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Industrial Electrical Engineering and Automation

Descriptive Assessment and Amendment of the Simple Treat Model

Modelling of Organic Chemicals in Sludge for Soil Application

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Abstract

Large quantities and numbers of organic compounds (OCs) from industries and domestic sources enter the wastewater treatment plants (WWTPs) everyday, which is an ever-increasing issue in modern society. In WWTPs, the pollutants are either degraded or emitted to the air, the effluent (water) or the sludge (biosolids). Even though the sludge may contain toxic contaminants and heavy metals, there is an incentive of recycling sewage sludge as a fertiliser to preserve the phosphorus that is a limiting resource. To ensure the quality of the sludge, the WWTPs can certify their work according to the Swedish certification system, REVAQ that includes setting up an *upstream action* plan (uppströmsarbete in Swedish) by which to improve the sludge. Nevertheless, the overall environmental risk of OCs, i.e. from entering the WWTP to exposing the sludge containing OCs to soil processes, has so far not been taken into consideration in the upstream action.

This master's thesis is carried out at SWECO Environment AB in association with the umbrella project "Organic compounds in sludge recycling, evaluation and prioritisation" for the Swedish Water & Wastewater Association, in cooperation with four Swedish wastewater treatment plants: Ellinge, Käppala, Ryaverket and Sjölunda.

The main objective of the thesis is to develop a methodology to predict the fate of organic chemical pollutants in sludge after being exposed to soil processes by applying and amending the easy accessible modelling tool SimpleTreat 3.1. However, further investigation of how the soil processes will affect the removal of the OCs in soil will not be assessed in this thesis. The SimpleTreat will as well be adapted to existing known parameters of generic Swedish WWTPs that have not been included in the original SimpleTreat. In addition, the applicability of the modified model for four generic Swedish WWTP configurations will be validated by comparing the predicted results of effluent and sludge with measurements from the IVL-database (Swedish Environmental Research Institute). Furthermore, by simulating measured chemicals in the influent, a chemical list with expected concentration ranges in Swedish effluent and sludge can be obtained, especially when many of the emerging chemicals' presence, frequency of occurrence or source may be unknown. Since two input parameters from Ellinge are missing, this WWTP has consequently been left out of the investigation. The old and new sections of Käppala have different plant configurations and are therefore treated as two separate plants.

In summary, a stepwise methodology presented to predict the distribution of OCs to water and sludge, which comprises of a plant description, chemical data collection, calibration and validation. The OCs that are investigated and measured in WWTPs are mostly hydrophobic and their emissions to air are thus negligible. Moreover, the SimpleTreat model was modified and proved to be applicable for predicting the fate of organic pollutants with regard to a number of factors: 1) the model structure, 2) the model parameters and 3) the data quality. Firstly, the structure of the modified SimpleTreat is limited to a primary settler, an activated sludge system (anaerobic, anoxic and aerobic zones) and a secondary clarifier. Secondly, the physico-chemical parameters are preferably experimentally measured but estimated values from EPI (Estimation Programs Interface) Suite™ are equally satisfactory. Thirdly, the data of influent, effluent and sludge has to be measured at the right location within a reasonable time frame and employing the same sampling and analysis method. To improve the results for a specific compound, it is

suggested to measure the partition coefficient K_p in raw sewage, primary settler, aeration tank and secondary clarifier to gain a more precise prediction of the partitioning in the defined WWTP.

In conclusion, a total of 84 chemicals were modelled in the modified SimpleTreat with the four plant configurations respectively; the chosen WWTPs attested representative overall pollution removal rates via effluent and sludge when compared with typical concentrations ranges of the IVL-database. Predictions of the concentrations' order of magnitude in Swedish effluent using the modified SimpleTreat proved to have 92% accuracy and in Swedish sludge 56% accuracy. However, further analysis of the chemicals must be carried out to classify the risk of the chemical in soil amendment. Finally, the information that can be acquired by applying all steps in the methodology is which substances that do not pose a threat to the environment and human health despite being recycled with sludge, supposing that the concentration level of toxicity is known.

***Keywords**: SimpleTreat, organic compounds, REVAQ, soil amendment, methodology, WWTP, fugacity and steady-state model*

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As a conclusion of my master's studies in environmental engineering, this report is the final product at the Division of Industrial Electrical Engineering and Automation (IEA) in the Faculty of Engineering, Lund University. The thesis work was carried out at SWECO Environment AB, where the topic was initiated.

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Acronyms

Abbreviation	*English*	*Swedish*
BASL4	Biosolids-Amended Soil: Level IV	Namnet på en slammodell
CFC	Chlorofluorocarbon	Klorfluorkolväte
CO_2	Carbon dioxide	Koldioxid
CSTR	Continued stirred tank reactor	Kontinuerligt omrörd tank reaktor
DDT	Dichloro-diphenyl-trichloroethane	Diklor-difenyl-triloroetan
EPA	Environmental Protection Agency	Miljöskyddsnämnd
EPI	Estimation Programs Interface	Estimeringsprogram gränssnitt
ETBE	Ethyl tert-butyl ether	Etyl-tert-butyleter
EUSES	European Union System for the Evaluation of Substances	Europeiska unionens system för utvärdering av ämnen
HRT	Hydraulic retention time	Uppehållstid
H_2O	Water	Vatten
IVL	Swedish Environmental Research Institute	Svenska Miljöinstitutet
OC	Organic compound	Organisk förening
PAH	Polycyclic aromatic hydrocarbon	Polyckliska aromatiska kolväten
PCB	Polychlorinated biphenyl	Polyklorerade bifenyler
REVAQ	Pure plant nutrients from sewage	Ren växtnäring från avlopp
POP	Persistent organic pollutant	Persistent organisk föreorening
STP	Sewage treatment plant	Reningsverk
Swedish EPA	Swedish EPA	Naturvårdsverket
SWWA	Swedish Water & Wastewater Association	Svenskt Vatten
VOC	Volatile organic chemical	Flyktiga organiska ämnen
WWTP	Wastewater treatment plant	Avloppsreningsverk

Table of Contents

1 Introduction

1.1 Background

There are approximately 143,000 chemicals registered in the European Union (European Chemical Agency, 2008), whereof over 30,000 are in daily used (EC, 1990; Schwarzenbach et al., 2006). Large quantities and numbers of organic compounds (OCs) from industries and domestic sources enter wastewater treatment plants (WWTPs) everyday, which is an ever-increasing issue in modern society. Since most of the investigated and measured OCs in WWTPs are hydrophobic, their emissions to air are thus negligible and they will leave the WWTPs with the effluent (water) or the sludge (biosolids) (see Figure 1). Besides OCs, the biosolids also contain phosphorus which can be recycled as a fertiliser on agricultural land or be used for land cover etc. Phosphorus is a limiting resource; hence, land application of biosolids will gradually become more of an important option for sustainable nutrient management (Clarke & Smith, 2010).

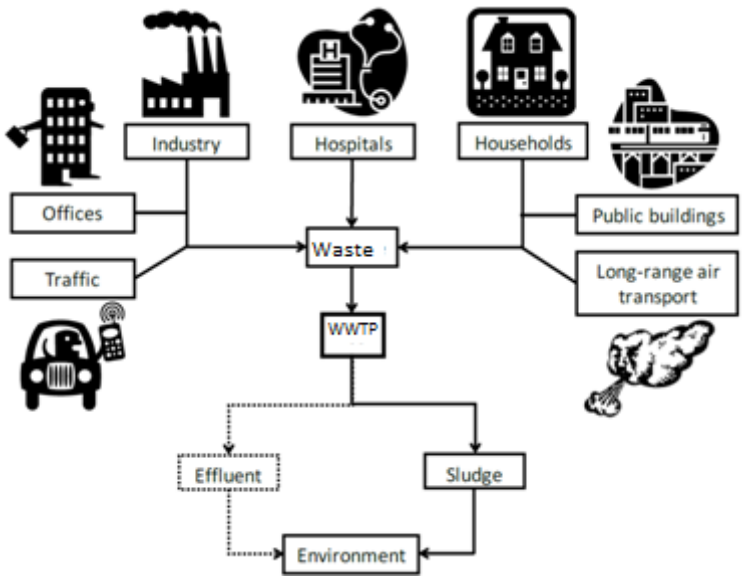


Figure 1. Schematic of the chemical substances' mass flows from different source (Olofsson, 2012).

A REVAQ certificate can be employed to ensure the quality of the biosolids for soil application from a WWTP, which includes setting up an *upstream action* plan (uppströmsarbete in Swedish) to decrease the inflow of potentially harmful substances. Nevertheless, the overall environmental risk of OCs, i.e. from entering the WWTP to exposing the sludge containing OCs to soil processes, has so far not been taken into consideration in the upstream action. This includes the effects of soil processes to the OCs in sludge, such as decomposition, accumulation, drainage or plant uptake. Hence, some toxic OCs in the sludge do not necessary pose a risk since they may be rapidly degraded when processed in soil environment.

Current general risk assessment of chemicals can be performed for example with the computational tool from the European Commission, EUSES (European Union System for the Evaluation of Substances) that incorporates the spreadsheet based model, SimpleTreat 3.1. For simplification, SimpleTreat 3.1 is from here on referred to as SimpleTreat. The primary use of

SimpleTreat in this study is to predict the concentrations of OCs in effluent and sludge after being treated in a WWTP.

This master's thesis is carried out at SWECO Environment AB in association with the project "Organic compounds in sludge recycling, evaluation and prioritisation" for the Swedish Water & Wastewater Association (SWWA), in cooperation with four Swedish wastewater treatment plants that are owned by VA SYD, Käppala Association and Gryaab AB.

1.2 Legislation, Regulation and Certification

Legislation, regulation and certification concerning the matter of recycling biosolids are presented here.

1.2.1 European Sewage Sludge Directive

The sewage sludge directive issued by the European Commission, 86/278/EEC, has two purposes: it is, firstly, to provide protection for humans, animals, plants and the environment from the potential risk that comes with spreading sewage sludge on agricultural land; it is, secondly, to encourage the correct application of sewage sludge (Ecologic Institute EU, 2009).

1.2.2 Swedish Environmental Goal

In Sweden, the 15th national environmental goal, "A good built environment", from 2010 states that by 2015 at least 60 % of the phosphorus in sludge from municipal wastewater treatment plants shall be reused on biologically productive land, whereof at least half of the amount on arable land (Carlgren & Reinfeldt, 2010). This phosphorus goal has, however, been dismissed until the Swedish EPA (Naturvårdsverket in Swedish) along with other authorities have investigated and suggested improvements of how to recycling phosphorus (Berglund, 2012).

1.2.3 REVAQ

The Swedish Water & Wastewater Association is the sole owner of the certification system, REVAQ. REVAQ was developed in accordance with the Swedish parliament's 15th environmental goal "A good built environment". By certifying a WWTP according to REVAQ, the WWTP is in agreement of ensuring the qualitative work of recycling sludge on agricultural land which includes impelling an active upstream action and continuously working to improve the WWTP and the quality of sludge in an open and transparent way. The persistent organic pollutants (POPs), nonylphenol, PCB and PAH, are already regulated within REVAQ.

1.3 SWECO Project

This thesis work is carried out under an umbrella project named "Organic compounds in sludge recycling, evaluation and prioritisation" performed by SWECO. The task of the project is to investigate the path of OCs from influent to WWTP, through its processes, to the sludge and on to agricultural land through sludge recycling, by applying a WWTP model and a soil model that simulate the fate of chemicals in a WWTP and soil, respectively. The purpose is to firstly evaluate those chemical substances that do not pose a threat to the environment and human health after soil application and secondly establish a priority list of chemicals that can support the upstream action for the water and wastewater industry.

1.4 Thesis Objective

The main objective of the thesis is to develop a methodology to predict the fate of organic compounds in sludge after being exposed to soil processes by applying and amending the easy accessible modelling tool SimpleTreat 3.1 (Struijs, 1996). However, further investigation of how the soil processes will affect the removal of the OCs in soil will not be assessed in this thesis. The SimpleTreat will as well be adapted to existing known parameters of generic Swedish WWTPs that have not been included in the original SimpleTreat. In addition, the applicability of the modified model for four generic Swedish WWTP configurations will be validated by comparing the predicted results of effluent and sludge with measurements from the IVL-database. Additionally, by simulating measured chemicals in the influent, a chemical list with expected concentration ranges in Swedish effluent and sludge can be obtained, especially when many of the emerging chemicals' presence, frequency of occurrence or source may be unknown.

The target audience of the thesis are SWECO, SWWA, the water and wastewater industries, environmental, chemical and civil engineers whom are interested in the subject of modelling of organic compounds in a WWTP.

The work is carried by reading relevant articles and books regarding the topic, collecting process data by contacting the involved WWTPs, searching data in databases, consulting the handbook of SimpleTreat and the supervisors.

1.5 Thesis Outline

An overview of the study is presented in Figure 2. The first chapter introduces the background and motivation of the thesis including legislation, description, certification of the master project by SWECO and the thesis objective. The second chapter presents of how to prioritise organic compounds and its important factors and properties as well as the background theory of mass balance models, which are a necessity to understand what is presented in this document. The third chapter comprises the principles of the mass balance model, SimpleTreat 3.1, which is the applied computational tool to determine the fate of chemicals in a WWTP. The fourth and the fifth chapters are the contributions to the umbrella project in which the fourth chapter presents a methodology of how to determine the fate of chemicals and a case study to demonstrate its application, where the case study consists of modelling ethyl tert-butyl ether (ETBE) in the old and new Käppala and simulating oxazepam in Ryaverket. The fifth chapter is composed of an outlook with comparisons of modelled and measured chemical ranges modelled the plant configurations of Käppala (old and new), Ryaverket and Sjölunda, respectively. The sixth chapter presents conclusions of the thesis.

The first appendix specifies the modifications altered in the SimpleTreat model. Since an additional sheet named "chemical" was added in the model to simplify simulating several OCs simultaneously, relevant input parameters as well as results of the simulation is explained in the second appendix. In the third appendix, the plant configurations of Ellinge, Käppala (old and new), Ryaverket and Sjölunda needed for performing simulations with the SimpleTreat are presented. The fourth appendix consists of macro codes used for connecting the "chemical" sheet with the rest of the model. In the fifth appendix, the results of the case study are summarised in a table. The sixth appendix contains the full list of predicted concentrations of OCs in effluent and sludge, which is the result of chapter five.

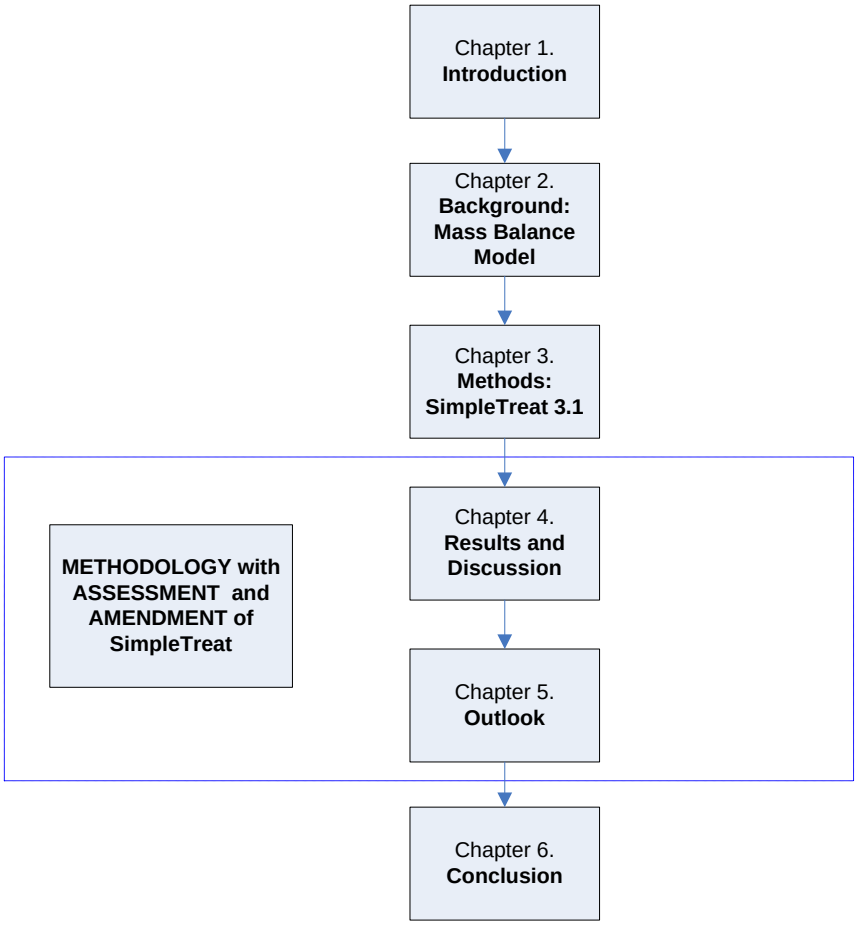


Figure 2. Outline of the thesis.

2 Theory

2.1 Organic Chemicals

Some fundamental knowledge of the risk factors, as well as the essential properties and factors which determine the risk and fate of a chemical are introduced in this chapter.

2.1.1 Identify Prioritised Chemicals

To identify chemicals that are of priority, i.e. may pose a threat to the human and environment, from a raw list of chemicals is a difficult task. Decision of whether a chemical is of priority is typically depending on the following factors (Mackay, 2001):

- Quantity
- Persistence
- Bioaccumulation
- Toxicity
- Potential for transport to distant locations
- Other adverse effects

Quantity

A central citation quoted from the Swiss-German scientist Paracelsus (Hargrave, u.d.) is that "the dose makes the poison", which states the importance of the chemical quantity. Similarly, it also implies that all chemicals are safe as long they exist in sufficiently small doses. A small fraction of a chemical that is considered toxic may for instance not give a significant adverse effect to the environment while a large amount of an ordinary bulk chemical might give arises to unpredicted effects (Mackay, 2001).

Persistence

Persistence is referring to the lifetime, half-life or residence of a chemical in the environment. Typical persistent chemicals, such as DDT or PCBs, have a high resistance against biological and physical degradation. They may be spread extensively and exist in nature for several years and eventually result in accumulating into highly concentrated areas. As an example, the accumulation of the persistent CFCs through migration of CFCs from earth to the stratosphere results in depleting the ozone layer. The amount of a chemical can thus be correlated to the environmental exposure and effects of that chemical. The persistence of a chemical is, however, difficult to determine due to the surroundings, temperature, sunlight, presence of degrading microorganisms and acidity etc (Mackay, 2001).

Bioaccumulation

Bioaccumulation is defined as the uptake of chemicals by organisms. Note that bioaccumulation is a phenomena and not an effect, which occurs when an organisms absorbs a chemical at a rate faster than at which the substance is lost. Bioaccumulation is an increasing concerning matter in particular when an organism or a predator/consumer of that organism (food chain effect) is adversely affected by the concentrated chemical. Chemicals that are hydrophobic tend to partition to organic media and then bioaccumulate in fatty tissues, e.g. concentration of PCBs in

fish may reach factors of 100,000 times the concentration in the surrounding water (Mackay, 2001).

Toxicity

Toxicity is most easily demonstrated by testing of acute toxicity, where the concentration level is sufficiently high to kill 50% of an aquatic organism population within a measured time frame. Another type of toxicity test is chronic or sub lethal test that is both expensive and controversial. The difference from estimating acute toxicity is to measure the concentration or dose that will result in adverse effects to the organism, such as growing more slowly, becoming sterile, behaving more abnormal etc. This will ultimately lead to shortened life span. The harmful chemical that causes the adverse effect is also ironically an essential nutrient in many cases. Determination of whether a chemical is carcinogenic, mutagenic or teratogenic is the most difficult test. These types of chemicals are often highly ranked on priority lists, and concerns have in particular been raised towards endocrine disrupting substances. The foremost difficulty to analyse the toxicity of a chemical is that these effects may be latent for long periods before they are revealed or that the concerned chemical only play one role in a series of biochemical reactions. In addition, there is a great uncertainty of the exposure to humans from diverse sources e.g. smoking, drugs and environment. In a world full of chemicals, the exposure to toxic substances is inevitable where they can act in synergism and antagonism. Considerations of both the chemical's inherent toxicity and its exposure to the environment are important when classifying a chemical (Mackay, 2001).

Long-Range Transport

Chemicals that can transport long-distances are a transboundary issue which involves worldwide nations. An example of this is the sulphur dioxide that is a gaseous pollutant and can acidify lakes with poor buffering capacity at remote places. It requires political incentives in order to regulate the emissions of long-range transportable pollutants. It is thus indeed vital to identify those chemicals as well as apply international treaty (Mackay, 2001).

Other Effects

Concerns regarding other adverse effects from chemicals have been raised and to mention a few of them: disruption of atmospheric chemistry, shift of pH, foam in rivers and formation of toxic metabolites or degradation products (Mackay, 2001).

2.1.2 Key Properties and Factors

Introduction of central concepts of properties and factors for modelling of WWTP are presented in this chapter.

Definition of Partition Coefficient

Partition, distribution or sorption coefficient, K_p or K_d, is defined as the ratio of a chemical's concentration in two chemical phases at equilibrium (Leo, et al., 1971). In other words, the partition coefficient is a measure of the solubility difference in two environmental media. For hydrophobic compounds, the partition coefficients can be estimated from solubility, vapour pressure, octanol-water partition coefficient (K_{OW}) and acid (basic) dissociation constant ($K_{a(b)}$).

Physico-chemical Properties

In order to gain a somewhat better understanding in how partitioning of a chemical work in the environment, its behavioural attributes in an air-water-octanol (1-octanol) system is observed. Since the C:H:O-ratio of octanol is similar to regular lipids and the fact that octanol is also hydrophobic, octanol can act as a substitute for lipids as well as natural organic matter in soils and sediments (Mackay, 2001).

In Figure 3, the logarithmical K_{OW}, is plotted against the logarithmical air-water partition coefficient, log K_{AW}, where the dots represent 233 different chemicals that are listed in table 3.5 in Mackay, (2001). K_{AW} is also referred to as the dimensionless Henry's law constant, K_H. Note that Henry's constant with the unit of Pa m^3 mol^{-1} is denoted as H. The 45° lines are the constant K_{OA} that is equal to the division of K_{OW} and K_{AW}. In the upper left region of the figure the volatile compounds e.g. benzene can be found, in the lower left are the water soluble compounds e.g. benzaldehyde and in the lower right region are the hydrophobic chemicals e.g. PCBs (Mackay, 2001).

Typical OCs that end up in WWTPs are predominantly hydrophobic. They have a tendency to sorb onto organic matter in the sludge (Webber & Goodin, 1992), if they are freed into the aqueous phase they have a high probability of accumulating in organisms (Andersson et al., 2010). Hydrophobic chemicals most likely partition in lipids, organic or fat phases, hence, hydrophobicity can be described with K_{OW}. The value of K_{OW} approximately equals the ratio between the chemical concentration in an organic medium and water which it is in contact with. The term hydrophobicity is often confused with lipophilicity. In fact, the majority of OCs is more or less equally soluble in fat (lipohilic), but varies differently when solved in water (hydrophobic). Hydrophobicity is the description of the behaviour or affinity in water and not solubility in water (Mackay, 2001). Moreover, water soluble compounds remain in the aqueous phase and are usually biodegradable, while compounds with lower water solubility leave the aqueous phase (Andersson et al., 2010).

Evaporation of a chemical is controlled by its vapour pressure that can be described as the maximum pressure where a pure chemical solves or partitions from its chemical phase to gas phase. Vapour pressure can be regarded as the solubility of the chemical in gas phase and can easily be converted to solubility by dividing it with the gas constant, R (8.314 J K^{-1} mol^{-1}), and the absolute temperature, T (K). As a matter of fact, if the values of K_a and K_b are insignificantly small, K_{AW} or K_H can be deduced:

$$K_{AW} = \frac{(VP/RT)}{WS}$$

where VP is the vapour pressure (Pa) and WS is the water solubility (mol m^{-3}). The vapour pressure differs greatly between different organic chemicals and similarly their boiling points (Mackay, 2001). Readily volatile organic compounds (VOCs), e.g. solvent compounds that have high vapour pressures, are volatilised into the air through treatment in WWTP and land spreading. VOCs do not generally present a threat to the soil environment and humans (Webber & Goodin, 1992) which is also confirmed by an experiment (Wilson et al., 1994). However,

volatile organic pollutants may still contribute a risk to the atmosphere or stratosphere (Andersson, et al., 2010).

