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**SimpleTreat 3.0: a model to predict the  
distribution and elimination of chemicals  
by sewage treatment plants**

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**DISCLAIMER**

This report describes an improved version of SimpleTreat. It employs results of scientific papers and reports, but also suggestions to improve SimpleTreat. These suggestions have been made by several experts at numerous occasions. Although both this report and the spreadsheet model on a diskette have been prepared with care, they are not claimed to be free of errors. Use of the results obtained by means of these materials is the full responsibility of the user. Use of the model is encouraged and feedback is welcomed. However, other than by means of this document, no technical support for users is being offered.

**FOREWORD**

Many suggestions to improve the model SimpleTreat proved worthwhile and have been experienced as an incentive to develop SimpleTreat 3.0. Comments on SimpleTreat appeared very constructive and were appraised as a confirmation that the theoretical understanding of the chemical fate in sewage treatment plants is sufficiently developed to allow the use of this type of models. Also the necessity to use these models in order to be able to estimate exposure concentrations in the receiving environment, has been appreciated.

Of the experts who contributed to the development of SimpleTreat 3.0 I will name only a few. in alphabetical order: Ron Birch (Unilever, UK), Han Blok (BKH, NL) Chris Cowan (P&G, USA), Tom Feijtel (P&G, B) and last but not least: Jørgen Mikkelsen (National Environmental Research Institute, DK) and Niels Nyholm (Technical University of Denmark).

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## ABSTRACT

This report describes the spreadsheet SimpleTreat 3.0, a model to predict the DIstribution and ELimination of chemicals by sewage treatment. SimpleTreat 3.0 is an improved version of SimpleTreat, applied in the Netherlands in the Uniform System for the Evaluation Substances (USES version 1.0, 1994). Although in the very beginning strong reservations were encountered, soon it has become accepted as a useful tool for *generic* exposure assessment. It is now recognized that the accuracy of exposure assessment, in particular for the water compartment in urban regions, is largely determined by the accuracy with which the chemical fate in sewage treatment plants (STP) can be predicted. SimpleTreat has been scrutinized the last 6 years by several experts on 1) assumptions as to the composition and the daily amount of communal wastewater per person, 2) the optional modes of operation of the sewage treatment plant and 3) descriptions of the interactions between the chemical and its engineered environment, in particular biodegradation.

Suggestions expressed at several expert meetings of the European Community, were combined with new insights reported in the open and the "grey" literature. Recommendations were made to extend its applicability to the European Union. Most of them have been adopted in this completely revised model; it therefore has been given the new name, SimpleTreat 3.0.

This model includes a wider range of operation modes of wastewater purification in order to account for the variety of communal wastewater scenarios across the EU.

In SimpleTreat 3.0, chemical transport and transformation processes cover a wider range of compound properties and scenarios. Emission of substances via sludge production was modified to account for the presence and absence of primary sedimentation. The first scenario suits the urban areas where usually large installations purify the raw wastewater; the second is more representative for rural regions where a high percentage is connected to treatment installations, for example Denmark. Mathematical expressions of individual processes, a chemical may undergo in a STP, were critically reviewed. Emission to the air compartment, due to stripping in the aeration tank, has been re-assessed by taking into account the gas phase resistance. This correction is necessary to better predict the behaviour of semi-volatile chemicals. However, the input of biodegradation data and the way this information is processed have been altered most. Modifications are partly motivated by the discussions in the course of developing a risk assessment system for "new" and "existing" chemicals in the European Community. Also results, presented in recent literature, have been implemented.

A second version of USES is currently being developed to be applied in the EU. As a sewage treatment chemical fate model should cover many scenarios to play its key role in exposure assessment, it was decided to apply SimpleTreat 3.0 for this purpose in USES 2.0, in stead of SimpleTreat. This report may serve as a reference manual of SimpleTreat 3.0. The spreadsheet file on diskette that goes with this report, is written in MicroSoft EXCEL.



## SAMENVATTING

Dit rapport beschrijft het spreadsheet SimpleTreat 3.0, een model waarmee de distributie en eliminatie van chemicaliën door een rioolwaterzuiveringsinstallatie (rwzi) kan worden voorspeld. SimpleTreat 3.0 is een verbeterde versie van SimpleTreat, dat ten behoeve van het Uniform Beoordelingssysteem Stoffen (UBS versie 1.0, 1994) in Nederland wordt toegepast. Ofschoon aanvankelijk t.o.v. dit model de nodige reserves bestonden, werd het al spoedig geaccepteerd als een nuttig instrument voor *generieke* blootstellingsbeoordeling. Thans wordt onderkend dat de nauwkeurigheid van exposure assessment, met name voor het compartiment water, grotendeels wordt bepaald door de nauwkeurigheid waarmee de emissie door rwzi's kan worden voorspeld. SimpleTreat is de afgelopen zes jaar door verscheidene deskundigen onderzocht op 1) aannames over de aard en hoeveelheid van afvalwater die per persoon dagelijks wordt geproduceerd, 2) de keuzemogelijkheden t.a.v. bedrijfsvoering van de rwzi en 3) de afzonderlijke procesbeschrijvingen van de interactie tussen de stof en zijn omgeving, met name voor biodegradatie.

Suggesties ter verbetering van het model, voorgesteld tijdens verscheidene bijeenkomsten van deskundigenoverleg van de Europese Gemeenschap, werden gecombineerd met recent in de open en "grijze" literatuur gerapporteerde inzichten. Aanbevelingen werden gedaan om de toepasbaarheid van het model te vergroten zodat het geschikt wordt voor de Europese Unie. De meeste aanbevelingen werden overgenomen in dit volledig herziene model. Deze houden ondermeer in een aanzienlijk grotere keuzemogelijkheid t.a.v. de bedrijfsvoering van rwzi's, teneinde rekening te kunnen houden met de grote verschillen in afvalwaterbehandeling die in de EU bestaan.

In SimpleTreat 3.0 hebben de geformuleerde transport- en omzettingsprocessen van een chemische verbinding een breder toepassings gebied. Emissie van stoffen door een rwzi via slibproductie werd gemodificeerd teneinde rekening te kunnen houden met de aan- dan wel de afwezigheid van voorbezinking. Primaire bezinking wordt veel toegepast in stedelijke gebieden, waar meestal zeer grote installaties het afvalwater verwerken. Afwezigheid van voorbezinking komt meer voor in landelijke gebieden waar het overgrote deel gezuiverd wordt, zoals in Denemarken. Mathematische formuleringen voor de afzonderlijke lotgevallen van een stof in een rwzi werden herzien. Voor emissie naar lucht als gevolg van het beluchtingsproces in de aeratietank, is een verbeterde schatting gemaakt rekening houdend met de gas-film weerstand. Dit is meer correcte beschrijving van het gedrag van semi-vluchtige verbindingen. De invoer en de verwerking van biodegradatiegegevens hebben echter de meeste veranderingen ondergaan. Modificaties zijn gedeeltelijk ingegeven door de discussies die hebben plaatsgevonden tijdens de ontwikkeling van het risicobeoordelingssysteem voor "nieuwe" en "bestaande" stoffen voor Europese Gemeenschap. Ook recent gepubliceerde resultaten werden toepassing gebracht.

Momenteel wordt voor de EU een tweede versie van UBS voorbereid (USES 2.0). Aangezien de modelmatige beschrijving van het lot van stoffen in rwzi een sleutelrol speelt bij de blootstellingschatting, is besloten om voor dit doel een verbeterde versie van SimpleTreat aan te wenden. Dit rapport dient als naslagwerk voor SimpleTreat 3.0. De spreadsheet-file op diskette aan dit rapport toegevoegd werd geschreven in MicroSoft EXCEL.

## 1. INTRODUCTION

Quantitative risk assessment of chemicals is a tiered process in which each higher tier requires more data. It relies upon the comparison of exposure assessment and effect assessment. Obviously, also the availability and accuracy of exposure data have different stages: initial (screening, or tier-1), refined (tier-2) or comprehensive (tier-3). The higher the stage of risk assessment the more information is necessary to properly conduct exposure assessment. At the highest tier, this may include measured environmental concentrations. The lower the tier, the more it relies upon model calculations, in particular for exposure from chemicals released by communal wastewater treatment plants. This approach is typical for the Uniform System for the Evaluation Substances (USES version 1.0, 1994) in the Netherlands.

Many chemicals used domestically, commercially, industrially as well as non-agricultural pesticides, are discharged to sewer systems. In urban regions, most of these sewer systems are connected to biological sewage treatment plants (STP), or will be in the near future (Council Directive 91, 271, EEC). The mathematical model, SimpleTreat (Struijs et al. 1991), can be applied to estimate the *relative* emission of a chemical from a STP to the environmental compartments. For a readily biodegradable chemical, also the fraction eliminated due to biodegradation is calculated. In SimpleTreat all processes that determine the fate of a chemical are assumed linear, i.e. they occur at a rate proportional to the concentration in the different media. As the model was designed as an aid for regulatory risk assessment, the purpose was to obtain relevant output even if only those a few compound properties are known. Therefore, the model was customized to those few compound properties that are mandatory at the screening level of the notification procedure. At the screening level, SimpleTreat is the default calculation module in USES 1.0 to estimate the exposure concentration in the receiving water, soil and air in some "standard" emission scenario.

Relative emissions and elimination may be the desired information to explain differences in behaviour of chemicals in some "standard" STP. However, additional input is required for exposure assessment. Only base-set data *in combination* with an emission scenario may yield exposure data in terms of concentrations in purified wastewater flowing into waterbodies, produced sludge and the air above the plant. This emission scenario requires only two input data to be combined with data of the chemical, resulting in concentrations in water, soil and air:

- the emission rate of the chemical into the sewage system and
- the size of the STP, expressed as the number of inhabitants connected.

The model is constructed so that, according to the limited information at tier-1, it produces the required output from base-set characteristics of the chemical:

- molecular weight,
- water solubility,
- vapour pressure,
- hydrophobicity ( $\log K_{ow}$ ),
- results of "ready biodegradability" testing (OECD/EU): positive or negative.

Simplifications, especially for biodegradation which is of the "on or off" type and several other assumptions made, have been reasons for experts to consider this model with strong reservations. The limited choice of three "representative" STPs, equipped with a primary sedimentation tank (see Fig 1a), has been criticized. Nevertheless, in the course of technical-scientific dispute on its use in generic risk assessment, consensus on its use was reached - at least for the lower tier evaluations. Other approaches, such as categorizing according to ranges of  $\log K_{ow}$  and Henry's law constant ( $\approx$  the vapour pressure/water solubility) from which relative emissions are estimated appeared less suitable, if not inferior. Thus from the early days of quantitative risk assessment, when the model was given the benefit of the doubt, gradually the idea gained support that exposure assessment for urban regions could be considerably improved by means of such models. Several proposals on refining them were made (a.o. Cowan et al., 1993; Mikkelsen et al., 1995). It is obvious that, in principle, STP models could also be used at a higher tier evaluation, provided that more modes of operation of the STP are accounted for. Moreover, also improved process formulations have to be incorporated, in particular for biodegradation.

The development of a new version of SimpleTreat was necessary for reasons of scientific agreement on its use in risk assessment, not only at the screening but also the refined level. The approach to accomplish this is: 1) more options in defining the STP environment, and 2) improved formulations of the interaction between the chemical and the engineered STP environment. The greater flexibility makes the model suitable for a wide variety of wastewater scenarios in the EU.

More options may include the absence of primary sedimentation (see Fig 1b), a continuous scale on which the sludge loading rate can be chosen, and the sewage volume per inhabitant per day. These parameters, in combination with the chosen aeration technique, largely define the mode of operation of the plant. This has a significant influence on the fate of the modelled chemical.

