Work Package 2: Identification of target substances

Technical Report
Activity 2.2
Fate of substances during emission treatment

October 2019

HAZBREF

Interreg Baltic Sea Region

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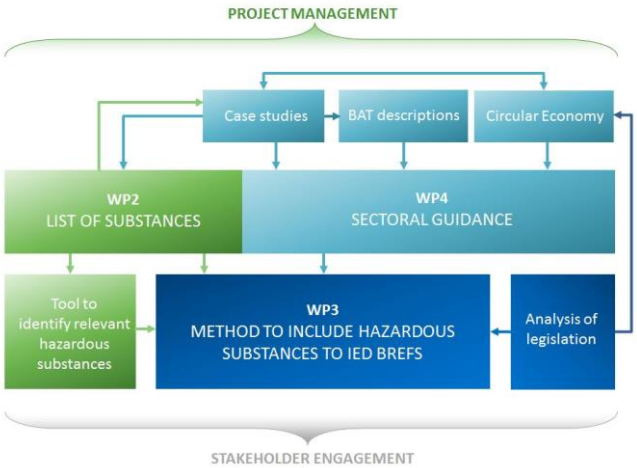
HAZBREF in Brief

This report is a product of the HAZBREF project *"Hazardous industrial chemicals in the IED BREFs"*. HAZBREF is funded by the EU Interreg Baltic Sea Region Programme and the implementation period is three years from October 2017 until September 2020.
The overall aim of HAZBREF is to increase the knowledge base of the industrial sources and the reduction measures of hazardous chemicals. HAZBREF will identify relevant chemicals used in industrial sectors, their use patterns, environmental characteristics and measures to prevent and reduce releases to environment.
On the EU level the main instrument to control industrial releases is the Industrial Emissions Directive (IED), particularly through the publication of BAT Reference documents (BREFs) and their key chapter: the BAT conclusions. However, these BAT conclusions in most cases do not address hazardous substances in a systematic and comprehensive way. HAZBREF aims to develop a systematic approach that will help to exchange and utilize the existing information about hazardous substances between different regulatory frameworks (IED, REACH, Water Framework Directive, Marine Strategy Framework Directive, EU provisions on Circular Economy, Stockholm POP Convention & HELCOM) in the preparation of BREFs.
When the use and risks of chemicals are better addressed in BAT Reference documents, the capacity to manage industrial chemicals will be enhanced among both authorities and operators. The information gathered in BREFs is also useful for the Baltic Marine Environment Protection Commission HELCOM in the development of actions to reduce the inputs of hazardous substances to the Baltic Sea. HAZBREF also promotes the circular economy by finding ways to include circular economy aspects in BREFs.
HAZBREF outputs target both the policy and the enforcement level. On policy level the outputs will strengthen the links between different regulatory frameworks and their key players. On enforcement level at industrial installations the project will identify and test model solutions for hazardous chemical management.
The activities will be carried out in four Work Packages:

- WP1 – Project management and administration (Lead Partner SYKE) including communication and dissemination of results;
- WP2 – Identification of target substances (Lead by UBA) that include:
  - 2.1 Identification and selection of target substances
  - 2.2 Fate of substances during emission treatment
- WP3 – Policy improvement (Lead by UBA) that include:
  - 3.1 Strengthening links between regulatory frameworks on different levels
  - 3.2 Developing method to include substance information into BREFs, improve communication and data flow
- WP4 – Best practices in chemicals management in industry (lead by IETU) that include:
  - 4.1 Sectoral guidance for three IED sectors (chemicals, textile, surface treatment of metals and plastics)
  - 4.2 Case studies in selected installations
  - 4.3 BAT descriptions and model permits
  - 4.4 Circular economy aspects.

The HAZBREF partnership includes 5 organisations from the Baltic Sea region: Finnish Environment Institute (SYKE) (Lead partner), German Environment Agency (UBA), Swedish Environmental Protection Agency (SWEPA), Institute for Ecology of Industrial Areas (IETU) and Estonian Environmental Research Centre (KLAB).
In addition 27 associated organisations and a wide range of other stakeholders will be involved in HAZBREF, such as ministries and governmental environmental and chemical agencies from several EU countries, permitting and supervision authorities as well as industries and environmental NGOs.

More information about HAZBREF can be found on our project website (www.syke.fi/projects/hazbref).



Overview of the design of the HAZBREF-project with its four work packages.

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Fate modelling

The substances of interest in the HAZBREF project are those with a probability to be released via the effluent from WWTPs. The purpose of Activity 2.2 is to obtain generic knowledge about the fate of a subset of industrial target substances in typical waste water treatment and feed information into Activity 2.1 and the creation of a decision tree for the identification of substances of concern for BAT candidates. Based on Activity 2.2 results and conclusions and presented methodology, substances that are likely to be released to wastewater treatment effluents may be identified in advance and thus trigger specific actions in industrial wastewater treatment plants (IWWTPs) or before that in modifying industrial processes (incl. use of chemicals containing the particular substance).

