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Application of SimpleTreat 4.0 in European substance regulations

For our Environment

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Application of SimpleTreat 4.0 in European substance regulations

by

Jaap Struijs

National Institute of Public Health and the Environment,
Bilthoven, The Netherlands

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Wörlitzer Platz 1
06844 Dessau-Roßlau
Tel: +49 340-2103-0
Fax: +49 340-2103-2285
info@umweltbundesamt.de
Internet: www.umweltbundesamt.de

/umweltbundesamt.de
/umweltbundesamt

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Abstract

SimpleTreat 4.0 is an exposure and emission model developed to estimate chemical emission from sewage treatment plants and exposure in surface water within the framework of risk assessment of chemicals. It is a revision of SimpleTreat 3.1 which supported the chemical act 25 years ago in the Netherlands and later in the European Union (EU). The revision was necessary to account for recent scientific insights with respect to behavior of the chemical in domestic sewage and activated sludge. This report is a guidance for substance regulators how to apply SimpleTreat 4.0 in accordance to REACh (Registration, Evaluation, Authorization and restriction of Chemicals) and other regulations of substances in the EU, such as biocides, medicines and plant protection products. It provides detailed instructions how to apply basic substance properties and other information present in the substance notification files according to substance regulations in the EU. The variety in basic physic-chemical properties and measured data about fate in the environment requires a hierarchy in data handling which is explained in this report. It is expected that some time will elapse before SimpleTreat 4.0 is the recommended model for risk assessment in the EU. Therefore the revised model has a provision to switch to output that would have been produced by SimpleTreat 3.1, despite the fact that for organic compounds that are (partly) ionized predictions do not reflect the technical-scientific state of the art.

Kurzbeschreibung

SimpleTreat 4.0 ist ein Expositions- und Emissionsmodell, das entwickelt wurde um die chemischen Emissionen aus Kläranlagen und die entsprechende Exposition in Oberflächengewässern im Rahmen der Risikobewertung von Chemikalien abzuschätzen. SimpleTreat wurde vor 25 Jahren entwickelt, um das damalige Chemiekaliengesetz (ChemG) in den Niederlanden und später in der europäischen Union zu unterstützen. Die vorliegende Version ist eine Überarbeitung von SimpleTreat 3.1. Eine Überarbeitung war notwendig, um jüngste wissenschaftliche Erkenntnisse zum Verhalten von Chemikalien in häuslichem Abwasser und Belebtschlamm zu implementieren. Der vorliegende Bericht ist eine Handlungsanleitung für Stoffregulatoren, wie das überarbeitete SimpleTreat 4.0 in REACh (Registrierung, Evaluierung und Autorisierung von Chemikalien) und in anderen Stoffvollzügen bei Bioziden, Arzneimitteln und Pflanzenschutzmitteln anzuwenden ist. Detaillierte Anweisungen zeigen, wie Stoffeigenschaften und andere Informationen aus den Stoffdossiers nach EU-Stoffverordnungen in SimpleTreat 4.0 anzuwenden sind. Die Vielfalt an physikalisch-chemischen Eigenschaften und gemessenen Daten zum Verhalten in der Umwelt erfordern eine Hierarchie in der Dateneingabe, die in diesem Bericht beschrieben wird. Bis SimpleTreat 4.0 das empfohlene Modell für die Risikobewertung in der EU wird, kann in SimpleTreat 4.0 per Schalter in die alte Version gewechselt werden. Hier ist aber darauf hinzuweisen, dass für dissoziierende organische Verbindungen die Vorhersagen nicht den wissenschaftlichen Stand der Technik widerspiegeln.

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List of abbrevations

B	organic base
BOD	biological oxygen demand
BPR	Biocidal Products Regulation
Dow	the apparent n-octanol-water partition coefficient at the actual pH
ECHA	European Chemicals Agency
EMA	European Medicines Agency
EU	European Union
Fn	neutral fraction of an organic acid or base in water at a specified pH
foc	Fraction organic carbon of particles
H	Henry constant
H‘	Dimensionless Henry constant (= Kaw)
HA	organic acid
HRT	hydraulic retention time, without specification referring to the aeration tank
Ka	acid dissociation constant
Kb	base dissociation constant
Kaw	air-water partition coefficient
Kp	solids-water partition coefficient
Kp_{as}	Kp for activated sludge also indicated as Kp (activated sludge)
Kp_{s}	Kp for raw or settled sewage also indicated as Kp (sewage)
Koc	organic carbon-water partition coefficient
Kow	n-octanol-water partition coefficient
OECD	Organisation for Economic Co-operation and Development
pKa	negative logarithm of the acid dissociation constant
pKb	negative logarithm of the base dissociation constant
PPP	Plant Protection Products
R	universal gas constant (8.314 J K-1 mol-1)
REACh	Registration, Evaluation, Authorization and restriction of Chemical
STP	Sewage treatment plant
SLR	Sludge loading rate
SRT	Sludge retention time
TGD	Technical Guidance Document

Summary

The exposure and emission model SimpleTreat 3.1 is applied to estimate the emission and exposure of chemical substances via sewage treatment plants in the framework of risk assessment as described by the guidance on REACh (Registration, Evaluation, Authorization and restriction of Chemical), biocides and human pharmaceuticals. The model was originally developed for industrial chemicals which are used by the public at large and by other sectors in the industrial society. During the 1980's chemical acts came into force to regulate substances. In substance evaluation systems to support substance regulation, exposure assessment is based on models like SimpleTreat and SimpleBox.

An important requirement in the model development was that the model input should consist of a limited number of physical-chemical properties. These so-called base-set data were defined as being mandatory for the notification procedure of a new chemical and were limited to water solubility, vapour pressure, the octanol-water partition coefficient and molecular weight. These physical-chemical property data can then be complemented with information obtained from standardized biodegradability laboratory and adsorption on sludge tests according to the OECD guidelines. The fate of a chemical is most often entirely determined by the level of biodegradability and hydrophobicity. The latter is characterized by the octanol-water partition coefficient which proved satisfactory to estimate sorption of a chemical at the particle-water interphase.

The popularity of the models used in generic exposure assessment evoked application in other substance regulations of the European Union. SimpleTreat 3.1 has gradually become a tool used in the regulation of biocides, medicinal products for human use, and (in the Netherlands) plant protection products.

A fair share of the chemicals under these regimes however, are organic and weak acids or bases and are partly ionized in water under conditions in biological treatment of communal wastewater. The multi-equilibrium approach applied in SimpleTreat 3.1 proved unsatisfactory in recent studies by Unilever UK, the National Institute of Public Health and Environment in the Netherlands (RIVM) and the German Federal Environment Agency (UBA).

Recently a new version of the model was launched. In SimpleTreat 4.0 new equations for sorption of organic acids and bases are applied. Furthermore, default parameters defining the operation mode of a sewage treatment plants have changed according to the technological development in the EU in the last two decades. Accompanying, a technical report on SimpleTreat 4.0 has been published by RIVM. The current report however, is meant as guidance for those who are involved in the admission and regulation of chemicals in the framework of the aforementioned substance regulations.

A description of differences in the new model with respect to SimpleTreat 3.1 is given. New rules for sorption of an ionized organic chemical onto sludge particles require different input. This is explained in view of different substance regulations. Not only for ionized but also for chemicals that exist solely in neutral state, SimpleTreat 4.0 produces different output, especially for chemicals that are prone to biodegradation and volatilization. Partly this is due to a different choice of default parameters. This is illustrated with some examples.

SimpleTreat has always practiced a hierarchy with respect to input substance characteristics. In the new version this hierarchy is expanded and made more explicit. This was necessary as some parameters have disappeared and some others are new. This is also illustrated with a series of examples.

Version 3.1 however, is still the recommended model in substance regulations and therefore version 4.0 has a provision which enables switching to output that would have been produced by SimpleTreat 3.1. It is expected that some time will elapse before SimpleTreat 4.0 is the recommended model for risk assessment in the EU. Despite the fact that version 3.1 for organic compounds that are (partly) ionized does not reflect the technical-scientific state of the art regarding the behaviour of acids and bases in sediment and sludge.

The core of this report consists of detailed instructions how to use chemical properties and related information from substance notification files according to substance regulations in the EU in the new SimpleTreat version. The interpretation of the results given in the output sheet is described in a separate chapter.

Zusammenfassung

Das Expositions- und Emissionsmodell SimpleTreat 3.1 schätzt die Emission und Exposition von chemischen Substanzen über Kläranlagen im Rahmen der Risikobewertung nach den Leitlinien von REACH (Registrierung, Evaluierung und Autorisierung von Chemikalien), Bioziden und Arzneimitteln ab. Das Modell wurde ursprünglich für Chemikalien entwickelt, die hauptsächlich in privaten Haushalten, aber auch im industriellen Bereich verwendet werden. In den 1980er traten Chemiekaliengesetze in Kraft um Stoffe zu regulieren. Die Expositionsbewertung zur Stoffregulierung basiert auf Modellen wie SimpleTreat und SimpleBox.

Eine wichtige Anforderung bei der Modellentwicklung war, dass die Modell-Inputparameter nur aus einer begrenzte Anzahl von physikalisch-chemischen Eigenschaften bestehen sollte. Dieser sogenannte Grunddatensatz wurde als verbindlich im Meldeverfahren für neue Chemikalien beschlossen und auf die Parameter Wasserlöslichkeit, Dampfdruck, Oktanol-Wasser-Verteilungskoeffizient und Molekulargewicht begrenzt. Diese physikalisch-chemische Daten können dann mit Informationen aus standardisierten Labortests zur biologischen Abbaubarkeit und Adsorption am Klärschlamm nach den OECD-Richtlinien ergänzt werden. Der Verbleib einer Chemikalie ist häufig vollständig durch die biologische Abbaubarkeit und Hydrophobie festgelegt. Letzteres wird durch den Oktanol-Wasser-Verteilungskoeffizienten charakterisiert, der nachweislich die Sorption einer Chemikalie an der Phasengrenze Partikel-Wasser vorhersagen kann.

Die Popularität von Modellen in der generischen Expositionsabschätzung führte zur Anwendung in anderen Stoffregulierungen der Europäischen Union und SimpleTreat 3.1 wurde schrittweise in den Vollzügen der Biozide, Humanarzneimittel und Pflanzenschutzmittel (in den Niederlanden) verwendet.

Viele Stoffe in diesen Vollzügen sind jedoch schwache organische Säuren oder Basen und liegen teilweise dissoziiert im Wasser vor unter den Bedingungen, die bei der biologischen Behandlung von kommunalem Abwasser vorherrschen. In neueren Studien von Unilever UK, dem National Institute of Public Health and Environment in the Netherlands (RIVM) und dem Umweltbundesamt (UBA) erwies sich der bestehende Ansatz in SimpleTreat 3.1 als unzureichend.

Kürzlich wurde eine neue Version des Modells eingeführt. In SimpleTreat 4.0 sind neue Gleichungen für die Sorption von schwachen organischen Säuren und Basen hinterlegt. Darüber hinaus wurden Betriebsparameter zur Beschreibung einer Kläranlage verändert, entsprechend der technologischen Entwicklung in der EU in den letzten zwei Jahrzehnten. Begleitend zur Version 4.0 wurde vom RIVM ein technischer Report veröffentlicht. Der vorliegende Leitfaden soll zusätzlich als Arbeitshilfe in der Zulassung und Regulierung der vorgenannten Stoffvollzüge dienen.

Der Leitfaden beschreibt die Unterschiede im neuen Modell im Vergleich zu SimpleTreat 3.1. Neue Gleichungen für die Sorption von dissoziierten organischen Chemikalien an Schlammpartikel erfordern die Eingabe unterschiedlicher Parameter. Dies wird für die verschiedenen Stoffvollzüge erläutert. Nicht nur für dissoziierte sondern auch für Chemikalien, die ausschließlich im neutralen Zustand vorliegen, modelliert SimpleTreat 4.0 unterschiedliche Ergebnisse insbesondere bei biologisch abbaubaren und leichtflüchtigen Chemikalien. Dies ist teilweise auf die unterschiedliche Wahl der Standardparameter zurückzuführen und wird an einigen Beispielen veranschaulicht.

In SimpleTreat gibt es eine Eingabehierarchie in Bezug auf Stoffeigenschaften. In der neuen Version wird diese Hierarchie erweitert und herausgestellt. Dies war notwendig, da einige

Parameter nicht mehr enthalten und neue dazugekommen sind. Auch diese Neuerungen werden an Hand einer Reihe von Beispielen veranschaulicht.

Version 3.1 ist jedoch immer noch das empfohlene Modell in den verschiedenen Stoffvollzügen. Daher ist in Version 4.0 ein Schalter integriert, um auch die Ergebnisse, die durch SimpleTreat 3.1 berechnet werden, anzuzeigen. Es ist jedoch nicht zu erwarten, dass SimpleTreat 4.0 in naher Zukunft das empfohlene Modell für die Risikobewertung in der EU wird, obwohl Version 3.1 bei teilweise dissoziiert vorliegenden Chemikalien nicht den wissenschaftlichen Stand der Technik widerspiegelt bezüglich des Verbleibs von Säuren und Basen in Sedimenten und Klärschlämmen.

Der zentrale Teil dieses Berichts besteht aus detaillierten Anweisungen, wie Stoffeigenschaften und die anderen Informationen aus den Stoffdossiers nach EU-Verordnung in SimpleTreat 4.0 anzuwenden sind. Auch die Interpretation der Ausgabemaske ist in einem separaten Kapitel beschrieben.

1 Application of SimpleTreat 4.0 in European substance regulations

1.1 Introduction

SimpleTreat is a model to predict the fate of a chemical in a communal wastewater treatment plant (Figure 1) in the EU (European Union). Recently a new version of the model (4.0) was launched (Struijs, 2014). Currently, version 3.1 is in use to estimate chemical emission and exposure in the framework of risk assessment as described by the Technical Guidance Document (TGD, 2003) and by the guidance on REACh (source: European Chemicals Agency, http://echa.europe.eu/). Except for chemicals under REACh, SimpleTreat 3.1 has gradually become a tool used in the following substance regulations:

- Biocidal Products Regulation (BPR, Regulation (EU) 528/2012) of the European Parliament and of the Council)
- Guideline on the environmental risk assessment of medicinal products for human use, regulated by the European Medicines Agency (EMA) (EMA/CHMP/SWP/4447/00)
- Plant Protection Products (PPP, 1107/2009)

Many chemical compounds under these regimes are organic and acids or bases and are (partly) ionized in water under conditions in biological treatment of communal wastewater. SimpleTreat 3.1 accounts for dissociation of organic acids and bases in chemical fate computation. However, the multi-equilibrium approach including an ionization equilibrium in water and partitioning of the neutral chemical between two adjacent media such as solids-water and air-water, is based on the assumption that the ionized chemical can exclusively exist in the water phase. Recent studies by Unilever (Franco et al., 2013), the National Institute of Public Health and Environment in the Netherlands and the German Federal Environment Agency (Struijs, 2013) showed that this approach erroneously ignores sorption of the ionized organic acid or base onto sludge particles.