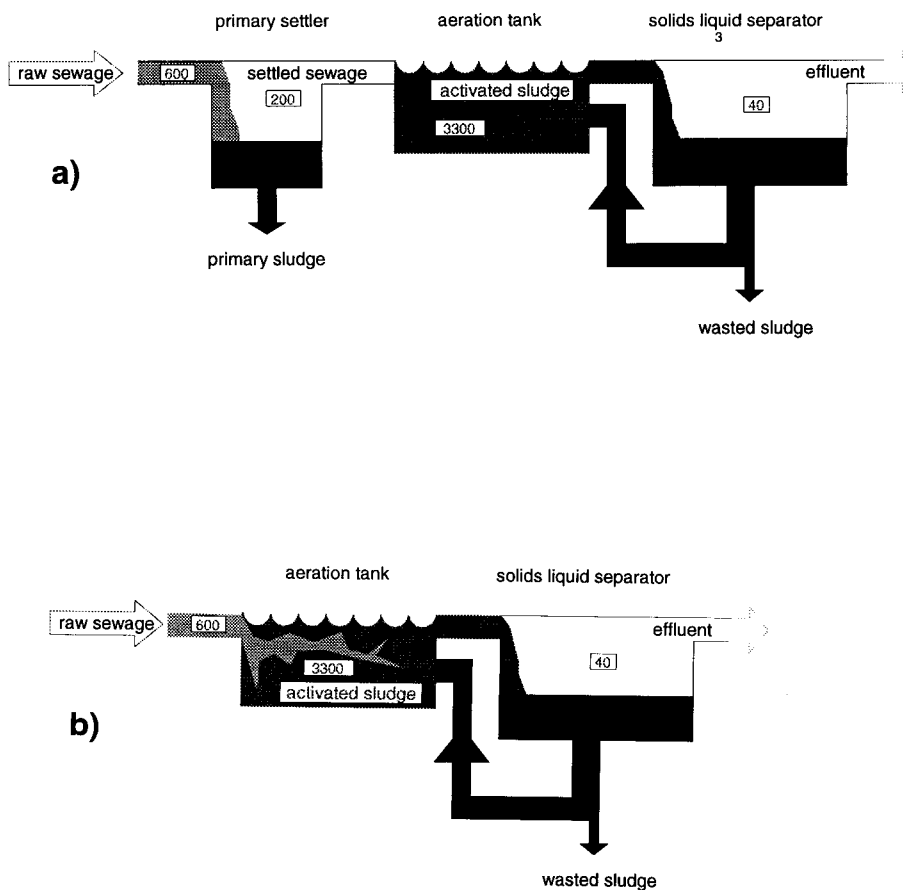
Process descriptions for air-water exchange were extended and biodegradation includes a simulation of non-linear Monod kinetics for microbial degradation.

The model is written in an EXCEL spreadsheet format and is primarily meant as a scientific tool to analyze the behaviour of a chemical in a STP and secondary as a default calculation module in the risk assessment system. It was decided to adhere to the multimedia box-model computation at the level of steady state non-equilibrium, also known as "Mackay level III" (see for example Mackay and Paterson, 1981). The design of the model is more systematic

than SimpleTreat, allowing sensitivity and uncertainty analysis easy to conduct. The structure, format and contents and so its applicability differ from SimpleTreat to such an extent that a new name is introduced: SimpleTreat 3.0, a chemical fate model to predict the **DIStribution and ELimination of chemicals by sewage treatment plants**.

This report contains all mathematical process descriptions and as such may serve as a reference manual of SimpleTreat 3.0.

*Fig 1. Schemes of communal biological sewage treatment plants; with (a) and without (b) primary sedimentation*



3300 = steady state concentration suspended solids

## 2. MODEL CONCEPT

The structure of a model is determined by its intended use. This general rule also applies to SimpleTreat 3.0 which was anticipated a computing tool to quickly calculate 1) the relative fate of a substance, provided that the chemical is persistent or degrades according to first order kinetics and 2) exposure concentrations in effluent (water), sludge (soil) and the air in the direct surroundings of the plant. The first requires basic compound properties, whereas for the second additional emission data are necessary. Emission may be specified as the release rate of the chemical into the sewage system of a certain urban population, expressed as the number of inhabitants connected to an STP. An additional requirement is transparency, facilitating sensitivity and uncertainty analysis.

SimpleTreat 3.0 has a modular set-up and consists of four sheets, named "input", "9-box", "6-box" and "output" (see Fig 2). Each sheet is subdivided in sections for different items, such as the mode of operation of the plant, different modes of interaction of the chemical with the environment of the different basins of the plant, etc. The spreadsheet format has been chosen because it allows interaction between the user and the model. A rather simple input sheet (see Appendix A) consists of three sections:

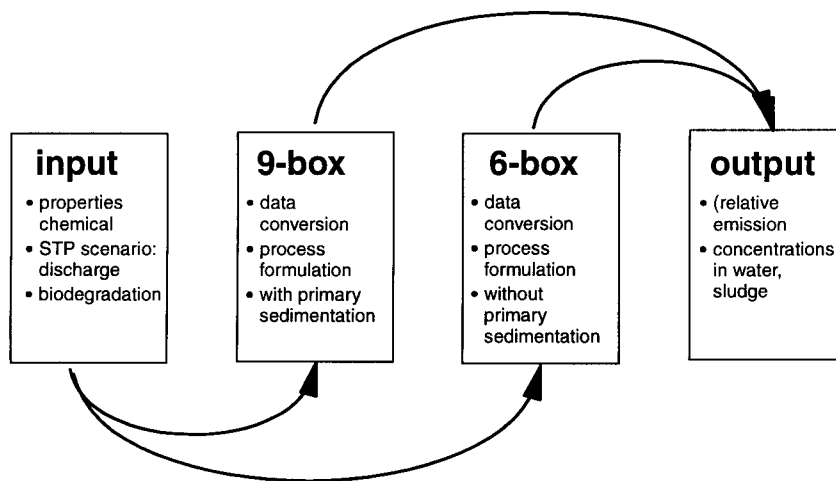
- Basic physico-chemical properties of the chemical
- Emission scenario
- Biodegradation in activated sludge

The sheets "9-box" and "6-box" are the calculation regions of the model. In "9-box", which may be regarded as an improved version of SimpleTreat, and in "6-box" the chemical fate is calculated in installations with and without primary sedimentation, respectively. As the names suggest, the box modelling approach implies that in all basins of the installation - three in "9-box" and two in "6-box" - the distinguished media are considered completely homogeneous. This assumption is considered valid in view of the controlled operation like forced aeration, which approximates complete mixing in the aeration tank, both in the aqueous and the solids phase. Also sludge recycling, typical for the activated sludge technique, contributes to well mixing in the distinguished media water, suspended and settled sludge. In most multimedia fate models for natural systems, the suspended solids phase in water is not included as a separate box because equilibrium partitioning inside the water column is assumed. In SimpleTreat 3.0 (Fig 3a,b) the suspended sludge phase is a separate box, as it was in SimpleTreat. This is convenient because the sludge recycling can easily be accounted for and diffusive transport processes between *settled* sediment and water can easily be inserted.

For generic exposure assessment, steady state over a certain period of time is an adequate representation of communal wastewater treatment. Equilibrium partitioning of the chemical over the different media, however, is less likely as the residence times of these media, carrying the chemical, are generally too short to reach equilibrium. Also in SimpleTreat 3.0 a steady state, non-equilibrium box model calculation is applied. It may be concluded that

releasing this concept for the purposes of relative fate calculation (f.i. comparing different chemicals with each other) and generic exposure assessment (f.i. comparing different emission scenarios for a certain chemical), would not provide more reliable results than inserting improved process formulations and offering the user more options for realistic modes of operation of the STP.

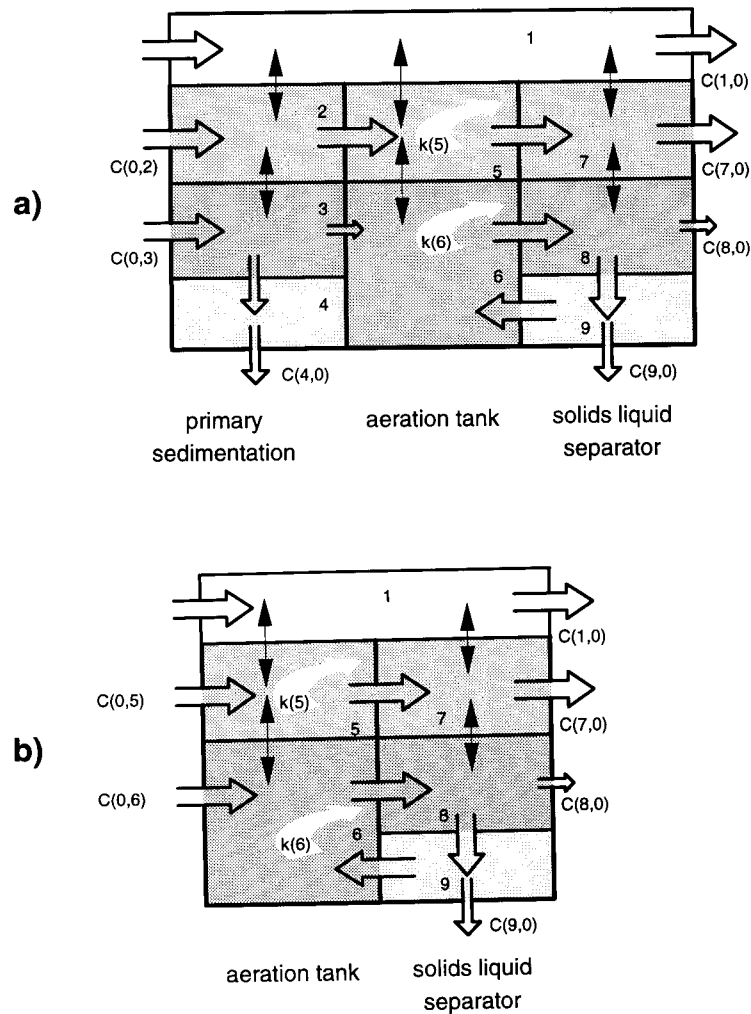
*Fig 2 Organization scheme of SimpleTreat 3.0*



In Fig 3 three different types of arrows represent the most relevant processes the chemical may undergo in a STP:

- 1) advective mass flow of the chemical (open arrows) from box  $i$  to  $j$ , as the result of media flow carrying the chemical; these are irreversible transport processes,
- 2) diffusive mass flow (two-headed arrows) driven by non-equilibrium concentrations in two adjacent boxes media  $i$  and  $j$ ,
- 3) degradation processes,  $k_i \cdot C(i) \cdot V_i$  [mol s<sup>-1</sup>] in the aqueous and, optionally, in the suspended particle phase of activated sludge, represented by the curved arrows in box 5 and 6.

