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USING THE SIMPLETREAT MODEL TO ESTIMATE POLLUTANTS REMOVAL IN WASTEWATER TREATMENT PLANTS

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Abstract: In order to analyze organic chemicals fate and removal by primary and secondary treatments in a wastewater treatment plant, the SimpleTreat model is used. The model estimates pollutants concentration in different basins of the treatment plant (primary clarifier, aeration tank and secondary clarifier). It is presented a comparative analysis of two categories of organic pollutants, the results in graphical form also indicating the removal efficiency, in %.
Keywords: SimpleTreat model, wastewater treatment plant, pollutants, adsorption, dissolution

1. INTRODUCTION. ORGANIC CHEMICALS FATE MODEL

As a result of using in personal care products or due to human ingestion, organic pollutants may enter the municipal wastewater as chemicals found in products as: cosmetics, detergents or pharmaceuticals [1]. Following primary and secondary treatment in wastewater treatment plants and depending on their biodegradability properties, these chemicals may be decomposed in non-toxic substances and eliminated [1]. Directive 76/464/EEC legislate the limit values of chemical substances disposal in the aquatic environment imposed by European community [2].

Several mathematical models were developed to study fate and removal efficiency in wastewater treatment plants of organic chemicals, as: SimpleTreat, WWTreat, Water9, Toxchem+, STP [3]. For availability reasons, in this study the "9-box" SimpleTreat model is used to estimate the removal efficiency of six organic pollutants depicted in municipal wastewaters.

The SimleTreat model was developed by the National Institute of Public Health and Environment in Netherlands (RIVM) [4]. It estimates the concentration of a pollutant (chemical compound) in a wastewater treatment plant consisting of primary settler (PS), aeration tank and secondary clarifier (SC), taking into account processes as advection, transport and diffusion [4-6]. A schematic representation of the SimpleTreat model compartments ("9-box") is given in figure 1 [4].

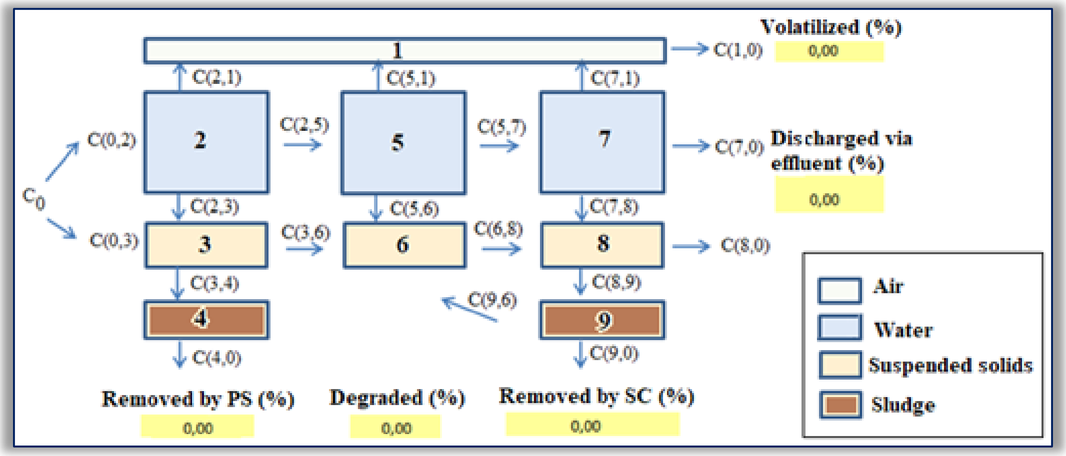

Figure 1. Graphical representation of "9-box" SimpleTreat model [4]

Each compartment represents a medium in the wastewater treatment plant, i.e: surrounding air (1), water (2, 5, 7), suspended solids (3, 6, 8) and sludge (4, 9). Also, primary clarifier is represented by boxes 2, 3 and 4, aeration tank by boxes 5 and 6, secondary clarifier by boxes 7, 8 and 9. In figure 1 are also represented the estimated concentrations C(i, j), in (mol/h) [4-6]. The pollutant (organic compound) may enter the wastewater treatment plant (concentration in influent, C_0) in two forms: dissolved in the liquid phase (water) – represented in figure 1 by concentration C(0,2) and adsorbed on the surface of the suspended solids – represented in figure 1 by concentration C(0,3) [4-6]. Also, pollutant removal efficiency is estimated in % after each treatment of primary settling, biodegradation and secondary clarification (figure 1).