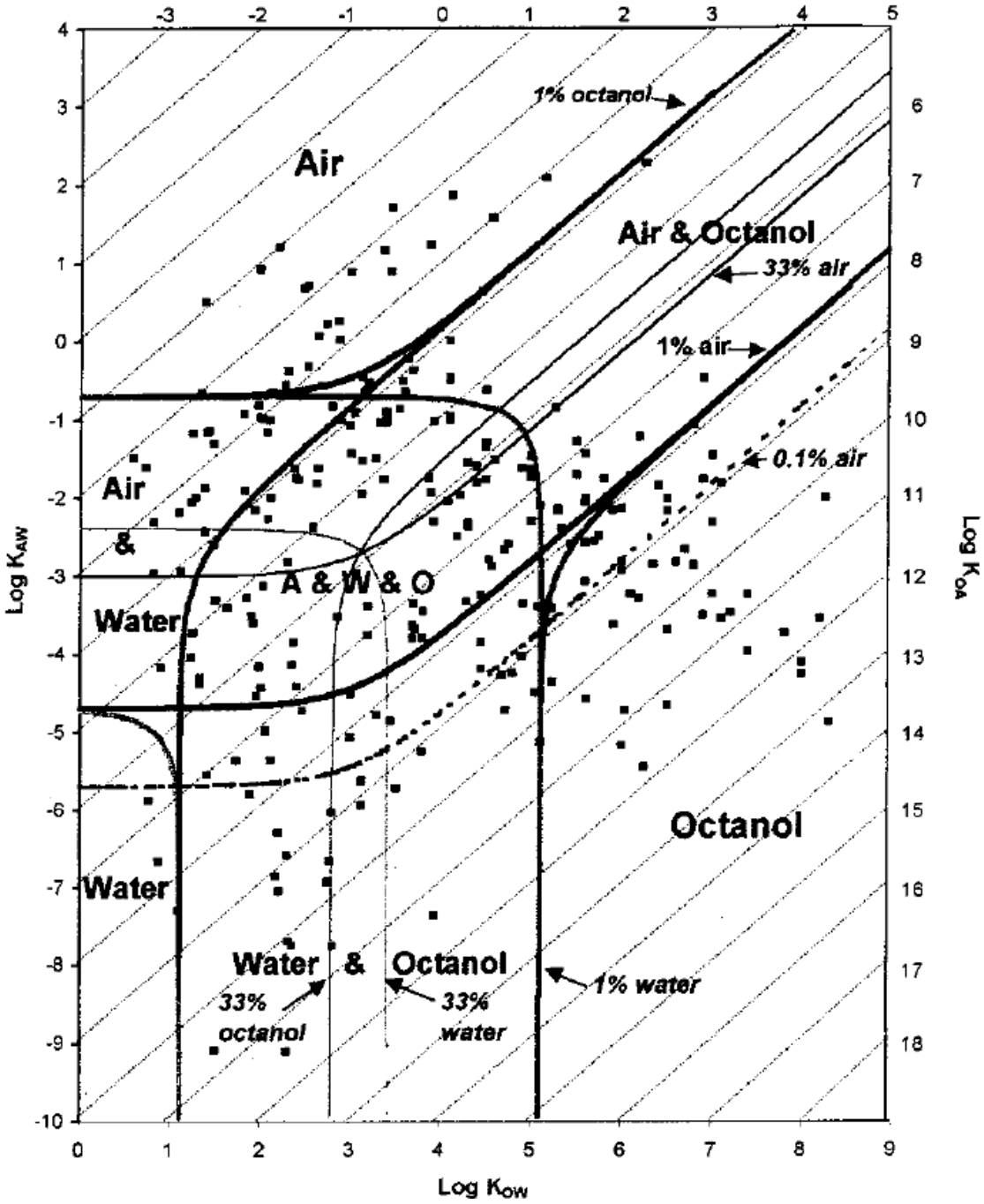


Figure 3. The log K_{OW}, is plotted against the log K_{AW}, where the dots represent the 233 different chemicals that are listed in table 3.5 in Mackay, 2001. The 45° lines are the constant K_{oa} that is equal to the division of K_{OW} and K_{AW}. The thick lines are the isolines of equilibrium phases in air, water and octanol (%), where it is assumed a volume ratio of 6565000:1300:1, respectively (Gouin, et al., 2000).

Important environmental factors to consider are the pH and the temperature. The behaviour of a substance can be affected by its surrounding pH, for example the mobility of a chemical can increase or become strongly sorbed onto particles and thus unavailable for microorganisms depending on the pH. Microorganisms thrive in pH 5 to 7 while outside this interval inhibits its metabolism (Andersson et al., 2010). At high pH, some organic acids will dissociate into their

ionic species in water solution e.g. phenols into phenolates, consequently, the acid/base dissociation constants are other factors that are important to take into account of (Mackay, 2001). Furthermore, temperature has as large influence on the metabolic activity of microorganisms that is favoured at ambient temperature of 10-30°C. Other temperature dependent parameters are the water solubility, vapour pressure, equilibrium constants and degradation (Andersson et al., 2010).

At last but not least, reactivity or persistence is another essential parameter in determining the behaviour of a chemical in the environment except for its partitioning properties. It is usually expressed as half-life, but this value is deceptive since reactivity is dependent on many other different factors such as the sunlight level, temperature etc (Mackay, 2001).

2.1.3 Environmental Fate

Due to the complexity of the environmental fate of a compound, it is difficult to predict its exact distribution in air, soil and water. Nevertheless, a general model of its fate is illustrated in Figure 4, which is based on the water solubility, vapour pressure and reactivity, e.g. degradation, volatilisation etc, of the compound (Andersson et al., 2010).

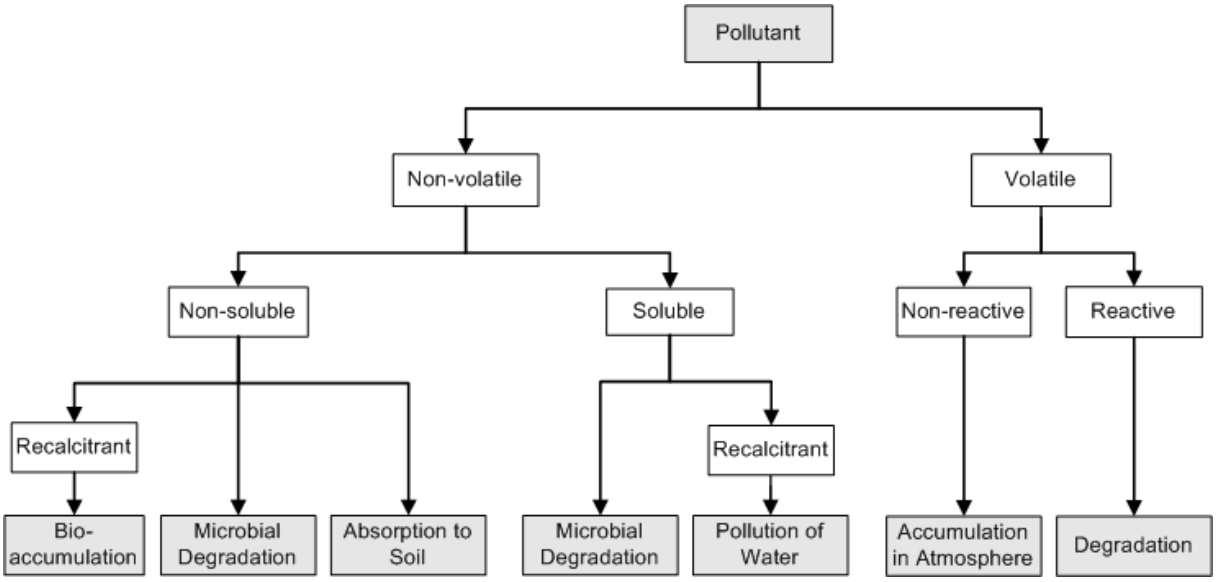


Figure 4. Environmental fate of a compound (Andersson et al., 2010).

2.2 Mass Balance Models

The principle of a *mass balance* model, in accordance to the mass conservation law; is that mass is neither created nor destroyed. Examples of mass balance models are the Sewage Treatment Plant (STP) Model and the SimpleTreat, which are described in more detail in chapter 3. The general purposes of a mass balance model are to (Mackay, 2001):

i. predict likely concentrations, used for e.g. monitoring purposes
ii. depict the relation between the removal processes, which helps defining the most significant process
iii. connect loadings to concentrations, used for identifying key sources and ultimately their effects
iv. estimate the recovery time or the response time
v. generate a general depiction of the system

2.2.1 Fugacity

As the STP Model and SimpleTreat employ the concept of fugacity, fugacity is also introduced in this chapter.

Chemical Potential

Before explaining fugacity, its relative, chemical potential, is equally important to understand. When a chemical diffuses from one phase to another phase, the chemical is attempting to strive for equilibrium. In this case, the free energy in the system will decrease until it reaches equilibrium i.e. the reaction is spontaneous and irreversible. Chemical equilibrium between two phases that are in contact with each other is simply achieved when the temperature, pressure and chemical potential of the chemical in the mixture is equal in all the phases. Chemical potential is defined as the partial molar Gibbs free energy. Hence, it is a derivate of Gibbs free energy, where every system seeks to achieve the minimum of free energy. If the chemical concentration in a phase is high, the chemical potential is thus high and vice versa. Since diffusion moves from high to low chemical potential, chemical potential can thus be used for calculating mass diffusion analogous to temperature for deducting heat transfer calculations (Mackay, 2001).

Introduction of Fugacity

The chemical potential is, however, difficult to manage in chemical equilibrium calculations and moreover to measure in absolute values. As a result, G.N. Lewis introduced a new term in 1901 (Mackay, 2001); fugacity *f* that can be considered as an adjusted partial pressure that replaces the chemical potential (Zacchi, 2000). Fugacity is logarithmically related to the chemical potential. For an ideal gas, the fugacity is equal to the partial pressure at low values of partial pressure (Mackay, 2001).

Application of Fugacity

As mentioned above, a system reaches equilibrium when the fugacity of a chemical is equally large in all phases, while the concentration does not have to be identical in the phases. Fugacity is thus better than the concentration at indicating equilibrium and in addition, similar to the chemical potential; the fugacity can be employed to calculate the diffusive fluxes as well as to determine the direction of the diffusion. An advice is to employ fugacity instead of the partial pressure for real gases at chemical equilibrium calculations.

The fugacity and the concentration of a chemical are proportional to each other at low concentration or low vapour pressure:

$$C = Zf$$

where C is the concentration (mol m^{-3}), Z is the proportional constant or fugacity capacity (mol m^{-3} Pa^{-1}) and f is the fugacity (Pa) (Arnot et al., 2005). Since various xenobiotics, i.e. artificial chemicals that are made by humans, in wastewater enter WWTP at low concentration, the above equation can be justified in WWTP models with the fugacity approach.

Fugacity Capacity

The fugacity capacity, *Z*, of a chemical is defined as the capacity of a phase, which is comparable with the heat capacity. A large value of *Z* for a given chemical thus indicates a high solubility of

that chemical in a chemical phase, i.e. a large volume of the chemical is sorbed to the phase (Mackay, 2001).

Since no interactions between compounds except for colliding events generally occur in the atmosphere, it is the simplest case to investigate the fugacity capacity of a chemical in the air phase. By applying the ideal gas law on the linear fugacity equation where the pressure is substituted with fugacity, one can deduct the following expression:

$$Z_A = \frac{1}{RT_A} = \frac{C_A}{f_A}$$

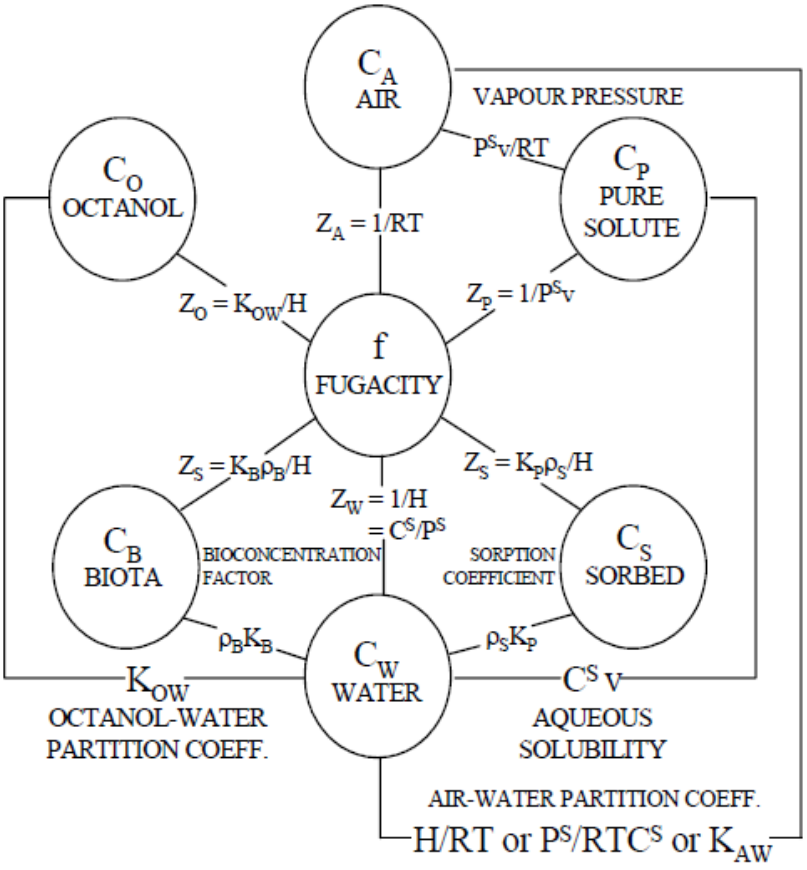
where the subscript A represents the air phase. From the definition of the partition coefficient, the partition coefficient for water and air at equilibrium can hence be expressed as:

$$K_{AW} = \frac{C_A}{C_W} = \frac{Z_A f_A}{Z_W f_W}$$

The air-water partition coefficient is measured at equilibrium i.e. f_A is equal to f_W, and is thus equivalent to the ratio of Z_A and Z_W. A general expression is hence described as:

$$K_{i,j} = \frac{Z_i}{Z_j}$$

A view of the relationship between fugacity, concentrations, partition coefficients and fugacity capacities in the various environmental media is illustrated in Figure 5 along with a summary of their definitions (Arnot et al., 2005).



Definition of Fugacity Capacities

Compartment	Definition of Z, mol/m³ Pa	
Air	1/RT	R = 8.314 Pa m³ / mol K T = temperature, K
Water	1/H or C^S/P^S	H = Henry's law constant, Pa m³ / mol C^S = aqueous solubility, mol/m³ P^S = vapour pressure, Pa
Solid Sorbent (e.g. soil, sediment, particles)	$K_P \rho_S$ / H	K_P = solid-water partition coefficient, L/kg ρ_S = density of solid, kg/L
Biota	$K_B \rho_B$ / H	K_B = biota-water partition coefficient, L/kg or bioconcentration factor (BCF), L/kg ρ_B = density of biota, kg/L (often assumed to be 1.0 kg/L)
Pure Solute	1 / P^S v	v = solute molar volume, m³/mol

Figure 5. Relationship between the fugacity capacities, Z, in different environmental media and definitions of the Z-values (Mackay, 2001).

3 Methods

3.1 SimpleTreat 3.1

A short summary of the multimedia mass balance model, SimpleTreat 3.1 is presented here, whereas its full description can be consulted in the handbook of Struijs (1996).

3.1.1 Model Concept

SimpleTreat is a spreadsheet (Excel®) based box model with fugacity approach, which predicts the fate of an organic xenobiotic in a WWTP. The SimpleTreat is comprised of four sheets: "input", "9-box", "6-box" and "output". The 9-box WWTP model consists of a primary settler, an aeration tank and a solids liquid separator (secondary clarifier), see Figure 6 (Boeije et al., 1998; Struijs, 1996).

The primary settler and secondary clarifier have the same function that is to settle the suspended contaminants of the influent in a large sedimentation basin, which is the mechanical treatment. In the aeration tank, the wastewater undergoes biological treatment to separate and decompose OCs with the help of microorganisms (Kemira Kemwater, 2003).

The biological processes can be separated: anaerobic, anoxic and aerobic decomposition. The model only consider the aerobic processes in the aeration tank, whereas generic Swedish WWTPs may also have an anaerobic reactor (absence of oxygen or nitrate) that increases the growth of phosphorus assimilating bacteria, and/or an anoxic reactor (similar to aerobic processes but uses the oxygen in nitrate instead of the dissolved oxygen) that denitrifies nitrate to nitrogen gas and degrades dissolved organic matter (Kemira Kemwater, 2003).

Besides from estimating the elimination of a compound, given that the chemical is either persistent or degrades according to first order kinetics, the model also calculates the distribution of the substance in air, water and sludge that are emitted to the surroundings of the WWTP (Boeije et al., 1998; Struijs, 1996).

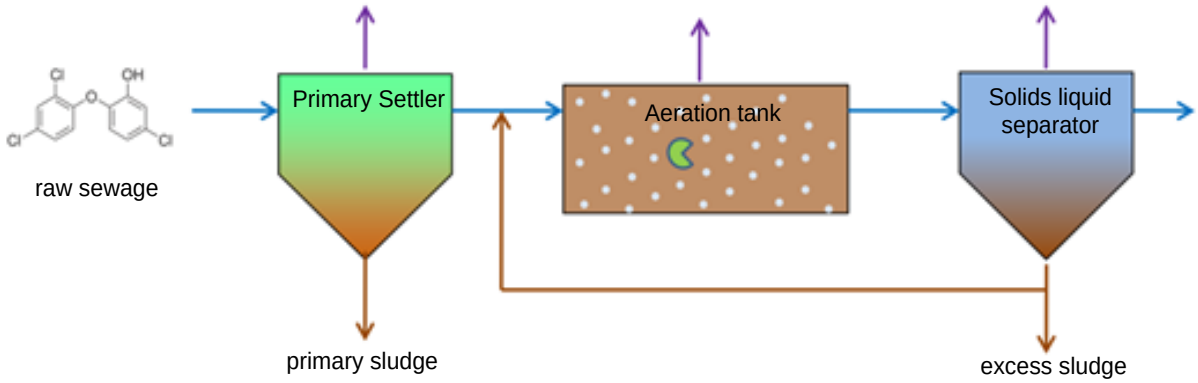


Figure 6. The schematic of a typical municipal wastewater treatment plant modelled in SimpleTreat 3.1 (Franco, et al., 2011).

In the SimpleTreat, the input sheet consists of the parameters describing the plant configuration, physico-chemical properties and influent (raw sewage) and the output of the simulation returns

the concentration in air, effluent and sludge, which is illustrated in Figure 7 (Boeije, et al., 1998; Struijs, 1996).

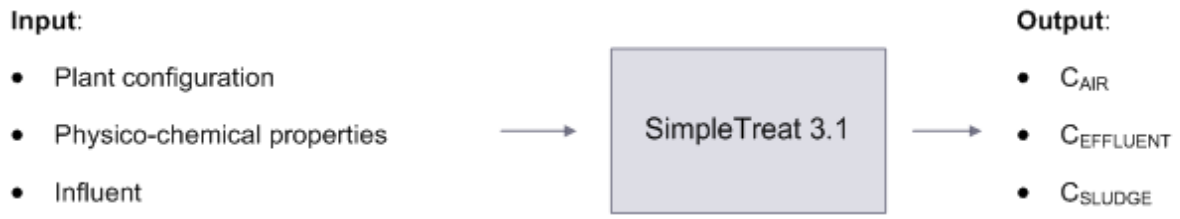


Figure 7. In- and output of SimpleTreat 3.1.

3.1.2 Biological and Physical Processes

The biological and physical processes that are included in the SimpleTreat are the degradation, advection and diffusion. Degradation takes place in the aeration tank. The advective mass flow (sedimentation, recycling of sludge etc) is the transportation through air, water and sludge, and the diffusive mass flow between water-solids (sorption) and water-air (volatilisation and stripping) (Franco et al., 2011; Struijs, 1996).

Organic contaminants are reduced through biodegradation processes, such as aerobic and anaerobic digestion and sludge composting.

Sorption is the collective name of absorption, adsorption and ion exchange where one chemical is attached to another (Struijs, 1996). When chemicals sorb onto particulate matter, it is usually unknown which of the sorption process that takes place, therefore, sorption is applied (Mackay, 2001). The most important chemical property for predicting the emission via sludge is the solids-water partition coefficient K_p (for hydrophobic compounds: K_{OW}), rather than the Henry's law constant, H, and the first order aerobic degradation rate, k_{deg}. Hence, the real partition coefficient K_p for each chemical will be necessary for accurately simulating new compounds such as surface active substances and dye stuffs. In the model, the partitioning of a chemical from one media to another (Struijs et al., 1991).

Another type of diffusive transport is volatilisation which is the transportation from water to air phase, which means that only chemicals that are present in the water may evaporate to air. The rate to volatilisation is determined by the difference of the actual concentrations and the equilibrium concentrations in the two phases at a constant temperature, which is the Henry's law and can thus be described with the dimensionless K_H. In addition, it is dependent on the total area of the primary settler and secondary clarifier. Volatilisation is simulated with the two films theory approach in the primary settler and secondary clarifier to derive the interphase mass transfer coefficients. Moreover, air stripping rely on the type of chemical technology that is utilised to transfer the volatile contaminant to an air stream (Struijs, 1996); surface aeration or bubble aeration can be selected in the model, where the surface aeration is more efficient than the bubble aeration (Struijs et al., 1991).

3.1.3 Model Structure

In SimpleTreat, a set of compartments (boxes) are used to represent a WWTP, where each box is assigned a chemical phase or an environmental media in a reactor of a plant. In the 9-box model

from Figure 8, box 1 represents the air above the WWTP. The primary settler comprises of boxes 2 (water), 3 (suspended solids) and 4 (settled solids), the aeration tank of boxes 5 (mixed liquor of water) and 6 (suspended particulate matter), and the solids liquid separator consists of boxes 7 (water), 8 (small volume of suspended solids) and 9 (settled sludge). Moreover, the 6-box model is the same as the 9-box model with the exception of the primary settler (Struijs et al., 1991). For each box i, a mass balance equation can be described:

$$V_i \cdot \frac{dC_i}{dt} = -k_i C_i V_i + \sum ADV_{i,j} \cdot C_i + \sum DIFF_{i,j} \cdot C_i$$

where V is the volume (m^3), C is the concentration (g m^{-3}), t is the time (s), k is the first order aerobic biodegradation constant rate (s^{-1}), ADV is the advective mass flow (mol s^{-1}) and $DIFF$ is the diffusive mass flow (mol s^{-1}). The advective flows are expressed individually and described more specifically in the handbook (Struijs, 1996). The diffusive exchange between box i and box j is expressed for both directions:

$$DIFF_{i,j} = DIFF_{j,i} = \frac{D_{i,j}}{Z_i}$$

where $D_{i,j}$ is the interphase mass transfer coefficients (mol s^{-1} Pa^{-1}) and Z_i is the fugacity capacity (mol m^{-3} Pa^{-1}). Hence, the fugacity concept enables the formulation and calculation of $DIFF$ (Mackay & Paterson, 1982). A total of nine linear mass balance equations are set up that are solved at steady state (Struijs et al., 1991).

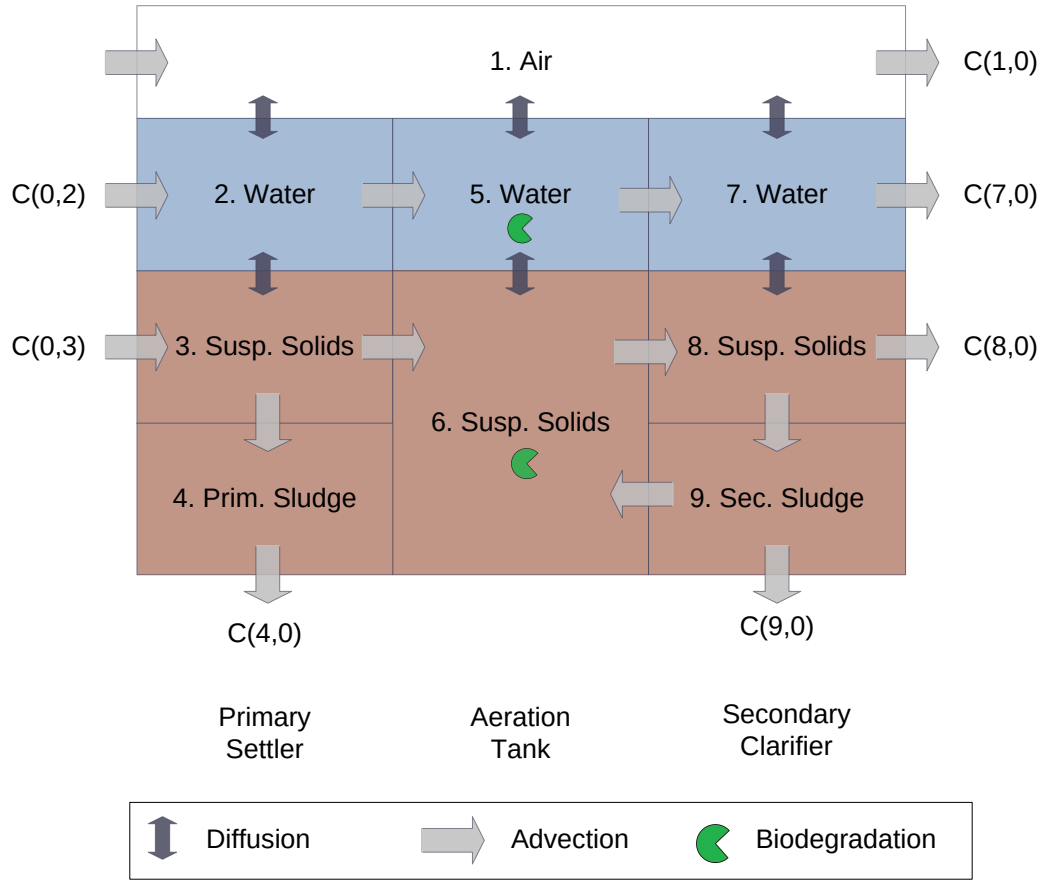


Figure 8. The 9-box model with primary settler, aeration tank and secondary clarifier (Struijs, 1996).

3.1.4 Model Assumptions

The primary intended use of SimpleTreat is to analyse the behaviour of an organic substance in a WWTP and the secondary use is to function as a default calculation module in the risk assessment sheet model, EUSES (Struijs, 1996). To apply the model, physico-chemical properties and a biodegradability profile of the organic substance are necessary.