In SimpleTreat 4.0 new equations for sorption of organic acids and bases are formulated. Furthermore, default parameters defining the operation mode of a sewage treatment plants (STP) have changed according to the technological development in the EU the last two decades.

This report is a user manual for those involved in the evaluation and admittance of substances under REACH and the regulations mentioned above. SimpleTreat 4.0 allows a wider definition of wastewater and the operation of the primary clarifier. The default settings however, are representative for the treatment of domestic sewage. Chemical fate and emission calculations with respect to treatment of industrial wastewater are beyond the scope.

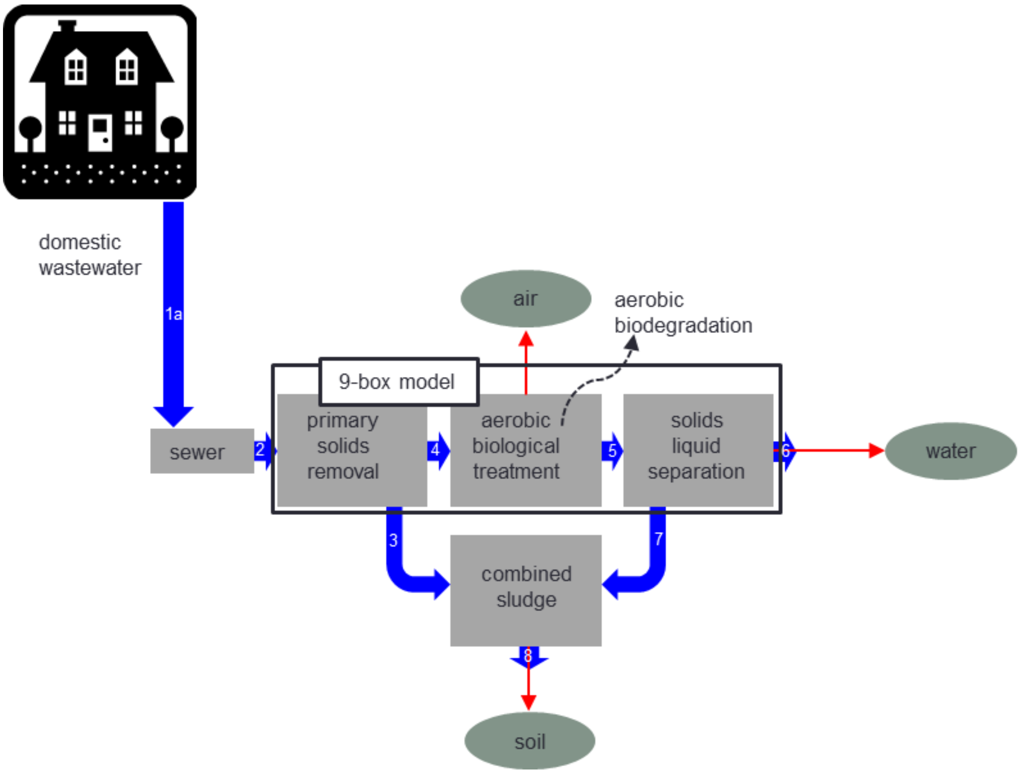
The consequences of the modifications are explained in section 3.2. Differences in model output between version 4.0 and version 3.1 of SimpleTreat are explained.

Section 3.3 describes in general terms how the model is applied in the evaluation of substances. It gives an outline of the hierarchy regarding input parameters in the model calculations. Chemical properties required as input for the calculations may be measured, derived from measured data or estimated from basic chemical properties such as water solubility, octanol-water partition coefficient. SimpleTreat 4.0 establishes a priority with respect to substance characteristics. Also in the estimation of biodegradation of the chemical, a certain hierarchy is practiced with respect to results of different standardized biodegradation tests.

Section 3.4 provides specific guidance on filling in the input part of the model. Interpretation of the output tables of the model is given.

Section 3.5 describes the switch in the model to convert version 4.0 into version 3.1. The latter is still in use in the framework of regulating substances.

Figure 1: Sewage treatment plant (STP) in its (communal) environment. The chemicals discharged into the sewer are emitted to air, water and soil or degraded in the aeration tank. The “9-box model” SimpleTreat model predicts the fate of a chemical in the three tanks of an STP.



1.2 Differences with respect to version 3.1

The model structure has not changed with respect to SimpleTreat 3.1. Version 4.0 is a non-equilibrium, steady-state multimedia model of the fate of a chemical (Figure 2). The modelled chemical is supposed to be submitted to the following processes: media flow carrying the chemical with it (open arrows indicate irreversible transport of the chemical), inter-media transport (two-headed arrows indicate reversible exchange of the chemical) and degradation (curved arrows indicate first order decay of the chemical).

The equilibrium partition coefficient, which is the ratio of equilibrium chemical concentrations in adjacent media, is the required parameter to compute reversible exchange processes of the chemical between adjacent media, such as air-water and solids-water. Rate and direction of reversible exchange (also called diffusive chemical mass transport) is driven by non-equilibrium concentrations. Net chemical mass transport occurs across the boundary of adjacent media if concentrations are not in equilibrium.

Box 1 (Figure 2) is the air column above the STP; boxes 2, 5 and 7 represent the aqueous phase in the primary clarifier, aeration tank and solids-liquid separator respectively. Boxes 3, 6 and 8 are suspended solids in the primary clarifier, aeration tank and solids-liquid separator. Boxes 4 and 9 represent settled solids (sediment) in the primary clarifier and the solids-liquid separator, respectively.

Table 1: Sludge loading rates (SLR) and related hydraulic retention time (HRT) and sludge retention time (SRT) for an STP with primary sedimentation tank. Default SLR in bold.

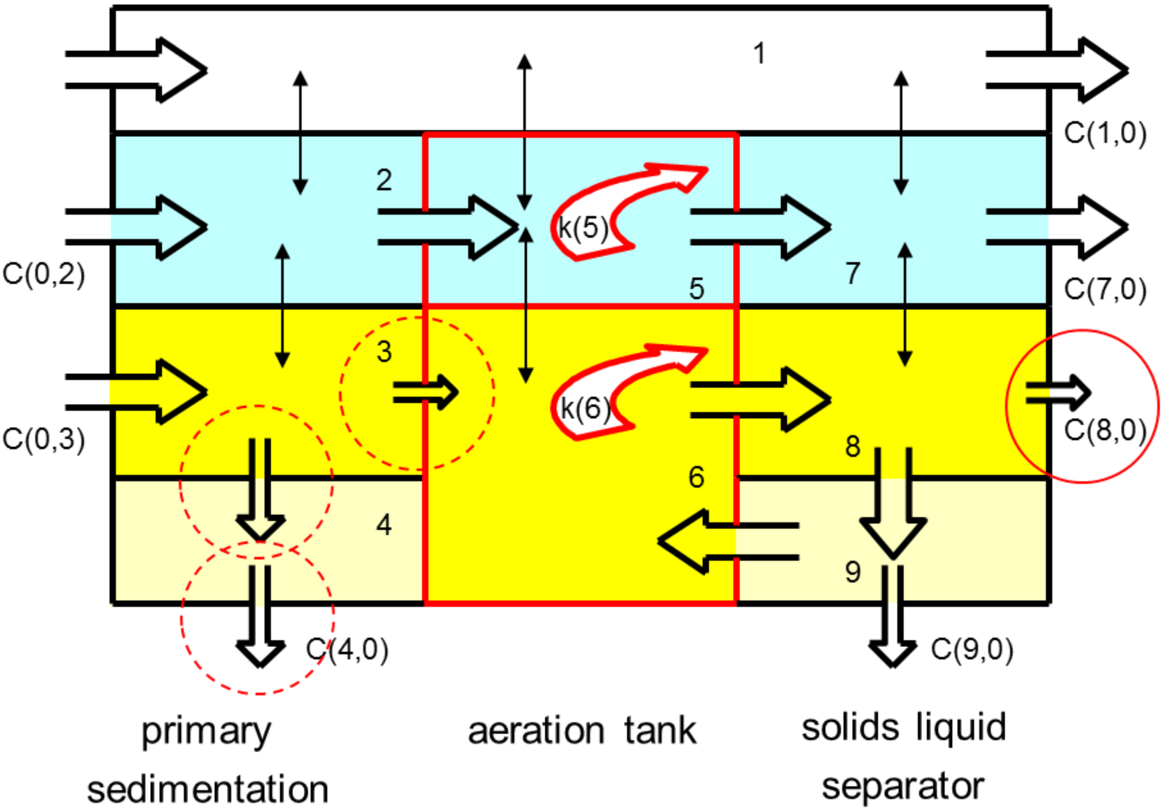
Sludge loading rate [kg BOD/kg solids/d]	Hydraulic retention time [hr]	Sludge retention time [d]
0.04 (low)	28.7	37.0
0.06 (low)	19.2	24.1
0.1 (low)	11.5	14.1
0.15 (medium)	7.7	9.2
0.2 (medium)	5.2	6.8
0.3 (high)	3.8	4.5
0.6 high)	1.9	2.2

Compared to SimpleTreat 3.1, the new model produces different output for ionized organic substances. Recently applied rules relating substance properties to the tendency of ionic chemicals to sorb onto sludge particles (Franco et al., 2013), were inserted in the model and described in detail by Struijs (2014). For neutral substances however, the equation for the solids-water partition coefficient has not changed. Nevertheless, the new version may give different output also for these chemicals because:

1. The input of biological oxygen demand (BOD) per person has increased from 54 to 60 g per day which has prolonged the hydraulic retention times (Table 1) compared to version 3.1;
2. Default settings for the sludge loading rate decreased from 0.15 to 0.1 kg BOD/kg solids/d;
3. Emission of suspended solids through the effluent is four times lower;

4. There are two modes to define first order kinetics for biodegradation in the aerator: occurring only in the water phase of the aeration tank (box 5) and occurring in both phases in activated sludge, i.e. water and the suspended solids phase (box 5 and 6). A third type of biodegradation kinetics, Monod kinetics, has been removed.

Figure 2: Multimedia (box) model representing the chemical fate in a sewage treatment plant which combines primary sedimentation and the activated sludge process (Struijs, 1996).



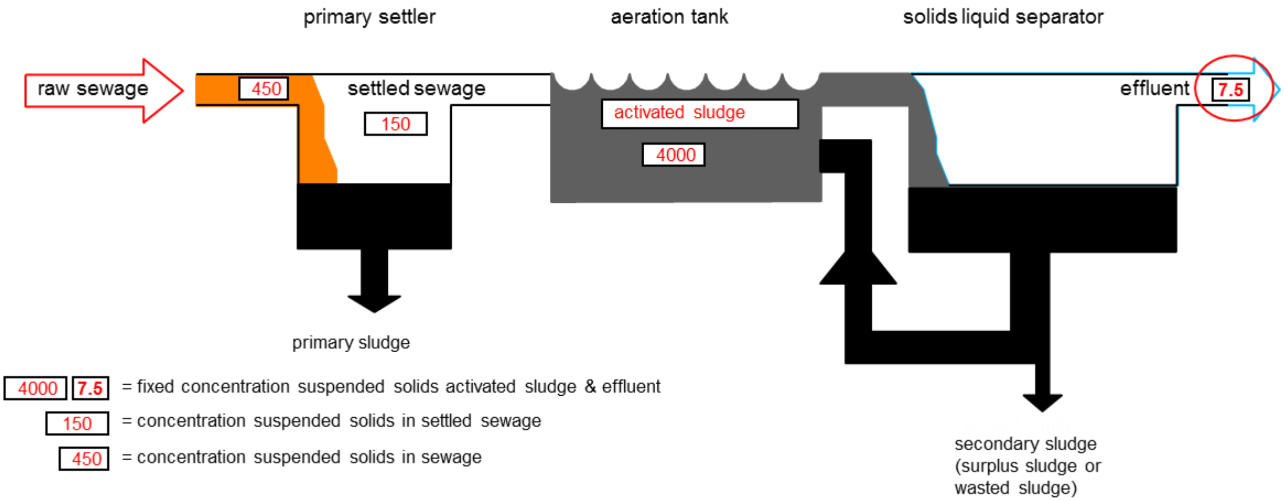
Modification 1 caused an increase in the volume of the aerator. This has the effect that the hydraulic retention time in the aeration tank is longer. With a fixed concentration of suspended solids in activated sludge not only the volume of the water phase (box 5) but also the volume of the suspended solids phase (box 6) will be larger.

In SimpleTreat 4.0, the default sludge loading rate (SLR) equals 0.1 (kg BOD/kg solids/d) which is lower than in SimpleTreat 3.1 (see Table 1). SLR is a measurement of the amount of biodegradable material in the influent (kg BOD/d) divided by the amount of microbial mass/activated sludge in the aeration tank (kg solids). The enhanced treatment rate in the EU results in a lower average loading of STPs. This justifies a lower default value for SLR. A lower SLR implies a longer hydraulic retention time which enables more volatilization and biodegradation to occur for the volatile and biodegradable chemicals.

The concentration of suspended solids in the effluent is 7.5 mg dry solids per liter in SimpleTreat 4.0 (see Figure 3) which is four times lower than in version 3.1. The suspended solids concentration of 7.5 mg/L better reflects the state of the art technology of wastewater treatment in Europe. This may reduce the emission of a chemical which tends to adsorb to particles. Chemical emission via effluent is calculated as the sum of chemical concentrations in the effluent: purely dissolved and associated to the suspended solids in effluent. In Figure 2 the circled arrow indicates irreversible chemical mass transport via sorption on suspended solids in effluent (out of box 8).

The dashed circles are only relevant for the chemical fate during treatment of industrial wastewater which is beyond the scope of this manual. The input parameters that determine irreversible media flow rates in the primary clarifier are not described here because default settings refer to communal wastewater treatment plants which is adequate for regulatory risk assessment of substances.

Figure 3: Steady state concentrations of suspended solids in raw sewage and the three STP basins. The suspended solids concentration in effluent is fixed at 7.5 mg/L. In SimpleTreat 3.1 it was 30 mg/L.