Fig 3. Box Schemes of the fate of a chemical un a communal wastewater treatment plant with (a) and without primary sedimentation (b)



A mass balance can be written for each box as follows:

$$V_i \cdot \frac{dC(i)}{dt} = - k_i \cdot C(i) \cdot V_i + \sum MED_{i,j} + \sum DIFF_{i,j} \quad (1)$$

with

- MED<sub>i,j</sub> : advective mass flow [mol s<sup>-1</sup>],
- DIFF<sub>i,j</sub> : diffusive mass flow [mol s<sup>-1</sup>],
- V<sub>i</sub> : volume of box i [m<sup>3</sup>]
- C(i) : concentration in box i [g m<sup>-3</sup>]
- t : time [s]
- k<sub>i</sub> : first order rate biodegradation rate constant in box i [s<sup>-1</sup>]



For steady state, i.e.  $dC(i)/dt = 0$ , the set of mass balance equations can easily be solved in a spreadsheet if mathematical expressions for  $MED_{i,j}$  and  $DIFF_{i,j}$  can be formulated as linear functions of  $C(i)$ . Obviously, the advective transport term is of the form:

$$MED_{i,j} = ADV_{i,j} \cdot C(i) \quad (2)$$

with

$ADV_{i,j}$  : flow rate of a medium irreversibly flowing from box i to j [ $m^3 s^{-1}$ ]

In a similar way, although the physical meaning is less apparent, diffusive transport from a source medium, box i, to a target medium, box j, can also be written in terms of a "volume flow rate" of some physical phase:

$$DIFF_{i,j} = XCH_{i,j} \cdot C(i) \quad (3)$$

with

$XCH_{i,j}$  : volume flow rate for diffusive transport from box i to j [ $m^3 s^{-1}$ ]

In the next chapters mathematical expressions for  $ADV_{i,j}$  and  $XCH_{i,j}$  are derived from base-set properties of the modelled chemical and parameters that are specific for a STP. If there is evidence for biodegradation during the activated sludge process, values higher than zero are assigned to  $k_i$ . Several approaches how to derive a value for  $k_i$  are described.  $V_i$  is a parameter which is also specific for the STP and dependent on the number inhabitants connected, and the mode of operation of the plant.

$C_i$  is obtained from multiple mass balance calculations and is standard output. This standard output is converted into customized output in the "output" sheet.

### 3 DEFINITION OF THE MODELLED CHEMICAL

#### 3.1 Physico-chemical properties

The molecular weight, the octanol-water partition coefficient, vapour pressure and water solubility are the minimal input parameters for which default values are taken if no data are given. The suggested default values are printed in the square brackets between the input column and the units column (see Fig 4). The acid and base dissociation constants,  $K_a$  and  $K_b$ , are optional and have such extreme defaults that at pH 7 only the neutral form of the chemical is assumed to exist in water. Therefore, specifying  $K_{a,b}$  should be omitted, unless there is evidence that the chemical dissociates at neutral pH.

From these four physico-chemical input parameters - and optionally  $K_{a,b}$  - Henry's law constant and the partition coefficients in raw sewage and activated sludge are calculated. For most organic chemicals these *calculated default* values, indicated as bold in between the square brackets in Fig 4, are satisfactory. Equations for these partition coefficients in terms of the minimal physico-chemical properties of the compound and some system parameters are given in 5.2 Diffusive volume flow rates. In case partition coefficients are available, direct input provides the user the opportunity to overrule the calculated defaults.

The last column displays the defined physico-chemical properties of the modelled chemical, in proper units, to be used in the calculation regions in "9-box" and "6-box".

Fig 4 Physico-chemical properties of the modelled chemical in the input sheet

Physico-chemical properties					
Molecular weight =		[ 1E+02 ]	g mol <sup>-1</sup>	0.1	kg mol <sup>-1</sup>
$K_{ow}$ =		[ 1E+03 ]	(-)	1000	(-)
Vapour pressure =		[ 1E+00 ]	Pa	1	Pa
Solubility =		[ 1E+02 ]	mg L <sup>-1</sup>	1	mol m <sup>-3</sup>
$K_a$ =		[ 1E-20 ]	(-)	1E-20	(-)
$K_b$ =		[ 1E-20 ]	(-)	1E-20	(-)
Henry constant (H) =		[ 1E+00 ]	Pa m <sup>3</sup> mol <sup>-1</sup>	1	Pa m <sup>3</sup> mol <sup>-1</sup>
$K_p$ (raw sewage) =		[ 1E+02 ]	L kg <sub>dwt</sub> <sup>-1</sup>	150	L kg <sub>dwt</sub> <sup>-1</sup>
$K_p$ (activated sludge) =		[ 2E+02 ]	L kg <sub>dwt</sub> <sup>-1</sup>	185	L kg <sub>dwt</sub> <sup>-1</sup>

### 3.2 Biodegradability

Persistency, or  $k_i = 0 \text{ s}^{-1}$ , is the default if no information on the biodegradability of the chemical can be provided. Biodegradation of a chemical is not only a property of the chemical but to a large extent also dependent on its environment. Nevertheless, the input sheet allows the user to interpret an OECD, EU or ISO standardized test result as a first order rate constant for biodegradation in the aqueous phase (Method I), if it were some sort of a compound property. The other two options, Method II and III, may be appropriate if more data of biodegradation research is available.

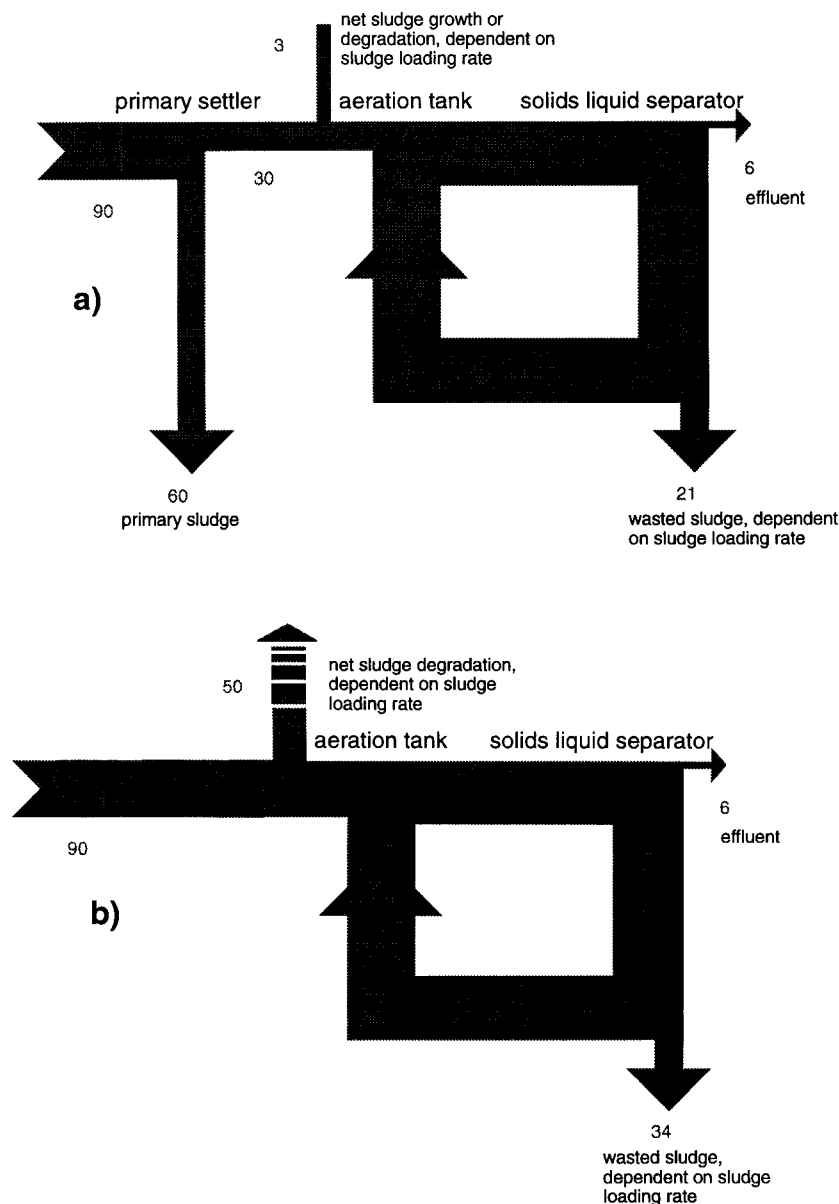
### 3.3 Concentration in raw wastewater

The emission rate of the chemical and the sewage flow determine the concentration in raw wastewater. Although this is usually not considered a property of a compound, this parameter is relevant if the option "Method III, Monod kinetics" for biodegradation is chosen, because the biodegradation first order rate constant, in this particular case, is dependent on the chemical concentration in raw waste water.

### 4 MODEL PARAMETERS FOR THE SEWAGE TREATMENT SCENARIO

The operation of a STP is considered a flow through system of continuous flows of water, suspended solids and settled solids. A proper definition of these media flows carrying the chemical, is fundamental for describing its fate in this engineered environment. From the size and the mode of operation of a STP, advective transport terms are obtained, so defining the advective volume flow rates  $ADV_{i,j}$ . In Fig 5, the daily sludge flow is schematically shown for an installation with (5a) and without (5b) primary sedimentation. In the following sections the parameters that are essential to describe the most relevant advective and diffusive transport processes are subdivided into fixed, input and derived parameters. In the STP defining regions of the the calculation sheets "9-box" and "6-box", the fixed parameters can be distinguished from the input and derived parameters, because in the comment column these fixed values are repeated, whereas the derived and input parameters have the attached comments "calc." and "input", respectively.

Fig 5. The daily sludge flow in a STP with (a) and without primary sedimentation (b)



#### 4.1 Fixed parameters

In Table 1 the fixed parameters are listed, subdivided into the categories raw sewage, primary sedimentation (only 9-box), aerator and solids liquid separation.

*Table 1. Fixed parameters for raw sewage and the operation of domestic waste water treatment.*

parameter	units	meaning	value
<i>raw sewage</i>			
BOD	$\text{g O}_2 \text{ PE}^{-1} \text{ d}^{-1}$	Mass of $\text{O}_2$ binding material per person per day	54
SOLIDS	$\text{kg}_{\text{dwt}} \text{ PE}^{-1} \text{ d}^{-1}$	Dry weight solids produced per person per day	0.09
$d_{\text{RS}}$	$\text{kg}_{\text{dwt}} \text{ L}^{-1}$	Density solids	1.500
$\text{foc}_{\text{RS}}$	-	Fraction organic carbon	0.3
<i>primary settler (9-box only)</i>			
$h_{\text{PS}}$	m	Depth	4
$\text{HRT}_{\text{PS}}$	hr	Hydraulic retention time	2
$d_{\text{PS}}$	$\text{kg}_{\text{dwt}} \text{ L}^{-1}$	Density suspended and settled solids	1.500
$\text{foc}_{\text{PS}}$	-	Fraction organic carbon solids	0.3
<i>activated sludge tank</i>			
$h_{\text{A}}$	m	Depth	3
$d_{\text{A}}$	$\text{kg}_{\text{dwt}} \text{ L}^{-1}$	Density solids of activated sludge	1.300
$\text{foc}_{\text{A}}$	-	Fraction organic carbon solids	0.37
CAS	$\text{kg}_{\text{dwt}} \text{ m}^{-3}$	Concentration solids of activated sludge	4
$\text{Cox}$	$\text{kg m}^{-3}$	Steady state $\text{O}_2$ concentration in activated sludge	0.002
G	$\text{m}^3 \text{ s}^{-1} \text{ PE}^{-1}$	Aeration rate bubble aeration	$1.31 \cdot 10^{-5}$
<i>solids liquid separator</i>			
$h_{\text{SLS}}$	m	Depth	3
$d_{\text{SLS}}$	$\text{kg}_{\text{dwt}} \text{ L}^{-1}$	Density suspended and settled solids	1.300
$\text{foc}_{\text{SLS}}$	-	Fraction organic carbon solids	0.37
CEF	$\text{kg}_{\text{dwt}} \text{ m}^{-3}$	Concentration solids in effluent	0.03
$\text{HRT}_{\text{SLS}}$	hr	Hydraulic retention time	6

## 4.2 Input parameters

Only four parameters may be specified if the user does not accept the default values (see Table 2). The sludge loading rate parameter,  $k_{SLR}$  ( $\text{kg BOD kg}_{dwt}^{-1} \text{ d}^{-1}$ ), is chosen in stead of the sludge retention time, SRT (d), to quantify the BOD loading of the installation. In principle also the hydraulic retention time, HRT (hr), could have been chosen for this purpose. For the relevant operation range of sewage treatment technology, these three parameters are depended according to certain empirical relationships. Table 1 of the input sheet (see Appendix A), may serve as a guidance for choosing an appropriate value for  $k_{SLR}$  if the user only is able to specify a desired SRT or HRT.

