1) Approach to get the elementary flows of COD and nutrients

The steps are the following:

A. We execute the design according to Metcalf&Eddy Aecom (2014) equations
B. Some extra calculations and inputs needed after executing the design to prepare for the elementary flows factors
C. Calculation of the elementary flows factors following the equations in Table 1.

2) Extra calculations and new inputs needed

Inputs needed:

- TSSef: Average effluent TSS concentration (from 5 to 35 mg/L); 35 mg/L is the limit established by the directive 91/271 EU. This will be imposed in the desing exercise; and from this one we will estimate VSSe.

Extra calculations:

Table 1. Extra calculations

Id	Description	Equation/Value	Source
VSSe	WWTP Effluent volatile suspended solids (g/m3)	= TSSef · 0.85	Metcalf % Eddy
Qwas	Wastage flow rate (m3/d	$Qw\,(\frac{m3}{d}) = \frac{\frac{V_{reactor} \times MLSS}{SRT} - TSS_{eff} \times Q_{in}}{-1 \times TSS_{eff} + TSS_{was}}$ V in m3, MLSS in g/m3, SRT in days, TSS in g/m3, Q in m3/d	Typical equation of SRT calculation (see metcalf and eddy)
Qin	Influent flow (m3/d)		
Qe	Effluent flow (m3/d)		

3) COD Influent fractionation (in red what is an input ; in green what is calculated)

Table 2. COD influent fractionation;

Inputs	Fractions		Equation/Value
TCOD	COD total (g/m3)		
sCOD	COD soluble (g/m3)		
BOD	This is the carbonaceous BOD5 (g/m3)		
	bCOD (g/m3)		bCOD = 1.6(BOD)
	nbCOD (g/m3)		nbCOD = TCOD - bCOD
	nbsCODe (g/m3)		nbsCODe = sCOD - 1.6·sBOD (a check in here is needed to make sure that nbsCODe is not negative !... if this is the case I would fix nbsCODe at 20 g/m3 and recalculate sCOD)
	nbpCOD (g/m3)	To calculate nbVSS	nbpCOD = TCOD - bCOD - nbsCODe
	VSSCOD (g/m3)	To calculate nbVSS	VSSCOD = (TCOD-sCOD)/VSS
	nbVSS (g/m3)	To calculate sludge production (non biodegr from the influent)	nbVSS = nbpCOD / VSSCOD
	rbCOD (g/m3)	Readily biodegradable COD	For raw wastewater: rbCOD = 20% of bCOD For primary effluent wastewater: rbCOD = 32% of bCOD
	VFA (g/m3)	Volatile fatty acids (acetate)	VFA = 0.15 · rbCOD

Comentario [I1]: Is this factor changing for raw or primary effluent wastewater?

Comentario [I2]: Taken from Yves spreadsheet

TSS	Total suspended solids (g/m3)		
VSS	Volatile suspended solids (g/m3)		
	iTSS (g/m3)	To calculate sludge production (inerts from the influent)	iTSS = TSS – VSS
	Px,bio (g/d)		$Px, bio\ (VSS) = \frac{QY_H(S_0 - S)}{1 + b_H(SRT)} + \frac{(f_d)(b_H)Q(S_0 - S)SRT}{1 + b_H(SRT)} + \frac{QY_N(NOx)}{1 + b_{AOB}(SRT)}$
	Px,vss (g/d)		PX,VSS = PX,bio + Q·nbVSS
	Px,TSS (g/d)		$P_{x,TSS} = \frac{Px, bio}{0.85} + Q(nbVSS) + Qin(TSS_{in} - VSS_{in})$

4) Nitrogen influent fractionation (in red what is an input ; in green what is calculated)

Table 3. N influent fractionation

Inputs	Fractions		Equation/Value
TKN (g/m3)			
	nbpON (g/m3)		nbpON = fN(nbVSS) ; fN=0.064 ;
	nbsON (g/m3)		= 0.3 g/m3 ;
	TKN_N2O (g/m3)		TKN_N2O = fN2O X TKN; fN2O= 0.001 gN-N2O/gN-TKN
	bTKN (g/m3)	Biodegradable TKN available for nitrification; this is the	bTKN = TKN - nbpON – nbsON – TKN_N2O

Comentario [I3]: This is the NOX from the BOD and nitrification exercise. Meaning, all ammonia which has been converted to nitrate. For the BOD removal technology this equals 0.