The data regarding relevant parameters (e.g., biodegradability, partition coefficient (K_{ow}), vapour pressure and water solubility) are generated by testing the chemicals individually with standardized and commonly agreed laboratory tests (e.g., OECD test guidelines) or by applying quantitative structure/activity relationship tools (QSAR tools). The generation of such data is in the responsibility of the producer of the chemicals, not the user (i.e. the operator of an industrial plant under IED) and generally available in Material Safety Data Sheets (MSDS) or chemicals databases. The environment in the waste water treatment plant/sewage treatment plant (WWTP/STP) is something completely different compared to the recipient, and hence, the data obtained by modelling or by QSAR analysis has to be used with caution and can only work as an *indication* if a substance may be problematic or not problematic for the environment and/or human health.. A rough estimate regarding the fate and behaviour of a particular substance in WWTP/STP may be performed by analyzing physical and chemical parameters, e.g., the partition coefficient (K_{ow}), vapor pressure and water solubility. But it is important to be aware of the uncertainties coupled to an analysis based solely on physical and chemical parameters.

The required information regarding fate and behaviour of substances in WWTP/STP can be obtained according to established and commonly used methods as outlined in the Reach Guidance on information requirements and Chemical Safety Assessment, Chapter R.16: Environmental exposure assessment. More specifically the methods are outlined in The European Union System for the Evaluation of Substances (EUSES). The fate of substances in WWTP/STP can be assessed in the SimpleTreat 4.0 model (https://www.rivm.nl/en/soil-and-water/simpletreat).

In order to obtain information regarding the fate of several substances (functional groups) that are representative of chemical categories/groups may be analysed with respect to their fate and behaviour. However, if data for a particular substance will be used to make predictions for other substances in a given chemical category, such data has to be interpreted with some caution if harmonized Guidance on Read across and QSAR analysis (available at ECHA) have not been used. When data is lacking for a particular substance, one may use data by read across and/or QSAR analysis from another substance. In such a case, it has to be sufficiently chemically similar in structure or sufficiently similar in biological mode of action in order to use read across and or QSAR analysis. Similarity in biological mode of action can be shown by similar action in so called Key Events in Adverse Outcome Pathways (AOPs) or by other means. The approach of using read across and QSAR analysis is not within the scope of WP 2.2, but can be a further step in other projects.

The fate of a subset of 25 substances in WWTP/STP has been assessed in the SimpleTreat 4.0 model. In the present report the outcome of the modelling is presented. The modelled substances have been selected based on their use in chemical, textile or STM sector and with respect to varying intrinsic properties but also if they have been prioritized e.g. within WFD (WFD Priority Substance or Priority Hazardous Substance) or REACH.

The necessary input data to the modelling (e.g., molecular weight, Kow, vapour pressure, solubility) has been taken mainly from registration dossiers at ECHA and in some cases from other sources, e.g. Pubchem.

The presented data in the results section may be used as examples on the behavior of substances with different properties and with potential relevance for substance categories/groups and with potential relevance in the context of HAZBREF project. Hence, the data may serve as indication if these substances could be taken into account already in the front loading process of relevant BATs/BREFs. It needs to be pinpointed and defined when a substance may pose a problem in the context of HAZBREF. Of vital importance in such analysis is of course the amounts released in the effluent. A trigger value of >10 % release in the effluent may be used. This has, however, to be coupled to the use volumes per year and how much of the use volume that is anticipated to be released from the industrial site, and hence, may reach the WWTP/STP. Furthermore, if a particular substance may be problematic if/when released via the effluent is also dependent on the intrinsic properties, e.g., persistence and environmental (ecotox) and human health hazard. It is also important to note that breakdown products (metabolites) are not addressed. These may potentially exhibit toxic properties in a more potent way compared to the mother substance.
In cases where the main fraction of a modelled chemical is ending up to the sludge, it is important to address the fate of the sludge according to agreed procedures outlined at e.g., regional-, national- and/or EU level, or elsewhere. As mentioned above, the data may serve as indication if also substances that to a large extent end up in sludge should be taken into account already in the front loading process of relevant BATs/BREFs.

Even though the modelling data presented here (and further modelling with more substances) may indicate that substance categories/groups may not be problematic or pose a problem in the context of HAZBREF, it may be recommended that, ideally, any industrial sector should model all their substances that they use with the SimpleTreat model or some other similar commonly accepted model.

It is important that the input data are inserted into the model in the correct way, e.g., log K_{ow} values need to be converted to K_{ow} values (10^x vs log), etc. It is also possible to adjust input parameters with respect to the mode of operation at a WWTP/STP. In the present modelling, default parameters set by the software (e.g., sewage flow, etc) for mode of operation have been used.

Results of the fate modelling in SimpleTreat

Substance group Volatile Organic Chemicals (VOC)

Dichloromethane, EC No: 200-838-9, CAS no: 75-09-2
Used in EU: 100 00 – 100 000 tonnes per year,
Readily biodegradable
Concern for endocrine disruption, under evaluation
H351: Suspected of causing cancer
EU WFD Priority Substance

Output Elimination percentages	Value	Unit
Elimination in the primary settler		
Volatilization	4,40	%
Via primary sludge	0,12	%
Total	4,52	%
Elimination in the aerator		
Stripping	23,90	%
Biodegradation	65,84	%
Total	89,74	%
Elimination in the solids liquid separator		
Volatilization	0,89	%
Via surplus sludge	0,00	%
Total	0,90	%
Total elimination from waste water	**95,15**	%
Total emission via effluent	**4,85**	%
Balance	**100,00**	%

Conclusion: The results of the modelling indicate that Dichloromethane may not be problematic within the scope of HAZBREF, since it is eliminated from waste water to an extent > 95% and is readily biodegradable.