Table 2 Input parameters characterizing size and the operation mode of the treatment plant.

parameter	units	meaning	default value
Q	$\text{m}^3 \text{ PE}^{-1} \text{ d}^{-1}$	sewage flow	0.2
N	PE	number inhabitants	6667
$k_{SLR}$	$\text{kg}_{BOD} \text{ kg}_{dwt}^{-1} \text{ d}^{-1}$	sludge loading rate	0.15
M	-	mode of aeration: surface (s) or bubble aeration (b)	s

## 4.3 Derived parameters

### 4.3.1 Raw sewage.

The concentration of solids in raw sewage is:

$$C_{ss, RS} = \frac{SOLIDS}{Q} \quad (4)$$

with

$$C_{ss, RS} \quad : \quad \text{solids concentration in raw sewage } [\text{kg}_{dwt} \text{ m}^{-3}]$$

### 4.3.2 Primary settler.

With a fixed  $HRT_{PS}$  and  $h_{PS}$ , the geometry of the primary settler is derived as follows:

$$VOL_{PS} = \frac{Q \cdot HRT_{PS}}{24} \quad (5)$$

$$AREA_{PS} = \frac{VOL_{PS}}{h_{PS}} \quad (6)$$

with

$$\begin{aligned} VOL_{PS} & : \quad \text{volume of the primary settler per person } [\text{m}^3 \text{ PE}^{-1}] \\ AREA_{PS} & : \quad \text{area of the primary settler per person } [\text{m}^2 \text{ PE}^{-1}] \end{aligned}$$

It is assumed that in the primary sedimentation tank 2/3 of the solids is withdrawn due to sedimentation. As a consequence, in the primary settler the steady state suspended solids concentration of so-called settled sewage is:

$$C_{ss, PS} = \frac{C_{ss, RS}}{3} \quad (7)$$

with

$C_{ss, PS}$  : solids concentration in settled sewage [ $\text{kg}_{\text{dwt}} \text{m}^{-3}$ ]

#### 4.3.3. Aeration tank.

Of the total BOD input in raw sewage a fraction 13/36 is assumed to be removed by primary sedimentation. Thus the concentration of oxygen binding substances flowing into the aerator, for which the term "oxygen requirement" is used, is depended on Q and whether or not the STP is equipped with a primary settler:

$$OxReq_{9\text{-box}} = \frac{1}{Q} \cdot \frac{23}{36} \cdot \frac{BOD}{1000} \quad (8)$$

$$OxReq_{6\text{-box}} = \frac{1}{Q} \cdot \frac{BOD}{1000} \quad (9)$$

with

$OxReq_{9,6\text{-box}}$  : oxygen requirement of settled (9-box) and raw (6-box) sewage [ $\text{kg}_{\text{BOD}} \text{m}^{-3}$ ]

The volume of the aerator per person depends on the sludge loading rate and the oxygen requirement of the (settled) sewage:

$$VOL_{A ; 9,6\text{-box}} = \frac{Q \cdot OxReq_{9,6\text{-box}}}{k_{SLR} \cdot CAS} \quad (10)$$

with

$VOL_{A ; 9,6\text{-box}}$  : volume of the aerator per person [ $\text{m}^3$ ]

With a fixed depth, the area of the aeration tank per person is:

$$AREA_{A ; 9,6\text{-box}} = \frac{VOL_{A ; 9,6\text{-box}}}{h_A} \quad (11)$$

with

$AREA_{A ; 9,6\text{-box}}$  : area of the aerator per person [ $\text{m}^2$ ]

Hence the hydraulic retention time,  $HRT_A = VOL_A/Q$ , is a function of the oxygen requirement, sludge loading rate, the suspended solids concentration and the presence or absence of the primary settler:

$$HRT_{A ; 9,6-box} = \frac{OxReq_{9,6-box} \cdot 24}{k_{SLR} \cdot CAS} \quad (12)$$

with

$HRT_{A ; 9,6-box}$  : hydraulic retention time aerator [hr]

#### 4.3.4 Solids liquid separator.

With a fixed  $HRT_{SLS}$  and  $h_{SLS}$ , the geometry of the solids liquid separator or secondary settler is derived as:

$$VOL_{SLS} = \frac{Q \cdot HRT_{SLS}}{24} \quad (13)$$

$$AREA_{SLS} = \frac{VOL_{SLS}}{h_{SLS}} \quad (14)$$

with

$VOL_{SLS}$  : volume of the solids liquid separator settler per person [ $m^3 PE^{-1}$ ]  
 $AREA_{SLS}$  : area of the solids liquid separator per person [ $m^2 PE^{-1}$ ]

#### 4.3.5 Sludge loading characteristics.

From the input parameter  $k_{SLR}$ , which is also known as the food to mass ratio (F/M), several parameters are derived that are typical for the operation of the plant. The fraction BOD removal has been reported by Mikkelsen (1995) to correlate with  $\ln k_{SLR}$  according to:

$$F_{BODrem} = 0.818 - 0.0422 \cdot \ln k_{SLR} \quad (15)$$

with

$F_{BODrem}$  : the fraction of the BOD removed in the aerator [-]

The yield of biomass per unit BOD degraded in the aeration tank also correlates (Mikkelsen, 1995) with the sludge loading rate:

$$Y_{BOD} = 0.947 + 0.0739 \cdot \ln k_{SLR} \quad (16)$$

with

$Y_{BOD}$  : yield of biomass (sludge growth) per BOD [ $kg_{dwt} kg_{BOD}^{-1}$ ]



Equations 15 and 16 were obtained using data from Henze (1992). The amount of surplus sludge daily produced, also known as wasted sludge, depends on the presence of primary sedimentation. The net production per capita is obtained after subtraction of the emitted solids via the effluent:

$$SURPLUS_{9,6-box} = Q \cdot (OxReq_{9,6-box} \cdot F_{BODrem} \cdot Y_{BOD} - C_{SLS}) \quad (17)$$

with

$SURPLUS_{9,6-box}$  : wasted (surplus) sludge [ $kg_{dwt} PE^{-1} d^{-1}$ ]

If equations 10 - 17 are combined, the dependence on the presence or absence of primary sedimentation disappears in deriving an expression for the sludge retention time, because the oxygen requirement cancels:

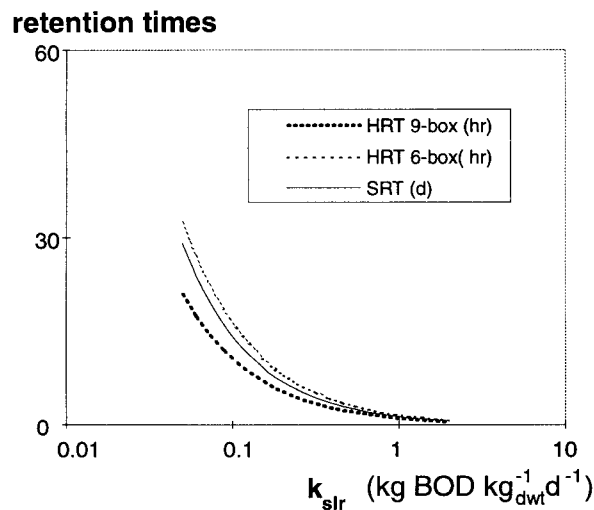
$$SRT = \frac{VOL_{A ; 9,6-box} \cdot CAS}{SURPLUS_{9,6-box} + C_{SLS} \cdot Q} = \frac{1}{k_{SLR} \cdot F_{BODrem} \cdot Y_{BOD}} \quad (18)$$

with

SRT : sludge retention time [d]

In Fig 6 the hydraulic retention time (hr) and the sludge retention time (d) are plotted against the sludge loading rate.

Fig 6. HRT, SRT vs  $k_{SLR}$  plot. Parameters used in the calculation are derived from Table 1.



## 5 DERIVING MEDIA FLOW RATES AS COEFFICIENTS FOR ADVECTIVE AND DIFFUSIVE TRANSPORT

### 5.1 Advective transport coefficients expressed as volume flow rates

#### 5.1.1. With primary sedimentation (9-box)

Air advection is dependent on the windspeed (input parameter) and the area of the plant:

$$ADV_{0,1} = ADV_{1,0} = h \cdot WS \sqrt{N \cdot AREA_{9\text{-box}}} \quad (19)$$

with

AREA <sub>9-box</sub>	:	AREA <sub>PS</sub> + AREA <sub>A; 9-box</sub> + AREA <sub>SLIS</sub> [m <sup>2</sup> PE <sup>-1</sup> ]
h	:	air mixing height [m] (fixed value: 10 m)
WS	:	windspeed [m s <sup>-1</sup> ] (default value: 3 m s <sup>-1</sup> )

The water volume flow rate into, inside and out of the installation is proportional to the sewage flow, Q, according to:

$$ADV_{0,2} = ADV_{2,5} = ADV_{5,7} = ADV_{7,0} = \frac{N \cdot Q}{24 \cdot 3600} \quad (20)$$

The volume flow rate of solids into, inside and out of the primary settler is given by the following three equations:

$$ADV_{0,3} = \frac{N \cdot SOLIDS}{1000 \cdot d_{RS} \cdot 24 \cdot 3600} \quad (21)$$

$$ADV_{3,4} = ADV_{4,0} = \frac{2}{3} ADV_{0,3} \quad (22)$$

$$ADV_{3,6} = \frac{1}{3} ADV_{0,3} \quad (23)$$

The solids flow in volume per time into the solids liquid separator is given by eqn 22:

$$ADV_{6,8} = \frac{N \cdot Q}{24 \cdot 3600} \frac{CAS}{1000 \cdot d_A} \quad (24)$$

The solids flow due to sedimentation (eqn 25) and recycling (eqn 26) is:

$$ADV_{8,9} = ADV_{6,8} - ADV_{8,0} \quad (25)$$

$$ADV_{9,6} = ADV_{8,9} - ADV_{9,0} \quad (26)$$

The emission of particulate matter as wasted (surplus) sludge and as suspended particulates to the receiving surface water, expressed as volume dry matter per time, is given by eqs 27 and 28, respectively:

$$ADV_{9,0} = \frac{N \cdot SURPLUS_{9\text{-box}}}{24 \cdot 3600 \cdot 1000 \cdot d_{SLS}} \quad (27)$$

$$ADV_{8,0} = \frac{N \cdot Q}{24 \cdot 3600} \frac{CEF}{1000 \cdot d_{SLS}} \quad (28)$$

### 5.1.2. Without primary sedimentation (6-box)

The air flow rate above the plant is given by:

$$ADV_{0,1} = ADV_{1,0} = h \cdot WS \sqrt{N \cdot AREA_{6\text{-box}}} \quad (29)$$

with

$$AREA_{6\text{-box}} : AREA_{A; 6\text{-box}} + AREA_{SLS} \text{ [m}^2 \text{ PE}^{-1}\text{]}$$

The water volume flow rates  $ADV_{0,5}$ ,  $ADV_{5,7}$  and  $ADV_{7,0}$  are calculated according to eqn 20, and the volume flow rate of solids in raw sewage entering the aeration tank,  $ADV_{0,6}$ , according to eqn 21. The sludge cycling in the activated sludge process, expressed as volume flow rates of dry solids is represented by three equations which are identical to 24, 25 and 26. Only one term appearing in eqn 26, i.e.  $ADV_{9,0}$  representing the volume flow rate related to the wasted or surplus sludge, is different. In the expression for  $ADV_{9,0}$  (eqn 27)  $SURPLUS_{9\text{-box}}$  has to be replaced with  $SURPLUS_{6\text{-box}}$ . The emission of solids in the effluent, expressed as volume dry matter per time,  $ADV_{8,0}$ , is identical to eqn 28.