This study aims analyzing by SimpleTreat model of municipal wastewater common pollutants removal efficiency in function of their solubility and biodegradability properties.

2. CASE STUDY. RESULTS AND DISCUSSIONS

The case study refers to six pollutants identified in the influent of municipal wastewater treatment plants [6, 7]. These are organic compounds contained in products as: *cosmetics* - Tonalide (AHTN), Decamethylcyclopentasiloxane (D5) and Edetic Acid (EDTA), *detergents* - Benzalkonium chloride (BAC) or *pharmaceuticals* - Permethrin (PMT) and Atenolol (A). Thus these pollutants can enter the wastewater as a result of their use in personal care products or as a result of human ingestion. Table 1 lists physico-chemical properties of these pollutants used as input data in the SimpleTreat model [6-8].

Table 1. Properties of analyzed compounds identified as pollutants in municipal wastewaters [6-8]

No.	Organic compound	Chemical formula	CAS No.	Molecular weight (g/mol)	Solubility at 25 °C (Pa)	Biodegradability k_{bio} (h^{-1})*
1.	Tonalide (AHTN)	$C_{18}H_{26}O$	1506-02-1	258.40	1.25	0
2.	Permethrin (PMT)	$C_{21}H_{20}Cl_2O_3$	52645-53-1	391.29	0.006	0.3
3.	Decamethylcyclo pentasiloxane (D5)	$C_{10}H_{30}O_5Si_5$	541-02-6	370.77	0.017	0
4.	Edetic Acid (EDTA)	$C_{10}H_{16}N_2O_8$	60-00-4	292.24	1000	0
5.	Benzalkonium chloride (BAC)	$C_{21}H_{38}ClN$	8001-54-5	340	22.47	1
6.	Atenolol (A)	$C_{14}H_{22}N_2O_3$	029122-68-7	266	13300	0.3

* not biodegradable: k_{bio}=0 h^{-1}; biodegradable: k_{bio}=0,1-0,3 h^{-1}; naturally biodegradable: k_{bio}=1 h^{-1}

For comparison some parameters (taken as default values in the model [5, 6]), are considered for all organic compounds, i.e.: pollutant mass flow entering the wastewater treatment plant ($\dot{m}_c = 1\ kg/day$), wastewater volume flow ($\dot{V}$ = 0.2 m^3/day·person), solids mass flow entering the wastewater treatment plant ($\dot{m}_s$ = 0.09 kg/day·person) and number of inhabitants (N = 60 000). Thus for all pollutants is considered the same value of nominal concentration in the influent C_0 = 0.083 mg/l, calculated with relation $C_0 = \frac{\dot{m}_c \cdot 1000}{\dot{V} \cdot N}\ [\frac{mg}{l}]$ [5]. Table 2 lists others parameters considered in the SimpleTreat model in function of the location in the wastewater treatment plant (WWTP).

Table 2. Parameters considered in the SimpleTreat model [5]

Location in the WWTP	Solids concentration $\left(\frac{kg}{m^3}\right)$		Solids density $\left(\frac{kg}{m^3}\right)$	Depth (m)	Volume $(m^3/person)$	Hydraulic retention time (h)
	Formula	Value				
Influent	$\frac{\dot{m}_s}{\dot{V}}$	0.45	1500	-	-	-
Primary settler (PS)	$\frac{1}{3}\frac{\dot{m}_s}{\dot{V}}$	0.15	1500	4	0.0167	2
Aeration tank	default	4	1300	3	0.0862	10
Secondary clarifier (SC)	default	0.03	1300	3	0.05	6
Effluent	default	0.03	1300	-	-	-

Table 3. Estimations of pollutants distribution in the influent, correlation with figures 2 and 3

No.	Compound	(~ %) dissolved in liquid phase	(~ %) adsorbed on solids surface
1.	Tonalide (AHTN)	13	87
2.	Permethrin (PMT)	3	97
3.	Decamethyl-cyclopentasiloxane (D5)	0	100
4.	Edetic Acid (EDTA)	100	0
5.	Benzalkonium chloride (BAC)	92	8
6.	Atenolol (A)	98	2

Also, both air surrounding the WWTP and wastewater temperatures are considered of 15ºC, wind speed of 3 m/s and water pH=7 [5].

Estimations by SimpleTreat model of analyzed pollutants distribution in the influent are given in Table 3. Given these estimations, further analysis is done on pollutants grouped in two categories: those adsorbed on solids surface in high proportion (AHTN, PMT and D5) and those dissolved in liquid phase in high proportion (EDTA, BAC and A). Results of removal efficiency for both pollutant categories are shown in figures 2 and 3, respectively.

