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ANALYSIS OF ORGANIC COMPOUNDS REMOVAL FROM WASTEWATER

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Abstract: Objective of this study is estimating the removing efficiency of Tonalide organic compound (AHTN) from wastewater in a sewage treatment plant consisting of: primary clarifier, aeration tank and secondary clarifier. The compound enters the treatment plant by two ways: being adsorbed on the solids surface and dissolved in the liquid phase. SimpleTreat v4.0 software is used to determine the compound concentration in effluent considering processes taken place during wastewater treatment (solids sedimentation, aeration, biodegradation).
Keywords: biodegradable organic compound, Tonalide, wastewater treatment, SimpleTreat model

1. INTRODUCTION. THE SIMPLETREAT MODEL

Domestic wastewaters contain a wide variety of pollutants including organic compounds that are found as chemicals in products like: soaps, personal care products, detergents, cleaning or pharmaceutical products [1]. Since 1979 the European community legislated the chemical substances disposal in the aquatic environment imposing limit values by Directive 76/464/EEC [2]. Currently exists an elaborated informational system regarding chemicals under European Chemicals Agency (ECHA) [3]. ECHA helps companies to comply with the European legislation and provides information on chemicals [3].

Also, for evaluating the chemicals exposure risk to human health and environment a general methodology is used, namely EUSES model (European Union System for the Evaluation of Substances) [3]. The model predicts concentrations in air, water and soil of studied chemicals at regional and continental levels. SimpleTreat model was adapted to EUSES with options defining wastewater treatment plants. So, the SimpleTreat model predicts chemicals emissions to air (surrounding the wastewater treatment plant), water (effluent) and soil (sludge) from wastewater during treatment [4, 5].

The National Institute of Public Health and Environment in the Netherlands (RIVM) developed the SimleTreat model [5]. Figure 1 shows version 4.0 of the model.

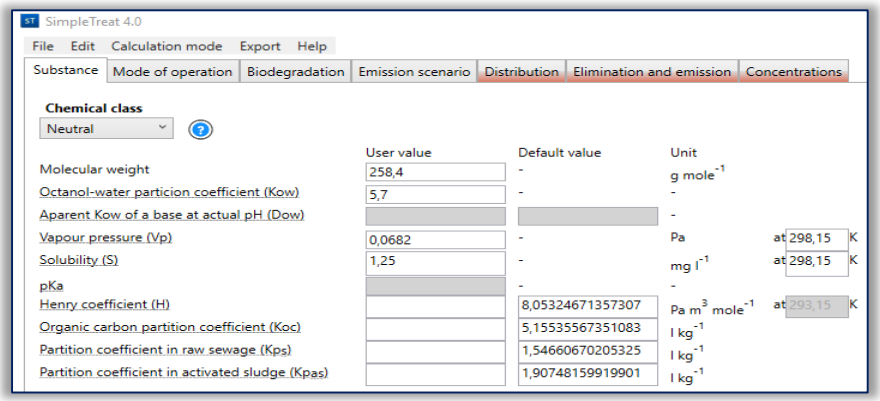


Figure 1. Main menu of SimpleTreat v4.0 software

Main menu contains four windows for input values (Substance, Mode of operation, Biodegradation and Emission scenario) and three windows for output values (Distribution, Elimination and emission, Concentrations), figure 1.

This study aims estimating Tonalide organic compound fate in wastewater treatment plant using SimpleTreat model. The removing efficiency is evaluated by calculating Tonalide concentration in the effluent after wastewater treatment in primary clarifier, aeration tank and secondary clarifier (solids liquid separator) using the SimpleTreat v.4.0 software.

2. CASE STUDY OF TONALIDE REMOVAL FROM WASTEWATER

Tonalide (AHTH) is an organic compound from tetralins class with chemical formula $C_{18}H_{26}O$ and CAS number 21145-77-7 [3, 6]. It is used in air care products, biocides (e.g. disinfectants, pest control products), washing and

cleaning products or cosmetics and personal care products [3]. These uses of Tonalide lead to its occurrence in the sewage wastewater.

In the SimpleTreat model presented further is considered that Tonalide enters the wastewater treatment plant through two ways: dissolved in the liquid and adsorbed on the solids (sludge) surface. Firstly, as input values were given the physico-chemical properties of Tonalide and presented in table 1 [6, 7].

Table 1. Physico-chemical properties of Tonalide (AHTN) [6, 7]

Property	Value
Chemical class	Neutral
Molecular weight	258.4 g/mole
Octanol-water partition coefficient, log(K_{ow})	5.7
Vapour pressure at 25°C, p_V	0.0682 Pa
Water solubility at 25°C, S	1.25 mg/l
First order degradation constant, K_{bio}	0.023 h^{-1} (slowly biodegradable)

Also, other measures were defined as suggested default values [5]: $\dot{m}_c = 1\ \mathrm{kg/day}$ Tonalide mass flow entering the wastewater treatment plant; $\dot{V} = 0.2\ m^3/(day \cdot person)$ wastewater volume flow and N = 60 000 number of inhabitants. Thus the value of nominal concentration in the influent of Tonalide, calculated with relation $C_{c,in} = \frac{\dot{m}_c \cdot 1000}{\dot{V} \cdot N}\ [\frac{mg}{l}]$ [5], is: $C_{c,in} = 0.083$ mg/l.