### 5.2 Diffusive transport coefficients expressed as volume flow rates

Diffusive transport processes are driven by non-equilibrium concentrations in adjacent phases. In the model these are the particles-water and air-water systems. In principle, partition coefficients for solids-water ( $K_p$ ) and air-water ( $K_H$ ) should be input parameters as they are necessary to quantify to which extent the actual concentrations deviate from the equilibrium concentration ratios given by these partition coefficients. Diffusive transport across the interphase is proportional to the excursion from the equilibrium concentration. Unfortunately, they are usually not available as they do not form part of the base-set data of a chemical. In

the next paragraph partition coefficients are estimated from base-set input chemical properties (Fig 4).

### 5.2.1. Partition coefficients

$K_p$  or  $K_H$  pertain to the neutral form of chemicals, both in the aqueous phase and the non-aqueous phase. As a consequence, if the chemical dissociates into ionic species, the partition coefficient is considered to exclusively refer to the neutral form. This may imply that for organic acids or bases these parameters should have been determined at such extreme pH values that the dissolved chemical is predominantly in the neutral form. When partition coefficients are estimated from base-set compound properties also these base-set properties have to be determined under such extreme pH conditions. The water solubility and the  $K_{ow}$  should also pertain to the neutral chemical. It is assumed that the dominant sorption mechanism depends on the availability of the undissociated (neutral) chemical in the aqueous phase and that the concentrations associated with the sludge and air phase are exclusively in the neutral form. For practical reasons *overall* partition coefficients were evaluated as the ratio of the total concentration in air or solids (only neutral) and in water, in which the total concentration is the sum of neutral and ionized species. The overall partition coefficients used in SimpleTreat (Struijs et al., 1991) are derived only for pH = 7. In SimpleTreat 3.0 a more generalized expression as a function of  $[H^+]$ , the ionization constant of water ( $K_w$ ) and  $K_{a,b}$  is used, modified for the temperature dependence of the ionization degree of water.

Sludge-water. In Table 3 relevant fixed parameters are listed that are defined in the calculation sheets. The default values for the acid and basic dissociation,  $K_{a,b}$  constants are  $10^{-20}$ , meaning that the chemical is entirely in the neutral form if no  $K_{a,b}$  is specified.  $K_b$  is considered specified if it is higher than  $10^{-20}$ . The sludge-water partition coefficients for the various sludges in raw sewage (RS), settled sewage (PS), activated sludge (A) and effluent (SLS) has the following form:

$$K_p (RS, PS, A, SLS) = K_{emp} \cdot f_{oc} (RS, PS, A, SLS) \cdot K_{ow} \frac{K_w}{K_w + K_b \cdot [H^+]} \quad (30)$$

If the chemical is an organic acid, i.e.  $K_b \leq 10^{-20}$  and  $K_a$  is specified to be higher than  $10^{-20}$ :

$$K_p (RS, PS, A, SLS) = K_{emp} \cdot f_{oc} (RS, PS, A, SLS) \cdot K_{ow} \frac{[H^+]}{[H^+] + K_a} \quad (31)$$

with

$K_p$  : solids-water partition coefficient in raw sewage (RS) and the STP basins (PS, A, SLS) [ $L \text{ kg}^{-1}$ ]

The value of the empirical constant is,  $K_{emp}$ , is given in Table 3. The water dissociation constant, expressed as  $pK_w$ , is dependent on the water temperature according to a correlation reported by Mikkelsen, 1995:

$$pK_w = 25.35757 - 0.03818 \cdot T_{water} \quad (32)$$

with

$T_{water}$  : the water temperature in K

Analogously, the pH dependency of the air-water partition coefficient for an organic base and acid is given by eqs 33 and 34:

$$K_H = \frac{H}{R T_{air}} \frac{K_w}{K_w + K_b \cdot [H^+]} \quad (33)$$

$$K_H = \frac{H}{R T_{air}} \frac{[H^+]}{[H^+] + K_a} \quad (34)$$

with

$H$  : Henry's law constant [ $\text{Pa m}^3 \text{ mol}^{-1}$ ]  
 $R$  : gas constant [ $8.314 \text{ J K}^{-1} \text{ mol}^{-1}$ ]  
 $T_{air}$  : temperature in air [K]

Henry's law constant,  $H$ , is estimated from base-set data:

$$H = \frac{P}{S} \quad (35)$$

$P$  : vapour pressure of the chemical [Pa]  
 $S$  : water solubility of the non-dissociated chemical [ $\text{mol m}^{-3}$ ]

Expressions for the fugacity capacity of each compartment or box can be derived as follows (Mackay & Paterson, 1982):

$$Z_{air} = Z_1 = \frac{1}{R T_{air}} \quad (36)$$

$$Z_{\text{water}} = Z_2 = Z_5 = Z_7 = \frac{1}{H} \quad (37)$$

$$Z_{\text{primarysludge}} = Z_3 = Z_4 = \frac{K_{p, PS} \cdot d_{PS}}{H} \quad (38)$$

$$Z_{\text{solids A, SLS}} = Z_6 = Z_8 = Z_9 = \frac{K_{p, A, SLS} \cdot d_{A, SLS}}{H} \quad (39)$$

### 5.2.2. Concentration in raw sewage: equilibrium partitioning

Although the retention time in the sewer can be relatively short and equilibrium may not be reached, solids-water equilibrium partitioning of the chemical in raw sewage seems a reasonable approximation. Concentrations in the aqueous and solids phase are derived using the relationship  $K_{p, RS} = C_{s, RS}/C_{w, RS}$  (L/kg), in which  $C_{s, RS}$  is the concentration in solids (g/kg) and  $C_{w, RS}$  is the dissolved concentration (g/L). The input *customized* model input concentrations (in  $\text{g m}^{-3}$ ) are written in terms of emission scenario parameters (E, Q and N), the partition coefficient ( $K_{p, RS}$ ), the dry weight density ( $d_{RS}$ ) and the concentration ( $C_{ss, RS}$ ) of suspended solids in raw sewage:

$$C(0,2)_{9\text{-box}} = C(0,5)_{6\text{-box}} = \frac{1000 \cdot E}{Q \cdot N} \cdot \frac{1}{1 + C_{ss, RS} \cdot \frac{K_{p, RS}}{1000}} \quad (40)$$

$$C(0,3)_{9\text{-box}} = C(0,6)_{6\text{-box}} = \frac{1000 \cdot E}{Q \cdot N} \cdot \frac{K_{p, RS} \cdot d_{RS}}{1 + C_{ss, RS} \cdot \frac{K_{p, RS}}{1000}} \quad (41)$$

with

E	:	emission rate of the chemical in the sewer [ $\text{kg d}^{-1}$ ]
C(0,i)	:	concentration in phase i of raw sewage entering the STP into box i [ $\text{g m}^{-3}$ ]

Input concentrations, C(0,i) as given by eqn 40 and 41, as well as internal chemical concentrations in the box model, C(i), are all in units of  $\text{g m}^{-3}$  ( $\text{mg L}^{-1}$ ).

### 5.2.3 Settled sewage (PS), activated sludge (A) and effluent (SLS): non-equilibrium in the suspended solids/water system

In all basins of the STP, non-equilibrium between suspended solids and water may drive diffusive transport, in particular in the activated sludge reactor. It is assumed that chemical

exchange between the suspended solids and aqueous phase can be expressed in terms of half-lives for uptake (sorption) and clearance (desorption), given by Table 3.

Table 3. Fixed parameters used in formulating partition coefficients and (de)sorption rates

parameter	units	meaning	value
[H <sup>+</sup> ]	mol L <sup>-1</sup>	H <sup>+</sup> concentration in water	10 <sup>-7</sup>
K <sub>emp</sub>	-	empirical constant	1
t <sub>1/2</sub> (PS)	s	half-live of (de)sorption in the primary settler	3600
t <sub>1/2</sub> (A)	s	half-live of (de)sorption in the aerator	360
t <sub>1/2</sub> (SLS)	s	half-live of (de)sorption in the solids liquid separator	3600
K <sub>air</sub>	m s <sup>-1</sup>	mass transfer coefficient in air	2.78·10 <sup>-3</sup>
K <sub>water</sub>	m s <sup>-1</sup>	mass transfer coefficient in water	2.78·10 <sup>-5</sup>

The approach of Mackay's concept of fugacity capacity (Mackay & Paterson, 1982) is employed to formulate coefficients for interphase transfer from box *i* to box *j*,  $D_{i,j}$ , in mass per time per pressure. Reversible solids-water exchange of the chemical in the different basins is represented by eqn 42. The different interphase transfer coefficients refer to, respectively, settled sewage (PS), represented by the combination of box 2 and 3 ( $D_{2,3} = D_{3,2}$ ), activated sludge (A) or box 5 and 6 ( $D_{5,6} = D_{6,5}$ ), and effluent (SLS) represented by box 7 and 8 ( $D_{7,8} = D_{8,7}$ ). The interphase transfer coefficients ( $D_{i,j}$ ) and the volumes of each box ( $V_i$ ) pertain to *N* persons:

$$D_{2,3; 5,6; 7,8} = D_{3,2; 6,5; 8,7} = \frac{\ln 2}{t_{1/2} (PS, A, SLS)} \cdot \frac{1}{\frac{1}{V_{2, 5, 7} \cdot Z_{2, 5, 7}} + \frac{1}{V_{3, 6, 8} \cdot Z_{3, 6, 8}}} \quad (42)$$

with

$$\begin{aligned} D_{i,j} &: \text{interphase transfer coefficient from box } i \text{ to box } j \text{ [mol s}^{-1} \text{ Pa}^{-1}] \\ V_i &: \text{the volume of box [m}^3] \end{aligned}$$

In Appendix B expressions are given for  $V_i$ .

#### 5.2.4 Reversible air-water transfer without aeration

Diffusive transport to the air is thought to occur exclusively from the water phase. In other words: only in the aqueous phase is the chemical available to participate in volatilization or

stripping processes. The rate of these processes depend on how far the actual concentrations deviate from the equilibrium concentrations in air and water. Both in the primary sedimentation and the solids liquid separator, air-water transport is simulated with a two layer model, applied by Liss & Slater (1974) and extended by Mackay & Leinonen (1975). According to Mackay et al. (1985) expressions for  $D_{i,j}$  are formulated for volatilization/gas absorption in basins without engineered aeration. As one equation for the three basins  $D_{i,j}$  would read:

$$D_{1,2; 1,5; 1,7} = D_{2,1; 5,1; 7,1} = \frac{A_{PS, A, SLS}}{\frac{1}{K_{air} \cdot Z_{air}} + \frac{1}{K_{water} \cdot Z_{water}}} \quad (43)$$

with

$A_{PS, A, SLS}$  : Area of the primary settler, aerator and the solids liquid separator for N persons [m<sup>2</sup>]

However, this type of air-water diffusive transfer only applies to non-aerated systems and therefore may underestimate the total interphase transport between water and air in the aeration tank. Stripping due to surface or diffuse aeration may exceed volatilization, especially for compounds with high H values. Before applying previously reported expressions for this particular diffusive process in terms of a first order rate constant (reciprocal time), in order to incorporate them in expressions for  $D_{i,j}$ , it is useful to first derive a first order rate constant for volatilization/gas absorption. This can easily be done by equating  $D_{i,j}$  in the form given by eqn 42, in which  $\ln(2)/t_{1/2}$  has been replaced with  $k_{vol/gasabs}$ , to the right hand side of eqn 43:

$$\frac{k_{vol/gasabs}}{\frac{1}{V_{air} \cdot Z_{air}} + \frac{1}{V_{water} \cdot Z_{water}}} = \frac{A}{\frac{1}{K_{air} \cdot Z_{air}} + \frac{1}{K_{water} \cdot Z_{water}}} \quad (44)$$

with

$k_{vol/gasabs}$  : first order rate constant for volatilization/gasabsorption [s<sup>-1</sup>]  
 A : area of the air-water interphase [m<sup>2</sup>]



It can easily be derived that:

$$k_{vol/gasabs} = \frac{\frac{1}{h} + \frac{K_H}{d_A}}{\frac{1}{K_{air}} + \frac{K_H}{K_{water}}} \quad (45)$$

In the following paragraph  $k_{vol/gasabs}$  is compared to first order rate constants reported for two different types of stripping processes.