Compared to version 3.1, the new input parameters have appeared into the “Characterization of the chemical” part of the input block. The chemical class has to be defined as “acid” or “base” if the chemical can occur in the ionized state (default is “neutral”). The organic carbon water partition coefficient (Koc) can be given directly as an input parameter. For organic bases Dow is the input parameter for the hydrophobicity of an organic chemical at the actual pH.

1.3 Input parameters: defaults and hierarchy

1.3.1 Default values

SimpleTreat can produce output solely on the basis of default data of a chemical and a default emission scenario. Default base-set chemical properties are 100 g/mol for the molecular weight, 1000 for the n-octanol-water partition coefficient, 1 Pa for the vapour pressure and 100 mg/L for the water solubility. All default values are shown between brackets in the column on the right of the shaded part of the input block. A default value for a compound property is overruled at the moment a number is inserted in the shaded input field (see Figure 4).

The model conducts the chemical fate computation on the basis of first order rate constants for degradation inside a medium and exchange between adjacent media. Quantification of inter-media transport of the chemical requires equilibrium partition coefficients regarding air-water and solids-water. For non-persistent chemicals, a first order biodegradation rate constant should be known. The default value for biodegradation rate constants is zero.

1.3.2 Hierarchy of input parameters

Equilibrium partition coefficients are primary input parameters but if they are not available an estimation is made on the basis of chemical properties (e.g. the n-octanol-water partition coefficient) and environmental characteristics (e.g. the organic carbon content of solids).

Measured equilibrium partition coefficients have the highest ranking. If these data are available, input chemical properties are not used to quantify inter-media transport rates. Most often however, these data are not known and estimation routines on the basis of chemical properties are needed to assess the indispensable equilibrium partition coefficients.

1.3.3 Ranking of estimation routines to estimate equilibrium partition coefficients

Non-numerical base set information of the chemical is “chemical class” which may be “acid”, “base” or nothing which means “neutral” (default). This label is decisive for how solids-water partition coefficients are calculated if no measured data are available.

Air-water Equilibrium partitioning of a chemical between air and water is given by Henry’s law constant (H) in appropriate units. If an experimentally determined H is not available, it is estimated as the ratio of the vapour pressure and the water solubility in appropriate units. When the organic chemical is an acid or base which may dissociate in water, water solubility pertains to the neutral form of the chemical.

Solids-water The partition coefficients for activated sludge (Kp_{as}) and (raw) sewage (Kp_s) have first priority. The following hierarchy is practiced in SimpleTreat 4.0:

1. If a partition coefficient of the chemical has been determined in slurry of activated sludge (Kp_{as}) but not in (raw) sewage (Kp_s) the latter is estimated from Kp_{as} as explained in Section 3.4.
2. If Kp_{as} is not known (assuming that also Kp_s is not known), they are estimated from another input parameter: the experimentally determined organic carbon-water partition coefficient (Koc).
3. In natural systems like freshwater (suspended) sediment or soil, the organic carbon content (foc) is most often low and usually in the range of 0.1 to 5 %. In sewage and activated sludge foc is much higher (30 to 40 %). Therefore, an experimentally deter-

mined Koc in activated sludge has priority over a Koc determined in a natural sediment or soil.

4. If there are no measured Koc data at all, Koc is estimated from quantitative structure (property) activity relationships derived for neutral chemicals, acids and bases (Struijs, 2014).
5. Estimation of Koc of an organic base requires the property Dow at ambient pH. Dow is the n-octanol-water partition coefficient measured at a specified pH. If a measured Dow at neutral pH is not available, it is estimated from two base-set chemical properties: the acid ionization constant and the n-octanol-water partitioning coefficient of the neutral chemical (Struijs, 2014).

1.3.4 Ranking biodegradability test results to estimate first order degradation rate constants

Several standardized biodegradability tests are included in the OECD Guidelines for testing of Chemicals (OECD, 2006). Both OECD Guidelines (2006) and the TGD (2003) practice some form of hierarchy. Generally, a result obtained from a simulation test has priority over results of screening test. In SimpleTreat 4.0 a hierarchy related to “biodegradability of a chemical” in the activated sludge process as observed in the OECD test system, is further elaborated in order to formulate first order degradation rate constants in the relevant media.

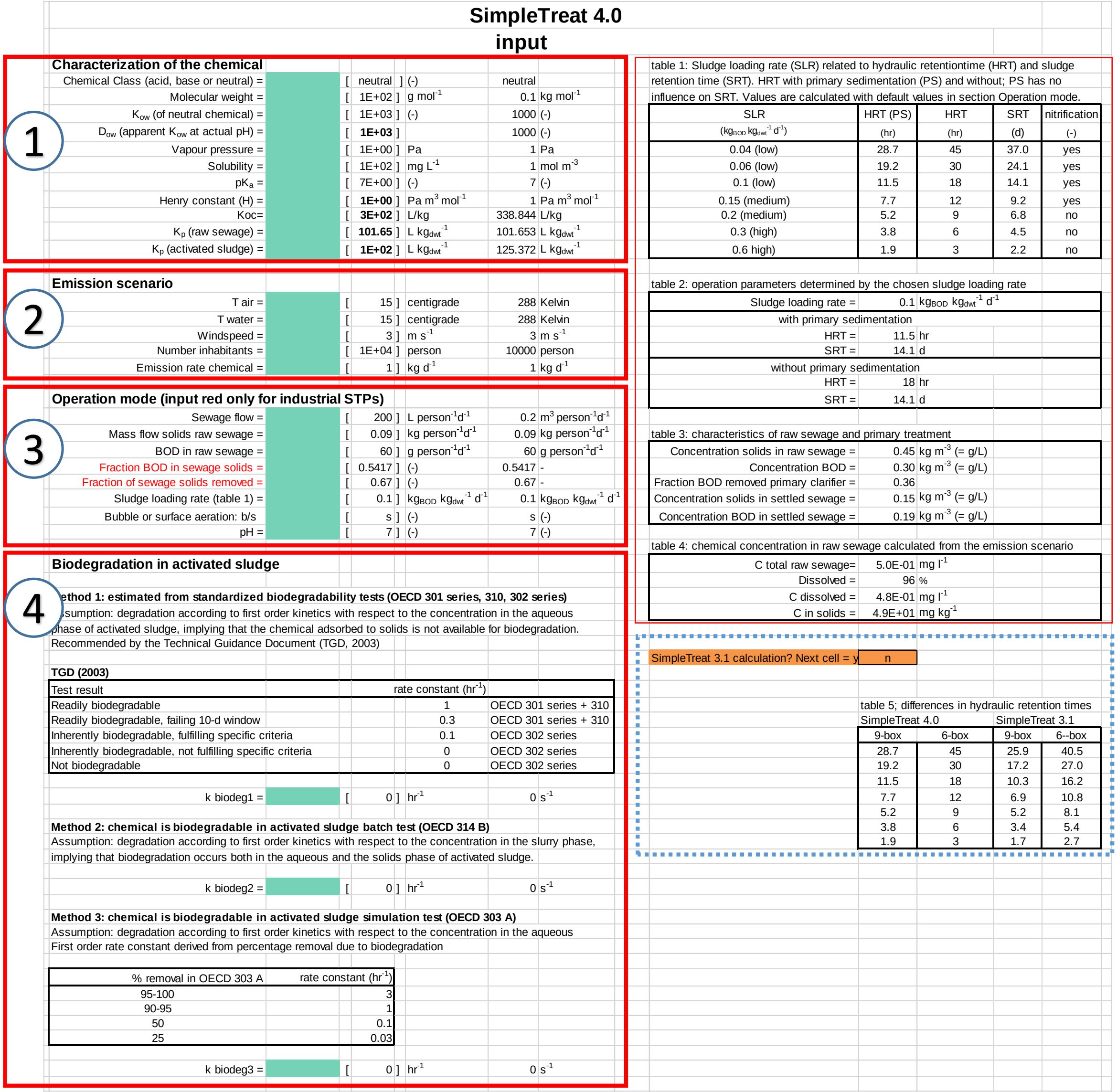
1.4 Input

The left part of the input sheet consists of four parts, indicated by four solid frames in Figure 4:

1. Characterization of the chemical
2. Emission scenario
3. Operation mode (of the communal sewage treatment plant)
4. Biodegradation in activated sludge

The thin frame on the right side in Figure 4 contains auxiliary information. Some tables display data which are dependent on input data in the left part of the input sheet.

Figure 4: Input part left is numbered 1 to 4, the explanatory part and the switch to 3.1 is right



SimpleTreat 4.0
input

Characterization of the chemical

Chemical Class (acid, base or neutral) =		[neutral]	(-)	neutral	
Molecular weight =		[1E+02]	g mol^{-1}	0.1	kg mol^{-1}
K_{ow} (of neutral chemical) =		[1E+03]	(-)	1000	(-)
D_{ow} (apparent K_{ow} at actual pH) =		[**1E+03**]		1000	(-)
Vapour pressure =		[1E+00]	Pa	1	Pa
Solubility =		[1E+02]	mg L^{-1}	1	mol m^{-3}
pK_a =		[7E+00]	(-)	7	(-)
Henry constant (H) =		[**1E+00**]	Pa m^3 mol^{-1}	1	Pa m^3 mol^{-1}
Koc=		[**3E+02**]	L/kg	338.844	L/kg
K_p (raw sewage) =		[**101.65**]	L kg$_{dwt}^{-1}$	101.653	L kg$_{dwt}^{-1}$
K_p (activated sludge) =		[**1E+02**]	L kg$_{dwt}^{-1}$	125.372	L kg$_{dwt}^{-1}$

Emission scenario

T air =		[15]	centigrade	288	Kelvin
T water =		[15]	centigrade	288	Kelvin
Windspeed =		[3]	m s^{-1}	3	m s^{-1}
Number inhabitants =		[1E+04]	person	10000	person
Emission rate chemical =		[1]	kg d^{-1}	1	kg d^{-1}

Operation mode (input red only for industrial STPs)

Sewage flow =		[200]	L person^{-1}d^{-1}	0.2	m^3 person^{-1}d^{-1}
Mass flow solids raw sewage =		[0.09]	kg person^{-1}d^{-1}	0.09	kg person^{-1}d^{-1}
BOD in raw sewage =		[60]	g person^{-1}d^{-1}	60	g person^{-1}d^{-1}
Fraction BOD in sewage solids =		[0.5417]	(-)	0.5417	-
Fraction of sewage solids removed =		[0.67]	(-)	0.67	-
Sludge loading rate (table 1) =		[0.1]	kg$_{BOD}$ kg$_{dwt}^{-1}$ d^{-1}	0.1	kg$_{BOD}$ kg$_{dwt}^{-1}$ d^{-1}
Bubble or surface aeration: b/s		[s]	(-)	s	(-)
pH =		[7]	(-)	7	(-)

Biodegradation in activated sludge

ethod 1: estimated from standardized biodegradability tests (OECD 301 series, 310, 302 series)
ssumption: degradation according to first order kinetics with respect to the concentration in the aqueous phase of activated sludge, implying that the chemical adsorbed to solids is not available for biodegradation.
Recommended by the Technical Guidance Document (TGD, 2003)

TGD (2003)

Test result	rate constant (hr^{-1})	
Readily biodegradable	1	OECD 301 series + 310
Readily biodegradable, failing 10-d window	0.3	OECD 301 series + 310
Inherently biodegradable, fulfilling specific criteria	0.1	OECD 302 series
Inherently biodegradable, not fulfilling specific criteria	0	OECD 302 series
Not biodegradable	0	OECD 302 series

k biodeg1 =		[0]	hr^{-1}	0	s^{-1}

Method 2: chemical is biodegradable in activated sludge batch test (OECD 314 B)
Assumption: degradation according to first order kinetics with respect to the concentration in the slurry phase, implying that biodegradation occurs both in the aqueous and the solids phase of activated sludge.

k biodeg2 =		[0]	hr^{-1}	0	s^{-1}

Method 3: chemical is biodegradable in activated sludge simulation test (OECD 303 A)
Assumption: degradation according to first order kinetics with respect to the concentration in the aqueous
First order rate constant derived from percentage removal due to biodegradation

% removal in OECD 303 A	rate constant (hr^{-1})
95-100	3
90-95	1
50	0.1
25	0.03

k biodeg3 =		[0]	hr^{-1}	0	s^{-1}

table 1: Sludge loading rate (SLR) related to hydraulic retentiontime (HRT) and sludge retention time (SRT). HRT with primary sedimentation (PS) and without; PS has no influence on SRT. Values are calculated with default values in section Operation mode.

SLR (kg$_{BOD}$ kg$_{dwt}^{-1}$ d^{-1})	HRT (PS) (hr)	HRT (hr)	SRT (d)	nitrification (-)
0.04 (low)	28.7	45	37.0	yes
0.06 (low)	19.2	30	24.1	yes
0.1 (low)	11.5	18	14.1	yes
0.15 (medium)	7.7	12	9.2	yes
0.2 (medium)	5.2	9	6.8	no
0.3 (high)	3.8	6	4.5	no
0.6 high)	1.9	3	2.2	no

table 2: operation parameters determined by the chosen sludge loading rate

Sludge loading rate =	0.1	kg$_{BOD}$ kg$_{dwt}^{-1}$ d^{-1}
with primary sedimentation		
HRT =	11.5	hr
SRT =	14.1	d
without primary sedimentation		
HRT =	18	hr
SRT =	14.1	d

table 3: characteristics of raw sewage and primary treatment

Concentration solids in raw sewage =	0.45	kg m^{-3} (= g/L)
Concentration BOD =	0.30	kg m^{-3} (= g/L)
Fraction BOD removed primary clarifier =	0.36	
Concentration solids in settled sewage =	0.15	kg m^{-3} (= g/L)
Concentration BOD in settled sewage =	0.19	kg m^{-3} (= g/L)

table 4: chemical concentration in raw sewage calculated from the emission scenario

C total raw sewage=	5.0E-01	mg l^{-1}
Dissolved =	96	%
C dissolved =	4.8E-01	mg l^{-1}
C in solids =	4.9E+01	mg kg^{-1}

SimpleTreat 3.1 calculation? Next cell = y | n

table 5; differences in hydraulic retention times

SimpleTreat 4.0		SimpleTreat 3.1	
9-box	6-box	9-box	6--box
28.7	45	25.9	40.5
19.2	30	17.2	27.0
11.5	18	10.3	16.2
7.7	12	6.9	10.8
5.2	9	5.2	8.1
3.8	6	3.4	5.4
1.9	3	1.7	2.7

The thin dashed frame contains a switch between version 4.0 and the former version 3.1. Hydraulic retention times (HRT) in table 1 in Figure 4 change if the switch is set from "*n*" (default) to "*y*" (SimpleTreat 3.1). Default in SimpleTreat 4.0 "*n*". Table 5 in Figure 4 shows the difference in HRT between versions 4.0 and 3.1.