In order to determine solids concentrations in different locations of the wastewater treatment plant (WWTP), is considered that solids mass flow entering the wastewater treatment plant is default value $\dot{m}_s$ = 0.09 kg/(day·person) [5]. In table 2 are given the calculated or default values [5].

Table 2. Solids concentration in different locations of the wastewater treatment plant (WWTP)

Location in the WWTP	Formula	Value
Influent	$C_{s,in} = \frac{\dot{m}_{s,in}}{\dot{V}}\ [\frac{kg}{m^3}]$	0.45 kg/m³ (450 mg/l)
Primary clarifier	$C_{s,1} = \frac{1}{3} C_{s,in}\ [\frac{kg}{m^3}]$	0.15 kg/m³ (150 mg/l)
Aeration tank	$C_{s,2}$ (default value)	4 kg/m³ (4000 mg/l)
Effluent	$C_{s,out}$ (default value)	0.03 kg/m³ (30 mg/l)

In table 2 and above, the flowing notations were made: *C* in [kg/m³] or [mg/l] is concentration; $\dot{m}$ in [kg/day] is mass flow and $\dot{V}$ in [m³/day] is volume flow. The subscripts of these measures represents as follows: *s* - solids; *c* - chemical; *1* - primary clarifier; *2* - aeration tank; *in* - influent; *out* – effluent.

A screen capture of SimleTreat model is presented in figure 2 showing solids concentrations through basins of the WWTP, in correlation with values given in table 2.

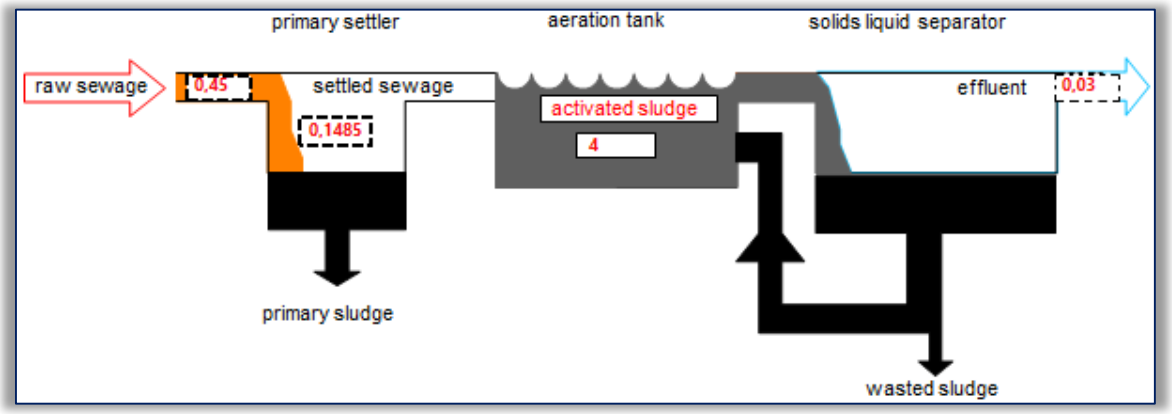


Figure 2. Solids concentration in different locations of the WWTP (SimpleTreat v4.0 screen capture)

Depth and retention time in different basins of the WWSP were also taken as default values and are given in table 3 [5].

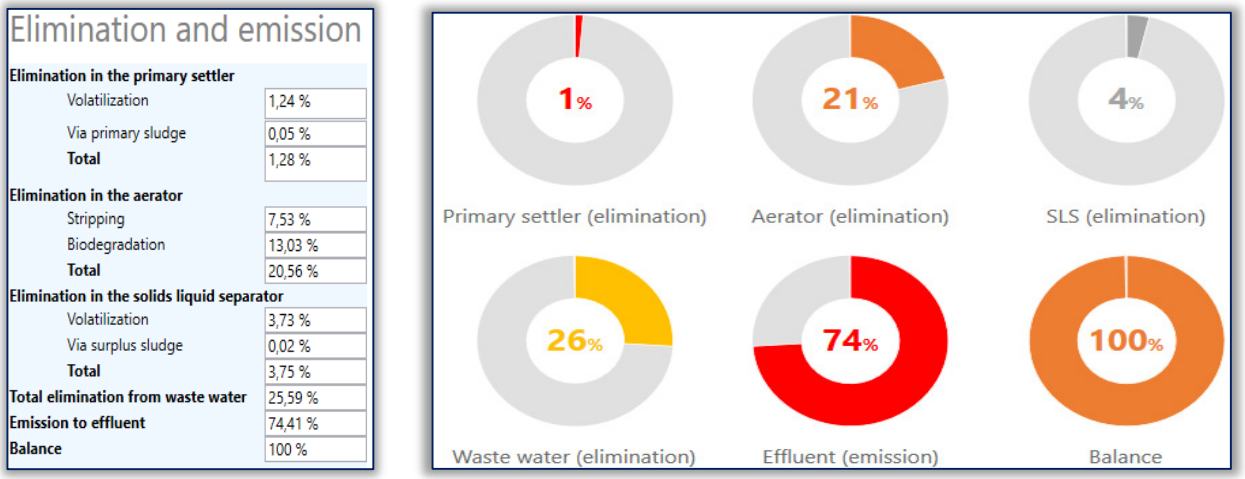
Table 3. Characteristics of basins of the WWTP [5]