Pentachlorophenol (PCP), EC No 201-778-6, CAS No 87-86-5
Restricted substance under REACH.
Not readily biodegradable
Production of PCP in the EU ceased in 1992. In 1996, 378 tonnes of NaPCP and 30 tonnes of PCP were imported from the USA (OSPAR Commission, 2001)
H301: Toxic if swallowed
H311: Toxic in contact with skin
H 315: Causes skin irritation
H319: Causes serious eye irritation
H330: Fatal if inhaled
H335: May cause respiratory irritation
H 351 Suspected of causing cancer
H 400: Very toxic to aquatic life.
H410: Very toxic to aquatic life with long lasting effects.
EU WFD Priority Substance

Output Elimination percentages	Value	Unit
Elimination in the primary settler		
Volatilization	0,01	%
Via primary sludge	47,21	%
Total	47,22	%
Elimination in the aerator		
Stripping	0,09	%
Biodegradation	0,00	%
Total	0,09	%
Elimination in the solids liquid separator		
Volatilization	0,05	%
Via surplus sludge	23,41	%
Total	23,45	%
Total elimination from waste water	**70,76**	%
Total emission via effluent	**29,24**	%
Balance	**100,00**	%

Conclusion: The results of the modelling indicate that Pentachlorophenol may pose a major problem in the context of HAZBREF, since it is present in the effluent in quantities of 30 %. However, it is a restricted substance and should not be used anymore.

2,5-dichlorophenol (2,5-DCP), EC No 209-520-4, CAS No 583-78-8
Intermediate use
Inherently biodegradable, not fulfilling specific criteria, data indicates a low inherent biodegradability (ECHA registration dossier)
H302: Harmful if swallowed.
H315: Causes skin irritation.
H319: Causes serious eye irritation.
H411: Toxic to aquatic life with long lasting effects.

Output **Elimination percentages**	**Value**	**Unit**
Elimination in the primary settler		
Volatilization	0,09	%
Via primary sludge	3,26	%
Total	3,35	%
Elimination in the aerator		
Stripping	0,68	%
Biodegradation	0,00	%
Total	0,68	%
Elimination in the solids liquid separator		
Volatilization	0,35	%
Via surplus sludge	1,69	%
Total	2,05	%
Total elimination from waste water	**6,08**	%
Total emission via effluent	**93,92**	%
Balance	**100,00**	%

Conclusion: The results of the modelling indicate that 2,5-dichlorophenol may pose a problem. It is released via the effluent to an extent of >90%. It is, however, for intermediate use, which may decrease the level of exposure.

N,N-dimethylacetamide, EC No: 204-826-4, CAS No: 127-19-5
Used in EU: 10 000 - 100 000 tonnes per year
REACH: Candidate list, Toxic for reproduction (Article 57c)
Readily biodegradable
H360: May damage fertility or the unborn child
H360D
H332: Harmful if inhaled.
H312: Harmful in contact with skin.

Output Elimination percentages	Value	Unit
Elimination in the primary settler		
Volatilization	0,00	%
Via primary sludge	0,08	%
Total	0,08	%
Elimination in the aerator		
Stripping	0,00	%
Biodegradation	77,40	%
Total	77,40	%
Elimination in the solids liquid separator		
Volatilization	0,00	%
Via surplus sludge	0,01	%
Total	0,01	%
Total elimination from waste water	**77,50**	%
Total emission via effluent	**22,50**	%
Balance	**100,00**	%

Conclusion: The results of the modelling indicate that N,N-dimethylacetamide may pose a problem. It is released via the effluent to an extent > 20 % and is used in high volumes.

Substance group Phtalates

Bis(2-methoxyethyl) phthalate (DMEP), EC No: 204-212-6, CAS 117-82-8
It is not clear whether the substance is used in the EU on an industrial scale. It should be assumed that the amounts offered are below one ton (Annex XV dossier, ECHA)
Readily biodegradable
REACH: Candidate list, Toxic for reproduction (Article 57c)
H360Df: May damage the unborn child. Suspected of damaging fertility

Output Elimination percentages	Value	Unit
Elimination in the primary settler		
Volatilization	0,00	%
Via primary sludge	0,09	%
Total	0,09	%
Elimination in the aerator		
Stripping	0,00	%
Biodegradation	91,89	%
Total	91,89	%
Elimination in the solids liquid separator		
Volatilization	0,00	%
Via surplus sludge	0,00	%
Total	0,00	%
Total elimination from waste water	**91,99**	%
Total emission via effluent	**8,01**	%
Balance	**100,00**	%

Conclusion: The results of the modelling indicate that Bis(2-methoxyethyl) phthalate (DMEP),, may not pose a problem , since it is present in the effluent in quantities < 10 %, and is readily biodegradable.

