Raw sewage and its treatment

|  |  |  |  |
| --- | --- | --- | --- |
| Symbol | meaning | equation | default |
| Q | Sewage flow |  | 0.2 |
| SO | Mass of sewage solids |  | 0.09 |
| BOD |  |  | 0.06 |
| FB | Fraction BOD in sewage solids |  | 0.5417 |
| FS | Fraction sewage solids removed by primary settler |  | 0.667 |
| focs | Fraction organic carbon in sewage solids |  | 0.3 |
| ds | Density of sewage solids |  | 1.5 |
| Cso,s | Conc. solids in raw sewage | $$^{SO}/\_{Q}$$ | 0.45 |
| CBOD,S | Conc. BOD in raw sewage | $$^{BOD}/\_{Q}$$ | 0.3 |

Defining the primary clarifier

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| --- | --- | --- | --- |
| Symbol | meaning | equation | default |
| hps | Depth of the PS tank |  | 4 |
| HRTPS | Hydraulic retention time |  | 2 |
| VOLPS | Volume PS per person | $$\frac{Q⋅HRT\_{PS}}{24}$$ | 1.67∙10-2 |
| AREAPS | Area PS per person | $$\frac{Q⋅HRT\_{PS}}{24⋅h\_{PS}}$$ | 4.167∙10-3 |
| CSO,PS | Conc. suspended solids in PS | (1-FS) ∙ Cso,s | 0.15 |
| FP | Fraction BOD removed by PS | FS∙FB | 0.36 |

Defining the activated sludge process

|  |  |  |  |
| --- | --- | --- | --- |
| Symbol | meaning | equation | default |
| hAS=hSLS | Depth of aeration tank and SLS |  | 3 |
| HRTSLS | Hydraulic retention time SLS |  | 6 |
| CSO,AS | Conc. suspended solids in activated sludge |  | 4 |
| CSO,SLS | Conc. suspended solids in effluent |  | 0.0075 |
| dAS | Density of activated sludge solids |  | 1.3 |
| focAS | Fraction organic carbon activated sludge |  | 0.37 |
| kSLR | Sludge loading rate |  | 0.1 |
| M | Aeration mode: surface (s) or bubble (b) |  | s |
| OxReq | Oxygen requirement | $$(1-FP)⋅\frac{BOD}{Q}$$ | 0.192 |
| VOLAS | Volume aerator per person | $$\frac{Q⋅OxReq}{k\_{SLR}⋅C\_{SO,AS}}$$ | 9.6∙10-2 |
| AREAAS | Area aerator per person | $$\frac{VOL\_{AS}}{h\_{AS}}$$ | 3.2∙10-2 |
| HRTAS | Hydraulic retention time aerator | $$\frac{VOL\_{AS}}{Q}⋅24$$ | 11.5 |
| VOLSLS | Volume SLS per person | $$\frac{Q⋅HRT\_{SLS}}{24}$$ | 5.0∙10-2 |
| AREASLS | Area SLS per person | $$\frac{VOL\_{SLS}}{h\_{SLS}}$$ | 1.67∙10-2 |

|  |  |  |  |
| --- | --- | --- | --- |
| Symbol | meaning | equation | default |
| FBODrem | Fraction BOD removed in activated sludge process | $$F\_{BODrem }=0.818-0.0422⋅ln⁡k\_{SLR}$$ | 0.915 |
| YBOD | Sludge growth | $$Y\_{BOD }=0.947-0.0739⋅ln⁡k\_{SLR}$$ | 0.777 |
| SU | Wasted sludge (surplus sludge) | $$SU=Q⋅\left( OxReq ⋅F\_{BODrem }⋅Y\_{BOD}-C\_{so,SLS }\right)$$ | 0.026 |
| SRT | sludge retention time | $$SRT=\frac{VOL\_{AS}⋅C\_{SO,AS}}{SU+C\_{SO,SLS}⋅Q}=\frac{1}{k\_{SLR}⋅F\_{BODrem}⋅Y\_{BOD}}$$ | 14.1 |