### 5.2.5 Reversible air-water transfer in the aeration tank

Air-water exchange of chemicals in the aerator depends on the mode of aeration. If mechanical or bubble aeration does not occur, the first order overall transfer rate constant is given by eqn 45. This rate constant and its related interphase transfer coefficient ( $D_{i,j}$ ) evaluated from the right hand side of eqn 44, may be regarded as the minimal mass transport coefficients for air-water exchange. At least for volatile chemicals ( $H > 50 \text{ Pa m}^3 \text{ mol}^{-1}$ ), aeration may cause higher removal rates due to stripping. Two types of stripping processes are distinguished in SimpleTreat and SimpleTreat 3.0: surface aeration and bubble aeration. Several expressions for first order rate constants have been reported.

Surface aeration. In SimpleTreat an expression for the first order rate constant for surface aeration was applied, as derived by Roberts et al. (1984). The gas phase resistance correction, however, was ignored. Instead, a proportionality constant equal to 0.6 was considered satisfactory, although it proved only valid for rather volatile chemicals. In the following equation this gas phase correction (GPC) is included. This equation reduces to the expression given by Roberts et al. (1984) and which was used in SimpleTreat if GPC is set equal to one (no gas phase resistance):

$$k_s = \psi \cdot GPC \frac{OxReq}{HRT_A \cdot \Delta O_2} \quad (46)$$

with

$k_s$	:	first order transfer rate constant for surface aeration [ $\text{s}^{-1}$ ]
$\psi$	:	empirical constant [0.6]
GPC	:	gas phase correction [-]
$\Delta O_2$	:	difference between saturation and actual $O_2$ concentration, $C_{ox,sat} - C_{ox}$ [ $\text{kg } O_2 \text{ m}^{-3}$ ]; default is $0.007 \text{ kg } O_2 \text{ m}^{-3}$ .

The approximation of  $GPC = 1$  has been shown a satisfactory if  $H$  exceeds  $250 \text{ Pa m}^3 \text{ mol}^{-1}$ , which means that liquid layer resistance controls the rate of interphase mass transfer. In order to extend the validity of eqn 46 to chemicals with  $H < 250 \text{ Pa m}^3 \text{ mol}^{-1}$ , the gas phase resistance should be taken into account. Munz and Roberts (1989) recommended to apply the following  $K_H$  dependency of GPC:

$$GPC = \frac{\frac{k_G a}{k_L a} \cdot K_H}{\frac{k_G a}{k_L a} \cdot K_H + 1} \quad (47)$$

with

$k_G a/k_L a$  : ratio of the mass transfer rates of the chemical in air and water [-]

A default value for  $k_G a/k_L a$  equal to 40 has been recommended as satisfactory (Munz & Roberts, 1989). Eqn 46 would produce the same value for systems with and without primary sedimentation. Although for a chosen mode of operation, both parameters OxReq and HRT have different values in 9-box and 6-box, their ratio is equal in both systems, being proportional to  $k_{SLR} \cdot CAS$  (see eqn 12).

Bubble aeration. If the oxygen supply is brought about by bubble or diffuse aeration, the first order rate constant of air-water exchange proposed by Hsieh et al. (1993) is:

$$k_b = 8.9 \cdot 10^{-10} \frac{G}{VOL_A} \cdot H^{1.04} \quad (48)$$

with

$k_s$  : first order transfer rate constant for bubble aeration [ $s^{-1}$ ]

This expression has an almost similar form as the relationship given by Blackburn et al. (1984), used in SimpleTreat. For most chemicals, however, eqn 48 would give a value being approximately a factor 1.8 higher than calculated by SimpleTreat. Note that here  $k_s$  is different for 9-box and 6-box as  $VOL_A$  is different for both systems.

For a certain sludge loading rate,  $k_{vol/gasabs}$ ,  $k_s$  and  $k_b$  are plotted versus  $K_H$  in Fig 7. For  $H < 60 \text{ Pa m}^3 \text{ mol}^{-1}$ , the first order constant related to the Liss & Slater approach,  $k_{vol/gasabs}$ , is higher than  $k_s$  and  $k_b$ . Therefore, Mikkelsen (1995) proposed to calculate the *overall* interphase transfer constant as the highest of surface volatilization and stripping. In SimpleTreat 3.0 surface volatilization is taken as the minimum rate constant to which the first order stripping constant  $k_s$  or  $k_b$  is added:

$$k_{aerator} = k_{vol/gasabs} + k_{s,b} \quad (49)$$

with

$k_{aerator}$  : first order overall transfer rate constant for surface or bubble aeration [ $s^{-1}$ ]

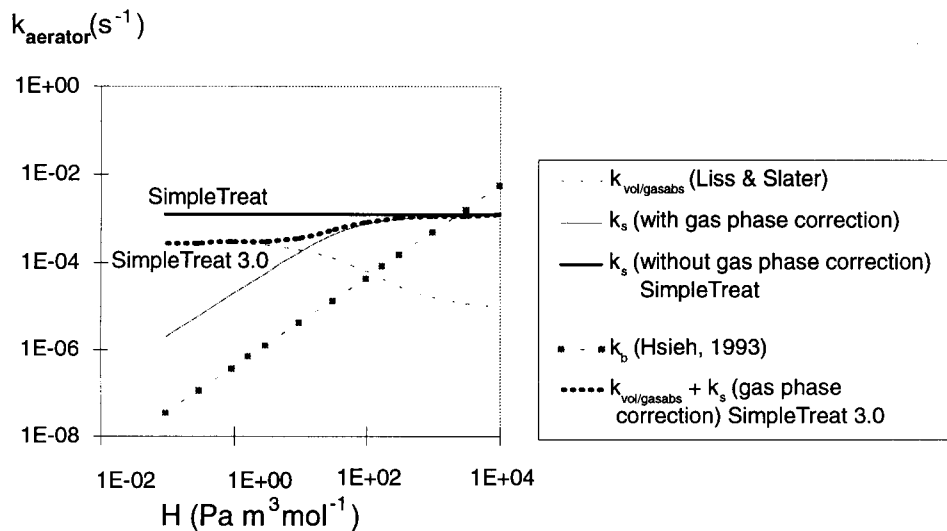
Expressions for  $D_{5,1}$  and  $D_{1,5}$  are obtained by replacing  $k_{vol/gasabs}$  with  $k_{aerator}$  in the numerator of the left part of eqn 44.

### 5.2.6 Diffusive exchange rates between two adjacent boxes

The diffusive exchange of the chemical between box  $i$  and box  $j$  is to be evaluated for both directions,  $XCH_{i,j}$  and  $XCH_{j,i}$ . With all interphase transfer coefficients,  $D_{i,j}$ , as derived in the former paragraphs, the mass transport coefficient from  $i$  to  $j$ , expressed as the volume flow rate from the source phase  $i$  into the direction of target phase  $j$ , is obtained as (Mackay & Paterson, 1982):

$$XCH_{i,j} = \frac{D_{i,j}}{Z_i} \quad (50)$$

Fig 7. First order air-water exchange rate constants for varying Henry's law constant



## 6 BIODEGRADATION IN ACTIVATED SLUDGE

Input of data and process description differs most from SimpleTreat. Three modes of data input have the following order of increasing priority:

- First order rate constant,  $k_{\text{biodeg}}(\text{I})$  in  $\text{hr}^{-1}$ , for biodegradation exclusively in the water phase. In the input sheet suggestions are made how to extrapolate results of standardized tests, according to the OECD/EU guidelines, to an input parameter;
- First order rate constants for degradation,  $k_{\text{biodeg}}(\text{II})$  in  $\text{hr}^{-1}$ , which refers to both the aqueous and the solids phase;
- Monod kinetic parameters ( $\mu_{\text{max}}$ ,  $K_s$ ). In the calculation sheets,  $k_{\text{biodeg}}(\text{III})$  is evaluated from the Monod constants, emission data and the sludge loading rate.

### 6.1 Standard OECD/EU tests

The only difference from SimpleTreat is that instead of "yes or no", which means that the first order  $k_{\text{biodeg}}(\text{I})$  is 3 or 0  $\text{hr}^{-1}$  - in the water phase of the aerator (box 5) - the user may choose a value. Suggestions are made, on the basis of the Technical Guidance Document for Environmental Risk Assessment of New and Existing Substances (1995), how to extrapolate a result of Ready or Inherent Biodegradability testing, according to the OECD/EU, to a value for  $k_{\text{biodeg}}(\text{I})$ , which in the model is converted into appropriate units of  $k_5$ .

### 6.2 Specifying one first order degradation rate constant which applies to both the aqueous and the solids phase

Cowan et al. (1993) proposed to assign one first order rate constant which applies to degradation in water as well as biodegradation in the sludge solids phase. They found better predictions for degradation of surfactants in the activated sludge reactor. In order to provide the user of SimpleTreat 3.0 with this option, method II is an option to specify  $k_{\text{biodeg}}(\text{II})$  in  $\text{hr}^{-1}$ . This value is converted into appropriate units to equally define  $k_5$  (water) and  $k_6$  (suspended solids). However no suggestions are made as to typical values of these constants.

### 6.3 Non-linear kinetics: biodegradation according to Monod

It has been found by Birch (1991) that the onset and extent of biodegradation during the activated sludge process is largely determined by the SRT and the concentration of the degradable chemical in wastewater. This can be understood from a model of growth kinetics for the competent microorganisms, capable to survive in the activated sludge process. From the actual growth rate, which has a maximum value for a given input concentration, and the decay of the specific degraders, it can be reasoned that the mean sludge retention time, SRT, determines whether or not these microorganisms may be present in activated sludge to a significant extent. It can be derived that below some SRT, called the critical sludge retention time ( $\text{SRT}_{\text{crit}}$ ), too slowly growing organisms will be washed out for any given influent concentration entering the aerator.