Di(ethylhexyl) phthalate (DEHP), EC No: 204-211-0, CAS No: 117-81-7
Used in EU: 10 000 - 100 000 tonnes per year
Readily biodegradable
REACH: Candidate list, Toxic for reproduction (Article 57c), Endocrine disrupting properties (Article 57(f) - environment), Endocrine disrupting properties (Article 57(f) - human health)
H360: May damage fertility or the unborn child

EU WFD Priority Hazardous Substance

Output	Output	Output	
Elimination percentages		**Value**	**Unit**
Elimination in the primary settler			
Volatilization		0,00	%
Via primary sludge		64,12	%
Total		64,12	%
Elimination in the aerator			
Stripping		0,00	%
Biodegradation		18,82	%
Total		18,82	%
Elimination in the solids liquid separator			
Volatilization		0,00	%
Via surplus sludge		14,46	%
Total		14,46	%
Total elimination from waste water		**97,40**	%
Total emission via effluent		**2,60**	%
Balance		**100,00**	%

Conclusion: The results of the modelling indicate that DEHP may not pose a major problem, since it is present in the effluent in quantities < 5 %, and is readily biodegradable. The substance is mainly removed from the effluent via sludge, due to high Kow, Koc, Kps and Kpas values Furthermore, it displays endocrine disrupting properties and may therefore be problematic.

Diisobutyl phthalate (DIBP), EC No: 201-553-2, CAS No: 84-69-5
Used in EU: 1 - 10 tonnes per year
REACH: Candidate list, Toxic for reproduction (Article 57c), Endocrine disrupting properties (Article 57(f) - human health)
Readily biodegradable
H360: May damage fertility or the unborn child
H360Df: May damage the unborn child. Suspected of damaging fertility, C ≥ 25 %.
H361f: Suspected of damaging fertility, 5 % ≤ C < 25 %
H400: Very toxic to aquatic life.
H410: Very toxic to aquatic life with long lasting effects

Output	Output	Output	
Elimination percentages		**Value**	**Unit**
Elimination in the primary settler			
Volatilization		3,45	%
Via primary sludge		8,89	%
Total		12,34	%
Elimination in the aerator			
Stripping		11,04	%
Biodegradation		70,14	%
Total		81,18	%
Elimination in the solids liquid separator			
Volatilization		0,87	%
Via surplus sludge		0,34	%
Total		1,21	%
Total elimination from waste water		**94,72**	%
Total emission via effluent		**5,28**	%
Balance		**100,00**	%

Conclusion: The results of the modelling indicate that Diisobutyl phthalate (DIBP), is eliminated from the waste water effluent to an extent of 95%, Hence only 5 % is released via the effluent.

However, it is very toxic to aquatic life, but is used in low volumes, and it is readily biodegradable according to registration dossiers at ECHA.

Substance group Alkylphenols and their ethoxylates

P-nonylphenol, EC No: 203-199-4, CAS No: 104-40-5
Used in EU: 1 - 10 tonnes per year
REACH restricted
Readily biodegradable
H302: Harmful if swallowed.
H314: Causes severe skin burns and eye damage.
H318: Causes serious eye damage.
H400: Very toxic to aquatic life.
H410: Very toxic to aquatic life with long lasting effects.
EU WFD Priority Hazardous Substance

Output		
Elimination percentages	**Value**	**Unit**
Elimination in the primary settler		
Volatilization	0,09	%
Via primary sludge	56,11	%
Total	56,20	%
Elimination in the aerator		
Stripping	0,13	%
Biodegradation	34,31	%
Total	34,44	%
Elimination in the solids liquid separator		
Volatilization	0,07	%
Via surplus sludge	5,93	%
Total	5,99	%
Total elimination from waste water	**96,63**	%
Total emission via effluent	**3,37**	%
Balance	**100,00**	%

Conclusion: The results of the modelling indicate that P-nonylphenol is eliminated from the waste water to an extent of 96 %. Hence, less than 4 % is released via the effluent It is used in low volumes and is readily biodegradable. It is, however, very toxic to aquatic life.

Substance group Siloxanes

Octamethylcyclosiloxane (D4), EC No: 209-136-7, CAS No: 556-67-2
Used in EU: 100 000 - 1 000 000 tonnes per year
REACH: Candidate list, PBT (Article 57d), vPvB (Article 57e)
Not biodegradable
H226: Flammable liquid and vapour.
H361: Suspected of damaging fertility or the unborn child
H413: May cause long lasting harmful effects to aquatic life.

Output Elimination percentages	Value	Unit
Elimination in the primary settler		
Volatilization	1,49	%
Via primary sludge	46,01	%
Total	47,50	%
Elimination in the aerator		
Stripping	47,02	%
Biodegradation	0,00	%
Total	47,02	%
Elimination in the solids liquid separator		
Volatilization	0,49	%
Via surplus sludge	2,42	%
Total	2,90	%
Total elimination from waste water	**97,42**	%
Total emission via effluent	**2,58**	%
Balance	**100,00**	%

Conclusion: The results of the modelling indicate that Octamethylcyclosiloxane (D4) is present in the effluent in quantities < 5 %. It may anyway pose a problem, since it is not biodegradable and is used in high volumes and is classified as H413: May cause long lasting harmful effects to aquatic life.
Decamethylcyclopentasiloxane (D5), EC No: 208-764-9 CAS No: 541-02-6
Used in EU: 10 000 - 100 000 tonnes per year
REACH: Candidate list, PBT, vPvB,
However, according to the registration dossier the substance is not PBT / vPvB
Not biodegradable

Output Elimination percentages	Value	Unit
Elimination in the primary settler		
Volatilization	0,23	%
Via primary sludge	63,72	%
Total	63,95	%
Elimination in the aerator		
Stripping	22,59	%
Biodegradation	0,00	%
Total	22,59	%
Elimination in the solids liquid separator		
Volatilization	0,27	%
Via surplus sludge	11,17	%
Total	11,44	%
Total elimination from waste water	**97,99**	%
Total emission via effluent	**2,01**	%
Balance	**100,00**	%

Conclusion: The results of the modelling indicate that Decamethylcyclopentasiloxane (D5) is present in the effluent in quantities < 5 %. It may anyway pose a problem, since it is not biodegradable and is used in high volumes. It has no harmonised classification.