Definition of the modelled chemical

Equilibrium partitioning constants

|  |  |  |  |
| --- | --- | --- | --- |
| Symbol | meaning | equation | default |
| SOS | Chemical concentration in sewage solids (raw and settled) |  |  |
| SOAS | Chemical concentration in activated sludge solids |  |  |
| W | Chemical concentration in water |  |  |
| A | Chemical concentration in air |  |  |
| KAW | Air-water equilibrium partition constant | $$\frac{A}{W}$$ |  |
| Kps | Sewage solids-water equilibrium partition constant | $$\frac{SO\_{S}}{W}$$ |  |
| KpAS | Activated sludge solids-water equilibrium partition constant | $$\frac{SO\_{AS}}{W}$$ |  |

$$H=\frac{P⋅MW}{W}=R⋅T⋅K\_{AW}$$

Henry’s law constant, H, has dimensions of Pa∙m3∙mol-1. P is the vapour pressure in Pascal (Pa) of the chemical in equilibrium with the aqueous concentration W, MW is the molecular weight of the chemical in g∙mol-1, R is the gas constant (8.314 J∙K-1∙1R -1) and T is the absolute temperature (K). KAW is also known as the dimensionless Henry constant.

Estimation methods for equilibrium partitioning constants

Neutral organic chemicals

From base-set data (Table 12) the air-water equilibrium partition coefficients of organic chemicals is estimated according to:

$$K\_{AW}=\frac{H}{R⋅T}=\frac{VP⋅\frac{MW}{SOL}}{R⋅T}$$



For the partitioning of the chemical between solids and the aqueous phase, a simple relationship is applied:

$$Kp=foc⋅Koc$$

With：

 Kp: partition coefficients [L∙kg-1] for sewage (KpS) or activated sludge (KpAS)

Koc: partition coefficient for organic [L∙kg-1]

foc: fraction organic carbon solids, focS =0.3 or focAS =0.37[-]

$$Koc=1.26⋅Kow^{0.81}$$

Organic acids and bases

$$Fn=\frac{1}{1+10^{γ}⋅(pH-pKa)}$$

In the case of acids, γ equals 1 and, in the case of bases, γ is -1

$$K\_{AW}=\frac{H}{R⋅T}⋅Fn=\frac{VP⋅\frac{MW}{SOL}}{R⋅T}⋅Fn$$

$$\begin{array}{c}\& Dow =\frac{C\_{n}^{0}+C\_{ion }^{o}}{C\_{n}^{W}+C\_{ion }^{W}}=\\\&=Fn⋅\frac{C\_{n}^{0}}{C\_{n}^{W}}+(1-Fn)⋅\frac{C\_{ion }^{0}}{C\_{ion }^{W}}=\\\&=Fn⋅ Kow +(1-Fn)⋅ Kow (ionized) ≅Fn⋅Kow\end{array}$$

Chemical fate processes

Mass balance equations

$$\begin{array}{c}\& box 1:C\_{1}⋅\left(XCH\_{1,2}+XCH\_{1,5}+XCH\_{1,7}+ADV\_{1,0}\right)-C\_{2}⋅XCH\_{2,1}-C\_{5}⋅XCH\_{5,1}-C\_{7}⋅XCH\_{7,1}=0\\\& box 2:C\_{1}⋅XCH\_{1,2}-C\_{2}⋅\left(XCH\_{2,1}+XCH\_{2,3}+ADV\_{2,5}\right)+C\_{3}⋅XCH\_{3,2}=-C(0,2)⋅ADV\_{0,2}\\\& box 3:C\_{2}⋅XCH\_{2,3}-C\_{3}⋅\left(XCH\_{3,2}+ADV\_{3,6}+ADV\_{3,4}\right)=-C(0,3)⋅ADV\_{0,3}\\\& box 4:C\_{3}⋅ADV\_{3,4}-C\_{4}⋅ADV\_{4,0}=0\\\& box 5: C\_{1}⋅XCH\_{1,5}+C\_{2}⋅ADV\_{2,5}-C\_{5}⋅\left(XCH\_{5,1}+XCH\_{5,6}+ADV\_{5,7}+k\_{5}⋅V\_{5}\right)+C\_{6}⋅XCH\_{6,5}=0\\\& box 6: C\_{3}⋅ADV\_{3,6}+C\_{5}⋅XCH\_{5,6}-C\_{6}⋅\left(XCH\_{6,5}+ADV\_{6,8}\right)+C\_{9}⋅ADV\_{9,6}=0\\\& box 7:C\_{1}⋅XCH\_{1,7}+C\_{5}⋅ADV\_{5,7}-C\_{7}⋅\left(XCH\_{7,1}+XCH\_{7,8}+ADV\_{7,0}\right)+C\_{8}⋅XCH\_{8,7}=0\\\& box 8: C\_{6}⋅ADV\_{6,8}+C\_{7}⋅XCH\_{7,8}-C\_{8}⋅\left(XCH\_{8,7}+ADV\_{8,0}+ADV\_{8,9}\right)=0\\\& box 9:C\_{8}⋅ADV\_{8,9}-C\_{9}⋅\left(ADV\_{9,6}+ADV\_{9,0}\right)=0\end{array}$$





