{1mol_{FeCl_3}}$$
 (molFe/d)

3.4. Moles of P available

$$P_{available} = P_{ti} - P_s - P_{ouse} - P_{obse}$$
 (mgP/L)

$$moles_P = \frac{Q \cdot P_{available}}{M_P}$$
 (molFe/d)

3.5. Fe/P mole ratio

$$Fe/P_{ratio} = \frac{moles_{Fe}}{moles_P}$$
 (molFe/molP)

3.6. Figure 6-13 Metcalf and Eddy 5th ed, page 484

Fe/P ratio	P_{se} (mgP/L)
8.00	0.01
4.90	0.02
4.50	0.03
4.20	0.04
3.90	0.05
3.80	0.06
3.70	0.07
3.50	0.08

Fe/P ratio	P_{se} (mgP/L)
3.35	0.09
3.30	0.10
2.60	0.20
2.10	0.30
2.00	0.40
1.70	0.50
1.50	0.60
1.20	0.70
1.10	0.80
1.00	0.90
1.00	1.00
0.20	2.00
0.10	3.00
0.10	4.00
0.01	5.00
0.01	6.00
0.005	7.00
0.001	8.00
0.001	9.00
0.0001	10.00

3.7. P removed by precipitation

$$P_{precipitation} = Q \cdot (P_{available} - P_{se})$$
 (kgP/d)

3.8. Extra iSS production by precipitation

$$F_{iSS_precipitation} = \frac{P_{precipitation}}{M_P} \left(M_{Fe_{1.6}H_2PO_4OH_{3.8}} + M_{Fe(OH)_3} \cdot (Fe/P_{ratio} - 1.6) \right) \quad \text{(kgiSS/d)}$$

4. Nitrification

4.1. Inputs

$$SF, f_{xt}DO, pH$$

4.2. Nitrifier kinetics

$$\mu_{Am} = 0.45$$
 (1/d)

$$\mu_{AmT} = \mu_{Am} (1.123)^{T-20} \tag{1/d}$$

$$K_O = 0.3 \tag{mgO/L}$$

$$\mu_{AmO} = \mu_{AmT} \frac{DO}{K_O + DO} \tag{1/d}$$

$$K_i = 1.13, K_{ii} = 0.3, K_{\text{max}} = 9.5$$

$$\mu_{AmpH} = \mu_{AmO}(2.35)^{pH-7.2} K_i \frac{K_{\text{max}} - pH}{K_{\text{max}} + K_{ii} - pH}$$
(1/d)

$$Y_A = 0.1 (gVSS/gN)$$

$$Y_{AT} = Y_A^{T-20}$$
 (gVSS/gNH4)

$$K_n = 1.0 (mgN/L)$$

$$K_{nT} = K_n (1.123)^{T-20}$$
 (mgN/L)

$$b_A = 0.04$$
 (1/d)

$$b_{AT} = b_A (1.029)^{T-20} (1/d)$$

4.3. Maximum design unaerated sludge mass fraction

$$f_{xm} = 1 - SF \frac{b_{AT} + \frac{1}{R_s}}{\mu_{AmpH}} \tag{\emptyset}$$

4.4. Minimum sludge age for nitrification

$$R_{sm} = \frac{1}{\frac{\mu_{AmpH}}{SF} (1 - f_{xt}) - b_{AT}}$$
 (d)

4.5. Effluent Ammonia concentration

$$N_{ae} = \frac{K_{nT}(b_{AT} + \frac{1}{R_s})}{\mu_{AmpH}(1 - f_{xt}) - b_{AT} - \frac{1}{R_s}}$$
 (mgN/L)

4.6. Nitrification capacity

$$N_c = N_{ti} - N_s - (N_{ae} + N_{ouse})$$
 (mgN/L)

4.7. ANO biomass

$$f_{X_{BA}} = \frac{Y_{AT}R_s}{1 + b_{AT} \cdot R_s}$$
 (gVSS·d/gNH4)

$$MX_{BA} = Q \cdot N_c \cdot f_{X_{BA}}$$
 (kgVSS)

$$X_{BA} = \frac{MX_{BA}}{V_p}$$
 (kgVSS/m³)

5. Denitrification

5.1. Inputs

$$a, DO_{RAS}$$
 alk_i

5.2. Denitrification kinetics

$$K_1^{20} = 0.72, K_2^{20} = 0.10, K_3^{20} = 0.10, K_4^{20} = 0.00$$
 (mgN/mgVSS·d)

$$K_{1T} = K_1^{20} (1.200)^{T-20}$$
 (mgN/mgVSS·d)

$$K_{2T} = K_2^{20} (1.080)^{T-20}$$
 (mgN/mgVSS·d)

$$K_{3T} = K_3^{20} (1.029)^{T-20}$$
 (mgN/mgVSS·d)

$$K_{4T} = K_4^{20} (1.029)^{T-20}$$
 (mgN/mgVSS·d)

5.3. Denitrification potential

$$D_{p1RBSO} = \frac{S_{bsi}(1 - f_{cv}Y_H)}{2.86}$$
 (mgN/L)

$$D_{p1BPO} = K_{2T} f_{xt} (S_{bi} - S_{nd}) f_{X_{RH}}$$
 (mgN/L)

$$D_{p1} = D_{p1RBSO} + D_{p1BPO}$$
 (mgN/L)

5.4. Optimum internal recirculation (a)

$$a_{opt} = \frac{-B + \sqrt{B^2 + 4AC}}{2A} \tag{\emptyset}$$

where:

$$A = \frac{DO}{2.86}$$

$$B = N_c - D_{p1} + \frac{(1 + RAS) \cdot DO + RAS \cdot DO_{RAS}}{2.86}$$

$$C = (1 + RAS) \cdot (D_{p1} - \frac{RAS \cdot DO_{RAS}}{2.86}) - RAS \cdot N_c$$

5.5. Minimum (optimum) effluent nitrate concentration

$$N_{ne_opt} = \frac{N_c}{a_{opt} + RAS + 1}$$
 (mgN/L)

5.6. Effluent nitrate (N_{ne})

 $if(a < a_{opt})$

$$N_{ne} = \frac{N_c}{a + RAS + 1}$$
 (mgN/L)

 $if(a > a_{opt})$

$$N_{ne} = N_c - D_{p1} + \frac{a \cdot DO + RAS \cdot DO_{RAS}}{2.86}$$
 (mgN/L)

5.7. Nitrogen gas production (FN_2)

$$FN_2 = Q(N_c - N_{ne})$$
 (kgN/d)

5.8. Oxygen recovered by denitrification and total oxygen demand corrected

$$FO_d = 2.86 \cdot Q \cdot (N_c - N_{ne})$$
 (kgO/d)

$$FO_t = FO_c + FO_n - FO_d (kgO/d)$$

5.9. Effluent alkalinity

$$alk_e = alk_i + 3.57 \cdot (N_{obi} - (N_s - N_{oupi})) - 7.14 \cdot N_c + 2.86 \cdot (N_c - N_{ne}) \text{ (mgCaCO3/L)}$$