Dodecamethylcyclohexasiloxane (D6), EC No: 208-762-8, CAS No: 540-97-6
Used in EU: 10 000 - 100 000 tonnes per year
REACH: Candidate list, PBT, vPvB
According to the registration dossier the substance is not PBT /vPvB. However, the criteria for persistence (P/vP) in the aquatic compartment are met. The screening criteria for persistence (P/vP) in the sediment compartment are met.
Not biodegradable

Output Elimination percentages	Value	Unit
Elimination in the primary settler		
Volatilization	0,05	%
Via primary sludge	66,36	%
Total	66,41	%
Elimination in the aerator		
Stripping	8,56	%
Biodegradation	0,00	%
Total	8,56	%
Elimination in the solids liquid separator		
Volatilization	0,11	%
Via surplus sludge	23,02	%
Total	23,13	%
Total elimination from waste water	**98,10**	%
Total emission via effluent	**1,90**	%
Balance	**100,00**	%

Conclusion: The results of the modelling indicate that Dodecamethylcyclohexasiloxane (D6) is present in the effluent in quantities < 5 %. It may anyway pose a problem, since it is not biodegradable and is used in high volumes. It has no harmonized classification.

Substance group Metal salts

Cobalt(II) sulphate

REACH: Candidate list, H302: Harmful if swallowed. H317: May cause an allergic skin reaction.
H319: Causes serious eye irritation.
H334: May cause allergy or asthma symptoms or breathing difficulties if inhaled.
H341: Suspected of causing genetic defects.
H350: May cause cancer by inhalation.
H360: May damage fertility or the unborn child
H373: May cause damage to organs
H400: Very toxic to aquatic life.
H410: Very toxic to aquatic life with long lasting effects.

The substance is not suitable to be run in SimpleTreat. Data on partition coefficient (K_{ow}) is lacking. Such a study technically not feasible. The substance is inorganic and the study was waived in the ECHA registration dossier.

Strontium chromate EC No: 232-142-6, CAS: 7789-06-2
Used in EU: 1 000 - 10 000 tonnes per year
REACH: Candidate list, Carcinogenic (Article 57a)
H302: Harmful if swallowed.
H330: Fatal if inhaled.
H335: May cause respiratory irritation.
H317: May cause an allergic skin reaction.
H361: Suspected of damaging fertility or the unborn child
H340: May cause genetic defects
H350: May cause cancer
H400: Very toxic to aquatic life

Inorganic, partition coefficient not available. Substance not modelled in SimpleTreat

Disodium tetraborate, anhydrous, EC No: 215-540-4, CAS No: 1330-43-4; 1303-96-4; 12179-04-3
Used in EU: 100 000 - 1 000 000 tonnes per year.
Readily biodegradable
H360: May damage fertility or the unborn child
H319: Causes serious eye irritation.

Output Elimination percentages	Value	Unit
Elimination in the primary settler		
Volatilization	0,24	%
Via primary sludge	0,00	%
Total	0,24	%
Elimination in the aerator		
Stripping	0,15	%
Biodegradation	91,61	%
Total	91,77	%
Elimination in the solids liquid separator		
Volatilization	0,08	%
Via surplus sludge	0,00	%
Total	0,08	%
Total elimination from waste water	**92,09**	%
Total emission via effluent	**7,91**	%
Balance	**100,00**	%

Conclusion: The results of the modelling indicate that Disodium tetraborate may not pose a major problem, since it is release in quantities < 10 % and is readily biodegradable.

Substance group Monomer unfluorinated

Acrylamide, EC number: 201-173-7 | CAS number: 79-06-1; 122775-19-3
Used in EU: 100 000 - 1 000 000 tonnes per year.
Readily biodegradable
REACH: Candidate list, Carcinogenic (Article 57a), Mutagenic (Article 57b)
H301: Toxic if swallowed.
H312: Harmful in contact with skin.
H332: Harmful if inhaled.
H315: Causes skin irritation.
H319: Causes serious eye irritation.
H317: May cause an allergic skin reaction.
H361: Suspected of damaging fertility or the unborn child
H340: May cause genetic defects
H350: May cause cancer
H372: Causes damage to organs

Output Elimination percentages	Value	Unit
Elimination in the primary settler		
Volatilization	0,01	%
Via primary sludge	0,00	%
Total	0,02	%
Elimination in the aerator		
Stripping	0,02	%
Biodegradation	77,45	%
Total	77,47	%
Elimination in the solids liquid separator		
Volatilization	0,01	%
Via surplus sludge	0,00	%
Total	0,01	%
Total elimination from waste water	**77,50**	%
Total emission via effluent	**22,50**	%
Balance	**100,00**	%

Conclusion: The results of the modelling indicate that Acrylamide, may pose a problem, since it is present in the effluent in quantities > 20 %, and is used in high volumes. It is classified as being carcinogenic, mutagenic and reprotoxic.