Table A1 Volumes of the nine boxes per inhabitant

|  |  |  |
| --- | --- | --- |
| Vi | Equation | default value(m3∙PE-1) |
| V1 | $$h⋅\left(AREA\_{PS}+AREA\_{AS}+AREA\_{SLS}\right)$$ | 0.53 |
| V2 | $$\frac{Q⋅HRT\_{PS}}{24}$$ | 1.67$⋅$10-2 |
| V3 | $$\frac{V\_{2}⋅(1-FS)⋅C\_{SO,S}}{1000⋅d\_{S}}$$ | 1.67∙10-6 |
| V4 | $$\frac{SO⋅FS⋅1(d)}{1000⋅d\_{S}}$$ | 4.17∙10-5 |
| V5 | $$\frac{Q⋅OxReq}{k\_{SLR}⋅C\_{SO,AS}}$$ | 9.58∙10-2 |
| V6 | $$\frac{V\_{5}⋅C\_{SO,AS}}{1000⋅d\_{AS}}$$ | 2.95∙10-4 |
| V7 | $$\frac{Q⋅HRT\_{SLS}}{24}$$ | 5.0∙10-2 |
| V8 | $$\frac{V\_{7}⋅C\_{SO,SLS }}{1000⋅d\_{AS}}$$ | 2.88∙10-7 |
| V9 | $$\frac{SU⋅1(d)}{1000⋅d\_{AS}}$$ | 1.67∙10-5 |

|  |  |  |
| --- | --- | --- |
| ADVi,j | Equation | default value |
| ADV0,1 | $$\begin{array}{c}\&h⋅WS\\\&⋅\sqrt{\left(AREA\_{PS}+AREA\_{AS}+AREA\_{SLS}\right)}\end{array}$$ | 6.9 m3∙s-1∙PE-½ |
| ADV1,0 | $$\begin{array}{c}\&h⋅WS\\\&⋅\sqrt{\left(AREA\_{PS}+AREA\_{AS}+AREA\_{SLS}\right)}\end{array}$$ | 6.9 m3∙s-1∙PE-½ |
| ADV0,2 | $$\frac{Q}{24⋅3600}$$ | 2.31∙10-6 m3∙s-1∙PE-1 |
| ADV2,5 | $$\frac{Q}{24⋅3600}$$ | 2.31∙10-6 m3∙s-1∙PE-1 |
| ADV5,7 | $$\frac{Q}{24⋅3600}$$ | 2.31∙10-6 m3∙s-1∙PE-1 |
| ADV7,0 | $$\frac{Q}{24⋅3600}$$ | 2.31∙10-6 m3∙s-1∙PE-1 |
| ADV0,3 | $$\frac{SO}{1000⋅d\_{RS}⋅24⋅3600}$$ | 6.94∙10-10 m3∙s-1∙PE-1 |
| ADV3,4 | $$\frac{FS⋅SO}{1000⋅d\_{RS}⋅24⋅3600}$$ | 4.63∙10-10 m3∙s-1∙PE-1 |
| ADV3,6 | $$\frac{(1-FS)⋅SO}{1000⋅d\_{RS}⋅24⋅3600}$$ | 2.31∙10-10 m3∙s-1∙PE-1 |
| ADV4,0 | $$\frac{FS⋅SO}{1000⋅d\_{RS}⋅24⋅3600}$$ | 4.63∙10-10 m3∙s-1∙PE-1 |
| ADV6,8 | $$\frac{Q⋅C\_{SO,AS}}{1000⋅d\_{AS}⋅24⋅3600}$$ | 7.12∙10-9 m3∙s-1∙PE-1 |
| ADV8,0 | $$\frac{Q⋅C\_{SO,SLS}}{1000⋅d\_{A}⋅24⋅3600}$$ | 1.34∙10-11 m3∙s-1∙PE-1 |
| ADV8,9 | $$\frac{Q⋅\left(C\_{SO,AS}-C\_{SO,SLS}\right)}{1000⋅d\_{AS}⋅24⋅3600}$$ | 7.11∙10-9 m3∙s-1∙PE-1 |
| ADV9,0 | $$\frac{SU}{1000⋅d\_{AS}⋅24⋅3600}$$ | 2.29∙10-10 m3∙s-1∙PE-1 |
| ADV9,6 | $$\frac{Q⋅\left(C\_{SO,AS}-C\_{SO,SLS}\right)-SU}{1000⋅d\_{AS}⋅24⋅3600}$$ | 6.88∙10-9 m3∙s-1∙PE-1 |
| Sludge decay | $$ADV\_{3,6}⋅\frac{d\_{S}}{d\_{AS}}+ADV\_{9,6}-ADV\_{6,8}$$ | 2.44∙10-11 m3∙s-1∙PE-1 |