Comentario [I4]: Factor from metcalf and Eddy

Comentario [I5]: Ref is ASM2d

Comentario [I6]: To be checked with modelers

Comentario [I7]: Yve can confirm this value, or provide a different value for each type of technology

Comentario [I8]: Comment from Yves: this fraction depends a lot on the process 0.005 Chandran et al. (2010)

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0.0001 to 0.112 Foley et al. (2015)
https://books.google.ca/books?hl=en&lr=&id=C4IbCgAAQBAJ&oi=fnd&pg=PP1&dq=foley+wastewater+n2o&ots=FiQ6OuQ-8q&sig=paR3bTLaXbNaQxPV44gUTlptuXo#v=onepage&q=foley%20wastewater%20n2o&f=false

N2O and CH4 Emission from Wastewater Collection and Treatment Systems: State of the Science Report and Treatment Report
By Jeff Foley, Zhiguo Yuan, Jurg Keller, Elena Senante, Kartik Chandran, John Willis, Anup Shah, Mark C. M. van Loosdrecht, Ellen van Voorthuizen

		fraction of N used for nitrification. We assume 100% of bTKN is hydrolyzed to Ammonia.	
Ne (g/m3)		Imposed ammonia concentration in the effluent	
NOx,e (g/m3)		This is the imposed NOX concentration at the effluent	
	NOx_nitri (g/m3)	Amount of nitrogen oxidized to nitrate	NOx_nitri = bTKN – Ne – 0.12·Px,bio/Q (g/m3)

5) Phosphorus influent fractionation (in red what is an input ; in green what is calculated)

Table 4. Influent P fractionation

Inputs	Fractions		Equation/Value
TP (g/m3)			
	nbpP (g/m3)		nbpP = fP·(nbVSS) ; fP=0.025 gP/gnbpVSS;
	nbsP (g/m3)		= 0 gP/m3
	aP (g/m3)	Available phosphorus to be accumulated in organisms ; this corresponds to the P in Metcalf and Eddy design	aP = TP – nbpP – nbs = PO4in

Comentario [I9]: Value provided by George

Comentario [I10]: Value provided by George.

		exercise.	
	aPchem (g/m3)	Available phosphorus for chemical P removal (we first use P for biomass growth and the remaining is going to be precipitated with chemicals)	aPchem = aP – (0.015 · Px,bio)/Qin

6) Elementary flows factors

Table 5. Elementary flows factors

For organic matter we provide the elementary flow based on COD; just one C balance based on COD. The BOD is included within the balance, but will not have a separate balance. The lower case "e" means effluent. All flows in m3/d; concentrations are in g/m3.

	Water (effluent) (g/d)	Air (g/d)	Sludge (g/d)
COD	CODwater = sCODe + biomass CODe $sCODe\left(\frac{g}{d}\right) = Q_e \times nbsCOD + Q_e \times \frac{k_S(1 + k_d \times SRT)}{SRT(Y_H - k_{d,H}) - 1}$ $biomass\ CODe\ (g/d) = Q_e \times VSSe \times 1.42\ gCOD/gVSS$	(negative COD goes to air in the form of oxygen; but this is accounted as oxygen demand, estimated from metcalf and Eddy equations;)	CODsludge = A + B $A = \left[\frac{Q \times Y_H \times (S_0 - S)}{1 + (k_{d,H} \times SRT)} + \frac{k_{d,H} \times f_d \times Q \times Y_H \times (S_0 - S) \times SRT}{1 + (k_{d,H} \times SRT)} + \frac{Q \times Y_A \times (NH_{x,0} - NH_x)}{1 + (k_{d,A} \times SRT)}\right] \times 1.42\ gCOD/gVSS$ $B = Q_{was} \times sCODe$
CO2	-	CO2 from BOD oxidation (includes COD removal under aerobic and under anoxic conditions, with the assumption	