4,4'-isopropylidenediphenol (Bisphenol, BPA), EC No 201-245-8. CAS No 80-05-7,
Used in EU: 1 000 000 - 10 000 000 tonnes per year.
Readily biodegradable
REACH: Candidate list, Toxic for reproduction (Article 57c), Endocrine disrupting properties environment and human health) (Article 57(f),
H318: Causes serious eye damage.
H317: May cause an allergic skin reaction.
H360: May damage fertility or the unborn child
H335: May cause respiratory irritation.
H411: Toxic to aquatic life with long lasting effects.

Output Elimination percentages	Value	Unit
Elimination in the primary settler		
Volatilization	0,00	%
Via primary sludge	6,16	%
Total	6,16	%
Elimination in the aerator		
Stripping	0,00	%
Biodegradation	86,05	%
Total	86,05	%
Elimination in the solids liquid separator		
Volatilization	0,00	%
Via surplus sludge	0,27	%
Total	0,27	%
Total elimination from waste water	**92,48**	%
Total emission via effluent	**7,52**	%
Balance	**100,00**	%

Conclusion: The results of the modelling indicate that Bispenol, BPA, is present in the effluent in quantities < 10 %, and is readily biodegradable. It may anyway be problematic, since it is used in high volumes and is toxic to aquatic life with long lasting effects, is toxic for reproduction and displays endocrine disrupting properties for the environment and human health.

Methyloxirane (Propylene oxide), EC No: 200-879-2, CAS: 75-56-9
Used in EU: 1 000 000 - 10 000 000 tonnes per year.
Readily biodegradable
REACH: Candidate list, Carcinogenic (Article 57a), Mutagenic (Article 57b)
H224: Extremely flammable liquid and vapour.
H302: Harmful if swallowed.
H311: Toxic in contact with skin.
H319: Causes serious eye irritation.
H335: May cause respiratory irritation.
H331: Toxic if inhaled.
H340: May cause genetic defects
H350: May cause cancer

Output Elimination percentages	Value	Unit
Elimination in the primary settler		
Volatilization	4,75	%
Via primary sludge	0,01	%
Total	4,76	%
Elimination in the aerator		
Stripping	73,74	%
Biodegradation	16,66	%
Total	90,39	%
Elimination in the solids liquid separator		
Volatilization	0,81	%
Via surplus sludge	0,00	%
Total	0,81	%
Total elimination from waste water	**95,96**	%
Total emission via effluent	**4,04**	%
Balance	**100,00**	%

Conclusion: The results of the modelling indicate that Methyloxirane may not pose a major problem, since it is present in the effluent in quantities < 5 %, and is readily biodegradable. It is, however, used in high volumes and is classified as being carcinogenic.

Substance group Biocides

Biocides are very diverse and there are 22 product types. Hence, physical and chemical parameters and (eco) toxicity vary considerably.

Diuron, EC No: 206-354-4, CAS No: 330-54-1
Used in EU: 100 - 1 000 tonnes per year, Diuron is a PT-substance but not a PBT substance
Not biodegradable
H410: Very toxic to aquatic life with long lasting effects.
H302: Harmful if swallowed.
H351: Suspected of causing cancer
H373: May cause damage to organs
EU WFD Priority Substance

Output Elimination percentages	Value	Unit
Elimination in the primary settler		
Volatilization	0,00	%
Via primary sludge	3,39	%
Total	3,39	%
Elimination in the aerator		
Stripping	0,00	%
Biodegradation	0,00	%
Total	0,00	%
Elimination in the solids liquid separator		
Volatilization	0,00	%
Via surplus sludge	1,78	%
Total	1,78	%
Total elimination from waste water	**5,17**	%
Total emission via effluent	**94,83**	%
Balance	**100,00**	%

Conclusion: The results of the modelling indicate that Diuron may pose a problem, since it is released via the effluent to an extent > 90 % and is not biodegradable and very toxic to aquatic life with long lasting effects.

Terbutryn, EC No: 212-950-5, CAS No: 886-50-0
This substance is being reviewed for use as a biocide, substance group: triazines
Use volume not specified, but use a biocide < 10 tonnes, or less than 100 tonnes.
Inherently biodegradable, slow biodegradation
H302: Acute Tox. 4
H317: Skin Sens. 1B
H400: Aquatic Acute 1, Very toxic to aquatic life
H410: Aquatic Chronic 1, Very toxic to aquatic life with long-lasting effects
EU WFD Priority Substance

Output Elimination percentages	Value	Unit
Elimination in the primary settler		
Volatilization	0,00	%
Via primary sludge	6,75	%
Total	6,75	%
Elimination in the aerator		
Stripping	0,00	%
Biodegradation	0,00	%
Total	0,00	%
Elimination in the solids liquid separator		
Volatilization	0,00	%
Via surplus sludge	3,53	%
Total	3,53	%
Total elimination from waste water	**10,28**	%
Total emission via effluent	**89,72**	%
Balance	**100,00**	%

Conclusion: The results of the modelling indicate that Terbutryn may pose a problem, since it is released via the effluent to an extent > 89 % and is very toxic to aquatic life with long lasting effects.