The calculations in SimpleTreat assume that the system is non-equilibrium and steady-state, which is illustrated in Figure 9c. As can be seen from Figure 9a and Figure 9c, the concentration ratio of benzene between the air and water flows leaving the compartment is not the same as in the compartment, i.e. a factor of 4 larger in the water phase. This factor is also known as the partition coefficient. What happens is that benzene has insufficient time to reach equilibrium before leaving the compartment. The model also assumes steady-state which means that all the concentrations are constant with time.

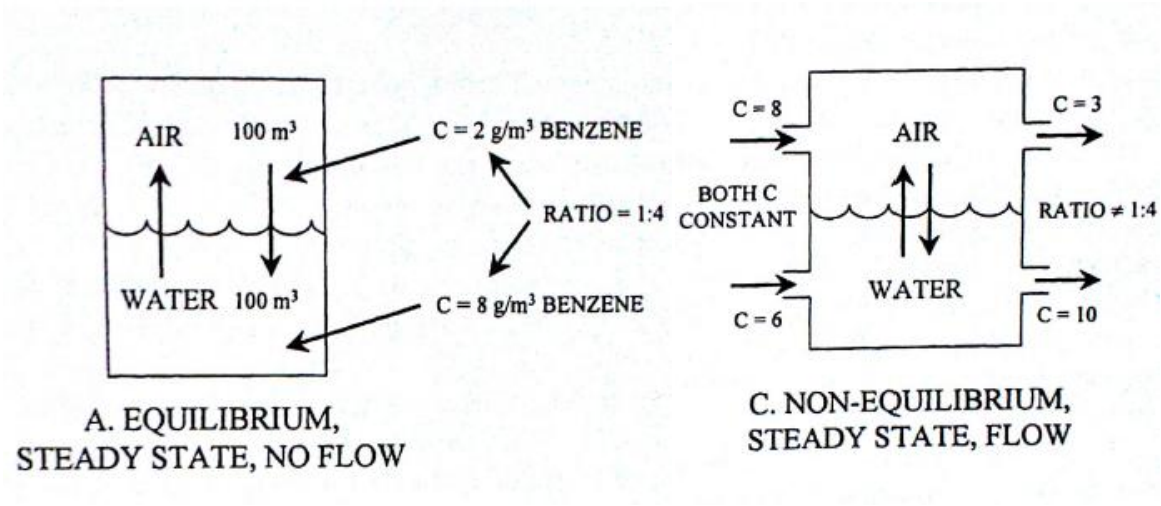


Figure 9. Difference between equilibrium and non-equilibrium system without and with flow (Mackay, 2001).

Other assumptions are that the compartments are considered homogenous and well-mixed systems similar to a continued stirred tank reactor (CSTR) and that biodegradation is a pseudo-first order that only takes place in the aeration tank. Pseudo-first order biodegradation can be justified for many fine chemicals, i.e. complex substances that are produced limited scale at a relatively high price, for example pharmaceuticals that enter with the wastewater at low concentration into the WWTP.

The model scenario does not consider all the chemical treatment units and processes in a WWTP such as phosphorus precipitation, microbial degradation in the settlers, parent compound formation/degradation products, abiotic decomposition for example hydrolysis, photolysis, oxidation and reduction etc (Franco et al., 2011). Moreover, the plant operates at pH 7 for optimal microbial activity which is reasonable. At this pH, the default values of the dissociation constants, K_a and K_b, are significantly small, which means that chemicals are assumed to only exist in its neutral form at pH 7 in water (Franco et al., 2011). For prediction of neutral and monovalent ionising species, there is a developed version of SimpleTreat (Franco et al., 2011).

3.1.5 Previous Studies

The developer of SimpleTreat also made his own analysis of the first version of SimpleTreat as he could conclude that for compounds with high volatility (H < 300 Pa m^3 mol^{-1}) and low hydrophobicity (log K_{OW} < 3), its emission to air is evidently dominant. In addition, the increase of volatility from 1 to 100 Pa m^3 mol^{-1} does not drastically affect the percentage emission via sludge increasing log K_{OW} from 1 to 6. Moreover, the biodegradation of a specified chemical decreased from 75% to 10% when the sorption coefficient K_p increased from 10^3 to 10^5 l kg^{-1}, which is an indication that the biodegradation is insignificant when the sorption to sludge is so strongly dependent of the sorption coefficients in this range (Struijs, et al., 1991).

In a previous research, the SimpleTreat has already been modified to take into account a more detailed description of sludge recycling and the anaerobic and anoxic stages. Surface volatilisation in all tanks and air stripping in the aerobic reactor were also assumed (Boeije et al., 1998). The additional parameters of the redox zones such as the degradation rates are, however, difficult to estimate. Since this model has a few more uncertain parameters than the original model, it loses its simplicity. Another study could confirm that the overall first order degradation rate (aerobic and anoxic) can be approximated to the first order aerobic degradation rate for compounds with longer aerobic half-life than 2 hours, which is valid for many chemicals (Fauser et al., 2002). The thesis will thus focus on altering the SimpleTreat as simple as possible by incorporating existing known parameters such as the dimensions and hydraulic retention time (HRT) of the anaerobic and anoxic tanks. Although, there are many uncertainties regarding the use of SimpleTreat, it has been concluded from another article that a steady-state model such as SimpleTreat can be used for estimating the effluent concentration, even though the SimpleTreat is altered (Fauser et al., 2002).

3.2 EPI Suite™

The EPI Suite™ (© 2000-2011 U.S. EPA, 2007) is a software suite with many different programs to estimate physico-chemical properties and environmental fate. The program is a product of the U.S. EPA and Syracuse Research Corporation.

3.2.1 Physico-chemical Properties

The EPI Suite™ can be used to excerpt experimental and estimation data of physico-chemical properties. The manual insertion of every chemical is needed to gain data of the molar weight in the program EPIWIN. As for the other properties, such as the water solubility can be obtained from WSKOWWIN, the vapour pressure from MPBPVP, the organic carbon partition coefficient or the soil adsorption coefficient from KOCWIN, the octanol-water partition coefficient from KOWWIN and the degradation rate from BIOWIN. The parameters are extracted through creating a batch text file with all the CAS-numbers (Chemical Abstracts Service) of chemicals that are of interest and then run them in the programs respectively. CAS-number is the unique assigned number of a chemical.

The parameters obtained from WKOWWIN, MPBPVP, KOCWIN and KOWWIN only requires a chemical structure to estimate it, but the subprograms also have a database with experimental values that is rather preferred than the estimated one. Among different biodegradation models in the BIOWIN, Biowin 3 was chosen to estimate the ultimate biodegradation time, which is calculating from taking into account of the molecular fragment and

the molar weight. Molecular fragment refers to how an organic molecule will specifically fragment depending on its functional group.

3.2.2 STPWIN

One of the environmental fate estimation software is the STPWIN which is a version of the STP model that was originally created by Mackay et al. at the University of Toronto (Clark et al., 1995). The model is only developed for the purpose of gaining generic information about the behaviour of a chemical and thus not to acquire the exact simulated data in a particular plant (U.S. Environmental Protection Agency, 2000).

The STP model is a mass balance model based on fugacity principles, similar to the SimpleTreat. The basis of STP Model is to predict the fate of an organic substance in a conventional WWTP using activated sludge secondary treatment. The chemical is removed by numerous processes such as biodegradation, evaporation, sorption to sludge and loss in the final effluent. The most crucial and uncertain parameters are those related to the biodegradation of the substance and the dependency of biomass concentration. The STPWIN solely uses the default operating conditions of a WWTP operating at 25ºC (see Table 1).

Table 1. The default system properties of STPWIN in EPI Suite™ (U.S. Environmental Protection Agency, 2000).

Parameter[a]	Tank 1 (primary)	Tank 2 (aerator)	Tank 3 (secondary)
Tank area (m^2)	266.7	800	727.3
Tank depth (m)	3.8	10	3.8
VSS conc (g/m^3)	50000	-	5500
VSS biomass (fraction)	0.005	0.0025	0.00055
Outflow MLVSS conc (g/m^3)	80.2	2500	15
VSS aeration rate (m^3/h)	-	8960	-
Fraction of influent flow recycled	-	-	0.8
Fraction of influent flow removed	0.0024	-	0.015

[a] Other system properties: influent total flow = 1000 m^3/h; influent VSS conc = 200 g/m^3; gas phase mass transfer phase coefficient = 5 m/h; liquid phase mass transfer coefficient = 0.05 m/h.

4 Results and Discussion

4.1 Methodology

Figure 10 shows a general scheme of the methodology on how to investigate chemicals' fate in a WWTP and as soil amendment with little available experimental data of the chemical, which is further described in more detail in this chapter. The methodology consists of five steps although the last step is not a part of the thesis.

STEP 1: The first step is to select a WWTP and thereafter collect necessary plant characteristics with regard to the selected model in *STEP 3*.

STEP 2: The second step is to select an organic compound that has been measured in sludge and will be used for soil application; either by searching in databases e.g. IVL-database, or measuring the chemical at the influent before the primary settler, the effluent after the secondary clarifier and both the primary and secondary sludge if possible. The primary sludge is defined as the sludge from the primary settler and the secondary sludge from the secondary clarifier. For every chemical of interest, relevant physico-chemical properties need to be specified. For this purpose, a suggestion is to apply the EPI Suite™ when reasonable measured values are not available.

STEP 3: The third step is to select a WWTP model that predicts the fate of a chemical in a WWTP, e.g. SimpleTreat or STP Model, depending on the selected WWTP and chemical. The WWTP model is simulated by inserting three essential input data: the plant configuration, the physico-chemical parameters and the influent, where the expected output is the predicted concentrations in air, effluent and sludge.

STEP 4: In this step, the modelled effluent is compared with the measured effluent. If these concentrations do not match well, the current model can either be modified or reselected. Another possible option is to run additional measurements of the chemical concentration in influent, effluent and sludge.

STEP 5: The last step is to select a soil model that simulates the soil processes using the predicted sludge concentration from the WWTP model to simulate the concentration in soil. If the predicted concentration of the OC after being processed in the soil is evaluated to be at an insignificant level by taking into consideration of its quantity, persistence, bioaccumulation, toxicity, potential for long-range transportation etc, then no further action is taken. In other cases, the chemical ought to be monitored in the WWTP and included in the work of upstream actions as a part of the REVAQ certification.

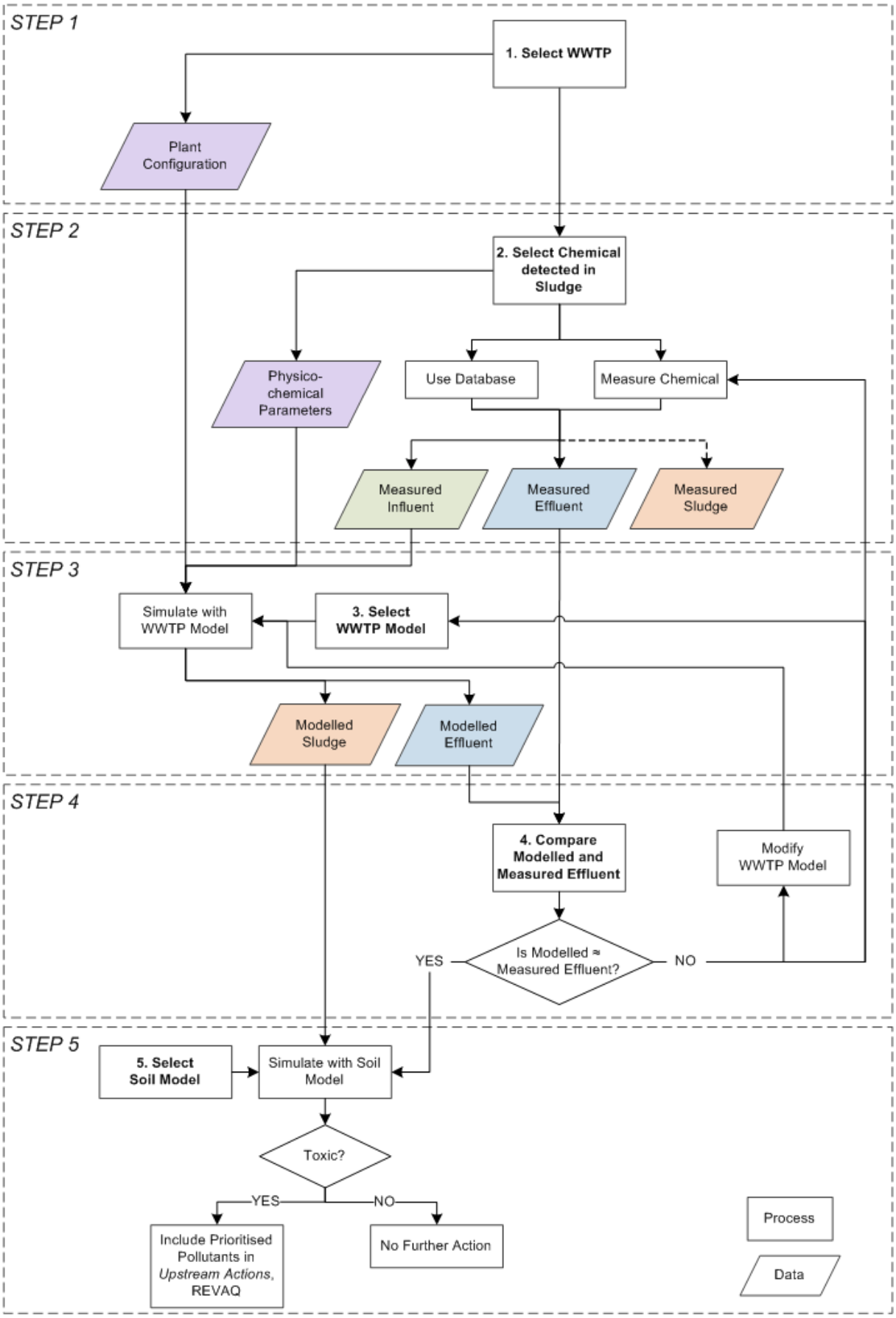


Figure 10. Methodology of how to predict the fate of a chemical in WWTP and soil.

4.2 Case Study

A case study using the methodology presented above is performed here.

4.2.1 Step 1: Select WWTP

For the case study, the chosen WWTPs were Ellinge, Käppala, Ryaverket and Sjölunda, which are also a part of the aforementioned umbrella project.

Wastewater Treatment Plants

A short description of the four Swedish WWTP representatives as well as their plant characteristics is presented below.

Ellinge WWTP

Ellinge WWTP is situated in Eslöv and is a part of VA SYD. The WWTP has two main incoming pipes; one from the inhabitants of the municipality and other connected industries which is seen in the upper part of Figure 11 and one from Procordia Food AB seen in the lower part of the same figure. The wastewater from the municipality and the industries are treated in the subsequent order: screen, grit removal, primary settler, anoxic tank, aeration tank, secondary clarifier, flocculation and phosphorus removal with ferric chloride. In this study, the inlet sewage flow from Procordia Food AB is neglected since the treatment process differentiates greatly from the model used in SimpleTreat. Moreover, the sludge is currently conveyed to an anaerobic digester for production of biogas (Eslöv Municipality, 2010).

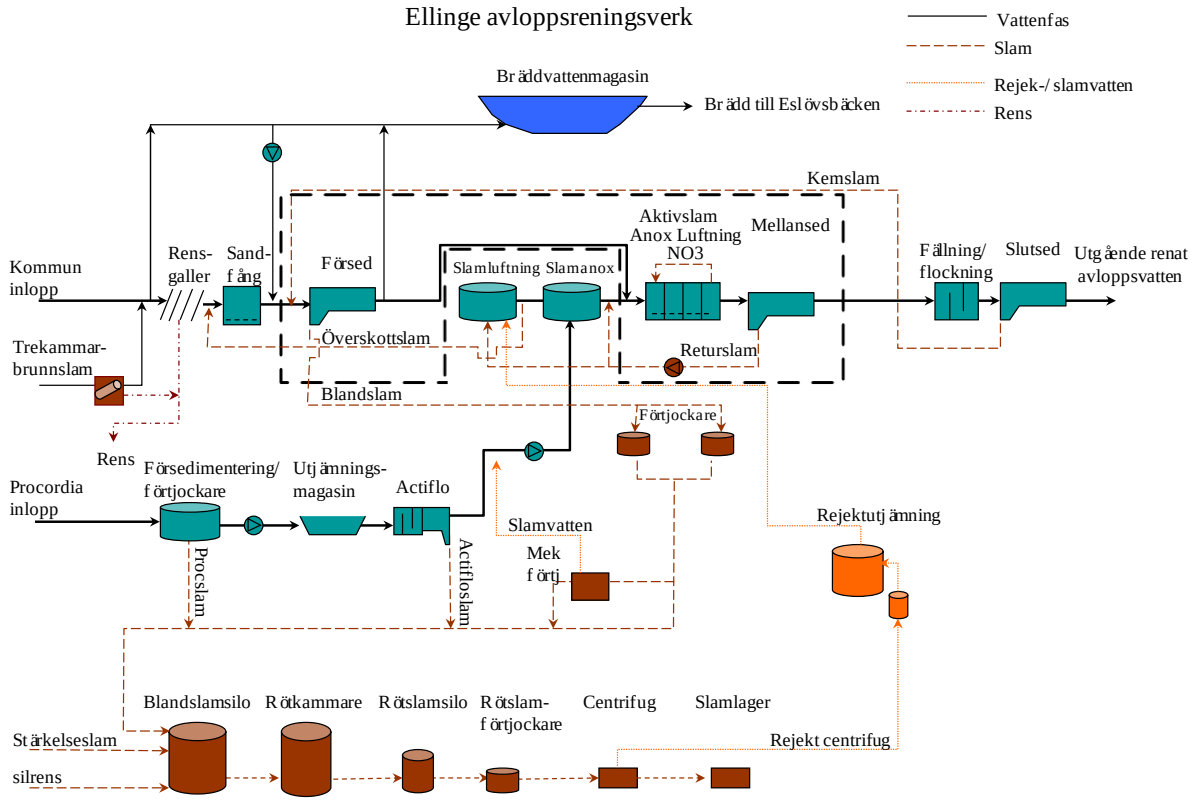


Figure 11. Process scheme of Ellinge WWTP, where the black dotted line is the system boundary for this work (Eslöv Municipality, 2010).

Käppala WWTP

Käppala WWTP is located in Lidingö and treats the wastewater from the neighbouring municipalities, Nacka and Värmdö as well as a part of the water from Järfälla municipality including Arla Dairy in Kallhäll. The owner of Käppala WWTP is the Käppala Association. The process scheme of the WWTP is displayed in Figure 12. Since Käppala has different plant configurations for the new and old section of Käppala, they are treated as two separate plants, see Figure 13. The wastewater undergoes numerous process steps: screen, grit removal, primary settler, activated sludge treatment with separate anaerobic, anoxic and aerobic tanks, secondary clarifier and sand filter. For phosphorus removal, ferrous sulphate is dosed twice; at the recycled sludge and before the sand filter. The sludge is partly recycled as fertiliser whereof the rest is for production of soil and soil amendment products, and is partly for production of biogas. The sludge applied for soil amendment is REVAQ certified (Käppalaförbundet, 2011).

Ryaverket WWTP

Ryaverket WWTP that is owned by Gryaab AB is situated in Göteborg and has two functions, firstly, to channel the water from the urban area to the WWTP and, secondly, to treat the wastewater. The influent mainly comes from the municipalities of Ale, Göteborg, Härryda, Kungälv, Mölndal and Partille, but also from industries such as Cleanpipe Sverige AB and Veolia Vatten AB. Figure 14 shows the process scheme of the WWTP, where the influent is treated in the following processes: coarse bars screen, grit removal, fine bars screen, primary settler, activated sludge (anaerobic, anoxic and aerobic zones), secondary clarifier and new installed disk filters. Removal of phosphorus is performed after the fine bars screen where polyaluminium chloride (PAC) is added to the water in a settler parallel to the primary settler. The application of sludge in Gryaab AB is the same as Käppala, where the sludge is certified as well (Gryaab AB, 2011).

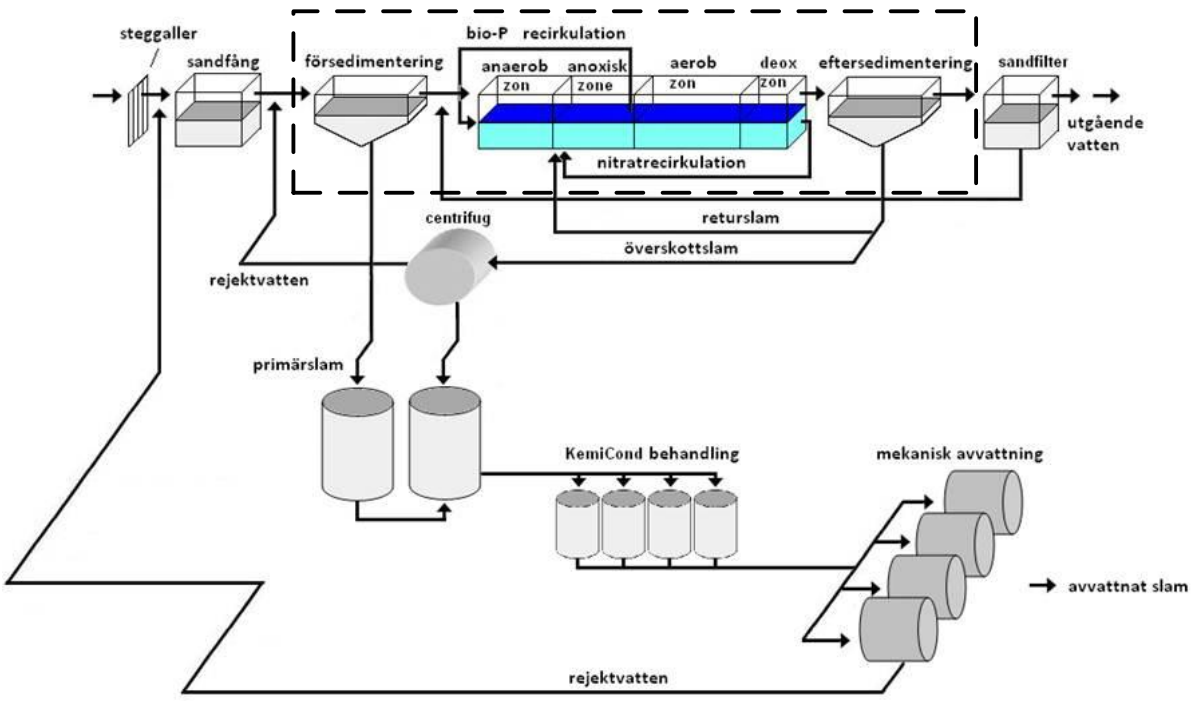


Figure 12. Process scheme of Käppala WWTP, where the black dotted line is the system boundary for this work (Käppalaförbundet, 2011).

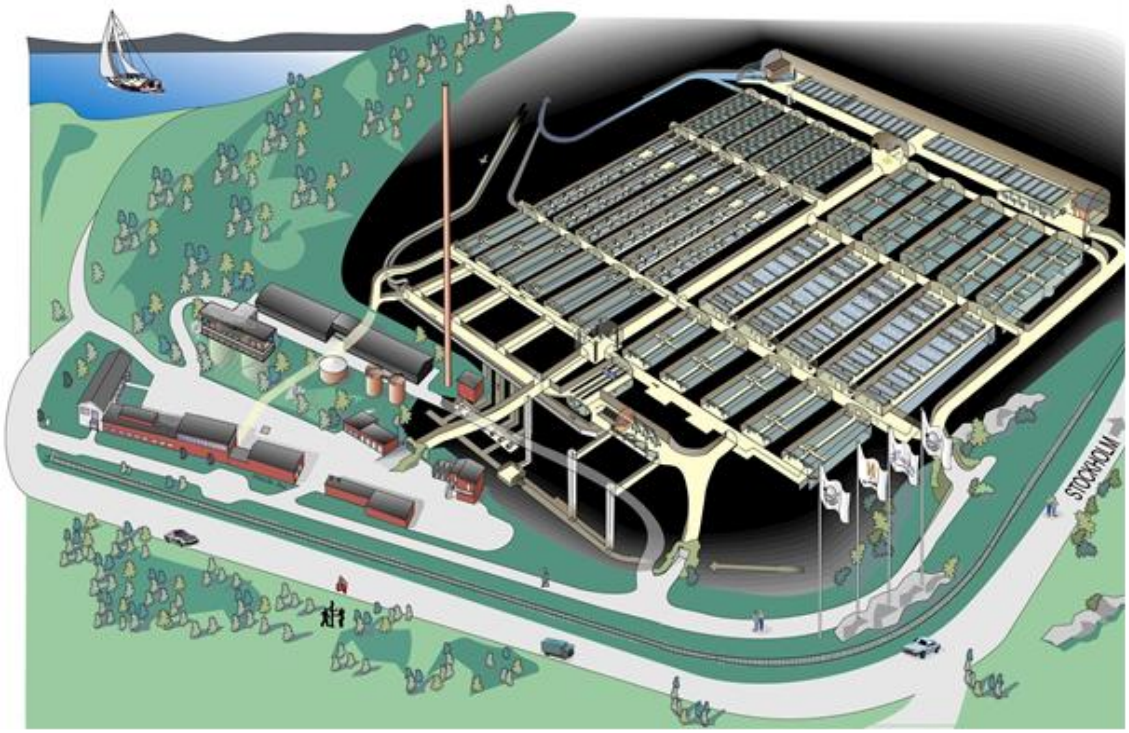


Figure 13. The old and new plant of Käppala where the old part is the six lines from atop and new part is the five lines on below (Käppalaförbundet, 2012).