Comentario [I11]: This is zero for the technology "BOD removal only "

		that yield in aerobic is same as anoxic) + CO2 from endogenous decay –CO2 consumed by nitrifiers $k_{\frac{CO2}{COD}} \times Q \times (1 - Y_H) \times (S_0 - S) + k_{CO2/biomass} \times \frac{Q \times Y_H \times (S_0 - S) \times (k_{d,H} \times SRT)}{1 + (k_{d,H} \times SRT)} \times (1 - f_d) - 4.49 \frac{gCO2}{gN\ nitrified} \times Nnitrified$ About 10% of this CO2 should be accounted as is non-biogenic! Should we account as well CO2 consumed by nitrifiers and the CO2 produced in the denitrification?	
CH4	-	$bCOD \times Qin \times 0.95$	-
TKN	- For the technology BOD removal only $TKNe\left(\frac{g}{d}\right) = (Q_{in} \times TKN_{in}) - (0.12 \times Px, bio) + (Q_e \times VSSe \times 0.12)$ - For any technology that involves nitrification TKNe = sTKNe + biomass N $sTKNe\left(\frac{g}{d}\right) = (N_e \times Q_e) + (nbsON \times Q_e)$ Ne is imposed by design input $TKNe\left(\frac{g}{d}\right) = (sTKN_e) + (Q_e \times VSSe \times 0.12)$	-	Nsludge = A + B $A = 0.12 \times Px, bio;$ $B = Q_{was} \times sTKNe$
NOx	- For technology BOD removal only; and BOD removal + nitrification:	-	$Q_{was} \times NOx_e$

Comentario [l12]: Nitrifiers are strict autotrophic bacteria that use only inorganic carbon for cell synthesis. That is, they consume CO_2 and thus deplete the levels of dissolved carbon dioxide (carbonic acid) in the wastewater. The equation representing this is shown below[1]:

$20CO_2 + 14 NH_4^+ = 10 NO_3 + 4C_5H_7O_2N + 24H^+ + 2H_2O$ ....(5)

Based on atomic weights, Equation 5 reveals that 4.49 kg of CO_2 is consumed per kg of N nitrified.

Comentario [l13]: (equation from Gori et al. (2011)

Comentario [l14]: In BOD only systems the Nnitrified is 0.

Comentario [l15]: The sludge production for this technology is calculated as

$nbpCOD \times Qin - bCOD \times Qin \times 0.05$

Comentario [l16]: Only applicable to the technology: anaerobic removal

0.95 has been provided by George

Yves says that the 0.95 would be ok for lagoons but probably not for intensive anaerobic treatment. TBD!

Comentario [l18]: $0.12 \frac{gN}{gbiomass}$ $(C5H7$

Comentario [l17]: $0.12 \frac{gN}{gbiomass}$ $(C5H7$

	$$NOx_e(\frac{g}{d}) = Q_e \times (bTKN - Ne) - 0.12 \times Px,bio$$ - For the technology BOD removal + nitrification + denitrification: NOx is Imposed by design input $$NOx_e(\frac{g}{d}) = (Q_e \times NOx)$$		
N2	-	Only for the technology that includes denitrification (= the technology that is named Nremoval). For the others N2 equals 0. $0.22 \times (NOx_{nitri} - NOx_e)$	-
N2O	-	This applies to all technologies (even BOD removal only?) $$Qin \times TKN\_N2O$$	-
TP	(in g/d) For non BioP and non ChemP→ $$PO4_e = PO4in$$ $$TPe = (Q_e \times PO4_e) + (Q_e \times VSSe \times 0.015)$$ For BioP → PO4e is Imposed by design input $$PO4_e = PO4in - P_{EBPR} - P_{synthesis}$$	-	(in g/d) **A+B** For non BioP→ $$\boldsymbol{A} = 0.015 \frac{gP}{gbiomass} \times P_{x,bio}$$ For BioP → $$\boldsymbol{A} = 0.015 \frac{gP}{gbiomass} \times P_{x,bio} + P_{EBPR}$$

Comentario [I19]: Question to modelers.