Imidazolidine-2-thione, EC No:202-506-9, CAS No: 96-45-7
Used in EU: 100 - 1 000 tonnes per year
Not biodegradable
REACH: Candidate list, toxic for reproduction,
H302: Harmful if swallowed.
H360: May damage fertility or the unborn child

Output Elimination percentages	Value	Unit
Elimination in the primary settler		
Volatilization	0,01	%
Via primary sludge	0,00	%
Total	0,01	%
Elimination in the aerator		
Stripping	0,06	%
Biodegradation	0,00	%
Total	0,06	%
Elimination in the solids liquid separator		
Volatilization	0,03	%
Via surplus sludge	0,00	%
Total	0,03	%
Total elimination from waste water	**0,10**	%
Total emission via effluent	**99,90**	%
Balance	**100,00**	%

Conclusion: The results of the modelling indicate that Imidazolidine-2-thione is present in the effluent in quantities > 99 %, and hence, may pose a problem, since it is not biodegradable.

Nitrobenzene, EC No: 202-716-0, CAS 98-95-3,
Intermediate Use Only
REACH: Candidate list, Toxic for reproduction (Article 57c), Concern for endocrine disruption but conclusion postponed.
Readily biodegradable
H351: Suspected of causing cancer
H360: May damage fertility or the unborn child
H301: Toxic if swallowed.
H331: Toxic if inhaled
H311: Toxic in contact with skin.
H372: Causes damage to organs
H412: Harmful to aquatic life with long lasting effects.

Output Elimination percentages	Value	Unit
Elimination in the primary settler		
Volatilization	0,24	%
Via primary sludge	1,05	%
Total	1,29	%
Elimination in the aerator		
Stripping	0,15	%
Biodegradation	90,62	%
Total	90,77	%
Elimination in the solids liquid separator		
Volatilization	0,07	%
Via surplus sludge	0,04	%
Total	0,12	%
Total elimination from waste water	**92,17**	%
Total emission via effluent	**7,83**	%
Balance	**100,00**	%

Conclusion: The results of the modelling indicate that Nitrobenzene may not pose a major problem, is present in the effluent in quantities < 10 %, is readily biodegradable, and is for intermediate use only.

Substance group Dyes

4,4'-methylenedianiline, EC No: 202-974-4, CAS No: 101-77-9
Used in EU: 10 000 - 100 000 tonnes per year
Not readily biodegradable
REACH: Candidate list, Carcinogenic (Article 57a)
H350: May cause cancer
H341: Suspected of causing genetic defects <
H370: Causes damage to organs
H373: May cause damage to organs
H317: May cause an allergic skin reaction.
H411: Toxic to aquatic life with long lasting effects.

Output Elimination percentages	Value	Unit
Elimination in the primary settler		
Volatilization	0,00	%
Via primary sludge	32,65	%
Total	32,65	%
Elimination in the aerator		
Stripping	0,00	%
Biodegradation	0,00	%
Total	0,00	%
Elimination in the solids liquid separator		
Volatilization	0,00	%
Via surplus sludge	16,63	%
Total	16,63	%
Total elimination from waste water	**49,28**	%
Total emission via effluent	**50,72**	%
Balance	**100,00**	%

Conclusion: The results of the modelling indicate that 4,4'-methylenedianiline may pose a problem. It is released via the effluent to an extent of 50%, and is not readily biodegradable and is classified as being a possible carcinogen, mutagen, may display target organ toxicity and is also toxic to aquatic life with long lasting effects

Substance group Solvents

1-Methyl-2-pyrrolidone (NMP), EC No: 212-828-1, CAS 872-50-4
Used in EU: 10 000- 100 000 tonnes per year,
Readily biodegradable
REACH: Candidate list, Toxic for reproduction (Article 57c)
H360: May damage fertility or the unborn child
H319: Causes serious eye irritation.
H315: Causes skin irritation.
H335: May cause respiratory irritation.

Output Elimination percentages	Value	Unit
Elimination in the primary settler		
Volatilization	0,00	%
Via primary sludge	0,01	%
Total	0,01	%
Elimination in the aerator		
Stripping	0,00	%
Biodegradation	91,97	%
Total	91,97	%
Elimination in the solids liquid separator		
Volatilization	0,00	%
Via surplus sludge	0,00	%
Total	0,00	%
Total elimination from waste water	**91,98**	%
Total emission via effluent	**8,02**	%
Balance	**100,00**	%

Conclusion: The results of the modelling indicate that 1-Methyl-2-pyrrolidone (NMP) may not pose a major problem, is present in the effluent in quantities < 10 %, and is readily biodegradable.

Substance group Foaming agent

Diazene-1,2-dicarboxamide (C,C'-azodi(formamide)) (ADCA), EC No: 204-650-8 | CAS: 123-77-3
Used in EU: 10 000 - 100 000 tonnes per year
Not biodegradable
REACH: Candidate list, Respiratory sensitising properties (Article 57(f) - human health)
H334: May cause allergy or asthma symptoms or breathing difficulties if inhaled

Octanol-water partition coefficient (K_{ow}): As low solubility in both n-octanol and water precluded the use of the shake-flask method, the partition coefficient was estimated using high performance liquid chromatography (HPLC) and was estimated to log10 P_{ow} < 1.0. Value used in SimpleTreat: 0,9

The low solubility may indicate that the substance can be taken care of by risk mitigation measures, even though the results of SimpleTreat shows hat 99,82 % is emitted via the effluent.