Characterization of the chemical and *Biodegradation in activated sludge* are the most important sections for the computation of the relative fate of the chemical and relative emission rates. Data block *Emission scenario* is needed to calculate the absolute emission rates and concentrations in water and sludge emitted by the STP. The chemical concentration in air may indicate occupational exposure but this falls beyond regulatory application of the model. *Operation mode STP* has default settings of the average STP in the EU. Only if special scenarios are considered, input parameters can be adjusted with respect to the sludge loading rate and the aeration mode. It is not recommended to change input parameters like *Fraction BOD in sewage solids* or *Fraction of sewage solids removed*. For regulatory risk assessment input should be avoided. These parameters are used to specify the fate of a chemical in the primary clarifier which may be necessary to simulate treatment of industrial wastewater. For application of SimpleTreat 4.0 in North America, changing parameters in the input block *Operation mode STP* is not adequate as special adaptations inside the model are necessary. This is also the case if the model is applied for chemical fate simulations in an industrial wastewater treatment plant. For regulatory application in the EU nothing should be changed in *Operation mode STP*.

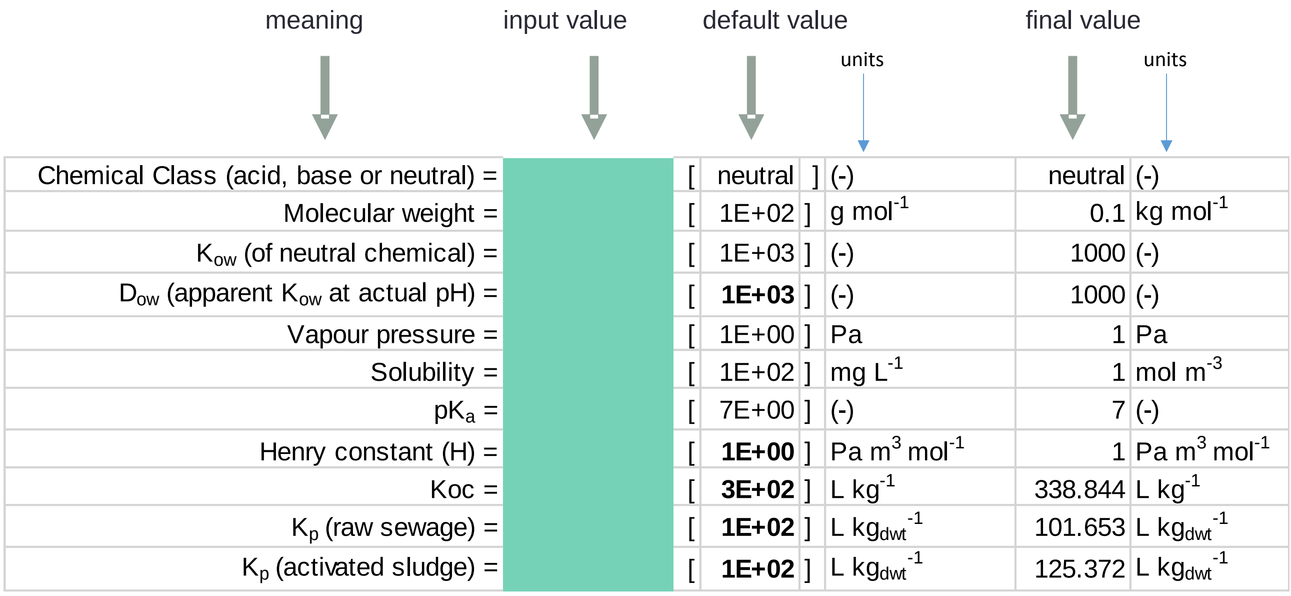
The thin frame of Figure 4 (upper right) contains several explanatory tables. In the input sheet, table 1 is an extended version of Table 1 in this manual. Tables 2 to 4 display the consequence of chosen input parameters by showing information on the mode of operation (tables 2 and 3) and the concentration and partitioning of the chemical in raw sewage (table 4).

The lower right part of the input sheet inside the dashed frame contains an input cell that functions as a switch between SimpleTreat versions 4.0 and 3.1. Differences in hydraulic retention times (HRT) between version 3.1 and 4.0 are given by table 5. Note that in version 4.0 the HRT is longer than in version 3.1. There is no difference in sludge retention times (SRT) between version 3.1 and 4.0. The SLR is only dependent on the chosen sludge loading rate. Default settings with regard to the version of SimpleTreat are "n" (no) which means that the model conducts a computation according to SimpleTreat 4.0. Chapter 5 gives a motivation and further details why the model contains this switch.

1.4.1 Characterization of the chemical

This part is concerned with the chemical properties (Figure 5). The first column contains the symbol or meaning of the chemical property. In the shaded 2nd column an input value has to be filled in with units as indicated by the default value column. The default value is either fixed or calculated (bold). If the input parameter is dimensionless, the final value equals the default value when the cell input value is empty, otherwise the input value is selected. Note that the final value may have different units than the input value. For example *Solubility* has an input value in mg/L whereas the final value is converted by the model into mol/m^3.

Figure 5: Chemical properties part of the input sheet in EXCEL™ format



Chemical Class (acid, base or neutral) =	🟩	[neutral]	(-)	neutral	(-)
Molecular weight =	🟩	[1E+02]	g mol^{-1}	0.1	kg mol^{-1}
K_{ow} (of neutral chemical) =	🟩	[1E+03]	(-)	1000	(-)
D_{ow} (apparent K_{ow} at actual pH) =	🟩	[**1E+03**]	(-)	1000	(-)
Vapour pressure =	🟩	[1E+00]	Pa	1	Pa
Solubility =	🟩	[1E+02]	mg L^{-1}	1	mol m^{-3}
pK_a =	🟩	[7E+00]	(-)	7	(-)
Henry constant (H) =	🟩	[**1E+00**]	Pa m^3 mol^{-1}	1	Pa m^3 mol^{-1}
Koc =	🟩	[**3E+02**]	L kg^{-1}	338.844	L kg^{-1}
K_p (raw sewage) =	🟩	[**1E+02**]	L kg_{dwt}^{-1}	101.653	L kg_{dwt}^{-1}
K_p (activated sludge) =	🟩	[**1E+02**]	L kg_{dwt}^{-1}	125.372	L kg_{dwt}^{-1}

1.4.1.1 Chemical class

Chemical Class (acid, base or neutral) =	🟩	[neutral]	(-)	neutral	(-)

If nothing is filled in, SimpleTreat 4.0 assumes that the chemical is neutral or not dissociated. If *acid* or *base* is inserted, decisions are made by the model regarding:

1. the computation of the fraction of the compound that is in the neutral state at pH = 7
2. the selection of the equation to calculate the organic carbon-water partition coefficient

1.4.1.2 Molecular weight

Molecular weight =	🟩	[1E+02]	g mol^{-1}	0.1	kg mol^{-1}

The default value of *Molecular weight* is 100 g per mol. Conversion into kg per mol is conducted by the model in the last column.

1.4.1.3 Kow (of a neutral chemical)

K_{ow} (of neutral chemical) =	🟩	[1E+03]	(-)	1000	(-)

Kow is the n-octanol-water partition coefficient of the chemical. It characterizes the hydrophobicity of the authentic chemical: not dissociated and neutral. If the chemical can exist only in the neutral state, input is straightforward. If the chemical is (partly) dissociated because it is an acid or base, *Kow* refers to conditions in which the chemical predominantly exists in the neutral state. This may imply that the *Kow* is experimentally determined under conditions considerably lower or higher than pH = 7, or calculated from QSARs.

1.4.1.4 Dow (apparent Kow at actual pH)

D_{ow} (apparent K_{ow} at actual pH) =		[	**1E+03**	]	(-)	1000	(-)

Dow is a new parameter in the SimpleTreat model and is only used if the chemical class is *base*. The Dow of an organic compound is the *apparent* n-octanol-water partition coefficient at the actual pH. This implies that determination of the n-octanol-water partition coefficient is not necessarily at a pH at which the chemical is largely in the neutral state. Dow is the n-octanol-water partition coefficient of all species of the chemical (neutral and ionized) at an actual pH. In sewage treatment systems the actual pH equals 7. If Dow of a base is not given, SimpleTreat 4.0 *calculates* a default value (printed in bold) from Kow (of the neutral molecule) and the pKa of a base. Appendix B gives an explanation.

1.4.1.5 Vapour pressure

Vapour pressure =		[	1E+00	]	Pa	1	Pa

The default value of *Vapour pressure* is fixed at 1 Pa. The final value has similar units.

1.4.1.6 Water solubility

Solubility =		[	1E+02	]	mg L^{-1}	1	mol m^{-3}

The default water *Solubility* is fixed at 100 mg/L. Note that the final value is converted into mol/m^3.

1.4.1.7 The negative logarithm of the acid dissociation constant, pKa

pK_a =		[	7E+00	]	(-)	7	(-)

In SimpleTreat 3.1 two different dissociation constants were distinguished as input parameters, Ka for acids and Kb for organic bases. In SimpleTreat 4.0 the required information concerning the ionic dissociation equilibrium has to be provided by the operator in a different way. Again two parameters are needed but now it is *Chemical Class* which determines if the chemical is an *acid* or *base* and the negative logarithm of the acid dissociation constant, pKa. This information is sufficient to calculate the fraction of the neutral species in water (see also Appendix A) for both acids and bases.

For a monovalent acid HA, partial dissociation results in two species: the neutral HA and the negatively charged A^-:

$$\mathrm{HA} \leftrightarrow \mathrm{H}^+ + \mathrm{A}^-$$

The acid dissociation constant (Ka) is defined as:

$$\mathrm{Ka} = \frac{[\mathrm{H}^+] \cdot [\mathrm{A}^-]}{[\mathrm{HA}]}$$

The pKa is the negative logarithm of Ka.

An organic base (B) dissociates according to:

$$\mathrm{B} + \mathrm{H_2O} \leftrightarrow \mathrm{BH}^+ + \mathrm{OH}^-$$

with the base dissociation constant:

$$\mathrm{Kb} = \frac{[\mathrm{BH}^{+}] \cdot [\mathrm{OH}^{-}]}{[\mathrm{B}]}$$

According to modern conventions, regarding organic base (B) only the conjugated acid (HB^+) is considered to define the ionic dissociation constant. HB^+ dissociates according to:

$$\mathrm{BH}^{+} \leftrightarrow \mathrm{B} + \mathrm{H}^{+}$$

The dissociation constant of the conjugated acid HB^+ of base B is also called Ka:

$$\mathrm{Ka} = \frac{[\mathrm{B}] \cdot [\mathrm{H}^{+}]}{[\mathrm{BH}^{+}]}$$

If only the Kb or pKb of a base is given, the required input parameter pKa of the conjugated acid HB^+ of base B is easily obtained:

$$\mathrm{pKa} = 14 - \mathrm{pKb}$$

1.4.1.8 Henry constant

Henry constant (H) =		[	**1E+00**	]	Pa m^3 mol^{-1}	1	Pa m^3 mol^{-1}

The Henry constant *H* is a measure for the partition of a chemical between air and water. If there is no measured *H* known, SimpleTreat 4.0 estimates H as the ratio of the vapour pressure (in Pa) and the water solubility (in mol/m^3). Note that with default values for vapour pressure (1 Pa), water solubility (100 mg/L = 100 g/m^3) and molecular weight (100 g/mol), the default value of H must be equal to 1 Pa·m^3/mol. Sometimes a “dimensionless Henry constant” is given, often indicated by symbols like H’ or Kaw (which is in fact the air-water partition coefficient). Conversion to H requires the absolute temperature (in K):

$$\mathrm{H} = \mathrm{Kaw} \cdot \mathrm{R} \cdot \mathrm{T} = \mathrm{H}^{'} \cdot \mathrm{R} \cdot \mathrm{T}$$

R is the universal gas constant (8.314 J·K^{-1}·mol^{-1}).

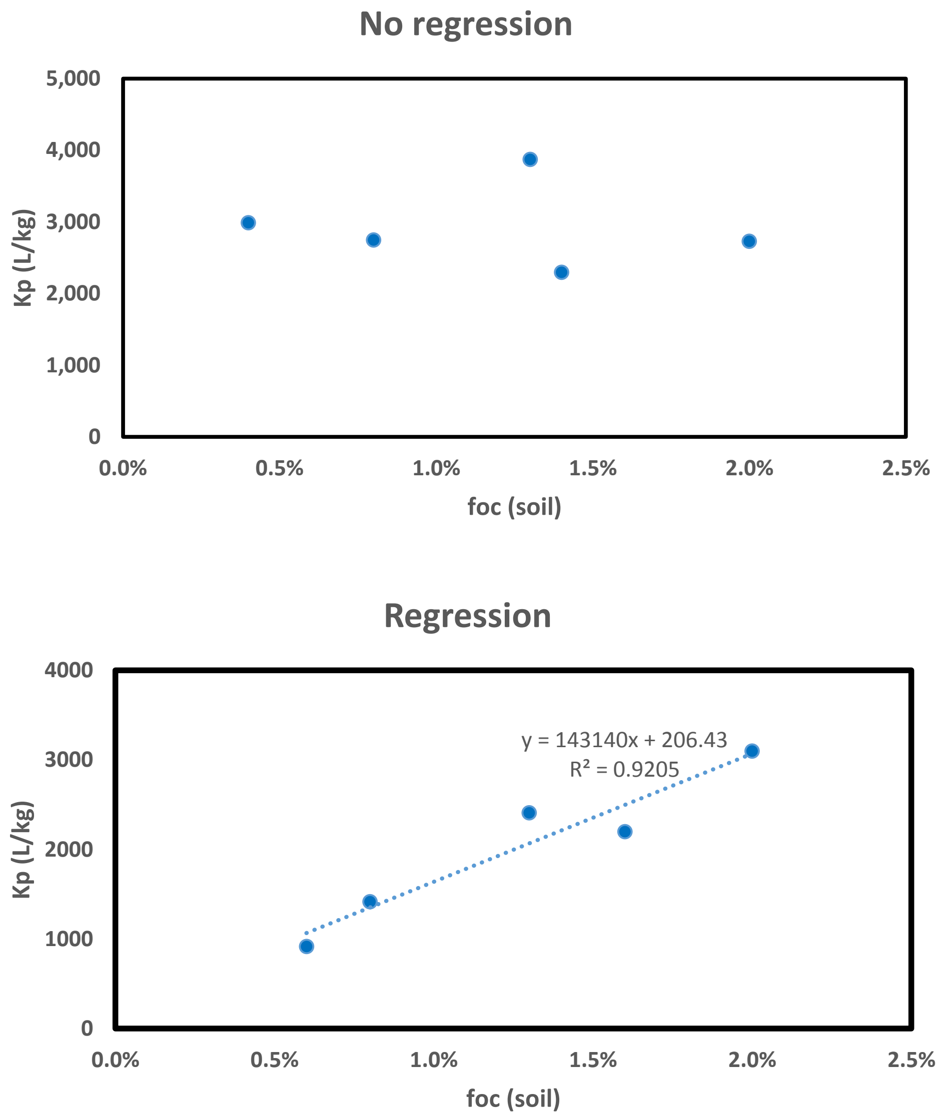
1.4.1.9 Koc

Koc =		[	**3E+02**	]	L kg^{-1}	338.844	L kg^{-1}

The property *Koc* is the organic carbon-water partition coefficient. It is also known as the “organic carbon normalized partition coefficient”. This means that the Koc equals the ratio of Kp, the solids-water partition coefficient (L/kg), and the organic carbon fraction (foc) of the solids. Both Kp and foc are determined directly. An experimentally determined Koc is always the result of two determinations: Kp and foc. If Koc has been determined experimentally, for example with OECD Test Guideline 106 (OECD, 2000), also a value of foc is available. The parameter Koc suggests that solids-water partitioning of an organic chemical is governed by the “organic carbon phase” in settled or suspended particles in water. Behaviour of organic chemicals in the real world is however complicated by several factors. Therefore we distinguish Koc related to sewage from Koc with respect to activated sludge and soil.