Comentario [I20]: 0.015 is the value from metcalf. Check against the value 0.025 provided in Table 4.

	$$P_{EBPR} = \frac{rbCOD}{rbCOD/P}$$ $P_{synthesis} = 0.015 \times Px, bio$ $$TPe = (Q_e \times PO4_e) + (Q_e \times VSSe \times (\frac{(PO4_e - PO4_{in})}{Px, vss}))$$ For chemP → PO4e is Imposed by design input $$TPe = (Q_e \times PO4_e) + (Q_e \times VSSe \times (\frac{(PO4_e - PO4_{in})}{Px, vss}))$$		$$P_{EBPR} = \frac{rbCOD}{rbCOD/P}$$ For chemP → $$A = 0.015 \frac{gP}{gbiomass} \times P_{x,bio} + (aPchem - PO4e) \times Qin$$ $\boldsymbol{B} = Q_{was} \times PO4e$
TS			

Comentario [l21]: We have implemented Fig 8-38 from Metcalf.

Comentario [l22]: Input from George needed.

INPUTS / OUTPUTS OF THE TOOL

Compound	**Influent (g/d)**	**Water (effluent) (g/d)**	**Air (g/d)**	**Sludge (g/d)**
COD				
CO_2				
TKN				
NO_x				
N_2				
N_2O				
TP				
TS				
CH_4				

WEB TAB WITH INPUTS REQUEST

Select technology

Options
BOD
BOD + nitrification
BOD + nitrification + denitrification
BOD + nitrification + denitrification + BioP
BOD + nitrification + denitrification + ChemP
BOD + ChemP

Primary treatment

Options	Purpose
Yes	If Yes, then for the influent COD fractionation we use the primary effluent wastewater
No	If No, then for the influent COD fractionation we use the raw wastewater

Wastewater flow and composition

Compound	**Units**	**Value**
Qin	m3/d	
TCOD	g/m3	
sCOD	g/m3	
BOD	g/m3	
TKN	g N/m3	
TP	g P/m3	
TS	g S/m3	
TSS	g/m3	
VSS	g/m3	
Temperature of wastewater	ºC	
Alkalinity	g CaCO3/m3	

Comentario [I23]: Sulfur compounds

Design choices

Compound	**Units**	Notes
Ne (effluent ammonia)	g N/m3	This one is only requested for the technologies including nitrification;
NOx,e (effluent nitrate)	g N/m3	This one is not requested for the following technologies: BOD; BOD+nitrification; BOD+chemP;
PO4,e (effluent phosphate)	g P/m3	This one is only requested for the technologies including ChemP or BioP

TSS,e (total suspended solids in the effluent)	g/m3	(default value= 35)
SRT (sludge retention time)	d	Only for the technologies not including nitrification (default value = 5d)
Zb (elevation of the WWTP above sea level)	m	
Diffuser depth	m	
Xr (MLSS concentration at the bottom of the settler)	g/m3	Default = 8000 g/m3
Anoxic mixing energy	?	
FeCl3 solution percentage	%	
FeCl3 solution unit weight	Kg/L	
Time for supply to be stored	d	

MASS BALANCE VERIFICATION

(row:column) from table 5

	Influent load (g/d) **(A)**	Wastewater Effluent load (g/d) **(B)**	Air load (g/d) **(C)**	Sludge load (g/d) **(D)**	Difference in the mass balance (g/d)
C balance	Qin X TCOD	(1:1)	(2:2)	(1:3)	A-B-C-D
N balance	Qin X TKN	(4:1) + (5:1)	(6:2)+(7:2)	(4:3) + (5:3)	A-B-C-D
P balance	Qin X TP	(8:1)	-	(8:3)	A-B-C-D
S balance	Qin X TS	(9:1)	-	(9:3)	A-B-C-D