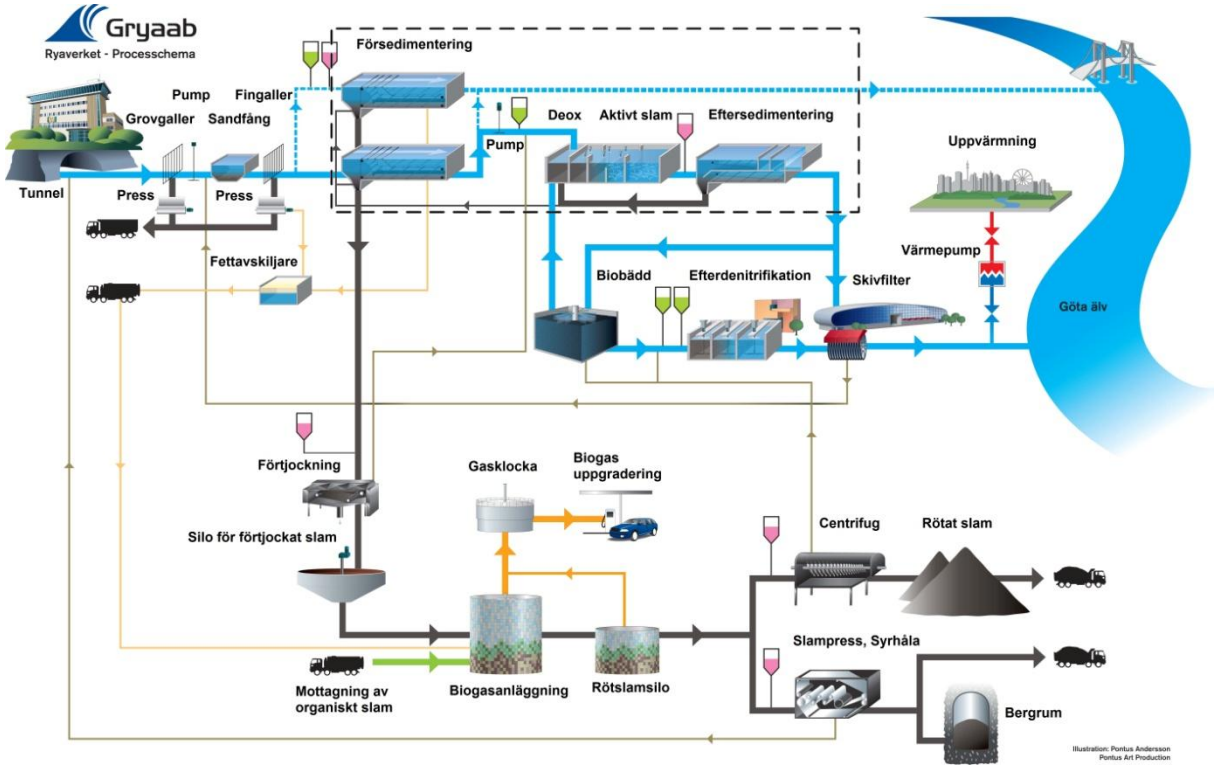


Figure 14. Process scheme of Ryaverket WWTP, where the black dotted line is the system boundary for this work (Gryaab AB, 2011).

Sjölunda WWTP

The location of Sjölunda WWTP is in Malmö and it is operated by VA SYD. The incoming wastewater comes from Malmö and Burlöv including parts of Lomma, Staffanstorp and Svedala municipalities. The treatment process of Sjölunda WWTP is illustrated in Figure 15 and is processed as: screen, grit removal, phosphorus removal with ferrous sulphate, primary settler, activated sludge (anoxic and anaerobic tanks), secondary clarifier, nitrification with trickling filter, solid bed process for denitrification and flotation. Sjölunda also produces biogas from sludge and uses sludge for land application, where they have certified their sludge with REVAQ. Sjölunda has two primary settlers which can be modelled as one since they are connected in series (VA SYD, 2010).

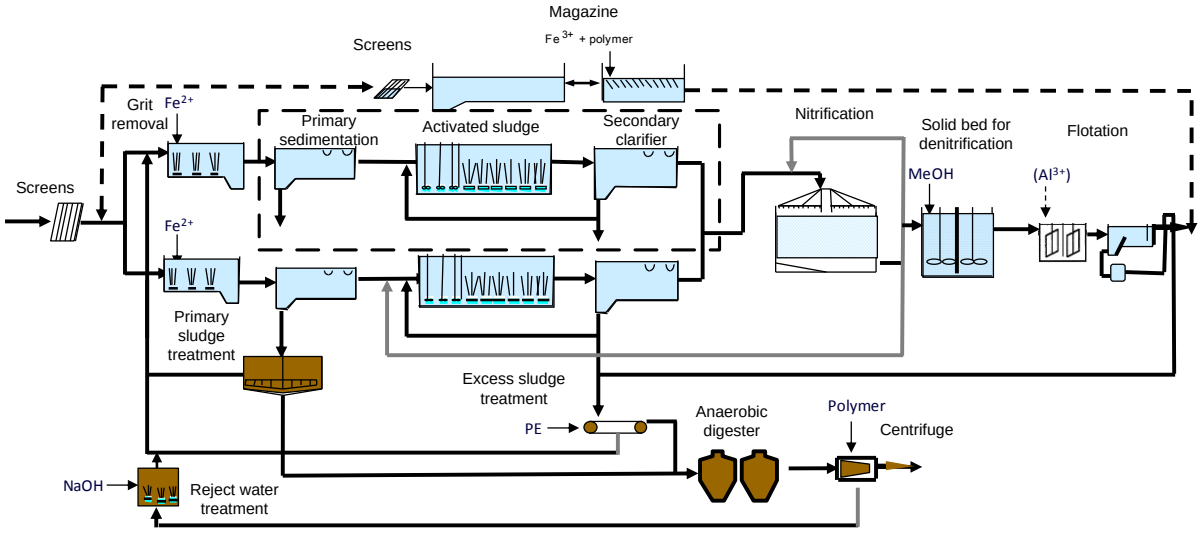


Figure 15. Process scheme of Sjölunda WWTP, where the black dotted line is the system boundary for this work (VA SYD, 2010).

Plant Configuration

A compilation of the plant configuration data from Ellinge, Käppala, Ryaverket and Sjölunda are tabulated in Table 2, while the full set of data is in Appendix 3. In the table, the parameters are divided into *emission scenario* and *system characteristics*, where the two model inputs are found in the sheets of "input" and "9-box" in SimpleTreat respectively. Since the input solids and fraction of organic carbon in the influent were not measured in the Ellinge plant, the modelling of Ellinge cannot proceed. Observe that many of the parameters are expressed per capita.

4.2.2 Step 2: Select Chemical

The chemical measurements were retrieved from the database of IVL on behalf of the Swedish EPA, where data from screening tests of environmental toxins in Sweden are gathered in the database. Measurements conducted by respective WWTPs were also collected, which however were inapplicable for this work. For selecting OCs, the following criteria were set:

1. The chemical has measured data of influent and effluent.
2. The chemical has measured data that are above the detection level.
3. The measured influent concentration has to be larger or equal to the effluent.
4. The effluent concentration compared to the influent measurement is approximately measured within in a reasonable time frame.

5. The chemical has measured data in all of the four WWTPs.
6. The chemical has many data measurements.
7. The total number of chosen chemicals has different properties and belongs to different groups.

Table 2. Fixed parameters of the plant configuration in Ellinge, Käppala (old and new), Ryaverket and Sjölunda.

Emission Scenario in "input"						
Parameter	*Ellinge*	*Old Käppala*	*New Käppala*	*Ryaverket*	*Sjölunda*	*Unit*
T air	15	8.3	8.3	10	15	^{o}C
T water	15	13.6	13.6	12	15	^{o}C
Wind speed	3	0	3	4	3	$m\ s^{-1}$
Sewage flow	358	270	270	514	424	$L\ PE^{-1}d^{-1}$
Number inhabitants	2.82E4	4.80E5	4.80E5	6.66E5	2.94E5	PE
Sludge loading rate	0.13	0.05	0.05	0.79	0.35	$kg_{BOD}\ kg_{dwt}^{-1}\ d^{-1}$
Bubble or surface aeration: b/s	b	b	b	b	b	(-)
System Characteristics in "9-box"						
raw sewage	*Ellinge*	*Old Käppala*	*New Käppala*	*Ryaverket*	*Sjölunda*	*Unit*
Input solids in raw sewage	No data	0.659	0.14	0.093	0.099	$kg_{dwt}\ PE^{-1}\ d^{-1}$
Fraction oc raw sewage	No data	0.85	0.85	0.3	0.5	(-)
BOD in raw sewage	101	60	60	54	70	$g_{BOD}\ PE^{-1}\ d^{-1}$
primary sedimentation						
HRT_{PS}	1.5	2.8	2.7	1.58	1.5	h
$Volume_{PS}$	0.1917	0.0519	0.0504	0.034	0.0269	$m^3\ PE^{-1}$
activated sludge tank						
HRT anaerobic	0	2.1	0	0	0	h
Volume anaerobic	0	0.0228	0	0	0	$m^3\ PE^{-1}$
HRT anoxic	5.31	13.4	17	0.9	0.945	h
Volume anoxic	0.0792	0.146	0.179	0.0459	0.0167	$m^3\ PE^{-1}$
HRT aerator	6	13	15	0.7	2.89	h
Volume aerator	0.0838	0.146	0.179	0.0308	0.0511	$m^3\ PE^{-1}$
solids liquid separation						
HRT_{SLS}	8	6.5	7.6	2.7	5	h
$Volume_{SLS}$	0.483	0.123	0.143	0.108	0.0167	$m^3\ PE^{-1}$

When analysing the IVL-database, only the first four requirements were fulfilled: oxazepam measured in Käppala and ETBE in Ryaverket. The drug, oxazepam, is applied for treating anxiety, insomnia and controlling symptoms of alcohol withdrawal. It is classified as a possible carcinogen (IARC, 1996). Furthermore, ETBE is an additive for production of gasoline from crude oil. ETBE is the better alternative to ethanol since its emissions from gasoline combustion in vehicle engines which are precursors to ozone and particulate matter in the atmosphere, are less than that of the ethanol (EFOA, 2006).

Physico-chemical Properties

The physico-chemical data were obtained from EPI Suite™. Relevant physico-chemical properties are listed in Table 3. Observe that the water solubility is in the unit of mg l^{-1} and not mol m^{-3} and that the pressure given from the EPI Suite™ is in the unit of mmHg and not in the SI-unit, Pascal.

Table 3. Physico-chemical data.

Parameter	Unit	Explanation
MW	g mol^{-1}	Molecular weight
WS	mg l^{-1}	Water solubility
Tws	°C	Temperature of water solubility
VP	Pa	Vapour pressure
Tvp	°C	Temperature of vapour pressure
Koc	l kg^{-1}	Organic carbon partition coefficient
LogKow	-	Logarithmical octanol-water partition coefficient
kDeg	Days	First order aerobic biodegradation rate (ultimate)

There are two main degradation rates that can be simulated in the EPI Suite™: ultimate and primary degradation rate. The ultimate degradation is defined as the complete degradation of a substance to CO_2, biomass, H_2O and other inorganic components. The primary degradation refers to the minimal conversion that alters the physical structure of a chemical. Since the microbial activity is more optimised in a WWTP than in the natural environment, the ultimate degradation rate is thus employed (Seth & Webster, 2008). The ultimate aerobic biodegradation, *x*, obtained from BIOWIN 3 in EPI Suite™ is a value between 1 to 5, where the values correspond to the following time units: 5 – hours; 4 – days; 3 – weeks; 2 – months; 1- longer. It was therefore recalculated with a general conversion equation into the unit of days.

$$k_{deg} = t_{1/2} = 10^{-1.07x+4.2}$$

where $t_{1/2}$ is the aerobic biodegradation half-life. The equation does not, however, apply to chemicals that have a low value of *x* from BIOWIN i.e. the compound is estimated to be very persistent where a value of less than 0.85 corresponds to a half-life of 2190 days or 6 years (Arnot et al., 2005).

4.2.3 Step 3: Select WWTP Model

The mass balance model, SimpleTreat, was selected for predicting the fate of chemicals with the motivation that it is used by the European Commission and has been validated in a number of articles. From the data point of view, the necessary parameters of SimpleTreat correspond to the existing and available data from the WWTPs, EPI Suite™ and IVL-database. The plant configurations provided by the WWTPs were translated into appropriate units to fit the SimpleTreat, see Table 4. The black dotted lines of Figure 11, Figure 12, Figure 14 and Figure 15 are the system boundaries of the SimpleTreat.

Modifications of SimpleTreat

An additional sheet named "chemical" was included in the SimpleTreat, where unlimited chemicals can be simulated simultaneously, see Figure 16. Termination of the simulation occurs when there is an empty row or a value was set to zero. The input column is divided into three parts: *properties*, *measured concentrations* and *measured distribution*. In the *measured distribution* column, the distribution of water and sludge is calculated based on the input of *Effluent* and *MeanSludge* (or *PrimSludge* and *SecSludge*) from *measured concentrations*. The output column is divided into two sections: *predicted concentrations* and *predicted distribution*. The output is redirected from the sheet "output". A more detailed description of all the parameters is given in Appendix 2.

Additional new features of the modified model are the parameter inputs of anaerobic and anoxic tank: HRT, height and volume. The process scheme of the modified SimpleTreat is illustrated in Figure 17. The previous HRT, area and volume were only linked to the aeration tank but now it takes into regard all three tanks. It has been checked thoroughly that these changes will not interfere with volatilisation and air stripping processes that specifically occur in the aerobic tank.

Moreover, the pre-estimated values of volumes in the primary settler and secondary clarifier are replaced with fixed WWTP characteristics. As a result, the significance of HRT is decreased since HRT was mostly assisting in calculating the dimensions of the treatment units. Furthermore, the influent is usually measured as ng l^{-1} in field measurements and not in kg day^{-1} as the previous unit, the emission rate or *InRate* (kg day^{-1}) is, therefore, calculated by automatically multiplying the influent concentration (ng l^{-1}) with the sewage flow and number of inhabitants.

It was also discovered that the EUSES used K_{OC} instead of K_{OW}. This was changed back to K_{OW} for calculations of the K_p in the different medias, since other articles estimate K_p with the help of K_{OW} and most of the K_{OC} from EPI Suite™ are estimated while a majority of the K_{OW} are experimental values.

4.2.4 Step 4: Comparison

A selection of the chosen chemicals was further simulated in the modified SimpleTreat, which is presented in Table 4 and more results are found in Appendix 5. Since the data of oxazepam was measured in Käppala, the chemical was simulated with the plant configurations of both the old and the new Käppala.

4.2.5 Step 5: Select Soil Model and Conclusion

As for the choice of the soil model, the Biosolids-Amended Soil: Level IV (BASL4) was suggested in the umbrella project. However, this study will not perform any simulation with BASL4.

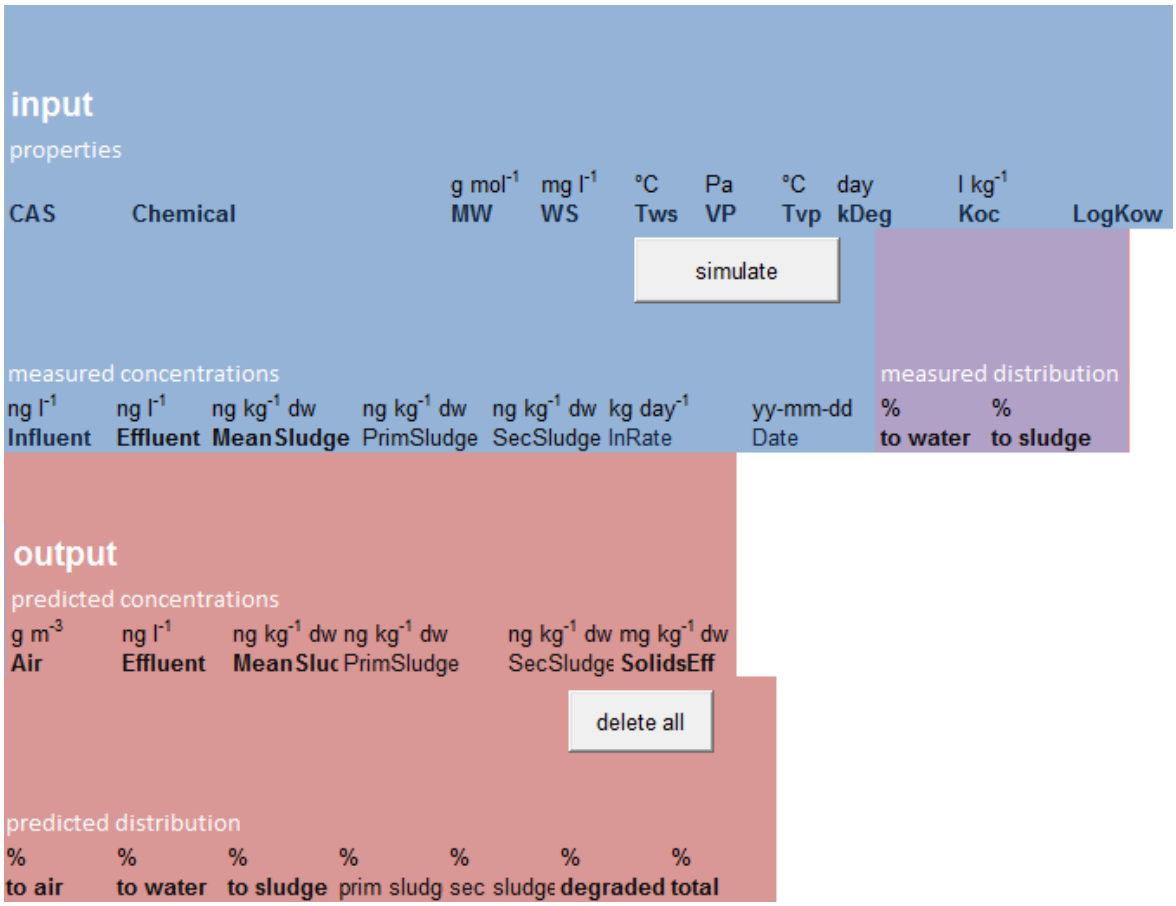


Figure 16. The additional input sheet "chemical" in SimpleTreat, where MW is the molar weight, WS is the water solubility, Tws is the temperature of the WS, VP is the vapour pressure, Tvp is the temperature of VP, kDeg is the degradation rate, Koc is the soil adsorption coefficient and LogKow is the logarithmic octanol-water coefficient.

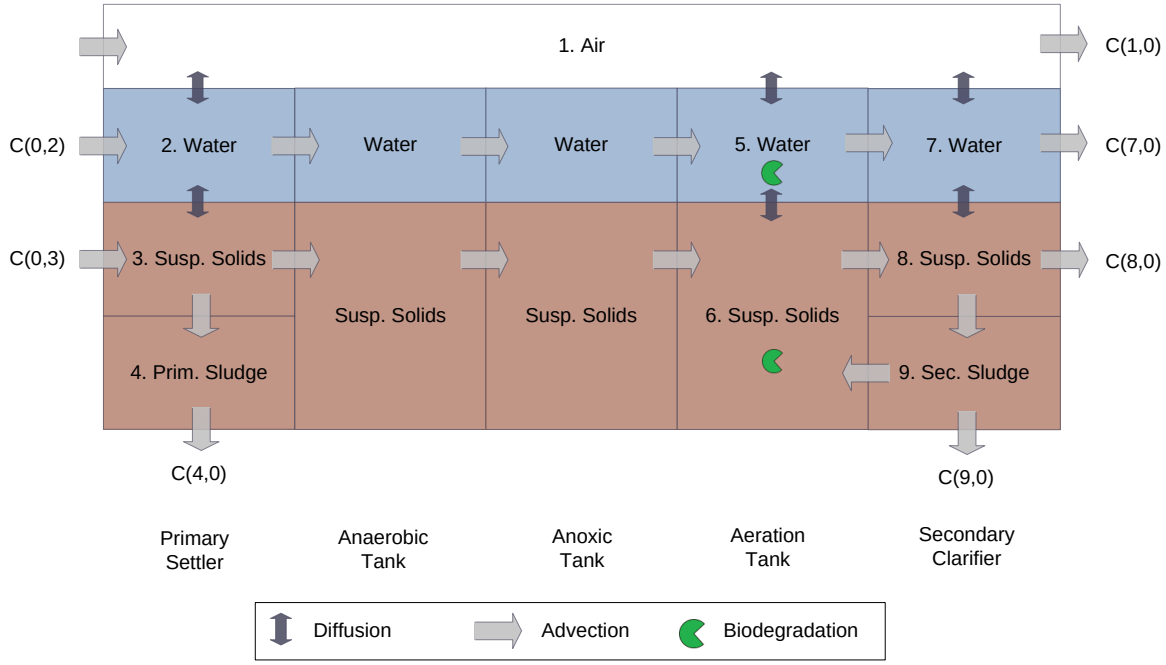


Figure 17. Process scheme of the modified SimpleTreat.

Table 4. The input data of the oxazepam and ETBE simulated in SimpleTreat including measured and predicted data. The numbers with asterisk are estimated values.

WWTP	Chemical	MW	WS at 25°C	VP at 25°C	kDeg	Koc	Log Kow	In (meas)	Eff (meas)	Eff (pred)
		g/mol	mg/l	Pa	day	l/kg	-	ng/l	ng/l	ng/l
Old Käppala	Oxazepam	287	179*	5.55E-10*	34.6*	176*	2.24	250	**220**	**175**
Old Käppala	Oxazepam	287	179*	5.55E-10*	34.6*	176*	2.24	210	**200**	**147**
Old Käppala	Oxazepam	287	179*	5.55E-10*	34.6*	176*	2.24	390	**290**	**273**
New Käppala	Oxazepam	287	179*	5.55E-10*	34.6*	176*	2.24	250	**220**	**196**
New Käppala	Oxazepam	287	179*	5.55E-10*	34.6*	176*	2.24	210	**200**	**165**
New Käppala	Oxazepam	287	179*	5.55E-10*	34.6*	176*	2.24	390	**290**	**306**
Ryaverket	ETBE	102	1.2E4	1.65E4	18.0*	40.7*	1.92*	31	**26**	**25.1**

4.3 Discussion

For most of the cases in Table 4 especially in the old and new Käppala, the predicted effluent concentration is lower than the measured effluent which may be due to a systematic error that either overestimates the degradation or the partitioning to sludge so that less amount of the chemicals is discharged with the effluent. Of the two options, it is more likely that the ultimate degradation rate is the reason for the systematic error.

Furthermore, the application of the methodology was analysed where the main uncertainties rely on 1) the model structure, 2) the model parameters 3) the data quality.

Firstly, the structure of the modified SimpleTreat is a simplification of reality since it does not take into consideration all the processes in the WWTP. For example, the effect of flotation, trickling filter and precipitation with PAC or ferrous sulphate are unknown in the removal of organic pollutants. Especially the screening process that filter sticks, hair, plastics etc and the grit removal that settles the sand, grit, stones and broken glass, can be neglected since their purpose is to mechanically remove larger objects from the wastewater and not OCs. The activated sludge process was extended with anaerobic and anoxic tanks, which, however, did not take into account degradation processes in these tanks. As mentioned before, the aggregated degradation rate (aerobic and anoxic) can be set equal to the aerobic degradation rate which thus partially validates the assumption. As for the anaerobic stage, the EPI Suite™ is also able to predict the anaerobic degradation rate just as the aerobic degradation rate; it will need a general equation to convert it into the unit of days. During anaerobic digestion of sludge, some compounds e.g. mono- and diethoxylates are degraded into 4-nonylphenol or just nonylphenol (Smith, 2009). For this specific case, it may be difficult to take into account parent compound formation/degradation products in a general model as the SimpleTreat only performs predictions of one chemical at a time.

As can be seen in Table 4, the predicted concentration of the new Käppala corresponds better to the measured concentration than the value of the old Käppala. From the results, one can

conclude that the plant configurations have a definite impact on the results. The measured and the predicted concentrations of ETBE in Käppala also correspond well.

When altering the SimpleTreat, the HRT was originally regarded as an important factor in the SimpleTreat. It was later revealed in the model equations that the HRT has little significance on the fate of the chemical after the modifications, such as changing some parameters into fixed values. In fact, the HRTs of the primary settler and secondary clarifier were only used to calculate the volumes respectively, which are not even a part of the modified version. Despite the fact that the HRT of the aerobic tank are incorporated in the surface aeration rate and in the Monod kinetics degradation rate, none of them are used during simulation.

Secondly, the model parameters refer to the physico-chemical parameters. The physico-chemical properties that were excerpted from the EPI Suite™ are a mixture of both experimental and estimated values. Since some values are estimated, the expected results from simulating a chemical may deviate from the measurements, especially those parameters that are important such as the K_{OW}. The K_{OW} of ETBE is estimated but the predictions are still not far from the measurements. The result of oxazepam is another example that proves that the predicted effluent concentration corresponds well to the measured concentration although a majority of the properties are estimated.

Thirdly, the consistency in sampling and the analysis method of the measurements from the IVL-database are doubtful, since their choice of methods are not described in the database. For this thesis, the sampling has to be made at specific measuring points of the WWTP within a realistic time frame. In addition, the accuracy of the instruments measuring nano grams and the small number of existing measurements are uncertain at these low values. For example, surface active detergents are not homogenously distributed in water and may require supplementary samplings. The comparison between the measured and predicted concentrations in the case study should be viewed critically because the values are compared in the units of ng l^{-1} or in the scale of 10^{-9}. However, it still demonstrates that the modelled values of SimpleTreat are fairly close to reality since they are in the same order of magnitude.