|  |  |
| --- | --- |
| XCHi,j | Equation |
| XCH1,2 | $$\frac{ AREA \_{PS}}{\frac{1}{K\_{air }}+\frac{K\_{AW}}{K\_{water }}}$$ |
| XCH2,1 | $$\frac{ AREA \_{PS}}{\frac{1}{K\_{air }⋅K\_{AW}}+\frac{1}{K\_{water }}}$$ |
| XCH2,3 | $$\frac{k\_{PS}}{\frac{1}{V\_{2}}+\frac{1}{V\_{3}⋅Kp\_{S}⋅d\_{S}}}$$ |
| XCH3,2 | $$\frac{k\_{PS}}{\frac{Kp\_{S}⋅d\_{S}}{V\_{2}}+\frac{1}{V\_{3}}}$$ |
| XCH1,5 | $$\frac{k\_{s,b}}{\frac{K\_{AW}}{V\_{5}}+\frac{1}{AREA\_{AS}⋅h}}$$ |
| XCH5,1 | $$\frac{k\_{s,b}}{\frac{1}{V\_{5}}+\frac{1}{AREA\_{AS}⋅h⋅K\_{AW}}}$$ |
| XCH5,6 | $$\frac{k\_{AS}}{\frac{1}{V\_{5}}+\frac{1}{V\_{6}⋅Kp\_{AS}⋅d\_{AS}}}$$ |
| XCH6,5 | $$\frac{k\_{AS}}{\frac{Kp\_{AS}⋅d\_{AS}}{V\_{5}}+\frac{1}{V\_{6}}}$$ |
| XCH1,7 | $$\frac{AREA\_{SLS}}{\frac{1}{K\_{air}}+\frac{K\_{AW}}{K\_{water}}}$$ |
| XCH7,1 | $$\frac{AREA\_{SLS}}{\frac{1}{K\_{air}⋅K\_{AW}}+\frac{1}{K\_{water}}}$$ |
| XCH7,8 | $$\frac{k\_{SLS}}{\frac{1}{V\_{7}}+\frac{1}{V\_{8}⋅Kp\_{AS}⋅d\_{AS}}}$$ |
| XCH8,7 | $$\frac{k\_{SLS}}{V\_{7}⋅d\_{AS}}+\frac{1}{V\_{8}}$$ |

Output

Emission to air

The fraction of the chemical emitted to air (Eair) by an STP of the size of N inhabitants is:

$$E\_{air }=3600⋅24⋅\frac{C\_{1}⋅ADV\_{1,0}⋅\sqrt{N}}{1000⋅E}$$

E: Emission rate of the chemical

Emission to water

The total concentration (CT in mg∙L-1) in effluent discharged into the receiving water body is:

$$C\_{T}=C\_{7}+C\_{8}⋅\frac{C\_{SO,SLS }}{1000⋅d\_{AS}}$$

The fraction (Eeff) of the chemical input that leaves an STP serving N inhabitants via effluent is:

$$E\_{eff}=\frac{C\_{T}⋅Q⋅N}{1000⋅E}$$

Emission via combined sludge

The concentration in combined sludge (Ccs in mg/kg dry weight) equals

$$\begin{array}{c}E\_{sludge }\&=\frac{C\_{4}⋅ADV\_{4,0}+C\_{9}⋅ADV\_{9,0}}{1000⋅E}⋅N\\\&=\frac{\frac{FS⋅SO}{1000⋅d\_{RS}}⋅C\_{4}+\frac{SU}{1000⋅d\_{AS}}⋅C\_{9}}{1000⋅E}⋅N\end{array}$$