Koc activated sludge. In principle, an experimentally obtained Koc is preferred over an estimated Koc. The organic carbon fraction (foc) of activated sludge is rather constant. It is in the range between 35 and 40 %. Partitioning of organic chemicals between suspended particles with a high carbon content and water is most often dominated by foc and less by other characteristics of activated sludge.

Figure 6: Measured Kp values of an organic chemical plotted versus foc in 5 soils with varying organic carbon contents



Koc soil. For Koc determined in soil, the situation is different. A measured Koc in soil cannot be used without reservations. The value of foc of (suspended) solids in raw sewage (0.3) and activated sludge (0.37) is much higher than in natural systems. In soil, foc is more than a factor of ten lower (f.i. 0.02) and in sediment it is around 0.05. Only in suspended solids in freshwater it can be as high as 0.1 (TGD, 2003), but it is still significantly lower than in activated sludge. Extrapolation from soil to activated sludge solids is therefore problematic. Koc derived from soil measurements with soil particles containing only 1 % organic carbon, may be flawed by the fact that a measured Kp can also be influenced by other factors than foc. For example, cat-ion exchange capacity, lumen content and pH may be more important than foc. As a result, the Koc of a chemical in soil, might be unreliable information with respect to Koc for activated sludge.

In the regulatory framework biocides, usually several Koc values have to be provided, most often five. Unfortunately, almost always Koc is determined in soil. It is therefore recommended to confirm that partitioning between soil particles and water is predominantly affected by the organic carbon content of soil particles. This can be done by plotting Kp versus foc as shown in Figure 6. If the dossier contains pairs of Koc and foc for each soil sample, the Kp for each soil is obtained as the product of Koc and foc. A test to recognize that foc is the dominating factor is conducted by plotting the Kp versus the organic carbon fraction in the soil, foc. Figure 6 illustrates how such plots may look like.

If there is no regression (upper part of Figure 6), Koc although experimentally determined, may not be the accurate input parameter. The Kp may be the result of other interactions between the chemical and soil particles than association with the organic carbon content of soil particles.

A positive correlation (lower panel of Figure 6) indicates the predominant role of the organic matrix in soil when a chemical partitions between soil solids and water. The average value of the ratio of Kp and foc may be used as input parameter for Koc.

1.4.1.10 Kp (raw sewage)

K_p (raw sewage) =	🟩	[	**1E+02**	]	L kg_{dwt}^{-1}	101.653	L kg_{dwt}^{-1}

OECD Test Guideline 106 (OECD, 2000) provides methods to obtain equilibrium adsorption coefficients for a chemical in various soils sediments and sludge. This equilibrium partition coefficient applies to both raw and settled sewage. Usually, this parameter is not an experimentally observed quantity but if available it should be used without restriction. Communal sewage resembles activated sludge, especially with respect to the high fraction organic carbon in the solids fraction (≈ 30 %). A measured Kp of raw or settled sewage is suitable as direct input but if absent, a measured Kp for activated sludge can be used. If Kp for activated sludge is available, Kp sewage is estimated by the model from multiplication of Kp activated sludge with the factor 0.3/0.37. This factor is the ratio of the foc (sewage) and foc (activated sludge). SimpleTreat 4.0 gives this approach a higher priority than Koc determined from soil measurements or other estimation methods.

1.4.1.11 Kp (activated sludge)

K_p (activated sludge) =	🟩	[	**1E+02**	]	L kg_{dwt}^{-1}	125.372	L kg_{dwt}^{-1}

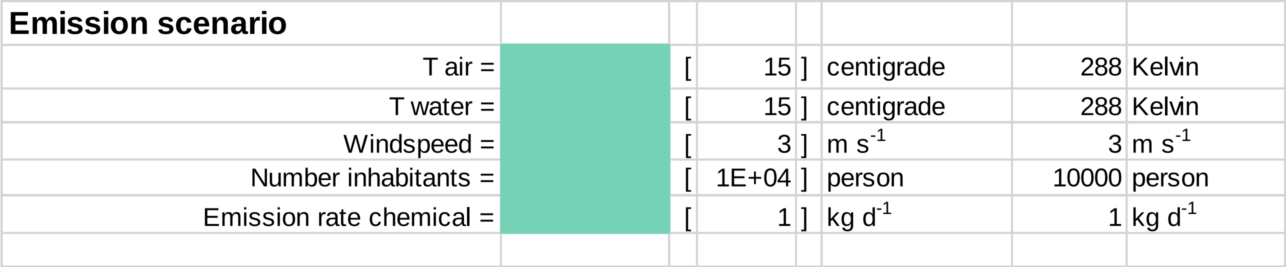
A measured partition coefficient of a chemical in activated sludge is of high value and can be used directly. It can also be applied to derive accurately a Kp for raw and settled sewage as explained above. If an experimental Kp activated sludge is not available, it is estimated from an experimentally determined Koc for that chemical, provided that there are no restrictions as illustrated by Figure 6, otherwise it is assessed from quantitative structure/property activity relationships for neutral and ionized organic chemicals (see RIVM report by Struijs, 2014).

1.4.2 Emission scenario

The *Emission rate chemical* (Figure 7) is required if absolute emission rates of the chemical to air, water and soil are desired. *Number inhabitants* determines the rates of discharge of effluent and production of sludge per day. These rates are necessary for real chemical concentrations in effluent and sludge.

The default temperature in air and water (*T air* and *T water*) and *Wind speed* reflects standard conditions as they are applied in generic exposure and risk assessment in the EU (TGD, 2003).

Figure 7: Emission scenario part of the input sheet in EXCEL™ format

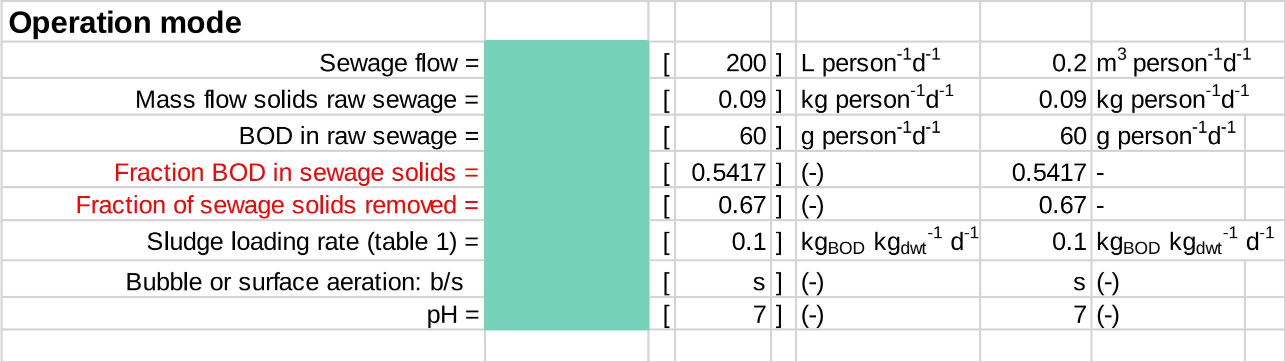


Emission scenario							
T air =		[	15	]	centigrade	288	Kelvin
T water =		[	15	]	centigrade	288	Kelvin
Windspeed =		[	3	]	m s^{-1}	3	m s^{-1}
Number inhabitants =		[	1E+04	]	person	10000	person
Emission rate chemical =		[	1	]	kg d^{-1}	1	kg d^{-1}

1.4.3 Operation mode of the sewage treatment plant

It is strongly recommended to accept all default values in this part of the input sheet. The first three input data (*Sewage flow*, *Mass flow solids raw sewage* and *BOD in raw sewage*) define the average communal sewage and sewage treatment in Europe. They are also used in generic exposure assessment at all scales (local and regional) in the EU (TGD, 2003). The parameters *Fraction BOD in sewage solids* and *Fraction of sewage solids* removed (printed in red) affect the operation of the primary clarifier. The default values are appropriate for exposure assessment of an average communal STP in the EU. The *Sludge loading rate* may deviate from the default value of 0.1 kg$_{BOD}$ per kg dry weight activated sludge per day. Also the aeration mode (*Bubble or surface aeration*) may be altered if justified by specific information on the local scenario. Values of the sludge loading rate exceeding the highest and lowest values in Table 1 should be avoided. There are no reasons to reject the default pH if communal sewage treatment is concerned.

Figure 8: Operation mode in the input sheet in EXCEL™ format



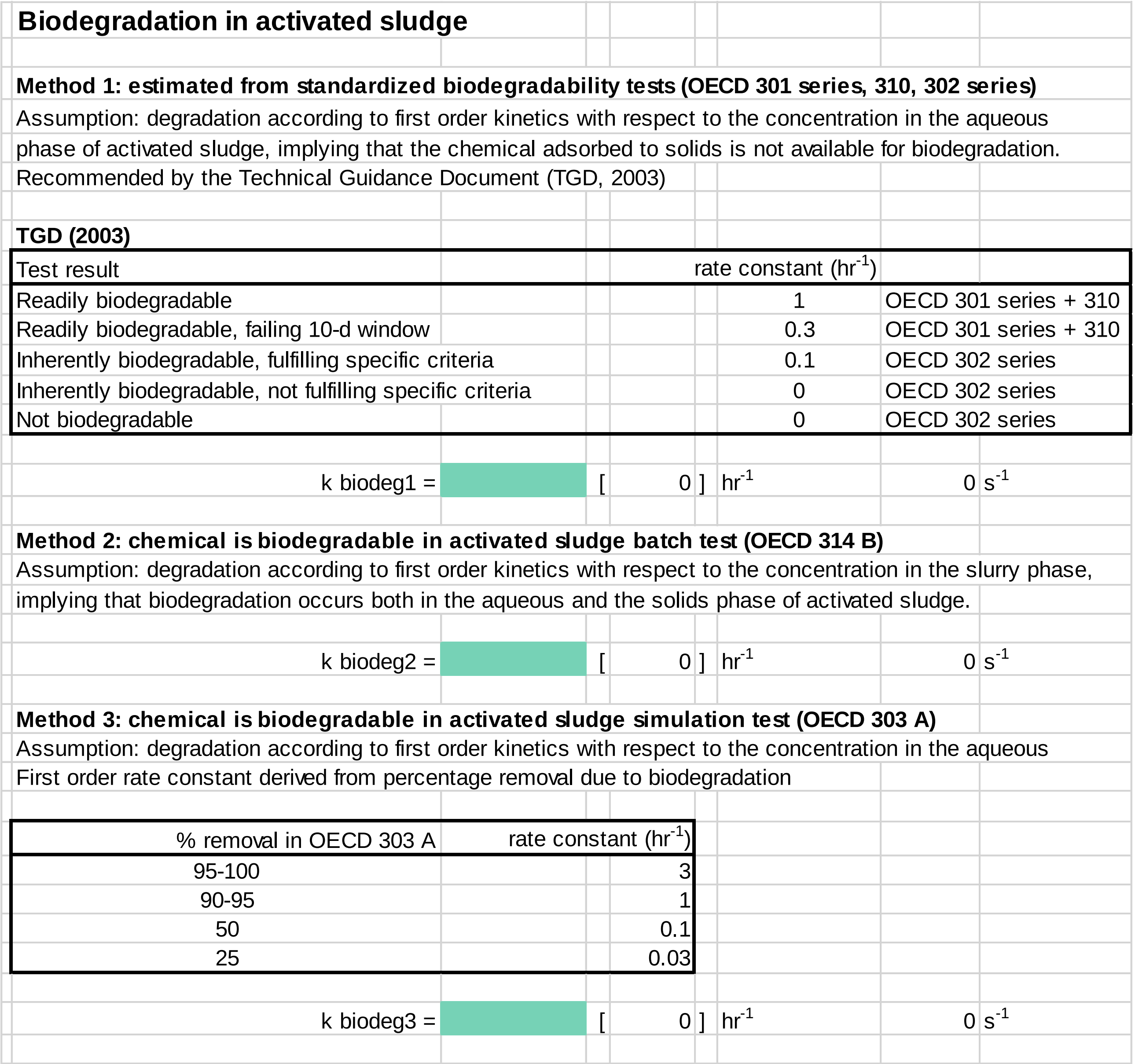
Operation mode							
Sewage flow =		[	200	]	L person^{-1}d^{-1}	0.2	m^3 person^{-1}d^{-1}
Mass flow solids raw sewage =		[	0.09	]	kg person^{-1}d^{-1}	0.09	kg person^{-1}d^{-1}
BOD in raw sewage =		[	60	]	g person^{-1}d^{-1}	60	g person^{-1}d^{-1}
Fraction BOD in sewage solids =		[	0.5417	]	(-)	0.5417	-
Fraction of sewage solids removed =		[	0.67	]	(-)	0.67	-
Sludge loading rate (table 1) =		[	0.1	]	kg$_{BOD}$ kg$_{dwt}^{-1}$ d^{-1}	0.1	kg$_{BOD}$ kg$_{dwt}^{-1}$ d^{-1}
Bubble or surface aeration: b/s		[	s	]	(-)	s	(-)
pH =		[	7	]	(-)	7	(-)

1.4.4 Biodegradation in activated sludge

SimpleTreat 4.0 subdivides the relevant standard tests in the OECD test system into three levels which differ in stringency, complexity (and costs) and predicting power. If more biodegradability tests results are given, the model assigns a first order degradation rate constant according to the priority:

Result Method 3 > Result Method 2 > Result Method 1

Figure 9: Biodegradation section in the input sheet in EXCEL™ format



Biodegradation in activated sludge

Method 1: estimated from standardized biodegradability tests (OECD 301 series, 310, 302 series)

Assumption: degradation according to first order kinetics with respect to the concentration in the aqueous phase of activated sludge, implying that the chemical adsorbed to solids is not available for biodegradation.