Finally, improvement of the results can be done by executing field measurements of various OCs which can be accessed for calibrating the model to the specific WWTP. To gain a deeper understanding of a specific chemical, another important parameter to measure is the partition coefficient K_p in the raw sludge and the different treatment units. To improve the model, a recommendation is to review the equations with for example HRT since some of the equations are replaced with fixed values and, moreover, perform a systematic comparison of the original SimpleTreat with the modified SimpleTreat.

5 Outlook

The intention of the outlook is to widen the current knowledge of OCs detected in influent wastewater by comparing their fates predicted for typical Swedish WWTP representatives with measurements of the IVL-database, i.e. what is expected to be found in Swedish sludge.

5.1 Comparison of Predictions and Data

In this chapter, OCs that have been measured in the incoming water of Swedish WWTPs from the IVL-database as well as predicting their expected concentration in the effluent and sludge are investigated by using the methodology in Figure 10.

STEP 1: Just as the case study, the chosen WWTPs were Käppala (old and new), Ryaverket and Sjölunda. As the fraction of organic carbon in raw wastewater is important in order to estimate the K_p and hence the chemical concentration in sludge, Ellinge has to measure this parameter in able to perform the simulations. The full set of plant configurations can be found in Appendix 3.

STEP 2: For the purpose of selecting chemicals found in the effluent of Swedish WWTPs, the IVL-database was applied. A total of 84 different OCs were selected (see Appendix 6) from year 2001 to 2012, which fulfilled the requirements of attaining at least a number of measurements:

- six influents
- three effluents
- three sludge

The concentrations that were below the detection level or measured 0 ng l^{-1} were excluded in the study. For the selected chemicals, the physico-chemical properties were obtained from the EPI Suite™ (see Table 3).

Chemicals that did not fulfil the requirements in *STEP* 2; they do not necessary pose a threat to the environment and human health. It is simply due to the fact that the measurements of those chemicals do not exist or are not sufficiently represented in the database.

STEP 3: As for selecting a WWTP model, the modified SimpleTreat from the case study was chosen. The modelling inputs are the four plant characteristics, the influent measurements and the physico-chemical data of the chosen chemicals. For every selected chemical, the minimum, average and maximum values of the influent was further simulated using the four plant characteristics with no regards to the location of where the chemicals were measured. The modified SimpleTreat generates estimated minimum, average and maximum concentrations of the effluent and sludge for the four plants.

STEP 4: Evaluation of the predicted minimum, average and maximum values in the effluent and sludge were determined by comparing if they were within the magnitude and range of the measured concentrations. Chemicals that fall within the range are evidently also within the order of magnitude. Substances that are considered within magnitude/range must have at least 6 of the predicted effluents and at least 6 of the predicted sludge out of 12, respectively (4 plant configurations multiplied with 3 of min-, mean- and max-values of a chemical). As a result, the number of values within the magnitude were 44 of which 15 were within the range (see Table 5).

The chemicals that were within range; their minimum and maximum measured concentrations and predicted concentrations in the effluent are shown in Table 6 and in the sludge in Table 7. All of the chemicals that have been simulated are found in Appendix 6.

Table 5. Number of chemicals (max. 84) that were within order of magnitude and/or range according to defined criteria. Substances that are considered within magnitude/range must have at least 6 predicted effluent concentrations and/or at least 6 predicted sludge concentrations out of 12 (4 plant configurations multiplied with 3 of min-, mean- and max-values).

Criteria for predicted conc. of a chemical when compared to measured conc.	Number of chemicals within magnitude (% of total)		Number of chemicals within range (% of total)	
≥6 effluents and ≥6 sludge	44	(52%)	15	(18%)
≥6 effluents	77	(92%)	51	(61%)
≥6 sludge	47	(56%)	25	(30%)

Table 6. The measured and predicted concentrations in the effluent for selected chemicals. The predicted concentrations that are marked in bold are within the range of the effluent measurements.

CAS	Chemical Application		Eff (meas) ng/l		Eff (pred) ng/l			
			Database (data points)		*Old Käppala*	*New Käppala*	*Rya-verket*	*Sjö-lunda*
80-05-07	**Bisphenol A**	min	5	(53)	2.04	2.95	**5.35**	4.43
	Plastics	max	3000		**1731**	**2504**	4550	3763
84-66-2	**Diethyl phthalate**	min	2	(33)	**76.9**	**86.7**	**150**	**135**
	Plasticizer	max	1500		**625**	**704**	**1215**	**1099**
117-81-7	**Di-(2-Ethylhexyl)-phthalate**	min	60	(36)	58.4	58.4	**177**	29.0
	Plasticizer	max	8300		**223**	**223**	**676**	**111**
114-07-8	**Erythromycin**	min	53	(12)	**63.7**	**93.7**	**123**	**112**
	Antibiotic	max	530		1029	1513	1990	1805
128-39-2	**2,6-Di-t-butyl-phenol**	min	0.450	(13)	0.0981	0.108	0.385	0.150
	UV stabilizer, antioxidant	max	3.80		**1.47**	**1.62**	5.77	**2.25**
140-66-9	**4-t-Octylphenol**	min	2.00	(62)	1.35	1.42	**5.27**	1.52
	Surface-active agent	max	290		**46.4**	**48.8**	**181**	**52.1**
738-70-5	**Trimethoprim**	min	50	(13)	**140**	**140**	**149**	**148**
	Antibacterial	max	510		1311	1308	1392	1380
84852-15-3	**4-nonylphenol, branched**	min	16	(61)	13.1	13.3	**47.0**	**29.7**
	Precursor to detergents	max	5500		11033	11261	39647	**129**
28159-98-0	**Irgarol 1051**	min	1.3	(13)	0.123	0.156	0.396	0.241
	Herbicide on boat coating	max	11		**2.88**	**3.65**	**9.24**	**5.63**
298-46-4	**Carbamazepine**	min	11	(35)	**41.7**	**49.0**	**68.3**	**64.1**
	Antiepileptic drug	max	1100		1526	1794	2500	2348
24219-97-4	**Mianserin**	min	4.1	(13)	1.01	1.22	3.41	1.90
	Antidepressant drug	max	61		11.1	13.4	37.6	21.0
59729-33-8	**Citalopram**	min	21	(44)	3.41	**45.2**	9.57	**50.5**
	Antidepressant drug	max	480		**284**	6867	798	7669
33704-61-9	**Cashmeran**	min	11	(12)	1.98	2.32	7.44	3.71
	Synthetic musk, drug impurity	max	310		**17.5**	**20.4**	**65.6**	**32.7**
1222-05-5	**Galaxolide**	min	40	(37)	2.12	2.16	7.35	1.47
	Synthetic musk	max	20000		**149**	**152**	**517**	**104**
21145-77-7	**Tonalide**	min	4.4	(37)	0.277	0.284	1.00	0.221
	Synthetic musk	max	1600		**15.9**	**16.4**	**57.7**	**12.7**

Table 7. The measured and predicted concentrations in the sludge for selected chemicals. The predicted concentrations that are marked in bold are within the range of the sludge measurements.

CAS	Chemical Application		Sludge (meas) ng/kg dw		Sludge (pred) ng/kg dw			
			Database (data points)		*Old Käppala*	*New Käppala*	*Ryaverket*	*Sjölunda*
80-05-07	**Bisphenol A**	min	5.00E-2	(53)	**2.06E3**	**5.26E3**	**3.51E3**	**1.25E3**
	Plastics	max	4.70E5		1.75E6	4.47E6	2.99E6	1.07E6
84-66-2	**Diethyl phthalate**	min	2.00E0	(5)	**2.27E4**	**2.87E4**	**1.29E4**	**5.26E3**
	Plasticizer	max	7.20E4		1.85E5	2.33E5	1.05E5	**4.28E4**
117-81-7	**Di-(2-Ethylhexyl)-phthalate**	min	5.70E6	(64)	9.58E5	3.79E6	**1.00E7**	1.57E6
	Plasticizer	max	1.00E12		3.66E6	**1.45E7**	**3.82E7**	**6.00E6**
114-07-8	**Erythromycin**	min	1.20E5	(4)	3.84E4	8.19E4	4.42E4	1.69E4
	Antibiotic	max	1.00E6		**6.20E5**	1.32E6	**7.13E5**	**2.73E5**
128-39-2	**2,6-Di-t-butyl-phenol**	min	2.00E3	(15)	7.38E2	**2.90E3**	**6.38E3**	1.15E3
	UV stabilizer, antioxidant	max	6.70E5		**1.11E4**	**4.35E4**	**9.57E4**	**1.73E4**
140-66-9	**4-t-Octylphenol**	min	3.90E4	(61)	1.37E4	**5.42E4**	**1.29E5**	2.20E4
	Surface-active agent	max	3.40E8		**4.73E5**	**1.86E6**	**4.44E6**	**7.57E5**
738-70-5	**Trimethoprim**	min	1.10E3	(5)	1.01E3	9.81E2	3.83E2	1.62E2
	Antibacterial	max	2.70E4		**9.44E3**	**9.15E3**	**3.58E3**	**1.51E3**
84852-15-3	**4-nonylphenol, branched**	min	6.90E-1	(61)	**1.79E5**	**7.06E5**	**1.79E6**	**7.60E0**
	Precursor to detergents	max	9.2E6		1.51E8	5.96E8	**1.51E9**	**3.29E1**
28159-98-0	**Irgarol 1051**	min	1.00E3	(18)	2.75E2	**1.01E3**	**1.33E3**	3.35E2
	Herbicide on boat coating	max	5.40E4		**6.42E3**	**2.35E4**	**3.11E4**	**7.81E3**
298-46-4	**Carbamazepine**	min	8.70E-2	(20)	**1.06E4**	**1.40E4**	**6.16E3**	**2.53E3**
	Antiepileptic drug	max	2.00E5		3.90E5	5.12E5	2.26E5	**9.25E4**
24219-97-4	**Mianserin**	min	1.10E4	(5)	2.83E3	1.06E4	**1.62E4**	3.73E3
	Antidepressant drug	max	9.40E4		**3.11E4**	1.17E5	1.79E5	**4.11E4**
59729-33-8	**Citalopram**	min	2.30E-2	(40)	**4.98E3**	**4.15E0**	**1.58E4**	**6.89E-1**
	Antidepressant drug	max	7.60E5		**4.15E5**	**6.30E2**	1.32E6	**1.05E2**
33704-61-9	**Cashmeran**	min	3.90E3	(23)	**8.46E3**	**3.26E4**	**5.96E4**	**1.22E4**
	Synthetic musk, drug impurity	max	2.50E6		**7.47E4**	**2.88E5**	**5.26E5**	**1.08E5**
1222-05-5	**Galaxolide**	min	8.70E3	(26)	**3.02E4**	**1.20E5**	**3.06E5**	**4.93E4**
	Synthetic musk	max	2.90E7		**2.13E6**	**8.42E6**	**2.15E7**	**3.47E6**
21145-77-7	**Tonalide**	min	8.80E4	(25)	3.68E3	1.46E4	3.66E4	5.99E3
	Synthetic musk	max	2.60E6		**2.12E5**	**8.38E5**	**2.11E6**	**3.45E5**

5.2 Discussion

The results of the modelling and simulation exercise are expected to provide typical concentration magnitudes/ranges of chemicals in Swedish sludge, where Käppala (old and new), Ryaverket and Sjölunda represent WWTPs from different parts of Sweden. More than 50% of the chemicals were within the magnitude/range of the measured concentrations, which implies that the modified SimpleTreat can be used as an estimation tool to predict the fate of these chemicals with default values. For other simulated chemicals that did not fall within the range in Appendix 6, the modified SimpleTreat is less applicable for simulating the fate of those chemicals in the effluent and sludge. This can be due to various reasons such as uncertainty regarding the

model structure, the model parameters and the measurements as already mentioned in the previous discussion (section 4.3).

Firstly, the structure of the modified SimpleTeat does not capture all the processes in a WWTP and thus the fate of a chemical. Secondly, the EPI Suite™ provides both experimental and estimated values of physico-chemical properties, where experimental results are preferred over estimated values. Similar to the results from the case study, chemicals that simulated good results consisted of both experimental and estimated physico-chemical properties; a further parameter analysis of the difference between experimental and estimated values should be carried out for verification. In terms of the outlook, thirdly, the data do not need to be plant specific or have exact values of the influent, effluent and sludge, since the main purpose is to distinguish between potentially harmful and harmless emerging chemicals that there is little knowledge of. Therefore, the data quality is not as important here as for calibrating the model. The results of the outlook should be primarily used as a first indicator of what chemicals in the sludge should be prioritised.

Finally, presuming that the model structure and the model parameters are reliable, the following statements can be made. In general, the modified SimpleTreat was better at predicting the concentration in the effluent than in the sludge, which was also the reason why many of the chemicals were not considered to fall within the magnitude/range. It could be due to the fact that the measured concentrations in sludge were not realistic in comparison to the influent measurements, or that the predicted magnitude/range covered the measured magnitude/range but was not accounted with the comparison method used. In addition, substances that have a negative logarithmic K_{OW} were predicted, as expected, poorly in sludge since the original SimpleTreat is mostly suited for predicting hydrophobic compounds. For such a simple fugacity model, the modified SimpleTreat still generated more than 90% accuracy in predicting the order of magnitudes of a chemical's fate in the effluent and 56% in the sludge; the modified SimpleTreat is better at predicting the effluent concentration than the sludge concentration of a chemical.

6 Conclusions

The summary and conclusions of the study are:

- The thesis presents a practical methodology to predict the distribution of OCs to sludge in a WWTP (section 4.1), which comprises of a plant description, chemical data collection, calibration, validation and continuation step to investigate the effect of soil processes.
- The modified SimpleTreat can be used to predict the fate of organic pollutants regard to a number of factors: 1) model structure, 2) model parameters and 3) data quality. Firstly, the structure of the modified SimpleTreat is limited to the primary settler, activated sludge system (anaerobic, anoxic and aerobic zones) and secondary clarifier. Secondly, the physico-chemical parameters are preferably experimental values although estimated values from EPI Suite™ are satisfactory. Thirdly, the influent, effluent and sludge data has to be measured at the correct location within a time frame that corresponds to the retention time of the chemical using the same sampling and analysis method.
- For a specific compound, it is suggested to measure the specific partition coefficient K_p in raw sewage, primary settler, aeration tank and secondary clarifier to gain a more precise prediction of the partitioning in the specified WWTP.
- A total of 84 chemicals were modelled in the modified SimpleTreat. The results for the selected WWTPs represent fairly well the overall pollution removal rates via the effluent and sludge when compared with the concentrations ranges of the IVL-database. Predictions of the concentrations' order of magnitude in Swedish effluent using the modified SimpleTreat proved to have a higher accuracy than in Swedish sludge.
- The information that can be acquired from the methodology supposing that further toxicity analysis of the chemical is performed is which potential substances that do not pose a threat to the environment and human health despite being recycled with sludge. However, additional analysis of the chemicals must be carried out to evaluate the overall risk of sludge when applied as soil amendment.

For future work:

- As a continuation of the thesis, the fate of the outlook chemicals in soil has to be investigated individually and subsequently evaluated for its potential risk to conclude whether the chemical is harmful or not to the environment and human health when the sludge is spread on agricultural land.
- Validate and calibrate the modified SimpleTreat by performing field measurements of different chemicals in the influent, effluent and sludge at specific WWTPs.
- Conduct sensitivity and uncertainty analysis of the modified SimpleTreat.

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Appendix 1: Modification of SimpleTreat

The "input" is from the "input" sheet in SimpleTreat and "9-box" is from the "9-box" sheet. The types of modification that was executed in the SimpleTreat can be divided into two types: the equation is altered (cell is marked with turquoise blue) or a new parameter (cell is marked with purple) is added in the sheet.

Fill in	*Equation changed*	*New parameter*
Input		
parameter	*unit*	*defaults and equations*
Characterisation of the chemical		
Name compound =		
Physico-chemical properties		
environment		
Molecular weight =	g mol^{-1}	1E02
K_{ow} =	(-)	1E03
Vapour pressure (env) =	Pa	2E00
Solubility (env) =	mg L^{-1}	5E02
K_a =	(-)	1E-20
K_b =	(-)	1E-20
Henry's constant =	Pa m^3 mol^{-1}	6E-01
K_p (raw sewage) =	L kg_{dwt}^{-1}	3E02
K_p (activated sludge) =	L kg_{dwt}^{-1}	2E02
Chemical class for K_{oc}-QSAR =	-	Non hydrophobics
K_{oc} =	L kg-1	6E02
Enthalpy of vaporisation =	kJ mol^{-1}	5E01
Enthalpy of dissolution =	kJ mol^{-1}	1E01
T (env) =	^oC	1E01
data set		
Vapour pressure at T vap =	Pa	
T vap =	^oC	3E01
Solubility at T sol =	mg L^{-1}	1E02
T sol =	^oC	1E-20
Emission scenario		
T air =	^oC	15
T water =	^oC	15
Windspeed =	m s^{-1}	3
Sewage flow =	L $PE^{-1}d^{-1}$	200
Number inhabitants =	PE	1E04
Sludge loading rate (table 1) =	kg_{BOD} kg_{dwt}^{-1} d^{-1}	0,15
Bubble or surface aeration: b/s	(-)	s

Emission rate chemical =		kg d^{-1}	1
Biodegradation in activated sludge			
k biodeg1 =		hr^{-1}	

9-box			
System characteristics			
general			
Height air column =		m	
Area of the plant =		m^2 PE^{-1}	
raw sewage			
Input solids in raw sewage =		kg_{dwt} PE^{-1} d^{-1}	0.09
Density solids raw sewage =		kg_{dwt} L^{-1}	1.5
C susp solids raw sewage =		kg_{dwt} m^{-3}	calc.
Fraction oc raw sewage =		(-)	0.3
BOD in raw sewage =		g BOD PE^{-1} d^{-1}	54
primary sedimentation			
Depth PS =		m	4
HRT PS =		h	2
Volume PS =		m^3 PE^{-1}	=Sewage_flow*HRTPS/24
Area PS =		m^2 PE^{-1}	=Volume_PS/Depth_PS
C susp solids PS =		kg_{dwt} m^{-3}	calc.
Fraction oc solids PS =		(-)	0.3
Density solids PS =		kg_{dwt} L^{-1}	1.5
activated sludge tank			
anaerobic tank			
Depth anaerobic =		m	-
HRT anaerobic =		h	=Volume_anaerobic/Sewage_flow*24
Volume anaerobic =		m^3 PE^{-1}	-
Area anaerobic =		m^2 PE^{-1}	-
anoxic tank			
Depth anoxic =		m	6
HRT anoxic =		h	=Volume_anoxic/Sewage_flow*24
Volume anoxic =		m^3 PE^{-1}	-
Area anoxic =		m^2 PE^{-1}	-
aerator			
Depth aerator =		m	3
HRT aerator =		h	=Volume_aerator/Sewage_flow*24

Volume aerator =		$m^3\ PE^{-1}$	=Sewage_flow*Oxygen_requirement/ (Sludge_loading_rate*C_activated_sludge)
Area aerator =		$m^2\ PE^{-1}$	=Volume_aerator/Depth_aerator
Oxygen requirement =		$kg\ BOD\ m^{-3}$	calc.
Oxygen concentration =		$kg\ O_2\ m^{-3}$	0.002
Aeration rate (1.31E-05) =		$m^3\ s^{-1}\ PE^{-1}$	0.0000131
C aerator =		$kg_{dwt}\ m^{-3}$	4
Fraction oc aerator =		(-)	0.37
Density solids aerator =		$kg_{dwt}\ L^{-1}$	1.3
total tanks			
HRT activated sludge =		h	calc. HRT
Volume activated sludge =		$m^3\ PE^{-1}$	calc. Volume
Area activated sludge =		$m^2\ PE^{-1}$	calc. Area
solids liquid separation			
Depth SLS =		m	3
HRT SLS =		h	6
Volume SLS =		$m^3\ PE^{-1}$	0.057825
Area SLS =		$m^2\ PE^{-1}$	=Volume_SLS/Depth_SLS
C susp solids SLS =		$kg_{dwt}\ m^{-3}$	0.03
Fraction oc solids SLS =		(-)	0.37
Density solids SLS =		$kg_{dwt}\ L^{-1}$	1.3
sludge loading characteristics			
F BOD removal =		(-)	calc.
Y BOD =		$kg_{dwt}kg_{BOD}^{-1}$	calc.
Surplus sludge =		$kg_{dwt}PE^{-1}\ d^{-1}$	calc.
Emitted solids in effluent =		$kg_{dwt}PE^{-1}\ d^{-1}$	calc.
SRT =		d	=Volume*C_activated_sludge/ (Surplus_sludgeC_susp_solids_SLS*Sewage_flow)
Sludge loading rate =		$kg_{BOD}\ kg_{dwt}^{-1}\ d^{-1}$	input

Appendix 2: Chemical Parameters

A new sheet named "chemical" was developed to simplify simulation of numerous chemicals simultaneously. The table below summarises the input and output of the modified SimpleTreat including their explanations and applications. The chemical parameters that are marked with italics are less important to include in the modelling than those not marked.

Parameter	*Unit*	*Explanation*	*Application*
Input			
properties			
CAS		CAS-number of chemical	
Chemical		Name of chemical	
MW	g mol^{-1}	Molar weight	
WS	mg l^{-1}	Water solubility	
Tws	°C	Temperature of water solubility	
VP	Pa	Vapour pressure	
Tvp	°C	Temperature of vapour pressure	
kDeg	day	First order degradation rate (half-life)	
Koc	l kg^{-1}	Organic carbon partition coefficient	
LogKow	-	Logarithmical octanol-water partitiion coefficient	
measured concentrations			
Influent	ng l^{-1}	Chemical concentration in influent	
Effluent	ng l^{-1}	Chemical concentration in effluent	
MeanSludge	ng kg^{-1} dw	Average of primary and secondary sludge concentration in dry weight	If MeanSludge not specified, not necessary for simulatation
PrimSludge	ng kg^{-1} dw	Chemical concentration in primary sludge	If PrimSludge and SecSludge not specified, use MeanSludge
SecSludge	ng kg^{-1} dw	Chemical concentration in secondary sludge	If PrimSludge and SecSludge not specified, use MeanSludge
Inrate	kg day^{-1}	Chemical inflow	Calculates automatically
Date	yy-mm-dd	Date of when the concentration was measured	Not necessary
measured distribution			
to water	%	Distribution of chemical to effluent	Calculates automatically
to sludge	%	Distribution of chemical to sludge	Calculates automatically
Output			
predicted concentrations			
Air	g m^{-3}	Chemical concentration in air	
Effluent	µg l^{-1}	Chemical concentration in effluent	
MeanSludge	ng kg^{-1} dw	Average of primary and secondary sludge concentration in dry weight	
PrimSludge	ng kg^{-1} dw	Chemical concentration in primary sludge	
SecSludge	ng kg^{-1} dw	Chemical concentration in secondary sludge	
predicted distribution			
to air	%	Distribution of chemical to air	
to water	%	Distribution of chemical to effluent	
to sludge	%	Distribution of chemical to average sludge	
prim sludge	%	Distribution of chemical to primary sludge	
sec sludge	%	Distribution of chemical to secondary sludge	
degraded	%	Distribution of chemical that are degraded	
total	%	The total distribution	

Appendix 3: WWTP Parameters

The "input" is from the "input" sheet in the modified SimpleTreat and "9-box" is from the "9-box" sheet. In the following table, a summary of all the plant configurations is presented here. The cells that are marked in orange are those parameters that were provided from Ellinge, Käppala (old and new), Ryaverket and Sjölunda, respectively, and those parameters also are a prerequisite for performing the simulation. Cells that are marked with turquoise blue have had their equation changed whereas cells that are coloured with purple are the additional new parameters.

