Document under development

UCT-ICRA wastewater MLE model

Implementation in Javascript

University of Cape Town (UCT)
Catalan Institute for Water Research (ICRA)

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1. State Variables

1.1. Inputs

$$Q \qquad \text{(ML/d)}$$

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

1.2. Total chemical oxygen demand (S_t)

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

and:

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

The components can be grouped as follows:

	S_s	S_p
S_b	S_{bs}	S_{bp}
S_u	S_{us}	S_{up}

So,

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

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

1.3. Default Mass ratio values for COD, N, P and C

State Variable	**COD (f_{cv})**	**N (f_N)**	**P (f_P)**	**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 (N_t)

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

where:

$$N_o = N_{obs} + N_{obp} + N_{ous} + N_{oup}$$
$$N_{obs} = S_{VFA} \frac{f_{N_{VFA}}}{f_{cv_{VFA}}} + S_{FBSO} \frac{f_{N_{FBSO}}}{f_{cv_{FBSO}}}$$
$$N_{obp} = X_{BPO} \frac{f_{N_{BPO}}}{f_{cv_{BPO}}}$$
$$N_{ous} = S_{USO} \frac{f_{N_{USO}}}{f_{cv_{USO}}}$$
$$N_{oup} = X_{UPO} \frac{f_{N_{UPO}}}{f_{cv_{UPO}}}$$
$$N_{active} = X_{OHO} \frac{f_{N_{OHO}}}{f_{cv_{OHO}}}$$

1.5. Total Phosphorus (P_t)

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

where:

$$P_o = P_{obs} + P_{obp} + P_{ous} + P_{oup}$$
$$P_{obs} = S_{VFA} \frac{f_{P_{VFA}}}{f_{cv_{VFA}}} + S_{FBSO} \frac{f_{P_{FBSO}}}{f_{cv_{FBSO}}}$$
$$P_{obp} = X_{BPO} \frac{f_{P_{BPO}}}{f_{cv_{BPO}}}$$
$$P_{ous} = S_{USO} \frac{f_{P_{USO}}}{f_{cv_{USO}}}$$
$$P_{oup} = X_{UPO} \frac{f_{P_{UPO}}}{f_{cv_{UPO}}}$$
$$P_{active} = X_{OHO} \frac{f_{P_{OHO}}}{f_{cv_{OHO}}}$$

1.6. Total Organic Carbon (C_t)

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

where:

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

1.7. Total suspended solids (X_T)

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

where:

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

2. Activated sludge

2.1. Inputs

$$T(^{o}C), V_p(m^3), R_s(days), RAS(ø)$$

2.2. Volatile suspended solids (VSS)

$$b_H = 0.24 \quad \text{(1/d)}$$

$$\theta_{bH} = 1.029 \quad \text{(1/d)}$$

$$b_{HT} = b_H \cdot (\theta_{b_H})^{T-20} \quad \text{(1/d)}$$

$$Y_H = 0.45 \quad \text{(gVSS/gCOD)}$$

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

$$k_{vT} = k_{v20} \cdot (\theta_{k_{v20}})^{T-20} \quad \text{(L/gVSS·d)}$$

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

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

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

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

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

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

$$X_V = \frac{MX_V}{V_p} \quad \text{(kgVSS/m}^3\text{)}$$

2.3. Total inert solids (iSS)

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

$$MX_{IO} = FiSS \cdot R_s + f_{iOHO} \cdot MX_{BH} + F_{iSS\_precipitation} \cdot R_s \quad \text{(kgiSS)}$$

2.4. Total suspended solids (TSS)

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

$$X_T = \frac{MX_T}{V_p} \quad \text{(kgTSS/m}^3\text{)}$$

2.5. Nominal hydraulic retention time

$$HRT = \frac{V_p}{Q} \qquad \text{(d)}$$

2.6. Wastage flowrate

$$Q_w = \frac{V_p}{R_s} \qquad \text{(ML/d)}$$

2.7. Effluent flowrate

$$Q_e = Q - Q_w \qquad \text{(ML/d)}$$

2.8. Nitrogen and Phosphorus required for sludge production

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

$$P_s = \frac{f_{P_{OHO}}(MX_{BH} + MX_{EH}) + f_{P_{UPO}} MX_I}{R_s \cdot Q} \qquad \text{(mgP/L)}$$

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

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

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

2.10. Wastage solids concentration

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

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

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

$$iSS_{was} = \frac{MX_{IO}}{V_p} \qquad \text{(mgiSS/L)}$$

2.11. Oxygen demand

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

$$FO_n = 4.57 \cdot Q \cdot N_{ae} \qquad \text{(kgO/d)}$$

$$FO_t = FO_c + FO_n \qquad \text{(kgO/d)}$$

$$OUR = \frac{FO_t}{V_p} \qquad (\mathrm{mgO/L \cdot h})$$

3. Chemical P removal

3.1. Inputs

$$mass_{FeCl_3}(kg/d)$$

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

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

3.4. Moles of P available

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

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

3.5. Fe/P mole ratio

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

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

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

3.8. Extra iSS production by precipitation

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

4. Nitrification

4.1. Inputs

$$SF(ø),\ f_{xt}(ø), DO(mg/L),\ pH(ø)$$

4.2. Nitrifier kinetics

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

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

$$K_O = 0.3 \qquad (mgO/L)$$

$$\mu_{AmO} = \mu_{AmT}\frac{DO}{K_O + DO} \qquad (1/d)$$

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

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

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

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

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

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

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

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

4.3. Maximum design unaerated sludge mass fraction

$$f_{xm} = 1 - SF\frac{b_{AT} + \frac{1}{R_s}}{\mu_{AmpH}} \qquad (ø)$$

4.4. Minimum sludge age for nitrification

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

4.5. Effluent Ammonia concentration

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

4.6. Nitrification capacity

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

4.7. ANO biomass

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

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

$$X_{BA} = \frac{MX_{BA}}{V_p} \qquad \text{(kgVSS/m}^3\text{)}$$

5. Denitrification

5.1. Inputs

$$a, DO_{RAS,} alk_i$$

5.2. Denitrification kinetics

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

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

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

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

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

5.3. Denitrification potential

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

$$D_{p1BPO} = K_{2T}\, f_{xt}(S_{bi} - S_{nd})\, f_{X_{BH}} \qquad \text{(mgN/L)}$$

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

5.4. Optimum internal recirculation (a)

$$a_{opt} = \frac{-B + \sqrt{B^2 + 4AC}}{2A} \qquad (ø)$$

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

$$N_{ne\_opt} = \frac{N_c}{a_{opt} + RAS + 1} \qquad \text{(mgN/L)}$$

5.6. Effluent nitrate (N_{ne})

$if\,(a < a_{opt})$

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

$if\,(a > a_{opt})$

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

5.7. Nitrogen gas production (FN_2)

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

5.8. Oxygen recovered by denitrification and total oxygen demand corrected

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

$$FO_t = FO_c + FO_n - FO_d \qquad \text{(kgO/d)}$$

5.9. Effluent alkalinity

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