The pollutants from first category, which tend to adsorb on suspended solids surface in wastewater (AHTN, PMT and D5), have similar fate, i.e. are mostly removed in primary and secondary clarifiers with evacuation of primary and secondary sludge. As can be observed in figure 2.a-c, these pollutants are removed by primary settler (PS) in proportion of about 60%, and by secondary clarifier (SC) in proportion of about 20%. As expected, removal by biodegradation in the aeration tank depends on pollutant properties (k_{bio} parameter given in table 1). So, AHTN and D5 being not biodegradable (k_{bio}=0 h^{-1}), in aeration tank the removal efficiency is zero (figure 2.a and c), while 7.29% of biodegradable PMT (k_{bio}=0.3 h^{-1}) is thus removed (figure 2.b).

Removal efficiency estimations with SimpleTreat model of pollutants from second category, which tend to dissolve in liquid phase of the wastewater (EDTA, BAC and A), are given in figure 3.a-c. Although, their removal is expected to take place in aeration tank by biodegradation, the EDTA organic compound is not biodegraded during this treatment with activated sludge (k_{bio}=0 h^{-1}), even if it is 100% dissolved in wastewater liquid phase (figure 3.a). As expected, the removal efficiency of this organic compound is very small [6]. BAC and A compounds, being biodegradable, may be eliminated in high proportion in aeration tank. Estimations presented in figure 3.b and c show removal of about 86% for BAC and 75% for A, respectively. As expected, removal of all dissolved pollutants by primary and secondary clarifiers is low, under 1% (figure 3.a-c).

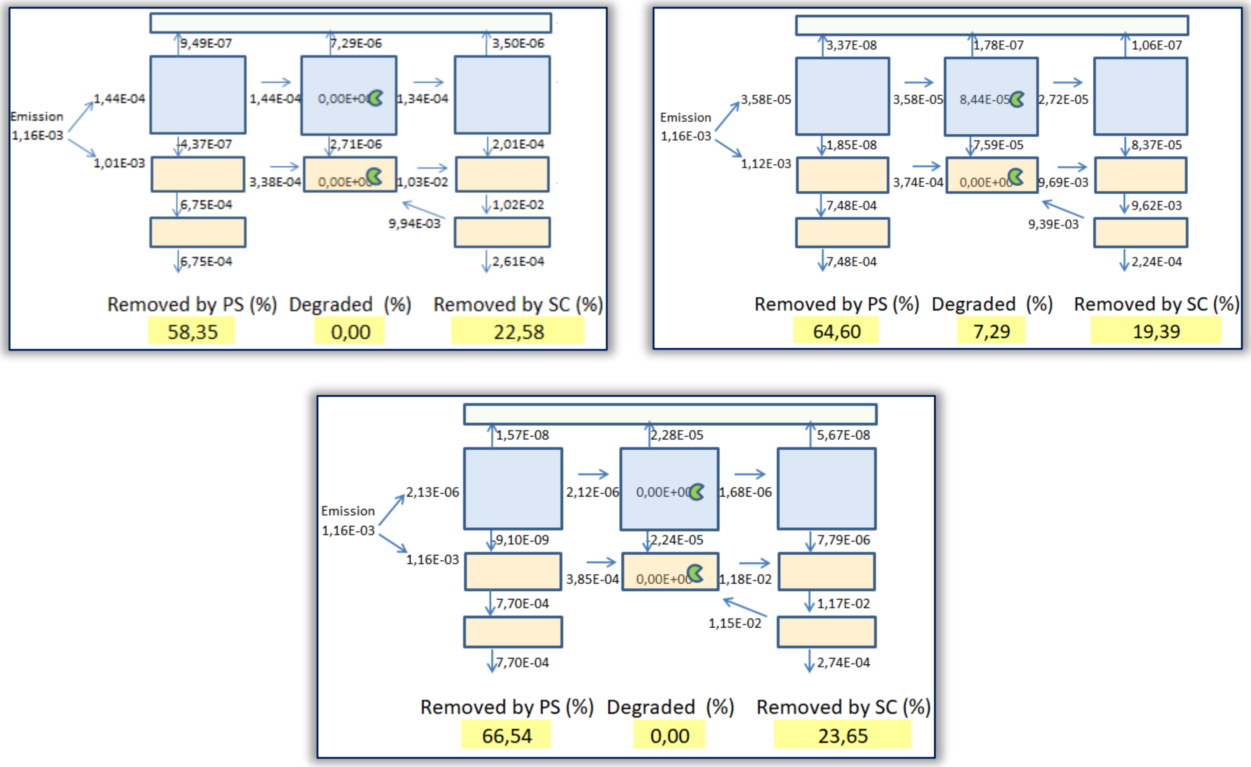

Figure 2. Estimations by SimpleTreat model of adsorbed pollutants removal efficiency
a) Tonalide (AHTN); b) Permethrin (PMT); c) Decamethyl-cyclopentasiloxane (D5)