Fill in	*Equation changed*	*New parameter*					
input							
Emission scenario							
	Ellinge	*Old Käppala*	*New Käppala*	*Rya-verket*	*Sjö-lunda*		*default*
T air =	15	8.3	8.3	10	15	^{o}C	15
T water =	15	13.6	13.6	12	15	^{o}C	15
Windspeed =	3	3	3	4	3	$m\ s^{-1}$	3
Sewage flow =	358	270	270	514	424	$L\ PE^{-1}d^{-1}$	200
Number inhabitants =	2.82E4	4.80E5	4.80E5	6.66E5	2.94E5	PE	1E04
Sludge loading rate (table 1) =	0.13	0.05	0.05	0.79	0.35	$kg_{BOD}\ kg_{dwt}^{-1}\ d^{-1}$	0.15
Bubble or surface aeration: b/s	b	b	b	b	b	(-)	s
Emission rate chemical =						$kg\ d^{-1}$	1
9-box							
System Characteristics							
general	*Ellinge*	*Old Käppala*	*New Käppala*	*Rya-verket*	*Sjö-lunda*		*default*
Height air column =	10	6	7.5	10	10	m	
Area of the plant =	0.251	0.103	0.0732	0.0553	0.0408	$m^2\ PE^{-1}$	
raw sewage							
Input solids in raw sewage =	No data	0.659	0.14	0.09	0.099	$kg_{dwt}\ PE^{-1}\ d^{-1}$	0.09
Density solids raw sewage =	4	1.5	1.5	1.5	0.236	$kg_{dwt}\ L^{-1}$	1.5
C susp solids raw sewage =	-	2.44	0.519	0.175	0.233	$kg_{dwt}\ m^{-3}$	calc.
Fraction oc raw sewage =	No data	0.85	0.85	0.3	0.5	(-)	0.3
BOD in raw sewage =	101	60	60	54	70	$g_{BOD}\ PE^{-1}\ d^{-1}$	54
primary sedimentation							
Depth PS =	2.5	2.6	3.6	4	1.41	m	4
HRT PS =	1.5	2.8	2.7	1.58	1.5	h	2
Volume PS =	0.192	0.0519	0.0504	0.0340	0.0269	$m^3\ PE^{-1}$	0.0315
Area PS =	0.0767	0.0200	0.0140	0.0085	0.0191	$m^2\ PE^{-1}$	0.00788
C susp solids PS =	-	0.814	0.173	0.0584	0.0778	$kg_{dwt}\ m^{-3}$	calc.
Fraction oc solids PS =	0.65	0.85	0.85	0.3	0.775	(-)	0.3
Density solids PS =	1.5	1.5	1.5	1.5	1.5	$kg_{dwt}\ L^{-1}$	1.5
activated sludge tank							

anaerobic tank							
Depth anaerobic =	0	6	0	0	0	m	
HRT anaerobic =	0	2.1	0	0	0	h	2.03
Volume anaerobic =	0	0.0228	0	0	0	$m^3 PE^{-1}$	
Area anaerobic =	0	0.00380	0	0	0	$m^2 PE^{-1}$	
anoxic tank							
Depth anoxic =	4.45	6	10	10	4	m	6
HRT anoxic =	5.31	13.4	17	0.9	0.945	h	13.0
Volume anoxic =	0.0792	0.146	0.179	0.0459	0.0167	$m^3 PE^{-1}$	
Area anoxic =	0.0178	0.0244	0.0179	0.00459	0.00417	$m^2 PE^{-1}$	
aerator							
Depth aerator =	4.45	6	10	10	4	m	3
HRT aerator =	6	13.0	15	0.7	2.89	h	13
Volume aerator =	0.0838	0.146	0.179	0.0308	0.0511	$m^3 PE^{-1}$	0.341
Area aerator =	0.0188	0.0244	0.0179	0.00308	0.0128	$m^2 PE^{-1}$	0.114
Oxygen requirement =	0.180	0.142	0.142	0.0671	0.105	$kg_{BOD} m^{-3}$	calc.
Oxygen concentration =	0.002	0.002	0.002	0.0023	0.002	$kg O_2 m^{-3}$	0.002
Aeration rate (1.31E-05) =	1.30E-5	1.81E-5	9.90E-6	4.26E-6	1.23E-5	$m^3 s^{-1} PE^{-1}$	1.31E-5
C aerator =	5.9	2.25	2	2.56	2.25	$kg_{dwt} m^{-3}$	4
Fraction oc aerator =	0.75	0.75	0.68	0.37	0.37	(-)	0.37
Density solids aerator =	1.3	1.3	1.3	1.3	1.3	$kg_{dwt} L^{-1}$	1.3
total tanks							
HRT activated sludge =	11.3	28.5	32	3.03	3.84	h	
Volume activated sludge =	0.163	0.315	0.358	0.107	0.0678	$m^3 PE^{-1}$	
Area activated sludge =	0.0366	0.0525	0.0358	0.0107	0.0170	$m^2 PE^{-1}$	
solids liquid separation							
Depth SLS =	3.5	4	6.1	3	3.5	m	3
HRT SLS =	8	6.5	7.6	2.7	5	h	6
Volume SLS =	0.483	0.123	0.143	0.108	0.0167	$m^3 PE^{-1}$	0.0578
Area SLS =	0.138	0.0307	0.0234	0.0361	0.00477	$m^2 PE^{-1}$	0.0193
C susp solids SLS =	0.015	0.01	0.01	0.016	0.004	$kg_{dwt} m^{-3}$	0.03
Fraction oc solids SLS =	0.65	0.75	0.68	0.146	1	(-)	0.37
Density solids SLS =	1.3	1.3	1.3	1.3	1.3	$kg_{dwt} L^{-1}$	1.3
sludge loading characteristics							
F BOD removal =	0.904	0.944	0.944	0.828	0.862	(-)	calc.
Y BOD =	0.796	0.726	0.726	0.930	0.869	$kg_{dwt}kg_{BOD}^{-1}$	calc.
Surplus sludge =	0.0411	0.0236	0.0236	0.0183	0.032	$kg_{dwt}PE^{-1} d^{-1}$	calc.
Emitted solids in effluent =	0.005	0.00270	0.00270	0.00822	0.00170	$kg_{dwt}PE^{-1} d^{-1}$	calc.
SRT =	20.7	27.0	27.3	10.3	4.55	d	27.0
Sludge loading rate =	0.13	0.05	0.05	0.79	0.35	$kg_{BOD}kg_{dwt}^{-1} d^{-1}$	Input

Appendix 4: Macro Codes

Below are the macro codes that were connected between the sheets of "chemical" and the two sheets "input" and "output". The first command button in "chemical" is named *simulate* in which the input parameters of "chemical" is automatically redirected to "input" and the results from the "output" is copied back to the output parameters in "chemical". This is done one row at a time. The second command button in "chemical" is named *delete* where all the filled-in cells are erased when pressed. The code starts erasing from the left cell to the right. The termination of the information in the cells is stopped whenever a cell is empty.

```
Private Sub CommandButton1_Click()
    Dim row As Integer
    Dim col As Integer
    row = 5

    Do Until IsEmpty(Cells(row, 11))
    '"Input
    "Properties
      'MW (g/mol)
      Sheets("input").Range("B8").Value = Sheets("chemical").Cells(row, 3).Value
      'WS (mg/l)
      Sheets("input").Range("B25").Value = Sheets("chemical").Cells(row, 4).Value
      'Tws (degC)
      Sheets("input").Range("B26").Value = Sheets("chemical").Cells(row, 5).Value
      'VP (Pa)
      Sheets("input").Range("B23").Value = Sheets("chemical").Cells(row, 6).Value
      'Tvp (degC)
      Sheets("input").Range("B24").Value = Sheets("chemical").Cells(row, 7).Value
      'kDeg (day)
      Sheets("input").Range("B62").Value = Log(2) / (Sheets("chemical").Cells(row, 8).Value)
      'Koc (l/kg)
      Sheets("input").Range("B18").Value = Sheets("chemical").Cells(row, 9).Value
      'logKow
      Sheets("input").Range("B9").Value = 10 ^ (Sheets("chemical").Cells(row, 10).Value)
    "Measured concentrations
      'Inrate (kg/day) Inrate=Influent*Sewageflow*Inhabitants*1e-3
      Sheets("chemical").Cells(row, 16).Value = 10 ^ -6 * (Sheets("chemical").Cells(row, 11).Value *
    Sheets("input").Range("G32").Value * Sheets("input").Range("G33").Value * 0.001)
      Sheets("input").Range("B36").Value = Sheets("chemical").Cells(row, 16).Value
    "Measured distribution
      'Measured dist to water (%) Effluent/Influent
      Sheets("chemical").Cells(row, 18).Value = 100 * Sheets("chemical").Cells(row, 12).Value /
    Sheets("chemical").Cells(row, 11).Value
      'Measured dist to sludge (%) (Prim*DenPS  Sec*DenSLS)/(2*Influent) or
    (MeanSludge/((DenPSDenSLS)/(2*Influent)
      If Sheets("chemical").Cells(row, 13).Value <> 0 Then
        Sheets("chemical").Cells(row, 19).Value = 100 * (Sheets("chemical").Cells(row, 13).Value *
    ((Sheets("9-box").Range("C27").Value  Sheets("9-box").Range("C65").Value) / 2)) /
    Sheets("chemical").Cells(row, 11).Value
      ElseIf Sheets("chemical").Cells(row, 14).Value <> 0 And Sheets("chemical").Cells(row,
    15).Value <> 0 Then
        Sheets("chemical").Cells(row, 19).Value = 100 * (Sheets("chemical").Cells(row, 14).Value *
    Sheets("9-box").Range("C27").Value  Sheets("chemical").Cells(row, 15) * Sheets("9-
    box").Range("C65")) / (2 * Sheets("9-box").Cells(row, 11))
      Else
```

```
            Sheets("chemical").Cells(row, 19).Value = 0
        End If

    '"Output
    "Predicted concentrations
        'Air (g/m3)
        Sheets("chemical").Cells(row, 20).Value = Sheets("output").Range("C34").Value
        'Effluent(ng/l)
        Sheets("chemical").Cells(row, 21).Value = 10 ^ 6 * Sheets("output").Range("C38").Value
        'MeanSludge (ng/kg dw)
        Sheets("chemical").Cells(row, 22).Value = 10 ^ 6 * Sheets("output").Range("C35").Value
        'PrimSludge (ng/kg dw)
        Sheets("chemical").Cells(row, 23).Value = 10 ^ 6 * Sheets("output").Range("D36").Value
        'SecSludge (ng/kg dw)
        Sheets("chemical").Cells(row, 24).Value = 10 ^ 6 * Sheets("output").Range("D37").Value
        'SolidsEff (mg/kg dw)
        Sheets("chemical").Cells(row, 25).Value = Sheets("output").Range("C41").Value
    "Predicted distribution
        'to air (%)
        Sheets("chemical").Cells(row, 26).Value = Sheets("output").Range("C26").Value
        'to water (%)
        Sheets("chemical").Cells(row, 27).Value = Sheets("output").Range("C27").Value
        'to sludge (%)
        Sheets("chemical").Cells(row, 28).Value = Sheets("output").Range("C28").Value
    Sheets("output").Range("C29").Value
        'via primary sludge (%)
        Sheets("chemical").Cells(row, 29).Value = Sheets("output").Range("C28").Value
        'via secondary sludge (%)
        Sheets("chemical").Cells(row, 30).Value = Sheets("output").Range("C29").Value
        'degraded (%)
        Sheets("chemical").Cells(row, 31).Value = Sheets("output").Range("C30").Value
        'total (%)
        Sheets("chemical").Cells(row, 32).Value = Sheets("output").Range("C31").Value
    row = row  1
    Loop
End Sub
```

Private Sub CommandButton2_Click()

```
    Dim r As Integer
    Dim HeaderRow As Long
    Dim rngRange As Range
    HeaderRow = 5
    msg = MsgBox("Do you want to delete all contents?", vbYesNo, "OBS!")

    If msg = vbYes Then
        With Sheets("chemical")
          Set rngRange = .Range _
            (.Cells(HeaderRow, 1), .Cells(.Rows.Count, 1)).EntireRow
        End With
        rngRange.Delete
    End If
End Sub
```

Appendix 5: Results of Case Study

The total results of the case study are presented here. The substances that were measured at Käppala were simulated for the old and new plant configurations. The table on below can be used to compare the measured and predicted concentration in the effluent. In the IVL-database, the sludge concentrations were not measured at the same date as the effluent, which has therefore been excluded in the table. The numbers with asterisk are estimated values of EPI Suite™.

WWTP	Chemical	MW	WS at 25°C	VP at 25°C	k Deg	Koc	Log Kow	In (meas)	Eff (meas)	Eff (pred)
		g/mol	mg/l	Pa	day	l/kg	-	ng/l	ng/l	ng/l
Old Käppala	Citalopram	324	31.1*	1.51E-5*	377*	6856*	3.74*	80	**67**	**22.7**
Old Käppala	Citalopram	324	31.1*	1.51E-5*	377*	6856*	3.74*	77	**58**	**21.9**
Old Käppala	Citalopram	324	31.1*	1.51E-5*	377*	6856*	3.74*	71	**59**	**20.2**
Old Käppala	Oxazepam	287	179*	5.55E-10*	34.6*	176*	2.24	250	**220**	**175**
Old Käppala	Oxazepam	287	179*	5.55E-10*	34.6*	176*	2.24	210	**200**	**147**
Old Käppala	Oxazepam	287	179*	5.55E-10*	34.6*	176*	2.24	390	**290**	**273**
Old Käppala	2.6-Diiso-propyl-phenol (propofol)	178	124*	1.07*	19.9*	2625*	3.79	21	**19**	**4.75**
New Käppala	Citalopram	324	31.1*	1.51E-5*	377*	6856*	3.74*	80	**67**	**31.7**
New Käppala	Citalopram	324	31.1*	1.51E-5*	377*	6856*	3.74*	77	**58**	**30.5**
New Käppala	Citalopram	324	31.1*	1.51E-5*	377*	6856*	3.74*	71	**59**	**28.1**
New Käppala	Oxazepam	287	179*	5.55E-10*	34.6*	176*	2.24	250	**220**	**196**
New Käppala	Oxazepam	287	179*	5.55E-10*	34.6*	176*	2.24	210	**200**	**165**
New Käppala	Oxazepam	287	179*	5.55E-10*	34.6*	176*	2.24	390	**290**	**306**
New Käppala	2.6-Diiso-propyl-phenol (propofol)	178	124*	1.07*	19.9*	2625*	3.79	21	**19**	**6.29**
Ryaverket	Benzene	78.1	1790	12639	38.8*	56.2	2.13	35	**7.3**	**26.6**
Ryaverket	Ethyl tert-butyl ether (ETBE)	102	12000	16532	18.0*	40.7	1.92*	31	**26**	**25.1**
Ryaverket	Toluene	92.1	526	3786	11.3*	117	2.73	1500	**280**	**1061**

Appendix 6: Results of Outlook

The results from the outlook are presented here, where the first table shows the results of predicted effluent concentrations and the second table the results of predicted sludge concentrations. CAS-numbers that are marked bolded are the predicted concentration of chemicals that fell within the measured magnitude and thus range.

CAS Bolded = within magnitude and range	**Chemical**	**MW** g mol^{-1}	**WS at 25 °C** mg l^{-1}	**VP at 25 °C** Pa	**kDeg** day	**Koc** l kg^{-1}	**Log Kow**		**In (meas)** ng l^{-1}	**Eff (meas)** ng l^{-1}	**Eff (pred)** ng l^{-1}			
									Database	*Database*	*Old Käppala*	*New Käppala*	*Rya-verket*	*Sjö-lunda*
000050-48-6	Amitryptiline	277	9.71	4.83E-5	73.4	27800	4.92	min	5.20E0	6.10E0	3.98E-1	4.33E-1	1.55E0	5.82E-1
								mean	1.90E1	1.74E1	1.45E0	1.58E0	5.66E0	2.12E0
								max	4.70E1	2.80E1	3.60E0	3.91E0	1.40E1	5.26E0
000052-86-8	Haloperidol	376	14	2.00E-8	701	3283	4.30	min	6.90E0	8.80E-1	1.12E0	1.35E0	3.80E0	2.07E0
								mean	2.15E1	1.01E1	3.49E0	4.20E0	1.18E1	6.43E0
								max	6.90E1	3.90E1	1.12E1	1.35E1	3.80E1	2.07E1
000057-83-0	Progesterone	314	8.81	3.59E-4	105	5370	3.87	min	4.00E0	1.00E0	9.88E-1	1.32E0	2.98E0	2.01E0
								mean	1.36E1	2.03E1	3.35E0	4.47E0	1.01E1	6.81E0
								max	3.00E1	1.10E2	7.41E0	9.90E0	2.24E1	1.51E1
000058-08-2	Caffeine	194	21600	9.77E-7	17.2	9.77	-0.07	min	1.50E1	9.20E1	1.12E1	1.06E1	1.45E1	1.39E1
								mean	6.80E4	1.48E4	5.08E4	4.82E4	6.58E4	6.28E4
								max	1.50E5	1.50E5	1.12E5	1.06E5	1.45E5	1.39E5
000058-73-1	Diphenhydramine	255	3060	7.73E-4	41.3	1780	3.27	min	6.50E0	7.40E0	2.43E0	3.56E0	5.90E0	5.00E0
								mean	4.27E1	2.33E1	1.60E1	2.34E1	3.87E1	3.28E1
								max	2.00E2	5.40E1	7.47E1	1.09E2	1.81E2	1.54E2
000060-87-7	Promethazine	284	15.6	1.37E-3	98.8	3969	4.81	min	1.20E1	1.10E1	1.04E0	1.15E0	4.00E0	1.62E0
								mean	6.60E1	4.06E1	5.73E0	6.32E0	2.20E1	8.91E0
								max	1.90E2	8.60E1	1.65E1	1.82E1	6.34E1	2.57E1
000064-75-5	Tetracycline	483	248900	4.12E-25	119	1.49	-3.70	min	1.00E0	8.00E-1	9.54E-1	9.44E-1	9.95E-1	9.88E-1
								mean	8.46E2	2.47E2	8.07E2	7.99E2	8.42E2	8.36E2
								max	4.50E3	1.40E3	4.29E3	4.25E3	4.48E3	4.45E3
000068-22-4	Norethindrone	298	7.04	3.15E-7	91.3	966	2.97	min	2.00E0	1.00E0	9.97E-1	1.42E0	1.90E0	1.74E0
								mean	1.21E1	7.47E0	6.02E0	8.59E0	1.15E1	1.05E1
								max	2.00E1	3.00E1	9.97E0	1.42E1	1.90E1	1.74E1
000068-88-2	Hydroxyzine	375	428	1.56E-9	175	496	2.36	min	5.90E0	1.60E0	4.42E0	5.26E0	5.82E0	5.67E0

								mean	2.02E1	1.12E1	1.52E1	1.80E1	1.99E1	1.94E1
								max	6.10E1	5.10E1	4.57E1	5.43E1	6.01E1	5.86E1
000076-57-3	Codeine	299	33900	2.55E-8	104	108	1.19	min	3.90E2	7.80E1	3.61E2	3.63E2	3.88E2	3.84E2
								mean	1.32E3	3.58E2	1.22E3	1.23E3	1.31E3	1.30E3
								max	4.20E3	7.80E2	3.89E3	3.91E3	4.17E3	4.13E3
000079-57-2	Oxytetracycline	460	313	1.21E-20	133	9.56	-0.90	min	6.00E-1	1.50E1	5.75E-1	5.70E-1	5.97E-1	5.94E-1
								mean	3.22E2	1.03E2	3.08E2	3.06E2	3.21E2	3.18E2
								max	7.90E2	2.60E2	7.57E2	7.50E2	7.87E2	7.82E2
000080-05-7	Bisphenol A	228	120	3.03E-5	26.5	6849	3.32	min	6.00E0	5.00E0	2.04E0	2.95E0	5.35E0	4.43E0
								mean	1.17E3	4.36E2	3.98E2	5.75E2	1.05E3	8.65E2
								max	5.10E3	3.00E3	1.73E3	2.50E3	4.55E3	3.76E3
000083-98-7	Orphenadrine	269	113	1.23E-2	56.5	3131	3.77	min	9.90E0	4.60E0	2.59E0	3.52E0	7.73E0	5.44E0
								mean	4.34E1	2.15E1	1.13E1	1.54E1	3.39E1	2.38E1
								max	1.80E2	8.10E1	4.70E1	6.41E1	1.41E2	9.88E1
000084-66-2	Diethyl phthalate	222	1080	2.80E-1	10.1	69.2	2.42	min	1.60E2	2.00E0	7.69E1	8.67E1	1.50E2	1.35E2
								mean	5.84E2	9.67E1	2.81E2	3.16E2	5.46E2	4.94E2
								max	1.30E3	1.50E3	6.25E2	7.04E2	1.22E3	1.10E3
000085-68-7	Butyl benzyl phthalate	312	2.69	1.10E-3	7.46	5248	4.73	min	1.00E2	1.50E1	8.35E0	8.94E0	3.51E1	1.44E1
								mean	2.87E2	5.20E1	2.40E1	2.57E1	1.01E2	4.13E1
								max	1.20E3	1.50E2	1.00E2	1.07E2	4.22E2	1.73E2
000088-18-6	2-t-Butyl-phenol	150	700	1.20E1	19.9	1048	3.31	min	3.00E0	7.50E-1	9.45E-1	1.36E0	2.63E0	2.17E0
								mean	1.57E1	2.88E0	4.95E0	7.13E0	1.38E1	1.13E1
								max	3.00E1	4.60E0	9.45E0	1.36E1	2.63E1	2.17E1
000096-76-4	2.4-Di-t-butyl-phenol	206	35.0	6.36E-1	45.5	9093	5.19	min	3.50E1	7.40E0	2.03E0	2.15E0	7.98E0	2.46E0
								mean	3.25E2	4.11E1	1.88E1	2.00E1	7.41E1	2.28E1
								max	2.20E3	1.70E2	1.28E2	1.35E2	5.02E2	1.55E2
000098-54-4	4-t-Butyl-phenol	150	580	5.08E0	19.9	1038	3.31	min	2.80E1	3.20E0	8.95E0	1.29E1	2.47E1	2.03E1
								mean	2.22E2	3.05E1	7.10E1	1.02E2	1.96E2	1.61E2
								max	1.90E3	7.50E1	6.07E2	8.73E2	1.68E3	1.38E3
000103-90-2	Paracetamol	151	14000	2.59E-4	13.6	30.73	0.46	min	3.60E4	1.10E1	2.51E4	2.36E4	3.45E4	3.26E4
								mean	1.35E5	3.03E3	9.44E4	8.88E4	1.30E5	1.22E5
								max	5.40E5	2.90E4	3.77E5	3.55E5	5.18E5	4.89E5
000104-40-5	4-n-nonylphenol	220	6.35	3.15E-3	9.96	26937	5.76	min	1.20E1	2.70E0	4.89E-1	4.98E-1	1.77E0	3.73E-1
								mean	2.10E3	2.10E2	8.55E1	8.71E1	3.09E2	6.53E1
								max	4.60E3	5.60E2	1.87E2	1.91E2	6.78E2	1.43E2
000107-51-7	Octamethyltrisiloxane	237	0.034	4.45E2	21.7	37579	6.60	min	2.50E0	3.00E-1	6.71E-2	6.24E-2	2.39E-1	3.68E-2
								mean	5.25E0	2.71E1	1.41E-1	1.31E-1	5.02E-1	7.72E-2
								max	1.30E1	8.00E1	3.49E-1	3.24E-1	1.24E0	1.91E-1
000114-07-8	Erythromycin	734	0.517	2.83E-23	746	120	3.06	min	1.30E2	5.30E1	6.37E1	9.37E1	1.23E2	1.12E2

								mean	5.26E2	1.96E2	2.58E2	3.79E2	4.99E2	4.52E2
								max	2.10E3	5.30E2	1.03E3	1.51E3	1.99E3	1.81E3
000117-81-7	Di-(2-Ethylhexyl)-phthalate	391	0.270	1.89E-5	5.78	87096	7.60	min	1.70E3	6.00E1	5.84E1	5.84E1	1.77E2	2.90E1
								mean	3.81E3	9.17E2	1.31E2	1.31E2	3.96E2	6.50E1
								max	6.50E3	8.30E3	2.23E2	2.23E2	6.76E2	1.11E2
000128-37-0	Butylhydroxytoluene	220	0.600	6.88E-1	59.1	10986	5.10	min	1.00E2	8.30E1	5.83E0	6.35E0	2.28E1	7.80E0
								mean	5.55E2	1.87E2	3.24E1	3.52E1	1.26E2	4.33E1
								max	2.70E3	4.40E2	1.57E2	1.71E2	6.13E2	2.11E2
000128-39-2	2.6-Di-t-butyl-phenol	206	2.50	9.39E-1	45.5	7734	4.92	min	1.40E0	4.50E-1	9.81E-2	1.08E-1	3.85E-1	1.50E-1
								mean	9.73E0	1.81E0	6.82E-1	7.53E-1	2.68E0	1.04E0
								max	2.10E1	3.80E0	1.47E0	1.62E0	5.77E0	2.25E0
000140-66-9	4-t-Octylphenol	206	4.82	6.37E-2	45.5	10134	5.28	min	2.50E1	2.00E0	1.35E0	1.42E0	5.27E0	1.52E0
								mean	1.31E2	3.68E1	7.07E0	7.44E0	2.76E1	7.95E0
								max	8.60E2	2.90E2	4.64E1	4.88E1	1.81E2	5.21E1
000141-62-8	Decamethyltetrasiloxane	311	0.00674	5.00E1	32.5	523118	8.21	min	2.80E0	5.90E-1	9.53E-2	9.50E-2	2.88E-1	4.70E-2
								mean	4.78E0	2.86E0	1.63E-1	1.62E-1	4.93E-1	8.04E-2
								max	6.90E0	8.90E0	2.35E-1	2.34E-1	7.11E-1	1.16E-1
000141-63-9	Dodecamethylpentasiloxane	385	0.0000660	1.36E1	48.6	5903370	9.61	min	2.20E1	5.90E-1	7.54E-1	7.53E-1	2.27E0	3.71E-1
								mean	4.55E1	1.22E0	1.56E0	1.56E0	4.70E0	7.67E-1
								max	8.40E1	1.70E0	2.88E0	2.88E0	8.67E0	1.42E0
000144-11-6	Trihexyphenidyl	301	17.95	7.48E-8	92.4	3979	4.49	min	6.20E-1	4.10E-1	7.89E-2	9.10E-2	2.85E-1	1.40E-1
								mean	2.20E1	1.14E1	2.80E0	3.23E0	1.01E1	4.96E0
								max	1.10E2	5.80E1	1.40E1	1.61E1	5.07E1	2.48E1
000298-46-4	Carbamazepine	236	112	1.17E-5	21.7	473	2.45	min	7.10E1	1.10E1	4.17E1	4.90E1	6.83E1	6.41E1
								mean	6.68E2	4.82E2	3.92E2	4.61E2	6.43E2	6.04E2
								max	2.60E3	1.10E3	1.53E3	1.79E3	2.50E3	2.35E3
000303-49-1	Clomipramine	315	0.294	2.01E-5	280	9121	5.19	min	3.20E0	8.10E-1	1.88E-1	2.00E-1	7.37E-1	2.27E-1
								mean	2.17E1	1.09E1	1.28E0	1.36E0	5.00E0	1.54E0
								max	7.20E1	4.90E1	4.23E0	4.50E0	1.66E1	5.10E0
000540-97-6	Dodecamethylcyclohexasiloxane	445	0.00510	3.00E0	67.5	7962510	9.06	min	5.50E1	1.10E1	1.88E0	1.88E0	5.68E0	9.27E-1
								mean	1.41E4	7.54E1	4.84E2	4.83E2	1.46E3	2.38E2
								max	8.50E4	2.70E2	2.91E3	2.91E3	8.77E3	1.43E3
000541-02-6	Decamethylcyclopentasiloxane	371	0.0170	2.67E1	45.0	1021175	8.03	min	5.10E1	4.40E2	1.73E0	1.72E0	5.25E0	8.55E-1
								mean	7.14E4	1.08E3	2.42E3	2.41E3	7.35E3	1.20E3
								max	3.10E5	2.30E3	1.05E4	1.05E4	3.19E4	5.20E3
000556-67-2	Octamethylcyclotetrasiloxane	297	0.00500	1.40E2	30.1	101007	6.74	min	2.40E2	6.00E1	6.84E0	6.45E0	2.34E1	3.65E0
								mean	1.85E4	1.37E2	5.27E2	4.97E2	1.80E3	2.82E2
								max	1.20E5	2.80E2	3.42E3	3.22E3	1.17E4	1.83E3
000564-25-0	Doxycycline	444	630	1.89E-21	87.0	13.70	-0.02	min	1.00E0	3.20E1	9.37E-1	9.25E-1	9.93E-1	9.84E-1