Recommended by the Technical Guidance Document (TGD, 2003)

TGD (2003)

Test result	rate constant (hr^{-1})	
Readily biodegradable	1	OECD 301 series + 310
Readily biodegradable, failing 10-d window	0.3	OECD 301 series + 310
Inherently biodegradable, fulfilling specific criteria	0.1	OECD 302 series
Inherently biodegradable, not fulfilling specific criteria	0	OECD 302 series
Not biodegradable	0	OECD 302 series

k biodeg1 = 🟩 [0] hr^{-1} 0 s^{-1}

Method 2: chemical is biodegradable in activated sludge batch test (OECD 314 B)

Assumption: degradation according to first order kinetics with respect to the concentration in the slurry phase, implying that biodegradation occurs both in the aqueous and the solids phase of activated sludge.

k biodeg2 = 🟩 [0] hr^{-1} 0 s^{-1}

Method 3: chemical is biodegradable in activated sludge simulation test (OECD 303 A)

Assumption: degradation according to first order kinetics with respect to the concentration in the aqueous

First order rate constant derived from percentage removal due to biodegradation

% removal in OECD 303 A	rate constant (hr^{-1})
95-100	3
90-95	1
50	0.1
25	0.03

k biodeg3 = 🟩 [0] hr^{-1} 0 s^{-1}

Method 1 For substance regulation it is recommended to apply the rate constants as shown in the table of TGD (2003) shown in the first table of this part of the input sheet. This category includes screening tests, both on the soft side for the selection of chemicals that are readily biodegradable (OECD 301 series and OECD 310) and on the hard side to identify persistent substances (OECD 302 series). The table in input block (Figure 9) displays the rate constants in reciprocal hours as recommended by the TGD (2003) and REACH (2006). These first order rate constants are rather conservative. For example, if a chemical degrades in an inherent biodegradability test (OECD 302 series) but “specific criteria” are not met, a rate constant equal to 0 is assigned. Although the chemical appears biodegradable, it is considered persistent. This approach is an incentive to conduct further testing, for example a simulation test such as the OECD 303 test for biodegradation during the activated sludge process. If the same chemical is biodegradable in the OECD 303 test and it is eliminated for more than 90 % exclusively due to biodegradation, a rate constant equal to 1 hr^{-1} is assigned in Method 3. In this example, the hierarchy above causes overruling the zero rate constant obtained in Method 1 by setting the first order biodegradation rate constant to 1 hr^{-1} derived from Method 3.

<u>Method 2</u> This is a simulation tests to assess the biodegradability of chemicals discharged in wastewater. This guideline describes a group of methods for determining the extent and kinetics of primary and ultimate biodegradation of organic chemicals whose route of entry into the environment begins with their discharge to wastewater. The second test, OECD 314B, is the most relevant test in this series. It evaluates biodegradation during a widely used form of biological sewage treatment. The other tests are focused on biodegradation in the sewer system, in the anaerobic reactor, in the mixing zone of receiving surface water etc. As input for SimpleTreat 4.0 only the results of OECD 314B should be considered.

<u>Method 3</u> OECD 303 describes the simulation of the two main types of aerobic biological waste water treatment (activated sludge and percolating, or trickling, filtration). OECD 303 A applies to the activated sludge system. The results obtained from this test can be interpreted according to the table in Figure 9 to obtain an input parameter.

1.4.5 Examples

In the following examples (exercises) an equation is used (see Appendix B) to calculate the neutral fraction (Fn) of an organic acid or base in water at a specified pH:

$$\mathrm{Fn} = \frac{C_n^w}{C_n^w + C_{ion}^w} = \frac{1}{1 + 10^{\gamma \cdot (\mathrm{pH} - \mathrm{pKa})}}$$

In this equation the concentration non-dissociated, C_n, and ionized, C_{ion}, refer to aqueous concentrations and the superscript w is here not really necessary. SimpleTreat 4.0 assigns a value of 1 to γ if the chemical is an acid. If it is a base γ is equal to -1.

In SimpleTreat 4.0, the estimation of Koc of a base only requires only the parameter Dow (Struijs, 2014 & Franco et al. 2013).

<u>Case 1</u>

A weak organic acid (**HA1**, molecular weight is 210 g/mol) ionizes in water according to pKa = 5. The water solubility (300 mg/L) and the vapour pressure (0.001 Pa) refer to the neutral chemical.

There are no measured values for partition coefficients such as Kp (solids-water) or Koc. The biodegradability is characterized as “readily biodegradable failing the 10-day time window”.

The n-octanol-water partition coefficient of the neutral chemical is not available. There are in the dossier however, two different experimental values for Kow referring to two different pH levels:

Kow (pH = 5) = 500

Kow (pH = 7) = 10

How can we obtain the appropriate input parameters for this chemical?

Answer: All parameters are available with the exception of Kow of the neutral chemical. At pH 5 and 7 the chemical is in the ionized state for 50 % or more as can be verified by means of the equation for Fn. In fact the reported Kow values are equivalent to Dow (pH = 5) and Dow (pH = 7) as Dow is the Kow at “ambient pH” which is here 5 and 7, respectively. Kow of the neutral chemical is evaluated according to the relationship (see Appendix B):

$$\mathrm{Dow(pH)} \approx \mathrm{Fn(pH)} \cdot \mathrm{Kow}$$

If pH is equal to 5, this equation is evaluated as:

$$\mathrm{Dow(pH = 5)} \approx \mathrm{Fn(pH = 5)} \cdot \mathrm{Kow}$$

It is easily derived that Fn (pH = 5) is exactly equal to ½. Hence the correct input value for Kow is 1000. This is Kow of the neutral form of the organic acid which is the required input in the model.

Is this congruent with Kow (pH = 7) equal to 10? Note that this is similar to Dow (pH = 7) = 10.

$$\mathrm{Dow(pH = 7)} \approx \mathrm{Fn(pH = 7)} \cdot \mathrm{Kow}$$

The answer is yes. The neutral fraction, Fn, at pH = 7 is approximately equal to 0.01. Also from this relation, it follows that Kow is approximately equal to 1000.

Now appropriate input parameters are complete for computation with SimpleTreat 4.0.

Case 2

A rather strong organic base (**B1**, mol weight = 100 g/mol) has a pKb equal to 4. The water solubility (of the neutral form) is 2 mg/L and the vapour pressure is 0.01 Pa; biodegradability is zero. There are no measured values for partition coefficients such as Kp (solids-water) or Koc. Kow is measured at different pH:

Kow (pH = 9) = 15

Kow (pH = 7) = 0.17

Are these measured Kow values consistent? How can we use these data in the model?

First, SimpleTreat 4.0 doesn’t recognize pKb. First, pKb of base B value has to be converted into pKa of the conjugated acid (HB+): pKa = 14 – pKb, hence pKa = 10. However, because the chemical is an organic base, only the Dow at pH = 7 is required. This is similar to Kow (pH = 7) which is equal to 0.17. This value can be used as input and the model estimates a Koc value from which the partition coefficients are derived.

The Kow of the neutral chemical is calculated from:

$$\mathrm{Dow(pH = 9)} \approx \mathrm{Fn(pH = 9)} \cdot \mathrm{Kow}$$

Fn (pH = 9) equals $1/(1+10^1) \approx 0.09$, hence Kow = $15/0.09 \approx 167$

This value is consistent with the result of the alternative computation:

Fn (pH = 7) equals $1/(1+10^3) \approx 0.001$, hence Kow = $0.17/0.001 \approx 170$

Case 3

A weak organic base (**B2**, mol weight = 350 g/mol) has a pKa equal to 5. The water solubility (of the neutral form) is 10 mg/L and the vapour pressure is 0.0001 Pa; biodegradability is zero. There are no measured values for partition coefficients such as Kp (solids-water) or Koc. Kow is known measured at different pH:

Kow (pH = 5) = 300

Kow (pH = 7) = 600

Are these measured Kow values consistent and how can we use these data in the model?

Answer: it is a base and Dow (pH = 7) is known because it is equal to Kow (pH = 7). For an organic base a value for pKa is not needed to estimate Koc, only Dow (pH = 7). Note that Kow at neutral pH approximates Dow (pH = 7) and that is sufficient for the estimation routine of Koc. Furthermore, at pH = 7 the chemical is predominantly in the non-dissociated form. At pH 5 however, the fraction neutral (Fn) is ½:

$$\mathrm{Dow(pH = 5)} \approx \frac{1}{2} \cdot \mathrm{Kow} = 300$$

It can be concluded that the measured Kow data at two different pH values are consistent and that Kow = 600 should be used which is equal to Kow (pH = 7).

Case 4

A rather strong organic acid (**HA2**, molecular weight is 110 g/mol) has a ionic dissociation constant pKa = 2.5. The water solubility (120 mg/L) and the vapour pressure (0.001 Pa) refer to the neutral chemical.

There are no measured values for partition coefficients such as Kp (solids-water) or Koc. The biodegradability is characterized as “inherently biodegradable fulfilling special criteria”, however in the OECD 303 simulation test the chemical is not detectable in the effluent.

The n-octanol-water partition coefficient of the neutral chemical is not available. Two different experimental Kow’s are mentioned in the dossier referring to two different pH levels:

Kow (pH = 3) = 500

Kow (pH = 5) = 7

What are the appropriate input parameters for this chemical?

Answer: Dow (pH = 3) is known because it is equal to Kow (pH = 3), being 500, from which Kow (neutral state) can be computed.

$$\mathrm{Dow(pH = 3)} \approx \mathrm{Fn(pH = 3)} \cdot \mathrm{Kow}$$

Fn (pH = 3) is $1/(1+10^{(3-2.5)}) = 1/(1+10^{0.5}) = 0.24$. Kow equals $500/0.24 = 2081$. This value can be used and is rather consistent with Kow (pH = 5) = 7. With Fn (pH = 5) = 0.00315 it can be derived that Kow of the neutral chemical would be equal to 2222. This value is close to 2081 considering the lack of precision in the determinations.

The water solubility requires special care as only at pH = 1 the chemical is dominantly in the neutral state.

The rate constant for biodegradation is 3 hr^{-1} to be filled in Method 3. SimpleTreat 4.0 automatically overrules 0.1 hr^{-1} assigned to the first order biodegradation rate constant according to Method 1.

Case 5

An organic base (pKa = 9) has a Dow (pH = 7) equal to 10,000. In 5 different soils the organic carbon fraction was measured. The measured partition coefficients (Kp) are shown in Table 2.

Table 2: Measured partition coefficients of an organic base with pKa = 9 in 5 different soils

foc soil measured [%]	Kp soil measured [L/kg]	Koc [L/kg]
2.10	2410	$1.15 \cdot 10^5$
0.20	920	$4.60 \cdot 10^5$
0.10	900	$2.90 \cdot 10^6$
2.50	780	$3.12 \cdot 10^4$
0.80	1420	$1.78 \cdot 10^5$

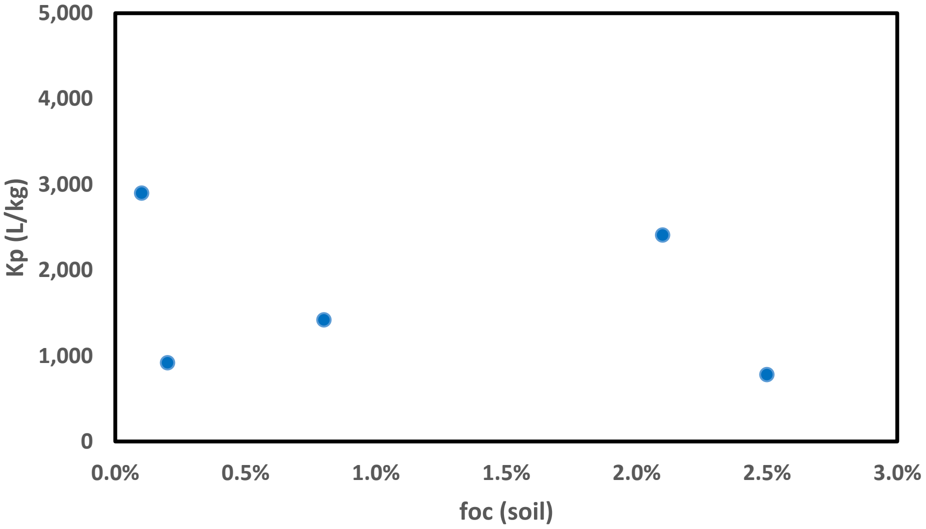
Which Koc value can be used as input?

Note that Koc values scatter over two orders of magnitude. The average of these five Koc's is $7.4 \cdot 10^5$, however the standard deviation is even higher $1.2 \cdot 10^6$. The coefficient of variation is high: 1.66 (= $1.2 \cdot 10^6 / 7.4 \cdot 10^5$). We suspect that partitioning between the soil organic carbon phase and water is not a good indicator for sorption and that the Koc derived from this dataset is not reliable. This is confirmed in a plot of Kp versus foc (Figure 10) which clearly shows that the measured soil-water partition coefficient is independent of foc.

If we reject a "measured Koc", what is then the alternative?

Answer: use only Dow (10,000) as input parameter and have confidence in the estimation of Koc by SimpleTreat 4.0. It appears that SimpleTreat 4.0 estimates Koc = $1.0 \cdot 10^4$ L/kg which is considerably lower than $7.4 \cdot 10^5$ and also half an order of magnitude lower than the lowest of the 5 soil Koc's.