To be able to calculate the  $SRT_{crit}$ , the total input concentration,  $C_{input}$ , of the biodegradable chemical has to be estimated for raw (6-box) or settled (9-box) sewage. To obtain the first is straightforward:

$$C_{input, 6-box} = \frac{1000 \cdot E}{Q \cdot N} \quad (51)$$

with

$C_{input, 6-box}$  : total concentration in raw sewage [ $g\ m^{-3}$ ]

The second is estimated from the emission scenario data  $E$ ,  $Q$ ,  $N$  and  $K_{p, RS}$  and the steady state concentration of suspended solids in raw sewage ( $C_{ss, RS}$ ). Of these solids 2/3 is removed during primary sedimentation. The total chemical concentration in the slurry flowing into the aerator after primary sedimentation - settled sewage - is:

$$C_{input, 9-box} = \left( \frac{1000 \cdot E}{Q \cdot N} \right) \frac{1 + \frac{1}{3} \frac{K_{p, RS} \cdot C_{ss, RS}}{1000}}{1 + \frac{K_{p, RS} \cdot C_{ss, RS}}{1000}} \quad (52)$$

with

$C_{input, 9-box}$  : total concentration in settled sewage [ $g\ m^{-3}$ ]

The critical sludge retention time and the steady state concentration in the aerator, i.e. the concentration in the mixed liquor flowing out of the aerator ( $C_{output}$ ), can be derived from the Monod function:

$$\mu_{act} = \frac{\mu_{max} \cdot C_{output}}{K_s + C_{output}} \quad (53)$$

with

$\mu_{act}$  : the actual growth rate of specific microorganisms [ $d^{-1}$ ]  
 $\mu_{max}$  : maximum growth rate of the specific microorganism [ $d^{-1}$ ]  
 $K_s$  : half saturation concentration [ $g\ m^{-3}$ ]  
 $C_{output}$  : total chemical concentration in activated sludge [ $g\ m^{-3}$ ]

and the mass balance for growth of the specific degraders:

$$\mu_{act} = K_{decay} + \frac{1}{SRT} \quad (54)$$

with

$K_{decay}$  : decay rate of the specific microorganism [ $d^{-1}$ ]

Eqn 54 states that the actual growth rate,  $\mu_{act}$ , is balanced by the decay rate and the sludge wastage rate ( $1/SRT$ ). The critical sludge retention time for any given input concentration, below which biodegradation should be set to zero, is evaluated according to Birch (1991):

$$\frac{1}{SRT_{crit}} = \frac{\mu_{max} \cdot C_{input, 6/9-box}}{K_s + C_{input, 6/9-box}} - K_{decay} \quad (55)$$

A reasonable approximation of the decay rate is  $0.5/SRT \text{ d}^{-1}$  (Blok & Struijs, 1996). If the actual sludge retention time (SRT) is longer than  $SRT_{crit}$ , biodegradation occurs at such a rate that the steady state concentration of the chemical in the aerator is entirely governed by the kinetic constants for microbial growth/decay and the sludge retention time. Assuming that  $K_{decay} = 0.5/SRT$  only  $\mu_{max}$ ,  $K_s$  and SRT are required data and assuming that the aerator is a well mixed system, this steady state concentration equals the output concentration ( $C_{output}$ ) of the aerator:

$$C_{output} = \frac{K_s(1 + SRT \cdot K_{decay})}{SRT (\mu_{max} - K_{decay}) - 1} \quad (56)$$

This equation states that the output concentration is independent of the input concentration. In addition to the Monod kinetic constants, only one major characteristic of the loading of the plant has to be known, i.e. SRT. Knowing SRT is important for two reasons:

- 1) to test whether or not  $SRT \leq SRT_{crit}$ ; if so, then persistency is assumed, resulting in  $k_5 = k_6 = 0$ ;
- 2) If  $SRT > SRT_{crit}$ ,  $C_{output}$  can be calculated according to eqn 56. This result is in the model approximated by calculating a first order biodegradation rate constant from a mass balance for the water phase of activated sludge, assuming that biodegradation is the only disappearance mechanism:

$$k_{monod} = \frac{C_{input, 6/9-box} - C_{output}}{C_{output} \cdot \frac{HRT}{24 \cdot 3600}} \quad (57)$$

with

$k_{monod}$  : first order rate constant for biodegradation in the aerator [ $s^{-1}$ ]

This implies that the first order degradation rate constant is dependent on the total concentration of the chemical in raw or settled sewage. Although the concentrations in eqn 57 refer to total concentrations in settled/raw (9/6-box) and activated sludge, the biodegradation rate constant presumably pertains to the aqueous phase only ( $k_6 = 0$ ):

$$k_5 = k_{biodeg(III)} = k_{monod} \quad (58)$$

#### 6.4 Priority of data evaluation and temperature dependency

The default values for  $k_{\text{biodeg}}(\text{I})$  and  $k_{\text{biodeg}}(\text{II})$  are zero and the defaults for Monod kinetics are  $\mu_{\text{max}} = 2 \text{ d}^{-1}$  and  $K_s = 0.5 \text{ mg L}^{-1}$ . If, however, no input data for  $\mu_{\text{max}}$  and  $K_s$  are given,  $k_{\text{biodeg}}(\text{III})$  is set to zero. The priority with which input data are treated is in the order III, II and I. Biodegradation is not taken into account in the model calculations, or  $k_5 = k_6 = 0$ , if the user has failed to provide any data. This is schematically shown in Fig 8. Either from input data or defaults,  $\mu_{\text{max}}$  and  $K_s$  are specified. In combination with emission data and plant operation data, the critical sludge retention time and, subsequently, the steady state output concentration and  $k_{\text{monod}}$  are evaluated according to eqs 56 and 57. Only if  $\mu_{\text{max}}$  and  $K_s$  are specified,  $k_{\text{biodeg}}(\text{III})$  is set equal to  $k_{\text{monod}}$ . With  $k_{\text{biodeg}}(\text{III}) = 0$ , but  $k_{\text{biodeg}}(\text{II}) > 0$ , i.e. input for method II is available, both  $k_5$  and  $k_6$  are set to equal values.

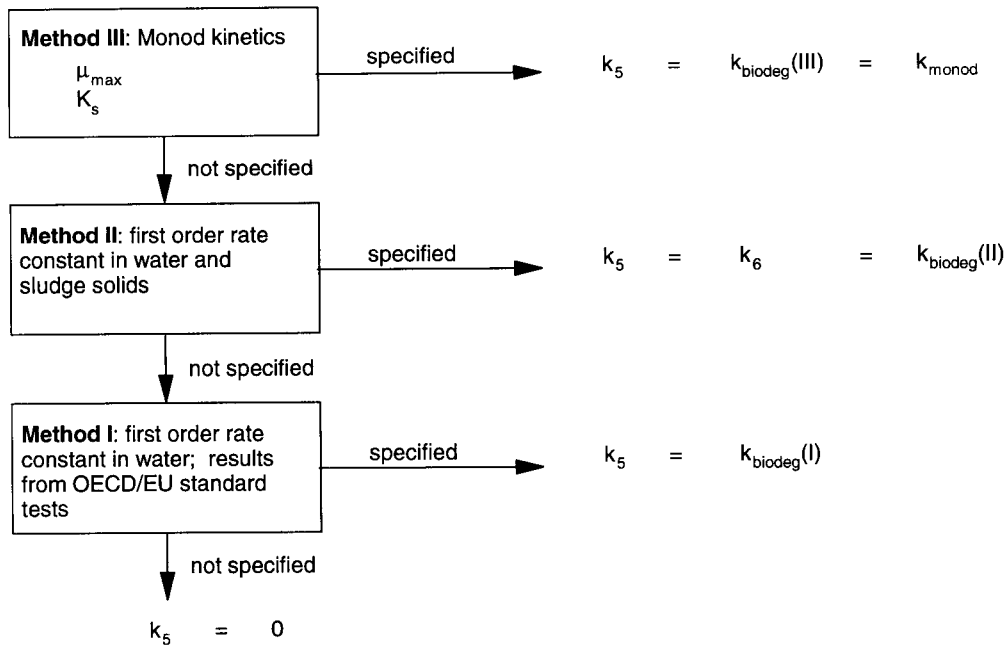
There is still no consensus among experts if the temperature dependence of the biodegradation process has to be taken into account, unless extreme low and high temperature are apparent. In particular for the activated sludge process, fed with (settled) sewage which has at least a non-freezing temperature, it is not yet clear if temperature dependence is relevant. Even in the winter in cold areas, the water temperature in the treatment plant basins is likely to have some elevated value as it comes from domestic sewage with a relatively high temperature. In a STP without primary sedimentation this flows directly into aerator, whereas in a primary sedimentation tank the short hydraulic residence time (usually ca 2 hr) may cause only a relatively temperature decrease. Therefore, the biodegradation section of the input sheet starts with the question if the temperature correction has to be made. If no answer is given, the default temperature correction factor with which  $k_{\text{biodeg}}$  is multiplied,  $F_T$ , is set equal to 1.  $F_T$  is calculated according to eqn 59, if temperature dependence is desired:

$$F_T = 1.072^{(T - T_{\text{ref}})} \quad (59)$$

with

T	:	water temperature [°C], derived from $T_{\text{water}}$ [K]
$T_{\text{ref}}$	:	temperature related to biodegradation input data [°C]

Fig 8 Priority of processing biodegradation data in SimpleTreat 3.0





## 7 DISCUSSION

SimpleTreat 3.0 predicts the chemical fate during primary sedimentation and subsequent activated sludge operation for a wide variety of operating conditions. The theoretical understanding of these processes is sufficiently developed to allow the use of mathematical models. Limited discharge data in combination with base-set compound properties are converted by the model into data that can be directly used for exposure assessment. The accuracy of exposure assessment in urban regions, in particular for the water compartment, is greatly affected by the accuracy with which the chemical fate in wastewater treatment systems can be predicted.

Domestic sewage and a significant part of industrial wastewater is a mixture which is also known as communal wastewater. In urban areas the major part of communal wastewater is, or will be, treated by the activated sludge reactor. Article 4 of Council Directive 91/271/EEC stipulates that, before 31 December 2000, urban wastewater discharged from agglomerations of more than 15000 population equivalent shall be subject to secondary treatment before being discharged to the environment. At present the percentage connection to sewage works is still quite diverse in the EU. Across the EU, taken as a whole, nearly 70 % of the municipal wastewater is treated at least in primary purification plants, i.e. solids BOD removal due to solely primary sedimentation. Some regions have connection percentages as high as 90 - 95 %, like Denmark and The Netherlands, some have yet low treatment percentages. In some mountainous areas of the EU the percentage will be technically limited to about 70 %.

Like in former versions of SimpleTreat the steady-state, non-equilibrium box modeling concept is applied, also known as Mackay level III. Suspended solids in the different basins are considered separated boxes, in between water and settled sediment. With this approach it is possible to account for sludge recycling in the activated sludge process. If appropriate, it can also be applied to simulate more complex systems, f.i. sludge stabilization tanks in between the settled solids in the solids liquid separator and the aeration tank or SPTs equipped with an anaerobic reactor. For the purpose of generic exposure modeling in the different regions of the EU, it is considered adequate to allow only for the presence and absence of primary sedimentation.

SimpleTreat 3.0 differs from earlier version of SimpleTreat in several aspects:

- The structure of SimpleTreat 3.0 is more systematic as it consists of modules. This facilitates model revisions by inserting new components or replacing mathematical expressions with improved proces descriptions.
- The mode of operation of the plant can be chosen on a continuous scale. The original version of SimpleTreat only allowed the user to choose "high", "medium" or "low" sludge

loading rate,  $k_{SLR}$ , equivalent to 2, 0.6 and 0.2 kg BOD/kg<sub>dwt</sub>/d, respectively (Struijs et al., 1991). The weakness may be illustrated by a minor revision, which has been considered necessary to account for a reduction of average BOD loading as a result of modernizing installations and increasing the percentage of connections. "High", "medium" or "low" has been shifted to 0.6, 0.2 and 0.06 kg BOD/kg<sub>dwt</sub>/d, which is equivalent to retention times of SRT = 1.7, 5.5 and 17 d and HRT = 3.1, 10.2 and 30 hr, respectively. This may be convenient for the Dutch situation where a treatment percentage as high as 92 % is associated with a low average  $k_{SLR}$ . However, although in the UK also a high percentage of wastewater is treated (83 % of which 74 % by secondary treatment; Feijtel, 1995), the average sludge loading rate is approximately a factor 10 higher compared to the Netherlands (Painter, 1995). Although the SRT range of 5 - 20 d and the HRT range of 4 - 16 hr is found typical for the EU (Feijtel, 1995), an exposure assessment model, applicable to all EU Member States, preferably spans a wider range of operation modes.