								mean	6.53E2	7.13E2	6.12E2	6.04E2	6.49E2	6.43E2
								max	2.30E3	3.10E3	2.15E3	2.13E3	2.28E3	2.26E3
000604-75-1	Oxazepam	287	179	5.55E-10	34.6	175	2.24	min	5.00E0	7.90E1	3.49E0	3.92E0	4.88E0	4.69E0
								mean	5.05E2	5.16E2	3.53E2	3.96E2	4.93E2	4.74E2
								max	1.80E3	1.20E3	1.26E3	1.41E3	1.76E3	1.69E3
000723-46-6	Sulfamethoxazole	253	610	1.73E-5	39.8	94.2	0.89	min	2.00E2	3.00E1	1.73E2	1.69E2	1.97E2	1.93E2
								mean	5.50E2	1.26E2	4.75E2	4.66E2	5.42E2	5.31E2
								max	1.50E3	2.90E2	1.30E3	1.27E3	1.48E3	1.45E3
000732-26-3	2,4,6-Tri-t-butyl-phenol	262	35.0	8.81E-2	104	41889	6.06	min	3.60E-1	5.10E-2	1.36E-2	1.38E-2	4.59E-2	8.66E-3
								mean	3.35E0	6.97E-1	1.27E-1	1.28E-1	4.27E-1	8.05E-2
								max	1.20E1	1.60E0	4.53E-1	4.59E-1	1.53E0	2.89E-1
000738-70-5	Trimethoprim	290	400	1.00E-6	104	238	0.91	min	1.50E2	5.00E1	1.40E2	1.40E2	1.49E2	1.48E2
								mean	4.30E2	2.17E2	4.03E2	4.02E2	4.27E2	4.24E2
								max	1.40E3	5.10E2	1.31E3	1.31E3	1.39E3	1.38E3
001222-05-5	Galaxolide	258	1.75	7.27E-2	85.3	15707	5.90	min	5.40E1	4.00E1	2.12E0	2.16E0	7.35E0	1.47E0
								mean	1.35E3	1.08E3	5.30E1	5.39E1	1.84E2	3.68E1
								max	3.80E3	2.00E4	1.49E2	1.52E2	5.17E2	1.04E2
001948-33-0	t-Butyl-hydroxyquinone	166	748	1.65E-2	18.9	1137	2.94	min	3.40E0	2.50E-1	1.43E0	1.95E0	3.17E0	2.82E0
								mean	3.63E1	7.27E0	1.52E1	2.08E1	3.39E1	3.01E1
								max	7.90E1	3.00E1	3.31E1	4.52E1	7.37E1	6.56E1
002078-54-8	2,6-Diiso-propyl-phenol (propofol)	178	124	1.07E0	19.9	2625	3.79	min	1.20E0	3.60E-1	2.71E-1	3.59E-1	9.08E-1	6.19E-1
								mean	4.73E1	3.38E1	1.07E1	1.41E1	3.58E1	2.44E1
								max	2.20E2	5.10E2	4.96E1	6.58E1	1.67E2	1.14E2
002082-79-3	Octadecyl 3-(3,5-di-tert-butyl-4-hydroxyphenyl)propionate	531	6.09E-9	4.51E-11	109	321514082	13.41	min	2.40E0	1.00E0	8.22E-2	8.22E-2	2.48E-1	4.05E-2
								mean	8.48E0	3.30E0	2.91E-1	2.91E-1	8.76E-1	1.43E-1
								max	1.60E1	7.10E0	5.48E-1	5.48E-1	1.65E0	2.70E-1
003380-34-5	Triclosan	290	10.0	6.20E-4	134	14028	4.76	min	1.80E1	8.00E0	1.66E0	1.85E0	6.32E0	2.65E0
								mean	7.90E3	6.24E1	7.30E2	8.10E2	2.77E3	1.16E3
								max	1.10E5	2.50E2	1.02E4	1.13E4	3.86E4	1.62E4
004130-42-1	2.6-Di-t-butyl-4-ethyl-phenol	234	2.12	2.89E-1	63.8	19827	5.52	min	5.20E-1	1.50E-1	2.36E-2	2.45E-2	8.83E-2	2.17E-2
								mean	2.19E0	9.58E-1	9.95E-2	1.03E-1	3.72E-1	9.17E-2
								max	7.40E0	1.90E0	3.36E-1	3.49E-1	1.26E0	3.10E-1
009016-45-9	4-nonylphenol-mono-ethoxylate	441	0.827	1.29E-10	32.2	804	4.48	min	1.30E2	3.30E0	1.62E1	1.85E1	6.01E1	2.93E1
								mean	1.96E3	1.16E3	2.43E2	2.78E2	9.04E2	4.41E2
								max	7.30E3	1.30E4	9.08E2	1.04E3	3.37E3	1.64E3
015307-86-5	Diclofenac	296	2.37	8.19E-6	56.7	431	4.51	min	1.10E0	3.20E0	1.35E-1	1.55E-1	4.96E-1	2.39E-1
								mean	6.98E2	4.52E2	8.58E1	9.82E1	3.15E2	1.52E2
								max	7.00E3	5.00E3	8.60E2	9.85E2	3.15E3	1.52E3
015574-96-6	Pizotifen	295	0.371	2.69E-5	81.0	34706	5.20	min	2.20E0	6.20E-1	1.28E-1	1.35E-1	5.01E-1	1.53E-1

								mean	8.24E0	6.36E0	4.78E-1	5.07E-1	1.88E0	5.73E-1
								max	3.50E1	2.20E1	2.03E0	2.15E0	7.97E0	2.43E0
015687-27-1	Ibuprofen	206	21.0	2.48E-2	10.8	308	3.97	min	1.30E0	2.70E0	2.29E-1	2.82E-1	8.82E-1	5.36E-1
								mean	5.13E3	2.11E3	9.05E2	1.11E3	3.48E3	2.12E3
								max	1.20E4	2.60E4	2.12E3	2.60E3	8.14E3	4.95E3
018323-44-9	Clindamycin	425	30.6	7.04E-15	62.2	29.9	2.16	min	3.70E1	3.10E1	2.84E1	3.17E1	3.64E1	3.55E1
								mean	8.84E1	1.38E2	6.78E1	7.56E1	8.70E1	8.47E1
								max	2.30E2	2.80E2	1.77E2	1.97E2	2.26E2	2.20E2
019982-08-2	Memantine	179	894	2.53E-2	71.7	398	3.28	min	9.30E0	6.50E0	3.62E0	5.35E0	8.47E0	7.22E0
								mean	2.75E1	2.38E1	1.07E1	1.58E1	2.51E1	2.14E1
								max	8.60E1	5.10E1	3.34E1	4.95E1	7.83E1	6.67E1
021145-77-7	Tonalide	258	1.25	6.83E-2	88	12763	5.70	min	6.60E0	4.40E0	2.77E-1	2.84E-1	1.00E0	2.21E-1
								mean	1.31E2	8.37E1	5.50E0	5.65E0	1.99E1	4.38E0
								max	3.80E2	1.60E3	1.59E1	1.64E1	5.77E1	1.27E1
022071-15-4	Ketoprofen	254	51.0	1.95E-4	11.7	214	3.12	min	3.90E0	3.30E0	1.27E0	1.76E0	3.51E0	2.95E0
								mean	2.08E3	1.02E3	6.77E2	9.38E2	1.87E3	1.57E3
								max	6.00E3	6.10E3	1.95E3	2.70E3	5.39E3	4.54E3
022204-53-1	Naproxen	230	15.9	1.69E-4	11.8	177	3.18	min	2.00E0	3.50E0	6.26E-1	8.73E-1	1.78E0	1.48E0
								mean	4.86E3	1.63E3	1.52E3	2.12E3	4.33E3	3.60E3
								max	2.10E4	1.50E4	6.57E3	9.17E3	1.87E4	1.56E4
024219-97-4	Mianserin	264	3.72	2.93E-4	107	4345	4.24	min	5.90E0	4.10E0	1.01E0	1.22E0	3.41E0	1.90E0
								mean	1.88E1	2.20E1	3.20E0	3.88E0	1.09E1	6.05E0
								max	6.50E1	6.10E1	1.11E1	1.34E1	3.76E1	2.10E1
025013-16-5	t-Butyl-4-hydroxy-anisole	180	213	3.12E-1	27.0	1010	3.50	min	3.30E1	5.70E-1	9.82E0	1.40E1	2.82E1	2.19E1
								mean	1.29E2	9.21E0	3.83E1	5.45E1	1.10E2	8.56E1
								max	2.90E2	3.50E1	8.63E1	1.23E2	2.48E2	1.93E2
026761-40-0	Diisodecyl phthalate	447	0.280	7.04E-5	34.1	1917123	10.36	min	3.00E2	3.00E2	1.03E1	1.03E1	3.10E1	5.06E0
								mean	1.54E3	4.20E2	5.29E1	5.29E1	1.59E2	2.60E1
								max	4.00E3	7.60E2	1.37E2	1.37E2	4.13E2	6.74E1
028159-98-0	Irgarol 1051	253	7.52	4.89E-4	143	329	4.07	min	6.00E-1	1.30E0	1.23E-1	1.56E-1	3.96E-1	2.41E-1
								mean	4.60E0	5.02E0	9.46E-1	1.20E0	3.03E0	1.85E0
								max	1.40E1	1.10E1	2.88E0	3.65E0	9.24E0	5.63E0
028553-12-0	Diisononyl phthalate	419	0.200	7.20E-5	29.3	560015	9.37	min	1.20E3	2.00E2	4.11E1	4.11E1	1.24E2	2.02E1
								mean	3.31E3	6.87E2	1.13E2	1.13E2	3.42E2	5.58E1
								max	6.40E3	3.90E3	2.19E2	2.19E2	6.61E2	1.08E2
029122-68-7	Atenolol	266	13300	1.03E-7	25.7	16.5	0.16	min	5.40E2	1.30E2	4.40E2	4.23E2	5.28E2	5.12E2
								mean	1.28E3	4.62E2	1.04E3	1.00E3	1.25E3	1.21E3
								max	4.90E3	9.20E2	3.99E3	3.84E3	4.79E3	4.64E3
033704-61-9	Cashmeran	206	5.94	5.37E-1	55.3	2032	4.49	min	1.70E1	1.10E1	1.98E0	2.32E0	7.44E0	3.71E0

								mean	7.23E1	5.13E1	8.44E0	9.85E0	3.16E1	1.58E1
								max	1.50E2	3.10E2	1.75E1	2.04E1	6.56E1	3.27E1
034911-55-2	Bupropion	240	140	4.40E-2	61.6	1064	3.85	min	1.20E1	2.70E0	2.94E0	3.93E0	9.02E0	6.10E0
								mean	3.03E1	1.91E1	7.42E0	9.91E0	2.27E1	1.54E1
								max	8.20E1	4.10E1	2.01E1	2.69E1	6.16E1	4.17E1
037350-58-6	Metoprolol	267	16900	3.84E-5	23.1	58.3	1.88	min	1.20E3	6.80E2	8.70E2	8.96E2	1.17E3	1.12E3
								mean	2.55E3	1.62E3	1.85E3	1.90E3	2.48E3	2.38E3
								max	6.80E3	2.80E3	4.93E3	5.08E3	6.61E3	6.34E3
052485-79-7	Buprenorphine	468	0.655	2.29E-11	2406	21900	4.98	min	7.40E1	1.00E1	5.36E0	5.81E0	2.08E1	7.51E0
								mean	2.53E2	2.72E1	1.83E1	1.99E1	7.14E1	2.57E1
								max	1.00E3	6.40E1	7.24E1	7.85E1	2.82E2	1.02E2
053179-11-6	Loperamide	477	0.0405	1.05E-13	730	30297	5.15	min	1.40E0	5.00E-1	8.54E-2	9.11E-2	3.35E-1	1.06E-1
								mean	6.38E0	7.91E0	3.89E-1	4.15E-1	1.52E0	4.83E-1
								max	2.10E1	2.80E1	1.28E0	1.37E0	5.02E0	1.59E0
054143-55-4	Flecainide	414	1.48	3.24E-6	1025	2057	3.78	min	4.80E1	1.90E1	1.33E1	1.83E1	3.76E1	2.66E1
								mean	1.91E2	1.23E2	5.27E1	7.29E1	1.50E2	1.06E2
								max	7.10E2	2.30E2	1.96E2	2.71E2	5.57E2	3.94E2
054910-89-3	Fluoxetine	309	60.3	3.36E-3	117	10245	4.05	min	8.20E0	5.20E0	1.71E0	2.18E0	5.48E0	3.37E0
								mean	6.12E1	3.40E1	1.28E1	1.63E1	4.09E1	2.52E1
								max	2.40E2	9.40E1	5.01E1	6.38E1	1.60E2	9.87E1
059729-33-8	Citalopram	324	31.1	1.51E-5	377	6856	3.74	min	1.20E1	2.10E1	3.41E0	4.52E1	9.57E0	5.05E1
								mean	1.69E2	1.39E2	4.81E1	2.45E3	1.35E2	2.73E3
								max	1.00E3	4.80E2	2.84E2	6.87E3	7.81E3	7.67E3
061869-08-7	Paroxetine	329	35.3	6.39E-6	151	3890	3.95	min	1.20E1	1.70E1	2.78E0	4.75E0	8.56E0	6.90E0
								mean	4.48E1	3.03E1	1.04E1	6.71E1	3.20E1	9.73E1
								max	1.30E2	5.60E1	3.01E1	3.96E2	9.28E1	5.75E2
065277-42-1	Ketoconazole	531	0.0866	8.55E-12	1300	7502	4.35	min	5.70E1	5.60E1	8.75E0	3.64E0	3.00E1	5.55E0
								mean	2.39E2	7.80E1	3.67E1	1.36E1	1.26E2	2.07E1
								max	1.20E3	1.20E2	1.84E2	3.95E1	6.33E2	6.01E1
066722-44-9	Bisoprolol	325	2240	3.93E-6	26.9	58.3	1.87	min	1.10E2	3.80E1	8.22E1	1.04E1	1.07E2	1.59E1
								mean	2.20E2	1.08E2	1.64E2	4.37E1	2.15E2	6.67E1
								max	5.60E2	2.50E2	4.18E2	2.19E2	5.46E2	3.35E2
079617-96-2	Sertraline	306	3.52	1.56E-4	99.3	33113	5.29	min	1.50E1	1.00E1	8.09E-1	8.50E1	3.15E0	1.03E2
								mean	5.11E1	2.19E1	2.75E0	1.70E2	1.07E1	2.07E2
								max	1.10E2	4.90E1	5.93E0	4.33E2	2.31E1	5.27E2
081103-11-9	Clarithromycine	748	0.342	3.09E-23	823	59.25	3.16	min	5.20E1	1.80E0	2.36E1	8.51E-1	4.86E1	8.99E-1
								mean	2.60E2	1.24E2	1.18E2	2.90E0	2.43E2	3.06E0
								max	4.80E2	7.80E2	2.18E2	6.24E0	4.49E2	6.59E0
081403-80-7	Alfuzosin	389	91.9	6.08E-11	203	540	1.86	min	1.60E1	1.80E1	1.41E1	3.52E1	1.59E1	4.32E1

								mean	6.74E1	5.52E1	5.95E1	1.76E2	6.70E1	2.16E2
								max	2.20E2	1.10E2	1.94E2	3.25E2	2.19E2	3.99E2
082626-48-0	Zolpidem	307	5.74	3.09E-8	63.4	6803	3.85	min	1.80E0	2.30E0	4.42E-1	1.51E1	1.35E0	1.57E1
								mean	1.49E1	1.12E1	3.66E0	6.35E1	1.12E1	6.62E1
								max	4.40E1	4.10E1	1.08E1	2.07E2	3.31E1	2.16E2
083366-66-9	Nefazodone	470	0.0602	6.93E-9	493	20999	5.00	min	1.10E0	8.10E-1	7.79E-2	5.91E-1	3.04E-1	9.16E-1
								mean	4.49E1	1.18E1	3.18E0	4.89E0	1.24E1	7.59E0
								max	2.20E2	7.00E1	1.56E1	1.44E1	6.07E1	2.24E1
083799-24-0	Fexofenadine	502	0.0236	5.04E-16	121	761	2.81	min	8.90E1	1.10E1	5.05E1	8.43E-2	8.59E1	1.08E-1
								mean	3.14E2	1.61E2	1.78E2	3.44E0	3.03E2	4.40E0
								max	1.10E3	3.70E2	6.24E2	1.69E1	1.06E3	2.16E1
084852-15-3	4-nonylphenol, branched	220	5000	1.26E-2	20.8	22111	5.77	min	3.20E2	1.60E1	1.31E1	6.92E1	4.70E1	8.06E1
								mean	1.35E4	5.10E2	5.53E2	2.44E2	1.99E3	2.84E2
								max	2.70E5	5.50E3	1.10E4	8.55E2	3.96E4	9.97E2
085721-33-1	Ciprofloxacin	331	30000	3.80E-11	141	3.15	0.28	min	3.00E1	1.00E1	2.87E1	1.33E1	2.99E1	9.90E0
								mean	8.80E1	3.12E1	8.43E1	5.65E2	8.76E1	4.19E2
								max	1.30E2	6.50E1	1.25E2	1.13E4	1.29E2	8.35E3
086386-73-4	Fluconazole	306	13660	3.89E-7	397	168	0.50	min	9.70E1	5.50E1	9.52E1	2.85E1	9.68E1	2.97E1
								mean	6.36E2	3.74E2	6.24E2	8.37E1	6.35E2	8.71E1
								max	2.10E3	1.10E3	2.06E3	1.24E2	2.10E3	1.29E2
088768-40-5	Cilazapril	17.5	27.5	2.08E-12	18.0	155	2.27	min	1.10E0	2.50E0	6.72E-1	9.52E1	1.06E0	9.66E1
								mean	1.36E1	8.70E0	8.28E0	6.24E2	1.30E1	6.33E2
								max	4.20E1	2.80E1	2.57E1	2.06E3	4.04E1	2.09E3
093413-69-5	Venlafaxine	277	267	3.28E-5	119	427	3.28	min	1.30E2	1.20E2	5.19E1	7.44E-1	1.19E2	9.94E-1
								mean	6.35E2	4.17E2	2.54E2	9.17E0	5.80E2	1.22E1
								max	2.20E3	7.00E2	8.79E2	2.84E1	2.01E3	3.79E1
106266-06-2	Risperidone	411	2.76	6.19E-9	392	26940	3.49	min	1.90E0	1.80E0	6.63E-1	7.73E1	1.66E0	1.02E2
								mean	3.62E1	3.67E1	1.26E1	3.77E2	3.16E1	4.96E2
								max	2.70E2	1.60E2	9.42E1	1.31E3	2.36E2	1.72E3
133040-01-4	Eprosartan	425	0.0195	4.47E-13	13.7	100138	6.37	min	2.70E1	1.20E1	9.70E-1	9.77E-1	3.12E0	1.33E0
								mean	3.42E2	2.40E2	1.23E1	1.86E1	3.95E1	2.53E1
								max	9.40E2	8.70E2	3.38E1	1.39E2	1.09E	1.89E2

CAS	Chemical	MW	WS at 25 °C	VP at 25 °C	kDeg	Koc	Log Kow		In (meas)	Sludge (meas)	Sludge (pred)			
		g mol^{-1}	mg l^{-1}	Pa	day	l kg^{-1}			ng l^{-1}	ng kg^{-1} dw	ng kg^{-1} dw			
									Database	*Database*	*Old Käppala*	*New Käppala*	*Rya-verket*	*Sjö-lunda*
000050-48-6	Amitryptiline	277	9.71	4.83E-5	73.4	27800	4.92	min	5.20	5.00E3	2.79E3	1.09E4	2.39E4	4.33E3
								mean	19.0	6.07E3	1.02E4	4.00E4	8.73E4	1.58E4
								max	47.0	7.80E3	2.52E4	9.90E4	2.16E5	3.91E4
000052-86-8	Haloperidol	376	14	2.00E-8	701	3283	4.30	min	6.90	3.70E3	3.37E3	1.28E4	2.03E4	4.54E3
								mean	21.49	5.12E3	1.05E4	3.98E4	6.33E4	1.41E4
								max	69.0	6.60E3	3.37E4	1.28E5	2.03E5	4.54E4
000057-83-0	Progesterone	314	8.81	3.59E-4	105	5370	3.87	min	4.00	1.70E4	1.73E3	6.00E3	6.57E3	1.84E3
								mean	13.6	9.17E4	5.85E3	2.03E4	2.23E4	6.25E3
								max	30.0	3.00E5	1.30E4	4.50E4	4.93E4	1.38E4
000058-08-2	Caffeine	194	21600	9.77E-7	17.2	9.77	-0.07	min	15.0	7.10E-2	1.06E1	9.90E0	3.99E0	1.68E0
								mean	67953	2.02E-1	4.82E4	4.49E4	1.81E4	7.59E3
								max	150000	5.60E-1	1.06E5	9.90E4	3.99E4	1.68E4
000058-73-1	Diphenhydramine	255	3060	7.73E-4	41.3	1780	3.27	min	6.50	9.80E3	2.18E3	5.41E3	3.44E3	1.25E3
								mean	42.7	1.50E4	1.43E4	3.55E4	2.26E4	8.20E3
								max	200	2.30E4	6.71E4	1.66E5	1.06E5	3.84E4
000060-87-7	Promethazine	284	15.6	1.37E-3	98.8	3969	4.81	min	12.0	4.50E4	6.37E3	2.49E4	5.24E4	9.73E3
								mean	66.0	5.98E4	3.50E4	1.37E5	2.88E5	5.35E4
								max	190	8.80E4	1.01E5	3.95E5	8.30E5	1.54E5
000064-75-5	Tetracycline	483	248900	4.12E-25	119	1.49	-3.70	min	1.00	1.40E4	1.68E-4	1.61E-4	6.28E-5	2.65E-5
								mean	846	1.28E6	1.42E-1	1.36E-1	5.31E-2	2.24E-2
								max	4500	3.60E6	7.57E-1	7.26E-1	2.83E-1	1.19E-1
000068-22-4	Norethindrone	298	7.04	3.15E-7	91.3	966	2.97	min	2.00	8.70E3	5.48E2	1.08E3	5.58E2	2.17E2
								mean	12.07	6.30E4	3.31E3	6.51E3	3.37E3	1.31E3
								max	20.0	2.10E5	5.48E3	1.08E4	5.58E3	2.17E3
000068-88-2	Hydroxyzine	375	428	1.56E-9	175	496	2.36	min	5.90	2.20E4	7.78E2	9.98E2	4.20E2	1.74E2
								mean	20.2	2.82E4	2.67E3	3.42E3	1.44E3	5.96E2
								max	61.0	3.90E4	8.04E3	1.03E4	4.34E3	1.80E3
000076-57-3	Codeine	299	33900	2.55E-8	104	108	1.19	min	390	9.50E3	4.94E3	4.84E3	1.90E3	8.01E2
								mean	1321	1.77E4	1.67E4	1.64E4	6.43E3	2.71E3
								max	4200	2.90E4	5.32E4	5.22E4	2.05E4	8.63E3
000079-57-2	Oxytetracycline	460	313	1.21E-20	133	9.56	-0.90	min	0.60	2.10E5	6.37E-2	6.11E-2	2.38E-2	1.00E-2
								mean	322	8.75E5	3.42E1	3.28E1	1.28E1	5.39E0
								max	790	1.40E6	8.39E1	8.04E1	3.13E1	1.32E1