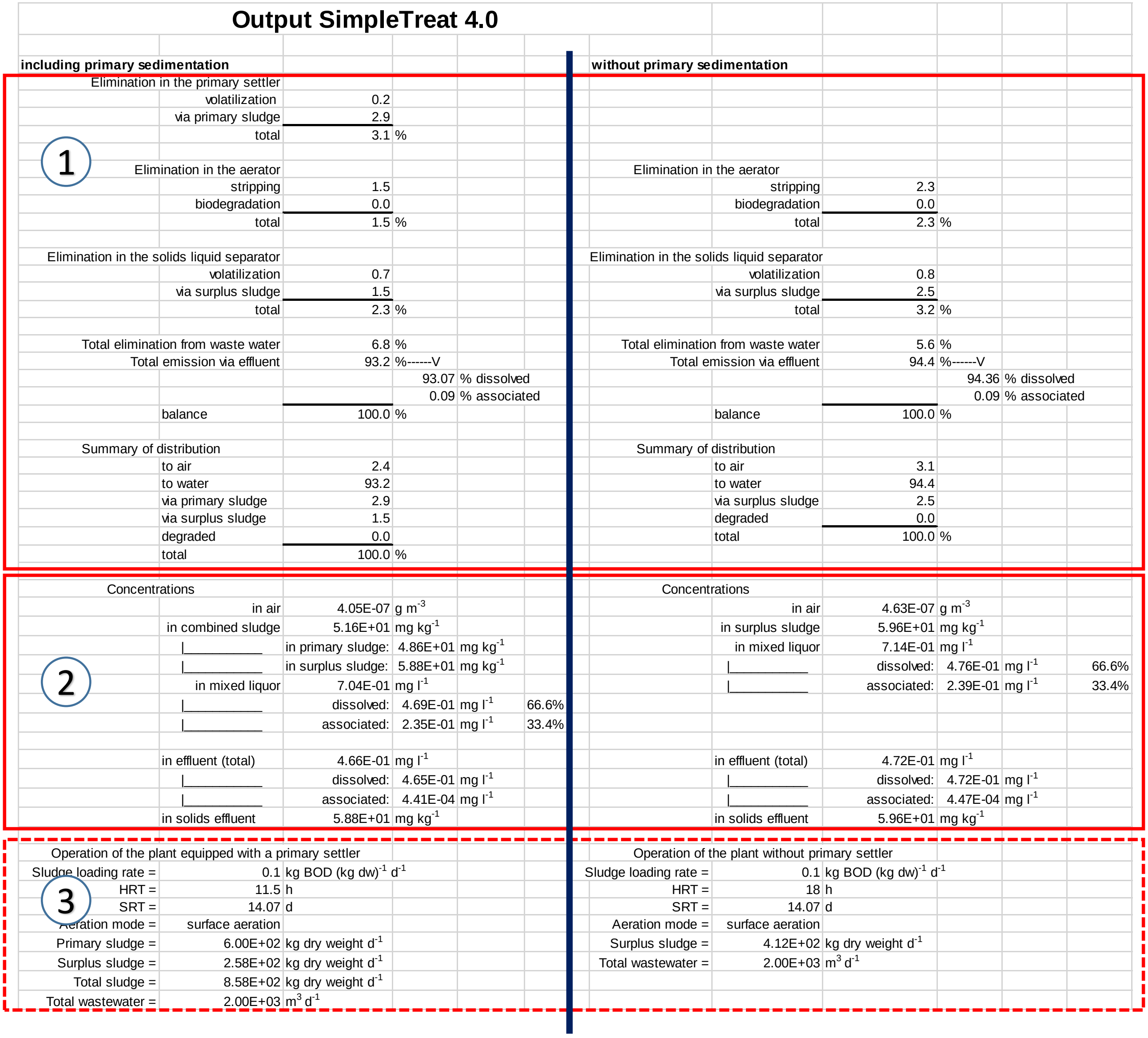
Figure 10: Measured Kp plotted versus measured foc



1.5 Output

The left part of the output sheet (Figure 11) displays the results with respect to an STP equipped with a primary sedimentation tank (9-box); the right hand part shows the output for an STP without a primary clarifier (6-box). Note that although the sludge loading rate of the latter is similar, the predicted relative emission rates are slightly different. The hydraulic retention time in the aerator that treats raw sewage without primary sedimentation, is longer due to the fact that the BOD input is higher than an STP equipped with a primary clarifier which not only removes solids but also BOD.

Figure 11: The output sheet. Part 1 gives relative emissions, part 2 the concentrations in the media that leave the STP and part 3 information on the operation mode of the STP



Output SimpleTreat 4.0

including primary sedimentation

Elimination in the primary settler					
	volatilization	0.2			
	via primary sludge	2.9			
	total	3.1	%		
Elimination in the aerator					
	stripping	1.5			
	biodegradation	0.0			
	total	1.5	%		
Elimination in the solids liquid separator					
	volatilization	0.7			
	via surplus sludge	1.5			
	total	2.3	%		
Total elimination from waste water		6.8	%		
Total emission via effluent		93.2	%------V		
			93.07	% dissolved	
			0.09	% associated	
	balance	100.0	%		
Summary of distribution					
	to air	2.4			
	to water	93.2			
	via primary sludge	2.9			
	via surplus sludge	1.5			
	degraded	0.0			
	total	100.0	%		
Concentrations					
	in air	4.05E-07	g m^{-3}		
	in combined sludge	5.16E+01	mg kg^{-1}		
	|__________	in primary sludge:	4.86E+01	mg kg^{-1}	
	|__________	in surplus sludge:	5.88E+01	mg kg^{-1}	
	in mixed liquor	7.04E-01	mg l^{-1}		
	|__________	dissolved:	4.69E-01	mg l^{-1}	66.6%
	|__________	associated:	2.35E-01	mg l^{-1}	33.4%
	in effluent (total)	4.66E-01	mg l^{-1}		
	|__________	dissolved:	4.65E-01	mg l^{-1}	
	|__________	associated:	4.41E-04	mg l^{-1}	
	in solids effluent	5.88E+01	mg kg^{-1}		
Operation of the plant equipped with a primary settler					
Sludge loading rate =	0.1	kg BOD (kg dw)$^{-1}$ d^{-1}			
HRT =	11.5	h			
SRT =	14.07	d			
Aeration mode =	surface aeration				
Primary sludge =	6.00E+02	kg dry weight d^{-1}			
Surplus sludge =	2.58E+02	kg dry weight d^{-1}			
Total sludge =	8.58E+02	kg dry weight d^{-1}			
Total wastewater =	2.00E+03	m^{3} d^{-1}			

without primary sedimentation

Elimination in the aerator					
	stripping	2.3			
	biodegradation	0.0			
	total	2.3	%		
Elimination in the solids liquid separator					
	volatilization	0.8			
	via surplus sludge	2.5			
	total	3.2	%		
Total elimination from waste water		5.6	%		
Total emission via effluent		94.4	%------V		
			94.36	% dissolved	
			0.09	% associated	
	balance	100.0	%		
Summary of distribution					
	to air	3.1			
	to water	94.4			
	via surplus sludge	2.5			
	degraded	0.0			
	total	100.0	%		
Concentrations					
	in air	4.63E-07	g m^{-3}		
	in surplus sludge	5.96E+01	mg kg^{-1}		
	in mixed liquor	7.14E-01	mg l^{-1}		
	|__________	dissolved:	4.76E-01	mg l^{-1}	66.6%
	|__________	associated:	2.39E-01	mg l^{-1}	33.4%
	in effluent (total)	4.72E-01	mg l^{-1}		
	|__________	dissolved:	4.72E-01	mg l^{-1}	
	|__________	associated:	4.47E-04	mg l^{-1}	
	in solids effluent	5.96E+01	mg kg^{-1}		
Operation of the plant without primary settler					
Sludge loading rate =	0.1	kg BOD (kg dw)$^{-1}$ d^{-1}			
HRT =	18	h			
SRT =	14.07	d			
Aeration mode =	surface aeration				
Surplus sludge =	4.12E+02	kg dry weight d^{-1}			
Total wastewater =	2.00E+03	m^{3} d^{-1}			

Figure 11 shows the output sheet which consists of three parts:

1. The upper (solid) frame shows elimination and emission of the chemical as percentage of the discharge rate of the chemical into the sewer system. In the part *Summary of*

distribution the relative fate of the chemical is summed up. Absolute emission and degradation rates are obtained by multiplication of these percentages with the total discharge rate of the chemical.

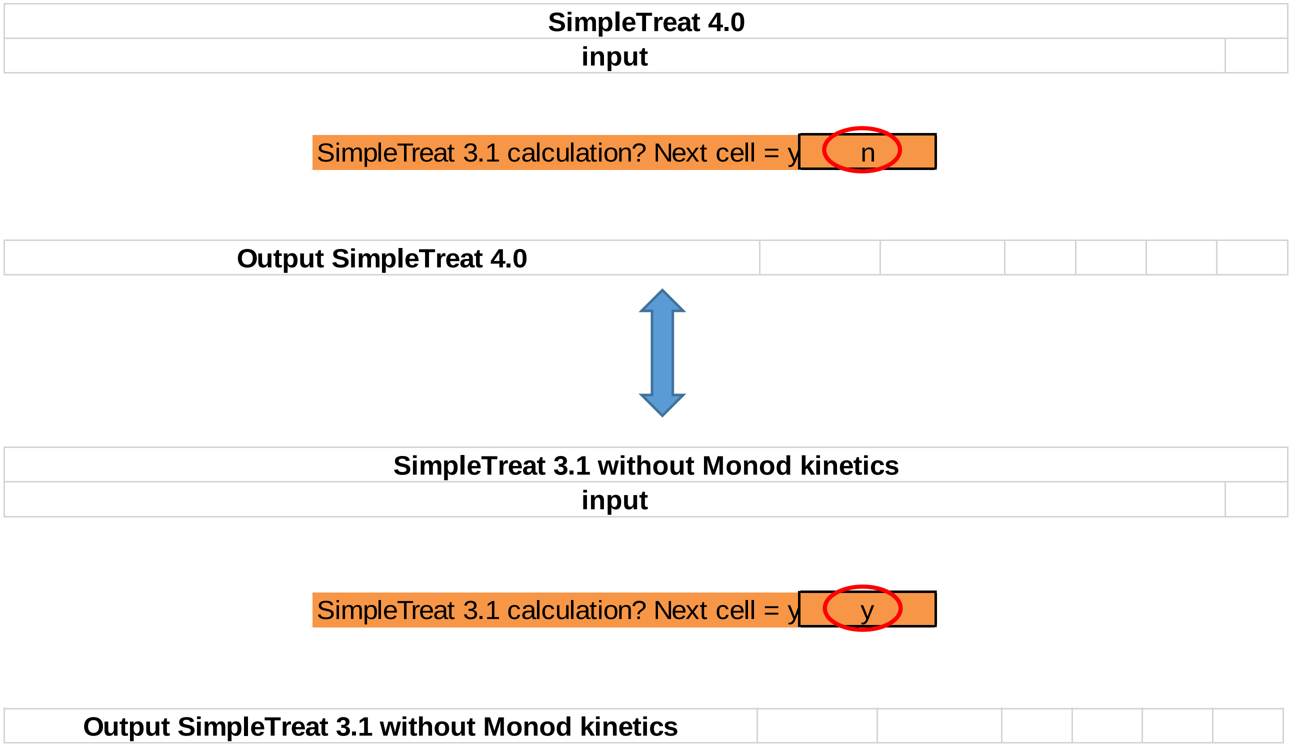
2. The solid middle frame contains concentrations in all media leaving the STP environment. These values are only real if the *Emission scenario* in block 2 in the input sheet has been filled in. The *total* concentration of the chemical in effluent is in mg/L ("nominal concentration") and is the sum of purely dissolved chemical and associated with suspended solids in the effluent column. Also the nominal concentration in mixed liquor (activated sludge) is given. This result may be useful in a comparison with toxicity tests for activated sludge.
3. The dashed frame below gives information as to the operation of the STP. Emission rates of primary and wasted sludge or combined sludge are presented.

1.6 Switch between SimpleTreat 4.0 and SimpleTreat 3.1

SimpleTreat 4.0 (Struijs, 2014) has been developed in response to evaluation studies by Franco et al. (2013) and Struijs (2013) which identified some weaknesses of SimpleTreat 3.1. Nevertheless, version 3.1 has still the status of “recommended model” for regulatory purposes. The risk assessor who runs the model SimpleTreat 4.0 may also want the output of SimpleTreat 3.1 even acknowledging that version 3.1 ignores new insights with respect to equilibrium partitioning of organic acids and bases (Franco et al., 2013). New equations for organic carbon-water equilibrium constants of organic acids and bases are being implemented into the multimedia environmental fate model SimpleBox 4.0. The SimpleBox model is also the model recommended by the EU for assessing exposure concentrations in the real world. It is expected that it will take some time before SimpleTreat 4.0 and SimpleBox 4.0 will replaced the former versions of exposure models recommended by the guidance on REACH.

It is therefore convenient to switch between version 4.0 and version 3.1 of the SimpleTreat model by using one input parameter. In the lower right part of the input sheet (Figure 4), this input parameter is default “n” which means that the 4.0 version is running according to the headings of the input and output sheet (upper part of Figure 12). If this parameter is set to “y” (lower part of Figure 12) the headings change to indicate that the system has changed to SimpleTreat 3.1.

Figure 12: Switch between version 4.0 and 3.1



SimpleTreat 4.0

input

SimpleTreat 3.1 calculation? Next cell = y n

Output SimpleTreat 4.0

SimpleTreat 3.1 without Monod kinetics

input

SimpleTreat 3.1 calculation? Next cell = y y

Output SimpleTreat 3.1 without Monod kinetics

Note that the hydraulic retentions times which are dependent on the sludge loading rate presented by table 1 of the input sheet (Figure 4) have changed after replacing “n” by “y”.

2 References

Franco A, Struijs J, Gouin T, Price O (2013). Evolution of the sewage treatment plant model SimpleTreat: applicability domain and data requirements. Integr Environ Assess Manag. 9: 560-568

OECD (2000) Test No. 106: Adsorption -- Desorption Using a Batch Equilibrium Method, Guidelines for the Testing of Chemicals, Section 1, Physical-Chemical properties

OECD (2001) Test No. 121: Estimation of the Adsorption Coefficient (Koc) on Soil and on Sewage Sludge using High Performance Liquid Chromatography (HPLC), Guidelines for the Testing of Chemicals, Section 1, Physical-Chemical properties

OECD (2006). Guidelines for the Testing of Chemicals, Revised introduction to the OECD guidelines for testing of chemicals, Section 3 Degradation and Accumulation. Part 1: Principles and strategies related to the testing of degradation of organic chemicals

REACH (2006). EG 1907/2006

Struijs J (2013). Evaluation of the SimpleTreat model. RIVM Report 607105001.