- SimpleTreat 3.0 allows to compute the chemical fate in a STP that is not equipped with a primary sedimentation tank. For the Danish situation, for example, where the nation wide treatment percentage is high (92 %), this may be useful because a significant part of the population is living in rural areas where sewer systems most often are connected to such installations.
- The sewage flow rate per capita is an input parameter; the default value is 200 L/person/d. As in the SimpleTreat 3.0 the hydraulic retention times of the sedimentation tanks are fixed, the volumes are adjusted accordingly. The volume of the aerator is calculated from the sewage flow rate, the fixed amount of BOD in raw sewage per capita per day and the chosen sludge loading rate. With these parameters the aerator volume of an installation without primary sedimentation is larger because raw sewage contains 36/23 more BOD than settled sewage (see eqs 8 - 10).
- Stripping due to surface aeration is formulated more accurately, taking the air phase resistance into account. This is necessary to avoid overestimation of stripping chemicals with  $H < 100 \text{ Pa m}^{-3} \text{ d}^{-1}$ . However, surface volatilization, expressed according Liss & Slater (1974), predicts higher removal than surface and bubble aeration for chemicals with  $H < 60 \text{ Pa m}^{-3} \text{ d}^{-1}$ . Thus either the first order stripping constant for surface or bubble aeration has to be overruled by a greater first order surface volatilization constant (Mikkelsen, 1995), or the sum of both has to be taken. In SimpleTreat 3.0 the latter approach is used. For the lower range of Henry's law constant, removal due to stripping - in particular for bubble aeration - is negligible compared to surface volatilization. On the other side of the log H scale, thus for highly volatile chemicals, surface volatilization would seriously underestimate water-air exchange. Adding surface volatilization to stripping counteracts the H dependency of the first order rate constant for surface aeration. As a result, the difference between SimpleTreat and SimpleTreat 3.0 (see Fig 7) is only significant - approximately a factor 3 - at  $H < 60 \text{ Pa m}^{-3} \text{ d}^{-1}$ .

- Unlike in former versions of SimpleTreat, settled solids-water exchange in the sedimentation tanks is neglected. The assumption that equilibrium partitioning applies to the chemical entering the sedimentation tank in combination with a short residence time of both water and solids, is part of the justification. Most of the solids-water exchange, driven by non-equilibrium concentrations, is thought to occur in the aeration tank with a very short half-life for sorption/desorption (see Table 3). Moreover, in this most relevant basin there is no settled sediment. However, this remains to be validated by sensitivity analysis.
- The most important modification is concerned with biodegradation in activated sludge. In SimpleTreat biodegradation is set to zero unless the user qualifies the chemical positive in a Ready Biodegradability Test, according to the OECD/EU. It was a matter of experience, although based upon a few chemicals, that a "readily biodegradable" compound is biodegraded in an activated sludge reactor at least to the extent BOD is degraded, even if biodegradation is the only removal mechanism. From correlating the hydraulic retention times with BOD removal percentages for three sludge loading conditions, it was derived that the first order rate constant for biodegradation - in the aqueous phase - should have at least the value  $3 \text{ hr}^{-1}$ . Thus in SimpleTreat  $k_{\text{biodeg}}$  is set equal to 0 or  $3 \text{ hr}^{-1}$ , by input "no" or "yes". The user was not offered the option to choose another rate constant. From the precautionary principle EU experts decided to apply a lower value in case the chemical is "ready". The modeling results in the Technical Guidance Document are based on  $k_{\text{biodeg}} = 1 \text{ hr}^{-1}$  for positive chemicals. In case the chemical is positive but only the stringent condition of the "10 days window" is not fulfilled,  $k_{\text{biodeg}}$  is set to  $0.3 \text{ hr}^{-1}$ . Calculations for "inherently biodegradable" chemicals were carried out with  $k_{\text{biodeg}} = 0.1 \text{ hr}^{-1}$ . In SimpleTreat 3.0 the user is free to choose any first rate constant. A first order biodegradation rate constant in both the particle and the water phase, at equal rates, can be specified according to method II. It has to be proved that this approach is a suitable one for generic exposure assessment. Method III is a simulation of non-linear degradation, by making the first order biodegradation rate constant dependent on the chemical concentration in raw or settled sewage. With this model the very high removal percentages reported for readily biodegradable high volume detergents can be accounted for, as well as observed rather low percentages for readily biodegradable substances entering the sewage works in concentrations that are orders of magnitude lower than those of consumer detergents. Validation research has been and is being conducted in several institutes. The non-linear degradation kinetic model predicts that the effluent concentration is independent on the influent concentration.

Future developments are focussed on experimental verification of the individual removal processes: via sludge withdrawal, volatilization/gas absorption and biodegradation. Validation of the model, combining all processes, will be carried out thereafter. Results are expected to be available within a few years.

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## Appendix 1 Input sheet

SimpleTreat 3.0 1996 (2/5/96)									
input									
<b>Characterization of the chemical</b>									
Name compound =	hypotheticum								
<b>Physico-chemical properties</b>					table 1:				
Molecular weight =	[ 1E+02 ]	g mol <sup>-1</sup>	0.1	kg mol <sup>-1</sup>	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 SR				
K <sub>ow</sub> =	[ 1E+03 ]	(-)	1000	(-)	SLR	HRT (PS)	HRT	SRT	nitrification
Vapour pressure =	[ 1E+00 ]	Pa	1	Pa	(kg <sub>BOD</sub> kg <sub>dw</sub> <sup>-1</sup> d <sup>-1</sup> )	(hr)	(hr)	(d)	(-)
Solubility =	[ 1E+02 ]	mg L <sup>-1</sup>	1	mol m <sup>-3</sup>	0.04 (low)	26.4	32.4	37.0	yes
K <sub>a</sub> =	[ 1E-20 ]	(-)	1E-20	(-)	0.06 (low)	17.6	27	24.1	yes
K <sub>p</sub> =	[ 1E-20 ]	(-)	1E-20	(-)	0.1 (low)	10.6	16.2	14.1	yes
Henry constant (H) =	[ 1E+00 ]	Pa m <sup>3</sup> mol <sup>-1</sup>	1	Pa m <sup>3</sup> mol <sup>-1</sup>	0.15 (medium)	7.1	10.8	9.2	yes
K <sub>p</sub> (raw sewage) =	[ 1E+02 ]	L kg <sub>dw</sub> <sup>-1</sup>	150	L kg <sub>dw</sub> <sup>-1</sup>	0.2 (medium)	5.3	8.1	6.8	no
K <sub>p</sub> (activated sludge) =	[ 2E+02 ]	L kg <sub>dw</sub> <sup>-1</sup>	185	L kg <sub>dw</sub> <sup>-1</sup>	0.3 (high)	3.5	5.4	4.5	no
					0.6 (high)	1.8	2.7	2.2	no
<b>Emission scenario</b>									
T air =	[ 20 ]	centigrade	293	Kelvin					
T water =	7 [ 20 ]	centigrade	280	Kelvin					
Windspeed =	[ 3 ]	m s <sup>-1</sup>	3	m s <sup>-1</sup>					
Sewage flow =	[ 200 ]	L person <sup>-1</sup> d <sup>-1</sup>	0.2	m <sup>3</sup> person <sup>-1</sup> d <sup>-1</sup>					
Number inhabitants =	[ 6667 ]	person	6667	person					
Sludge loading rate (table 1) =	[ 0.15 ]	kg <sub>BOD</sub> kg <sub>dw</sub> <sup>-1</sup> d <sup>-1</sup>	0.15	kg <sub>BOD</sub> kg <sub>dw</sub> <sup>-1</sup> d <sup>-1</sup>					
Bubble or surface aeration: b/s	[ ]	s	(-)	s					
Emission rate chemical =	[ 1 ]	kg d <sup>-1</sup>	1	kg d <sup>-1</sup>					
table 2: chosen operation parameters					table 3:				
Sludge loading rate =	0.15	kg <sub>BOD</sub> kg <sub>dw</sub> <sup>-1</sup> d <sup>-1</sup>	Concentration in raw sewage calculated from the default emission rate of the chemical						
with primary sedimentation									
HRT =	6.9	hr	C total raw sewage= 7.5E-01 mg l <sup>-1</sup>						
SRT =	9.2	d	Dissolved = 94 %						
without primary sedimentation									
HRT =	10.8	hr	C dissolved = 7.0E-01 mg l <sup>-1</sup>						
SRT =	9.2	d	C in solids = 1.1E+02 mg kg <sup>-1</sup>						
<b>Biodegradation in activated sludge</b>									
Temperature dependence (y/n)	[ ]	n	(-)	n					
<b>Method 1: estimated from OECD/EU standardized biodegradability tests (USES 2.0)</b>									
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.									
The following values are recommended:									
Readily biodegradable, fulfilling 10 d window criterion: range is 1 to 3 hr <sup>-1</sup> (TGD-EU: 1 hr <sup>-1</sup> )									
Readily biodegradable, <u>not</u> fulfilling 10 d window criterion: range is 0.3 to 1 hr <sup>-1</sup> (TGD-EU: 0.3 hr <sup>-1</sup> )									
Inherently biodegradable in MITI II and within 10 d in the Zahn-Wellens (window = 3 d): range is 0.1 to 0.3 hr <sup>-1</sup>									
Inherently biodegradable: range is 0.01 to 0.1 hr <sup>-1</sup> (TGD-EU: 0.1 hr <sup>-1</sup> )									
k biodeg1 =	[ 0 ]	hr <sup>-1</sup>	0	s <sup>-1</sup> , T water = 7 C					
<b>Method 2: chemical is biodegradable in activated sludge batch test (draft ISO test)</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 <sup>-1</sup>	0	s <sup>-1</sup> , T water = 7 C					
<b>Method 3: chemical is biodegradable in activated sludge, Monod Kinetics</b>									
Assumption: biodegradation in the aqueous phase of activated sludge, however, the rate constant is a function of the influent concentration, μ <sub>max</sub> and K <sub>s</sub> and the sludge retention time. Default values for μ <sub>max</sub> and K <sub>s</sub> pertain to readily biodegradable chemicals.									
μ <sub>max</sub> =	[ 2 ]	d <sup>-1</sup>	2	d <sup>-1</sup>					
K <sub>s</sub> =	[ 0.5 ]	mg L <sup>-1</sup>	0.5	mg L <sup>-1</sup>					

## Appendix 2

Expressions for  $V_i$  [m<sup>3</sup>]:

$$V_1 = AREA_{9,6-box} \cdot N \cdot h \quad (60)$$

$$V_2 = VOL_{PS} \cdot N \quad (61)$$

$$V_3 = \frac{V_2 \cdot C_{SS, PS}}{1000 \cdot d_{PS}} \quad (62)$$

$$V_4 = AREA_{PS} \cdot N \cdot sl_{PS} \quad (63)$$

with

$sl_{ps}$  : tickness sediment layer primary sedimentation tank [0.1 m]

$$V_5 = VOL_{A; 9,6-box} \cdot N \quad (64)$$

$$V_6 = \frac{CAS \cdot V_5}{1000 \cdot d_A} \quad (65)$$

$$V_7 = VOL_{SLS} \cdot N \quad (66)$$



$$V_8 = \frac{CEF \cdot V_7}{1000 \cdot d_{SLS}} \quad (67)$$

$$V_9 = AREA_{SLS} \cdot N \cdot sl_{SLS} \quad (68)$$

with

$sl_{SLS}$  : tickness sediment layer solids liquid separator [0.1 m]