000080-05-7	Bisphenol A	228	120	3.03E-5	26.5	6849	3.32	min	6.00	5.00E-2	2.06E3	5.26E3	3.51E3	1.25E3
								mean	1172	2.04E4	4.02E5	1.03E6	6.86E5	2.45E5
								max	5100	4.70E5	1.75E6	4.47E6	2.99E6	1.07E6
000083-98-7	Orphenadrine	269	113	1.23E-2	56.5	3131	3.77	min	9.90	8.80E3	4.12E3	1.37E4	1.37E4	4.06E3
								mean	43.4	1.34E4	1.80E4	6.02E4	6.02E4	1.78E4
								max	180	2.20E4	7.49E4	2.50E5	2.50E5	7.39E4
000084-66-2	Diethyl phthalate	222	1080	2.80E-1	10.1	69.2	2.42	min	160	2.00E0	2.27E4	2.87E4	1.29E4	5.26E3
								mean	584	5.39E3	8.30E4	1.05E5	4.70E4	1.92E4
								max	1300	7.20E4	1.85E5	2.33E5	1.05E5	4.28E4
000085-68-7	Butyl benzyl phthalate	312	2.69	1.10E-3	7.46	5248	4.73	min	100	1.20E4	5.08E4	1.96E5	4.15E5	7.79E4
								mean	287	3.07E5	1.46E5	5.63E5	1.19E6	2.24E5
								max	1200	8.70E5	6.10E5	2.35E6	4.98E6	9.35E5
000088-18-6	2-t-Butyl-phenol	150	700	1.20E1	19.9	1048	3.31	min	3.00	2.00E-3	1.02E3	2.56E3	1.72E3	6.13E2
								mean	15.7	9.71E-3	5.32E3	1.34E4	8.98E3	3.21E3
								max	30.0	4.90E-2	1.02E4	2.56E4	1.72E4	6.13E3
000096-76-4	2,4-Di-t-butyl-phenol	206	35.0	6.36E-1	45.5	9093	5.19	min	35.0	7.00E-3	1.91E4	7.54E4	1.77E5	3.05E4
								mean	325	1.77E0	1.78E5	7.00E5	1.64E6	2.83E5
								max	2200	3.70E1	1.20E6	4.74E6	1.11E7	1.92E6
000098-54-4	4-t-Butyl-phenol	150	580	5.08E0	19.9	1038	3.31	min	28.0	5.00E-3	9.50E3	2.40E4	1.60E4	5.73E3
								mean	222	3.83E-2	7.53E4	1.90E5	1.27E5	4.54E4
								max	1900	2.10E-1	6.45E5	1.63E6	1.09E6	3.89E5
000103-90-2	Paracetamol	151	14000	2.59E-4	13.6	30.73	0.46	min	36000	1.10E4	8.60E4	7.97E4	3.24E4	1.36E4
								mean	135200	3.30E4	3.23E5	2.99E5	1.22E5	5.10E4
								max	540000	7.30E4	1.29E6	1.20E6	4.85E5	2.04E5
000104-40-5	4-n-nonylphenol	220	6.35	3.15E-3	9.96	26937	5.76	min	12.00	1.00E4	6.68E3	2.64E4	6.70E4	1.09E4
								mean	2100	1.05E5	1.17E6	4.62E6	1.17E7	1.91E6
								max	4600	3.20E5	2.56E6	1.01E7	2.57E7	4.18E6
000107-51-7	Octamethyltrisiloxane	237	0.034	4.45E2	21.7	37579	6.60	min	2.50	8.10E3	1.30E3	5.07E3	1.41E4	2.20E3
								mean	5.25	1.24E7	2.74E3	1.06E4	2.97E4	4.61E3
								max	13.0	6.20E7	6.78E3	2.63E4	7.35E4	1.14E4
000114-07-8	Erythromycin	734	0.517	2.83E-23	746	120	3.06	min	130	1.20E5	3.84E4	8.19E4	4.42E4	1.69E4
								mean	526	4.55E5	1.55E5	3.32E5	1.79E5	6.85E4
								max	2100	1.00E6	6.20E5	1.32E6	7.13E5	2.73E5
000117-81-7	Di-(2-Ethylhexyl)-phthalate	391	0.270	1.89E-5	5.78	87096	7.60	min	1700	5.70E6	9.58E5	3.79E6	1.00E7	1.57E6
								mean	3810	7.16E+10	2.15E6	8.50E6	2.24E7	3.52E6
								max	6500	1.00E+12	3.66E6	1.45E7	3.82E7	6.00E6
000128-37-0	Butylhydroxytoluene	220	0.600	6.88E-1	59.1	10986	5.10	min	100	1.80E2	5.35E4	2.11E5	4.86E5	8.52E4
								mean	555	1.11E9	2.97E5	1.17E6	2.70E6	4.73E5
								max	2700	1.20E+10	1.45E6	5.70E6	1.31E7	2.30E6

000128-39-2	2,6-Di-t-butyl-phenol	206	2.50	9.39E-1	45.5	7734	4.92	min	1.40	2.00E3	7.38E2	2.90E3	6.38E3	1.15E3
								mean	9.73	1.01E5	5.13E3	2.02E4	4.43E4	8.03E3
								max	21.0	6.70E5	1.11E4	4.35E4	9.57E4	1.73E4
000140-66-9	4-t-Octylphenol	206	4.82	6.37E-2	45.5	10134	5.28	min	25.0	3.90E4	1.37E4	5.42E4	1.29E5	2.20E4
								mean	131	6.37E7	7.21E4	2.84E5	6.77E5	1.15E5
								max	860	3.40E8	4.73E5	1.86E6	4.44E6	7.57E5
000141-62-8	Decamethyltetrasiloxane	311	0.00674	5.00E1	32.5	523118	8.21	min	2.80	1.40E-3	1.57E3	6.23E3	1.65E4	2.58E3
								mean	4.78	6.09E2	2.69E3	1.06E4	2.81E4	4.41E3
								max	6.90	2.90E4	3.88E3	1.53E4	4.06E4	6.36E3
000141-63-9	Dodecamethylpentasiloxane	385	0.0000660	1.36E1	48.6	5903370	9.61	min	22.0	3.00E-3	1.24E4	4.91E4	1.29E5	2.03E4
								mean	45.5	4.44E3	2.56E4	1.01E5	2.68E5	4.20E4
								max	84.0	1.70E5	4.73E4	1.87E5	4.94E5	7.76E4
000144-11-6	Trihexyphenidyl	301	17.95	7.48E-8	92.4	3979	4.49	min	0.62	5.40E2	3.13E2	1.21E3	2.19E3	4.49E2
								mean	22.0	3.21E3	1.11E4	4.29E4	7.76E4	1.59E4
								max	110	9.00E3	5.56E4	2.14E5	3.88E5	7.97E4
000298-46-4	Carbamazepine	236	112	1.17E-5	21.7	473	2.45	min	71.0	8.70E-2	1.06E4	1.40E4	6.16E3	2.53E3
								mean	668	7.06E4	1.00E5	1.32E5	5.80E4	2.38E4
								max	2600	2.00E5	3.90E5	5.12E5	2.26E5	9.25E4
000303-49-1	Clomipramine	315	0.294	2.01E-5	280	9121	5.19	min	3.20	3.60E4	1.76E3	6.92E3	1.62E4	2.79E3
								mean	21.7	4.12E4	1.19E4	4.70E4	1.10E5	1.90E4
								max	72.0	4.60E4	3.95E4	1.56E5	3.64E5	6.28E4
000540-97-6	Dodecamethylcyclohexasiloxane	445	0.00510	3.00E0	67.5	7962510	9.06	min	55.0	3.00E-1	3.10E4	1.23E5	3.24E5	5.08E4
								mean	14126	6.30E4	7.96E6	3.15E7	8.31E7	1.30E7
								max	85000	2.50E6	4.79E7	1.90E8	5.00E8	7.85E7
000541-02-6	Decamethylcyclopentasiloxane	371	0.0170	2.67E1	45.0	1021175	8.03	min	51.0	3.40E0	2.86E4	1.13E5	3.00E5	4.70E4
								mean	71387	9.35E5	4.01E7	1.59E8	4.19E8	6.58E7
								max	310000	3.80E7	1.74E8	6.88E8	1.82E9	2.86E8
000556-67-2	Octamethylcyclotetrasiloxane	297	0.00500	1.40E2	30.1	101007	6.74	min	240	1.20E-1	1.27E5	4.96E5	1.37E6	2.14E5
								mean	18490	5.97E3	9.82E6	3.82E7	1.06E8	1.65E7
								max	120000	4.60E5	6.37E7	2.48E8	6.85E8	1.07E8
000564-25-0	Doxycycline	444	630	1.89E-21	87.0	13.70	-0.02	min	1.00	2.40E4	8.03E-1	7.69E-1	3.00E-1	1.27E-1
								mean	653.10	5.89E5	5.25E2	5.02E2	1.96E2	8.29E1
								max	2300	1.80E6	1.85E3	1.77E3	6.91E2	2.92E2
000604-75-1	Oxazepam	287	179	5.55E-10	34.6	175	2.24	min	5.00	1.40E-2	5.39E2	6.41E2	2.70E2	1.12E2
								mean	505	5.53E3	5.44E4	6.48E4	2.73E4	1.13E4
								max	1800	4.30E4	1.94E5	2.31E5	9.72E4	4.03E4
000723-46-6	Sulfamethoxazole	253	610	1.73E-5	39.8	94.2	0.89	min	200	8.80E3	1.28E3	1.23E3	4.87E2	2.05E2
								mean	550	1.06E4	3.53E3	3.38E3	1.34E3	5.65E2
								max	1500	1.20E4	9.63E3	9.23E3	3.65E3	1.54E3

000732-26-3	2,4,6-Tri-t-butyl-phenol	262	35.0	8.81E-2	104	41889	6.06	min	0.36	1.70E-4	2.02E2	7.99E2	2.06E3	3.30E2
								mean	3.35	2.14E-2	1.88E3	7.44E3	1.92E4	3.07E3
								max	12.0	2.30E-1	6.73E3	2.66E4	6.87E4	1.10E4
000738-70-5	Trimethoprim	290	400	1.00E-6	104	238	0.91	min	150	1.10E3	1.01E3	9.81E2	3.83E2	1.62E2
								mean	430	6.88E3	2.90E3	2.81E3	1.10E3	4.64E2
								max	1400	2.70E4	9.44E3	9.15E3	3.58E3	1.51E3
001222-05-5	Galaxolide	258	1.75	7.27E-2	85.3	15707	5.90	min	54.0	8.70E3	3.02E4	1.20E5	3.06E5	4.93E4
								mean	1352	7.59E6	7.57E5	2.99E6	7.65E6	1.23E6
								max	3800	2.90E7	2.13E6	8.42E6	2.15E7	3.47E6
001948-33-0	t-Butyl-hydroxyquinone	166	748	1.65E-2	18.9	1137	2.94	min	3.40	4.00E-3	8.99E2	1.68E3	8.83E2	3.44E2
								mean	36.3	2.54E-1	9.59E3	1.80E4	9.42E3	3.67E3
								max	79.0	2.80E0	2.09E4	3.91E4	2.05E4	7.99E3
002078-54-8	2,6-Diiso-propyl-phenol (propofol)	178	124	1.07E0	19.9	2625	3.79	min	1.20	1.00E-4	4.95E2	1.64E3	1.72E3	5.00E2
								mean	47.3	1.40E-2	1.95E4	6.47E4	6.75E4	1.97E4
								max	220	6.30E-2	9.07E4	3.01E5	3.14E5	9.17E4
002082-79-3	Octadecyl 3-(3,5-di-tert-butyl-4-hydroxyphenyl)propionate	531	6.09E-9	4.51E-11	109	321514082	13.41	min	2.40	6.20E2	1.35E3	5.35E3	1.41E4	2.22E3
								mean	8.48	6.99E3	4.78E3	1.89E4	4.99E4	7.84E3
								max	16.00	1.70E4	9.01E3	3.57E4	9.42E4	1.48E4
003380-34-5	Triclosan	290	10.0	6.20E-4	134	14028	4.76	min	18.00	1.10E-2	9.50E3	3.71E4	7.65E4	1.44E4
								mean	7898	5.00E6	4.17E6	1.63E7	3.36E7	6.32E6
								max	110000	4.30E7	5.81E7	2.27E8	4.68E8	8.80E7
004130-42-1	2,6-Di-t-butyl-4-ethyl-phenol	234	2.12	2.89E-1	63.8	19827	5.52	min	0.520	4.40E-4	2.88E2	1.14E3	2.81E3	4.67E2
								mean	2.19	2.06E-3	1.21E3	4.80E3	1.18E4	1.97E3
								max	7.40	7.00E-3	4.10E3	1.62E4	4.00E4	6.64E3
009016-45-9	4-nonylphenol-mono-ethoxylate	441	0.827	1.29E-10	32.2	804	4.48	min	130	1.10E0	6.50E4	2.50E5	4.54E5	9.34E4
								mean	1957	1.09E1	9.79E5	3.76E6	6.83E6	1.41E6
								max	7300	1.60E2	3.65E6	1.40E7	2.55E7	5.25E6
015307-86-5	Diclofenac	296	2.37	8.19E-6	56.7	431	4.51	min	1.10	4.00E3	5.56E2	2.15E3	3.94E3	8.03E2
								mean	698	2.81E4	3.53E5	1.36E6	2.50E6	5.09E5
								max	7000	7.70E4	3.54E6	1.37E7	2.51E7	5.11E6
015574-96-6	Pizotifen	295	0.371	2.69E-5	81.0	34706	5.20	min	2.20	9.00E2	1.21E3	4.76E3	1.11E4	1.92E3
								mean	8.24	2.20E3	4.52E3	1.78E4	4.17E4	7.20E3
								max	35.0	3.70E3	1.92E4	7.57E4	1.77E5	3.06E4
015687-27-1	Ibuprofen	206	21.0	2.48E-2	10.8	308	3.97	min	1.30	4.00E3	5.58E2	1.95E3	2.47E3	6.51E2
								mean	5130	8.45E4	2.20E6	7.70E6	9.76E6	2.57E6
								max	12000	3.10E5	5.15E6	1.80E7	2.28E7	6.01E6
018323-44-9	Clindamycin	425	30.6	7.04E-15	62.2	29.9	2.16	min	37.0	5.90E3	3.48E3	4.04E3	1.67E3	6.94E2
								mean	88.4	1.52E4	8.30E3	9.65E3	3.98E3	1.66E3
								max	230	2.10E4	2.16E4	2.51E4	1.04E4	4.32E3

019982-08-2	Memantine	179	894	2.53E-2	71.7	398	3.28	min	9.30	9.10E2	3.15E3	7.92E3	5.03E3	1.82E3
								mean	27.5	2.18E3	9.32E3	2.34E4	1.49E4	5.40E3
								max	86.0	3.10E3	2.91E4	7.32E4	4.65E4	1.69E4
021145-77-7	Tonalide	258	1.25	**6.83E-2**	88	12763	5.70	min	6.60	8.80E4	3.68E3	1.46E4	3.66E4	5.99E3
								mean	131	6.85E5	7.31E4	2.89E5	7.27E5	1.19E5
								max	380	2.60E6	2.12E5	8.38E5	2.11E6	3.45E5
022071-15-4	Ketoprofen	254	51.0	1.95E-4	11.7	214	3.12	min	3.90	5.00E3	1.17E3	2.52E3	1.49E3	5.59E2
								mean	2081	1.70E4	6.27E5	1.35E6	7.95E5	2.98E5
								max	6000	4.50E4	1.81E6	3.88E6	2.29E6	8.60E5
022204-53-1	Naproxen	230	15.9	1.69E-4	11.8	177	3.18	min	2.00	4.00E3	6.26E2	1.41E3	8.68E2	3.21E2
								mean	4858	2.57E4	1.52E6	3.43E6	2.11E6	7.80E5
								max	21000	1.50E5	6.57E6	1.48E7	9.12E6	3.37E6
024219-97-4	Mianserin	264	3.72	2.93E-4	107	4345	4.24	min	5.90	1.10E4	2.83E3	1.06E4	1.62E4	3.73E3
								mean	18.8	3.56E4	8.99E3	3.38E4	5.16E4	1.19E4
								max	65.0	9.40E4	3.11E4	1.17E5	1.79E5	4.11E4
025013-16-5	t-Butyl-4-hydroxy-anisole	180	213	3.12E-1	27.0	1010	3.50	min	33.0	3.00E-3	1.23E4	3.55E4	2.77E4	9.29E3
								mean	129	3.55E-2	4.80E4	1.39E5	1.08E5	3.62E4
								max	290	7.10E-2	1.08E5	3.12E5	2.44E5	8.16E4
026761-40-0	Diisodecyl phthalate	447	0.280	7.04E-5	34.1	1917123	10.36	min	300	6.60E6	1.69E5	6.69E5	1.77E6	2.77E5
								mean	1543	2.29E7	8.69E5	3.44E6	9.08E6	1.43E6
								max	4000	8.50E7	2.25E6	8.92E6	2.35E7	3.69E6
028159-98-0	Irgarol 1051	253	7.52	4.89E-4	143	329	4.07	min	0.60	1.00E3	2.75E2	1.01E3	1.33E3	3.35E2
								mean	4.60	1.47E4	2.11E3	7.73E3	1.02E4	2.57E3
								max	14.0	5.40E4	6.42E3	2.35E4	3.11E4	7.81E3
028553-12-0	Diisononyl phthalate	419	0.200	7.20E-5	29.3	560015	9.37	min	1200	1.30E6	6.76E5	2.68E6	7.06E6	1.11E6
								mean	3311	3.54E7	1.87E6	7.39E6	1.95E7	3.06E6
								max	6400	1.30E8	3.61E6	1.43E7	3.77E7	5.91E6
029122-68-7	Atenolol	266	13300	1.03E-7	25.7	16.5	0.16	min	540	1.20E4	6.52E2	6.13E2	2.45E2	1.03E2
								mean	1279	2.02E4	1.54E3	1.45E3	5.79E2	2.44E2
								max	4900	3.80E4	5.92E3	5.57E3	2.22E3	9.34E2
033704-61-9	Cashmeran	206	5.94	5.37E-1	55.3	2032	4.49	min	17.0	3.90E3	8.46E3	3.26E4	5.96E4	1.22E4
								mean	72.3	1.53E5	3.60E4	1.39E5	2.54E5	5.20E4
								max	150	2.50E6	7.47E4	2.88E5	5.26E5	1.08E5
034911-55-2	Bupropion	240	140	4.40E-2	61.6	1064	3.85	min	12.0	1.40E2	5.13E3	1.76E4	1.91E4	5.40E3
								mean	30.3	3.60E2	1.29E4	4.45E4	4.80E4	1.36E4
								max	82.0	6.10E2	3.51E4	1.21E5	1.30E5	3.69E4
037350-58-6	Metoprolol	267	16900	3.84E-5	23.1	58.3	1.88	min	1200	1.30E5	6.60E4	6.91E4	2.84E4	1.19E4
								mean	2550	2.24E5	1.40E5	1.47E5	6.03E4	2.52E4
								max	6800	4.10E5	3.74E5	3.92E5	1.61E5	6.72E4

052485-79-7	Buprenorphine	468	0.655	2.29E-11	2406	21900	4.98	min	74.0	2.10E4	4.00E4	1.57E5	3.49E5	6.25E4
								mean	253	6.34E4	1.37E5	5.39E5	1.19E6	2.14E5
								max	1000	1.40E5	5.41E5	2.13E6	4.71E6	8.44E5
053179-11-6	Loperamide	477	0.0405	1.05E-13	730	30297	5.15	min	1.40	4.50E3	7.67E2	3.02E3	6.99E3	1.22E3
								mean	6.38	8.98E3	3.49E3	1.38E4	3.18E4	5.53E3
								max	21.0	1.70E4	1.15E4	4.53E4	1.05E5	1.82E4
054143-55-4	Flecainide	414	1.48	3.24E-6	1025	2057	3.78	min	48.0	6.10E3	2.02E4	6.83E4	6.79E4	2.00E4
								mean	191	1.04E4	8.04E4	2.71E5	2.70E5	7.96E4
								max	710	1.40E4	2.99E5	1.01E6	1.00E6	2.96E5
054910-89-3	Fluoxetine	309	60.3	3.36E-3	117	10245	4.05	min	8.20	3.90E4	3.74E3	1.36E4	1.77E4	4.50E3
								mean	61.2	7.52E4	2.79E4	1.02E5	1.32E5	3.36E4
								max	240	1.60E5	1.09E5	3.99E5	5.18E5	1.32E5
059729-33-8	Citalopram	324	31.1	1.51E-5	377	6856	3.74	min	12.0	2.30E-2	4.98E3	4.15E0	1.58E4	6.89E-1
								mean	169	7.30E4	7.03E4	2.24E2	2.23E5	3.73E1
								max	1000	7.60E5	4.15E5	6.30E2	1.32E6	1.05E2
061869-08-7	Paroxetine	329	35.3	6.39E-6	151	3890	3.95	min	12.0	2.40E4	5.32E3	1.65E4	2.24E4	4.77E3
								mean	44.8	2.48E4	1.99E4	2.33E5	8.35E4	6.72E4
								max	130	2.60E4	5.76E4	1.38E6	2.42E5	3.97E5
065277-42-1	Ketoconazole	531	0.0866	8.55E-12	1300	7502	4.35	min	57.0	3.60E5	2.81E4	1.89E4	1.77E5	6.01E3
								mean	239	7.36E5	1.18E5	7.07E4	7.41E5	2.24E4
								max	1200	1.80E6	5.92E5	2.05E5	3.72E6	6.51E4
066722-44-9	Bisoprolol	325	2240	3.93E-6	26.9	58.3	1.87	min	110	2.80E3	5.94E3	1.07E5	2.54E3	3.86E4
								mean	220	5.36E3	1.19E4	4.50E5	5.09E3	1.62E5
								max	560	1.00E4	3.02E4	2.26E6	1.30E4	8.12E5
079617-96-2	Sertraline	306	3.52	1.56E-4	99.3	33113	5.29	min	15.0	8.00E-3	8.27E3	6.22E3	7.77E4	1.06E3
								mean	51.1	2.09E5	2.81E4	1.24E4	2.65E5	2.13E3
								max	110	1.70E6	6.06E4	3.17E4	5.70E5	5.42E3
081103-11-9	Clarithromycine	748	0.342	3.09E-23	823	59.25	3.16	min	52.0	1.40E3	1.65E4	3.26E4	2.19E4	1.32E4
								mean	260	5.23E3	8.22E4	1.11E5	1.09E5	4.51E4
								max	480	1.30E4	1.52E5	2.39E5	2.02E5	9.71E4
081403-80-7	Alfuzosin	389	91.9	6.08E-11	203	540	1.86	min	16.0	1.00E4	8.52E2	3.81E4	3.64E2	8.21E3
								mean	67.4	2.12E4	3.59E3	1.90E5	1.53E3	4.10E4
								max	220	3.40E4	1.17E4	3.51E5	5.00E3	7.58E4
082626-48-0	Zolpidem	307	5.74	3.09E-8	63.4	6803	3.85	min	1.80	2.00E-4	7.70E2	9.12E2	2.86E3	1.53E2
								mean	14.9	1.13E3	6.38E3	3.84E3	2.37E4	6.43E2
								max	44.0	8.30E3	1.88E4	1.25E4	6.99E4	2.10E3
083366-66-9	Nefazodone	470	0.0602	6.93E-9	493	20999	5.00	min	1.10	8.00E2	5.96E2	2.65E3	5.22E3	8.11E2
								mean	44.9	1.55E3	2.43E4	2.19E4	2.13E5	6.72E3
								max	220	2.90E3	1.19E5	6.47E4	1.04E6	1.98E4

083799-24-0	Fexofenadine	502	0.0236	5.04E-16	121	761	2.81	min	89.0	4.30E4	2.11E4	2.34E3	1.74E4	9.32E2
								mean	314	9.24E4	7.42E4	9.57E4	6.15E4	3.80E4
								max	1100	1.40E5	2.60E5	4.69E5	2.16E5	1.86E5
084852-15-3	4-nonylphenol, branched	220	5000	1.26E-2	20.8	22111	5.77	min	320	6.90E-1	1.79E5	3.65E4	1.79E6	6.96E3
								mean	13543	2.84E5	7.56E6	1.28E5	7.58E7	2.45E4
								max	270000	9.20E6	1.51E8	4.51E5	1.51E9	8.60E4
085721-33-1	Ciprofloxacin	331	30000	3.80E-11	141	3.15	0.28	min	30.0	6.80E4	4.80E1	7.06E5	1.80E1	2.91E5
								mean	88.0	4.29E6	1.41E2	2.99E7	5.28E1	1.23E7
								max	130	1.20E7	2.08E2	5.96E8	7.80E1	2.45E8
086386-73-4	Fluconazole	306	13660	3.89E-7	397	168	0.50	min	97.0	2.60E3	2.57E2	4.62E1	9.66E1	7.60E0
								mean	636	1.38E4	1.69E3	1.36E2	6.33E2	2.23E1
								max	2100	4.70E4	5.57E3	2.00E2	2.09E3	3.29E1
088768-40-5	Cilazapril	17.5	27.5	2.08E-12	18.0	155	2.27	min	1.10	1.10E3	1.24E2	2.49E2	6.33E1	4.08E1
								mean	13.6	1.54E3	1.53E3	1.63E3	7.81E2	2.68E2
								max	42.0	2.60E3	4.73E3	5.39E3	2.42E3	8.84E2
093413-69-5	Venlafaxine	277	267	3.28E-5	119	427	3.28	min	130	8.60E4	4.41E4	1.47E2	7.04E4	2.62E1
								mean	635	1.67E5	2.15E5	1.82E3	3.44E5	3.23E2
								max	2200	3.10E5	7.46E5	5.63E3	1.19E6	9.99E2
106266-06-2	Risperidone	411	2.76	6.19E-9	392	26940	3.49	min	1.90	6.60E2	7.16E2	1.11E5	1.57E3	2.55E4
								mean	36.2	1.32E3	1.36E4	5.44E5	3.00E4	1.25E5
								max	270	2.10E3	1.02E5	1.88E6	2.24E5	4.32E5
133040-01-4	Eprosartan	425	0.0195	4.47E-13	13.7	100138	6.37	min	27.0	1.00E4	1.52E4	2.09E3	1.57E5	5.31E2
								mean	342	1.27E4	1.92E5	3.99E4	1.98E6	1.01E4
								max	940	1.40E4	5.28E5	2.97E5	5.45E6	7.55E4