Struijs, J. (2014). SimpleTreat 4.0, a model to predict fate and emission of chemicals in wastewater treatment plants. Background report describing the equations. RIVM Report 601353005/2014.

3 Appendix A: Different output for neutral chemicals

Table 4 displays differences in output for chemicals with properties given by Table 3. If biodegradation is the only removal mechanism, SimpleTreat 4.0 predicts that the emission of a “readily biodegradable” chemical - according to the OECD guidelines (OECD, 2006) - to water has decreased from 12.6 % to 8.0 %. If sorption is the major removal mechanism however, emission to water decreased from 39.4 % to 34.1 % (chemical 3). For these chemicals, SimpleTreat 4.0 predicts a lower relative emission via effluent and obviously with lower concentrations in effluent.

Table 3: Physico-chemical properties of three hypothetical chemicals with molecular weight equal to 100 g/mol. Partition coefficients (air-water and solids-water) span five orders of magnitude

Chemical	Kow	Vapour pressure [Pa]	Water solubility [mg/L]	Readily biodegradable
1	1	100	0.1	No
2	1	0.1	100	Yes
3	10^5	1	100	No

Table 4: Version 3.1 compared to version 4.0: emission rates of chemicals listed in Table 3

Chemical	Emission to air [%]		Emission to water [%]	
	SimpleTreat 4.0	SimpleTreat 3.1	SimpleTreat 4.0	SimpleTreat 3.1
1	95.5	95	4.5	5
2	0.0	0.0	8.0	12.6
3	0.1	0.1	34.1	39.3

4 Appendix B: Estimation of Dow by SimpleTreat 4.0

If a measured value of Dow is not available it is estimated from Kow and the negative logarithm of the acid dissociation constant, pKa.

In the aqueous phase (concentration chemical in water is indicated as Cw), the fraction neutral (Fn) of an acid or base is.

$$\mathrm{Fn} = \frac{\mathrm{C_n^w}}{\mathrm{C_n^w} + \mathrm{C_{ion}^w}} = \frac{1}{1 + 10^{\gamma \cdot (\mathrm{pH} - \mathrm{pKa})}}$$

Cn and Cion are the concentrations of the neutral and ionized chemical, respectively. The pKa is the acid dissociated constant of an acid (γ = 1) or a base (γ = -1). The fraction ionized in water is equal to 1-Fn. The Dow of an organic compound is the apparent n-octanol-water partition coefficient at the actual pH and is based upon concentrations of the organic acid or base in both the n-octanol phase and in water (superscript o and w, respectively) of both the neutral and ionized of the chemical:

$$\mathrm{Dow} = \frac{\mathrm{C_n^o} + \mathrm{C_{ion}^o}}{\mathrm{C_n^w} + \mathrm{C_{ion}^w}} =$$

$$= \mathrm{Fn} \cdot \frac{\mathrm{C_n^0}}{\mathrm{C_n^w}} + (1 - \mathrm{Fn}) \cdot \frac{\mathrm{C_{ion}^o}}{\mathrm{C_{ion}^w}}$$

$$= \mathrm{Fn} \cdot \mathrm{Kow} + (1 - \mathrm{Fn}) \cdot \mathrm{Kow(ionized)} \approx \mathrm{Fn} \cdot \mathrm{Kow}$$

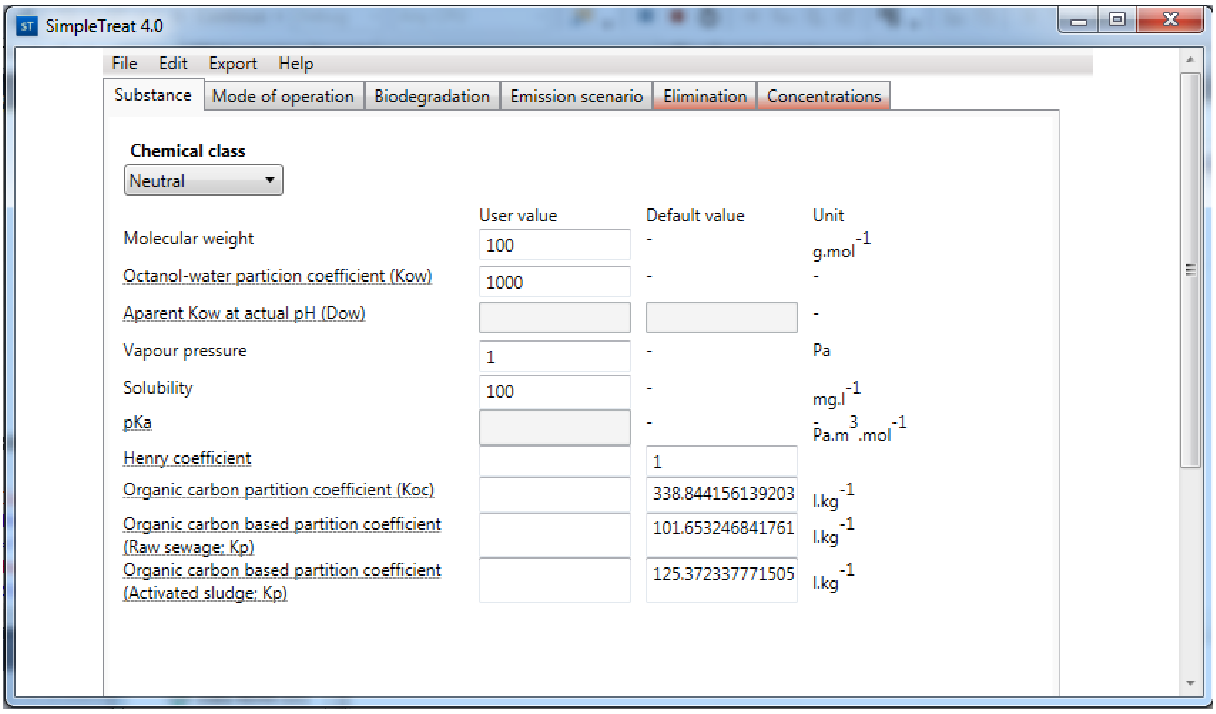
In this equation, the approximation is made that the concentration of an ionized organic compound in the n-octanol phase is zero and that Kow (ionized) is negligible.

5 Appendix C: Images of SimpleTreat 4.0 in .NET format

In 2014 a Windows application of SimpleTreat will be presented that will offer the same functionality. This application may replace the MS Excel spreadsheet model in the future. The application can be installed on any computer running Windows Vista or higher. The application will offer automatic updates, so users are assured there are always running the latest version of SimpleTreat, as authorized by RIVM.

Functionally, the application will be very much similar to the spreadsheet model described in this report. The figures in this appendix give an impression of the application.

Figure 13: SimpleTreat 4.0 substance properties input screen

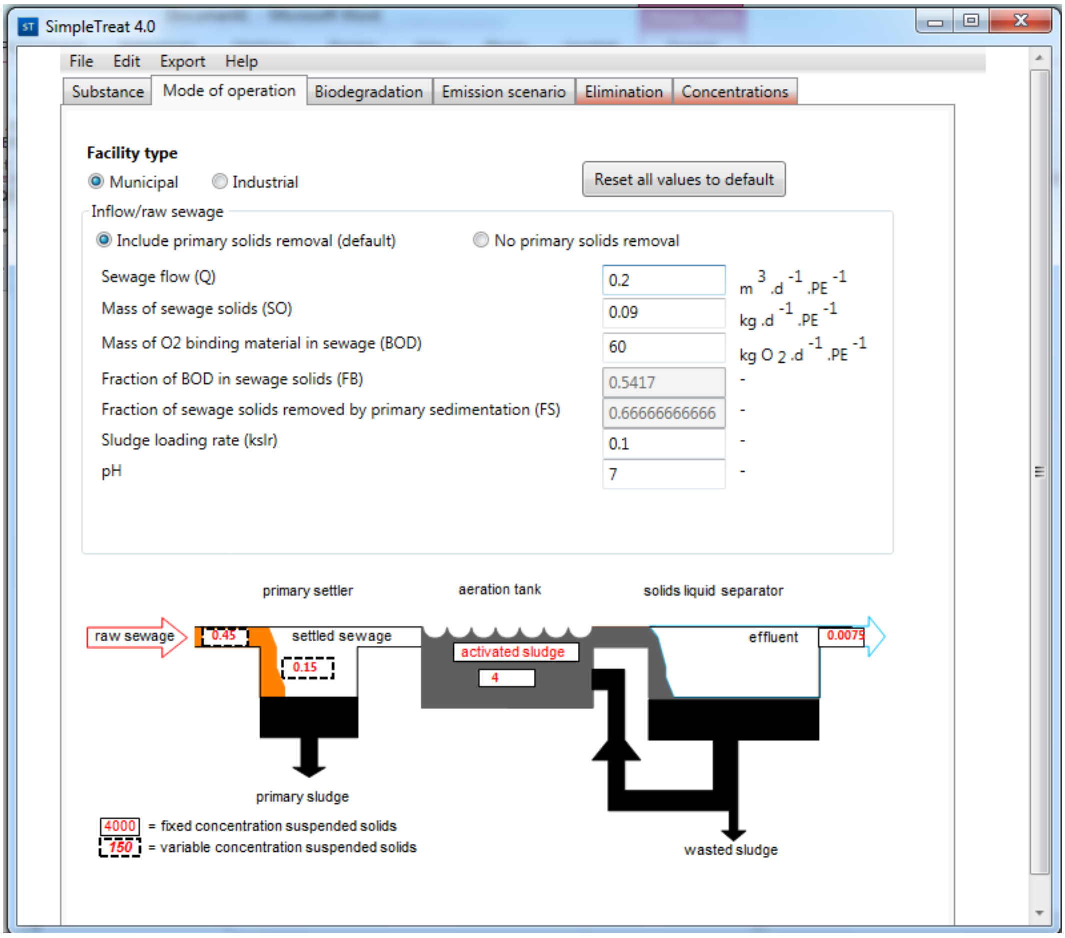


Chemical class

Neutral

	User value	Default value	Unit
Molecular weight	100	-	$g.mol^{-1}$
Octanol-water particion coefficient (Kow)	1000	-	-
Aparent Kow at actual pH (Dow)			-
Vapour pressure	1	-	Pa
Solubility	100	-	$mg.l^{-1}$
pKa		-	-
Henry coefficient		1	$Pa.m^{3}.mol^{-1}$
Organic carbon partition coefficient (Koc)		338.844156139203	$l.kg^{-1}$
Organic carbon based partition coefficient (Raw sewage: Kp)		101.653246841761	$l.kg^{-1}$
Organic carbon based partition coefficient (Activated sludge: Kp)		125.372337771505	$l.kg^{-1}$

Figure 14: SimpleTreat 4.0 mode of operation settings



Facility type

● Municipal ○ Industrial

Inflow/raw sewage

● Include primary solids removal (default) ○ No primary solids removal

Sewage flow (Q) 0.2 $m^3.d^{-1}.PE^{-1}$

Mass of sewage solids (SO) 0.09 $kg.d^{-1}.PE^{-1}$

Mass of O2 binding material in sewage (BOD) 60 $kg\,O_2.d^{-1}.PE^{-1}$

Fraction of BOD in sewage solids (FB) 0.5417 -

Fraction of sewage solids removed by primary sedimentation (FS) 0.66666666666 -

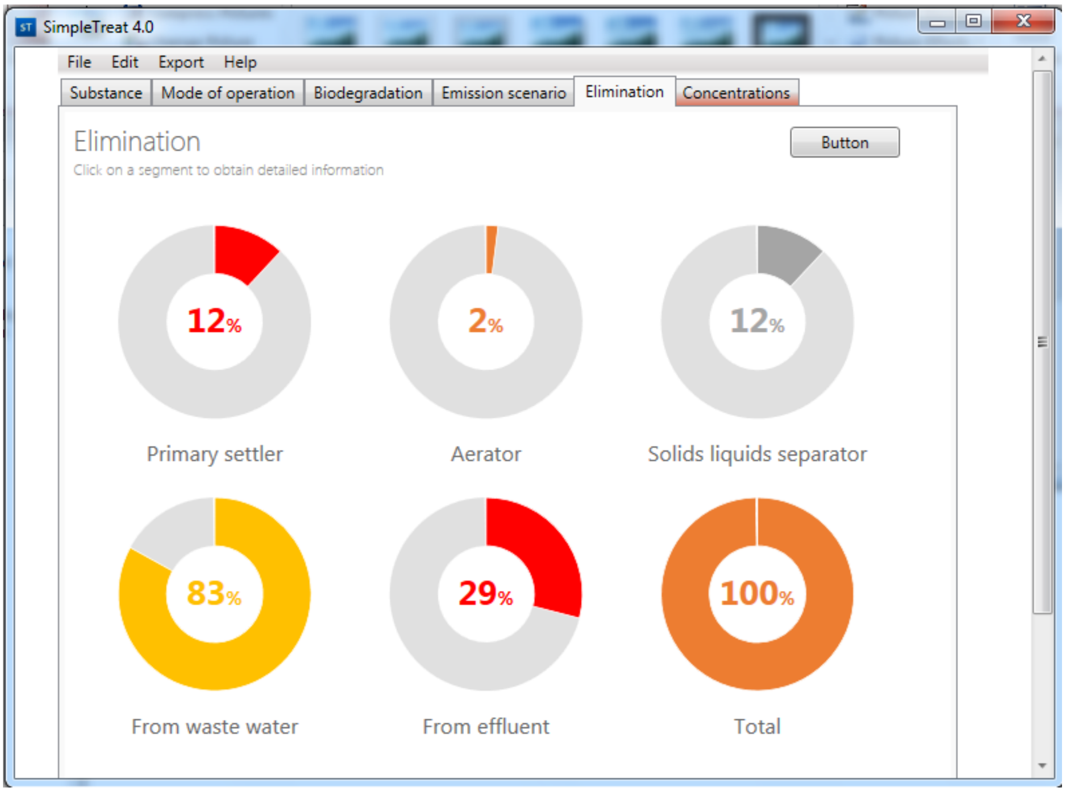
Sludge loading rate (kslr) 0.1 -

pH 7 -

4000 = fixed concentration suspended solids

150 = variable concentration suspended solids

Figure 15: Example of SimpleTreat 4.0 graphical output screen (elimination percentages)



Elimination

Click on a segment to obtain detailed information

Primary settler 12%

Aerator 2%

Solids liquids separator 12%

From waste water 83%

From effluent 29%

Total 100%