Basin	Depth [m]	Retention tine [h]
Primary clarifier	4	2
Aeration tank (bubble aeration)	3	11.5
Secondary clarifier	3	6

Other values for defining the SimpleTreat model were: air temperature surrounding the WWTP of 15°C, wind speed of 3 m/s and water pH=7 [5].

3. RESULTS AND DISCUSSIONS

Results regarding elimination and emission of Tonalide are presented in figures 3 and 4.



Elimination and emission	
Elimination in the primary settler	
Volatilization	1,24 %
Via primary sludge	0,05 %
Total	1,28 %
Elimination in the aerator	
Stripping	7,53 %
Biodegradation	13,03 %
Total	20,56 %
Elimination in the solids liquid separator	
Volatilization	3,73 %
Via surplus sludge	0,02 %
Total	3,75 %
Total elimination from waste water	25,59 %
Emission to effluent	74,41 %
Balance	100 %

Figure 3. SimpleTreat output values regarding elimination and emission of Tonalide

Following the obtained results, as presented in figure 3, 25.59% of Tonalide is expected to be eliminated during wastewater treatment, while 74.41% remains to be discharged by effluent to surface waters. These results are in agreement with the literature. For example, M. Carballa et al. [8] have done experiments of Tonalide removal from wastewater using coagulants, to favor sedimentation process in the aeration tank, and compared them with results obtained in experiments without any additive. The removal efficiencies were estimated as: 10% in experiments without additives, 50% with addition of 250 mg FeCl3 l^{-1} and 71% with addition of 300 mg $Al_2(SO_4)_3$ l^{-1} and 850 mg PAX l^{-1} [8]. M. Biel-Maeso et al. [9] also measured several chemicals concentration in influent and effluent of Jerez de la Frontera WWTP (SW Spain) over a period of 1 year. They have estimated the removal efficiency of Tonalide (fragrance) in summer of 25% [9].

Also from figure 3 it may be observed that elimination during wastewater treatment is about 0.07% via adsorption to solids (in the primary and secondary settlers), and about 13.03% via biodegradation (in the aeration tank). Moreover, 12.5% of Tonalide may be eliminated in the surrounding air by volatilization and stripping.

Concentrations		
Air	8,576e-07	g m^{-3}
Combined sludge (C_{sludge})	1,271e-01	mg kg^{-1}
Primary sludge	1,283e-01	mg.kg^{-1}
Surplus sludge	1,238e-01	mg.kg^{-1}
Raw sewage	8,333e-02	mg.l^{-1}
Dissolved	8,328e-02	mg.l^{-1}
Associated	5,773e-05	mg.l^{-1}
Settled sewage	8,226e-02	mg.l^{-1}
Dissolved	8,224e-02	mg.l^{-1}
Associated	1,905e-05	mg.l^{-1}
Mixed liquor	6,561e-02	mg.l^{-1}
Dissolved	6,511e-02	mg.l^{-1}
Associated	4,958e-04	mg.l^{-1}
Effluent ($C_{local_{effluent}}$)	6,2e-02	mg.l^{-1}
Dissolved	6,2e-02	mg.l^{-1}
Associated	3,713e-06	mg.l^{-1}
In solids effluent	1,238e-01	mg.kg^{-1}

Figure 4. SimpleTreat output values regarding Tonalide concentrations through wastewater treatment

The results of Tonalide concentrations are given in figure 4. If in influent (raw sewage) Tonalide had a concentration of 0.0833 mg/l (from which 0.0832 mg/l dissolved in liquid phase and $5.773 \cdot 10^{-5}$ mg/l adsorbed on solids), in effluent are found 0.062 mg/l.

Tonalide poor removal efficiency is expected due to its slowly biodegradation characteristic as the first order degradation constant K_{bio} has small value (see table 1).

4. CONCLUSIONS

The legislation adopted in the European community for organic compounds in detergents and personal care products requires them to be biodegradable under aerobic conditions [1]. This assures their decomposition in the aeration tank of the wastewater treatment plants and limiting emissions to surface waters.

For Tonalide organic compound a poor removal efficiency in wastewater treatment plant was estimated using SimpleTreat v.4.0 software. The result complies with low biodegradation characteristic of Tonalide. The removal efficiency may be improved by coagulants-flocculants addition or increasing the retention time [8].

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