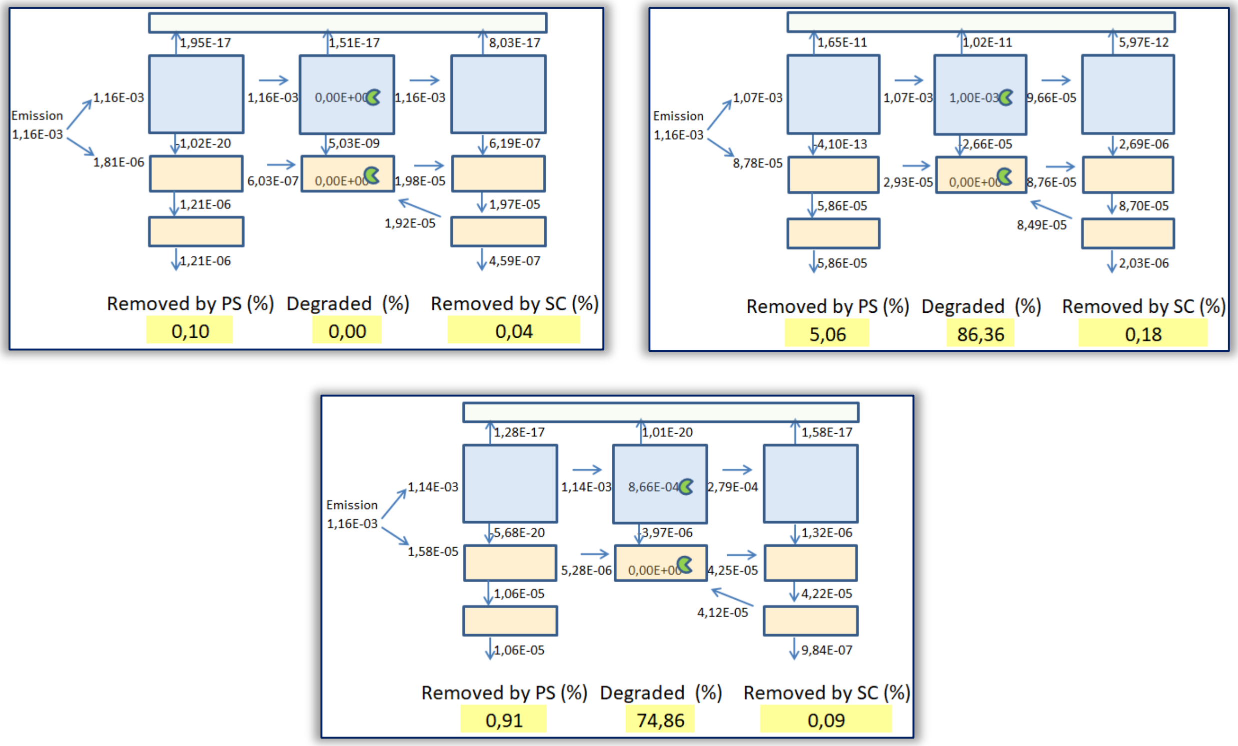

Figure 3. Estimations by SimpleTreat model of dissolved pollutants removal efficiency
a) Edetic Acid (EDTA); b) Benzalkonium chloride (BAC); c) Atenolol (A)

Although most wastewater treatment plants use activated sludge secondary treatment in aeration tanks, where pollutants removal is due to coagulation-flocculation and biodegradation processes, tertiary treatment may be used to improve the removal efficiency of organic compounds [7]. Tertiary treatment involves ozone and UV-based advanced oxidation processes or membrane filtration [7].

3. CONCLUSIONS

Removal efficiency of two categories of organic compounds found as pollutants in municipal wastewaters are analyzed using the SimpleTreat model. Each category comprises three pollutants which are either dissolved in the liquid phase or adsorbed on suspended solids of the wastewater treatment plant influent. From quantitative estimations using the SimpleTreat model it can be concluded that among organic compounds properties, solubility and biodegradability in the liquid phase, have major influence on their removal efficiency from wastewater.

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