Output Elimination percentages	Value	Unit
Elimination in the primary settler		
Volatilization	0,00	%
Via primary sludge	0,12	%
Total	0,12	%
Elimination in the aerator		
Stripping	0,00	%
Biodegradation	0,00	%
Total	0,00	%
Elimination in the solids liquid separator		
Volatilization	0,00	%
Via surplus sludge	0,06	%
Total	0,06	%
Total elimination from waste water	**0,18**	%
Total emission via effluent	**99,82**	%
Balance	**100,00**	%

Conclusion: The results of the modelling indicate that Diazene-1,2-dicarboxamide (C,C'-azodi(formamide)) (ADCA), may pose a problem , since it is present in the effluent in quantities > 99 %, and is not biodegradable.

Substance group Other

2-Methyl-1,2-thiazol-3(2H)-one - 5-chloro-2-methyl-1,2-thiazol-3(2H)-one, Polyacrylate,
EC No: 911-418-6, CAS number: 55965-84-9
Used in EU: 10 - 100 tonnes per year
Inherently biodegradable
H330: Fatal if inhaled.
H310: Fatal in contact with skin.
H301: Toxic if swallowed.
H314: Causes severe skin burns and eye damage.
H317: May cause an allergic skin reaction.
H410: Very toxic to aquatic life with long lasting effects.

Output Elimination percentages	Value	Unit
Elimination in the primary settler		
Volatilization	0,00	%
Via primary sludge	0,05	%
Total	0,05	%
Elimination in the aerator		
Stripping	0,00	%
Biodegradation	53,38	%
Total	53,39	%
Elimination in the solids liquid separator		
Volatilization	0,00	%
Via surplus sludge	0,01	%
Total	0,01	%
Total elimination from waste water	**53,45**	%
Total emission via effluent	**46,55**	%
Balance	**100,00**	%

Conclusion: The results of the modelling indicate that polyacrylate may pose a problem. It is released via the effluent to an extent > 45%. However, it is inherently biodegradable and is used in low volumes annually, which may decrease the level of concern.

Discussion

The present report shows the usefulness of modelling the fate of substances in WWTPs by using SimpleTreat. The substances have been chosen to serve as examples in order to estimate the fate of substances with a large variation in intrinsic properties such as biodegradation and physical/chemical parameters such as water solubility, vapour pressure, K_{ow}, etc. The operational parameters in WWTPs can be changed in order to reflect conditions at different industrial WWTPs.

The preferred choice when analysing fate is monitored data (measurements) if available. The second best option is to use established models such as SimpleTreat. The third option is to use standard phrases (or make estimation by looking directly at intrinsic properties) developed by analysing

results from modelling in relation to intrinsic properties. The level of uncertainty with respect to estimation of the fate of substances in WWTPs raises considerably from option one to option three.

In the present report the results of the modelling in SimpleTreat show (maybe not surprisingly) that substances with a high level of biodegradation, and/or high vapour pressure, and/or high K_{ow} and K_{oc} values are efficiently removed from the waste water and hence are not present in the effluent in any higher extent. In contrary, substances with low level of biodegradation, and/or low vapour pressure and/or low K_{ow}/K_{oc} values are released via the effluent at a high level, and hence, are relevant target substances in the context of HAZBREF.

Hence, the present report shows that modelling by SimpleTreat identifies substances (and identifies most important intrinsic properties) that are likely to be released to wastewater treatment effluents and hence, modelling data from SimpleTreat may be used in order to trigger specific actions in industrial wastewater treatment plants (WWTPs).
Furthermore, the data may serve as indication when substances could be taken into account already in the front loading process of relevant BATs/BREFs.

It is recommended that fate of substances in WWTPs are estimated by modelling in SimpleTreat. Only in cases when SimpleTreat cannot be used (for example for many inorganic substances and metals) estimations by using standard phrases and/or analysis of any available data with respect to intrinsic properties (e.g., physical and chemical data) may be used.

Annex I
SimpleTreat Export files

Dichloromethane, EC No: 200-838-9, CAS no: 75-09-2

SimpleTreat 4.0 Export file			
Calculation mode:	**SimpleTreat 4.0**		
Version:	**4.0.9**		
Date:	Monday, May 13, 2019		

Input			
Dichoromethane, EC No: 200-838-9, CAS no: 75-09-2	**User value**	Default value	Unit
Chemical class	**Neutral**		-
Molecular weight	**84,93**		g/mole
Octanol-water particion coefficient (Kow)	**17,78**		-
Aparent Kow at actual pH (Dow)			-
Vapour pressure	**58400**		Pa
Vapour pressure used (temp. corrected)	**4,090938E+04**		Pa
Temperature for determining vapour pressure	**293,15**	293,15	Kelvin
Solubility (S)	**13200**		mg/l
Solubility used (temp. corrected)	**1,229295E+04**		mg/l
Temperature for determining solubility	**293,15**	293,15	Kelvin
pKa			-
Henry coefficient (H)		2,826364E+02	Pam3/mole
Henry coefficient used (temp. corrected - only for user value)			Pam3/mole
Temperature for determining Henry coefficient (only for user value)	**293,15**	2,931500E+02	Kelvin
Organic carbon partition coefficient (Koc)		1,295522E+01	l/kg
Partition coefficient in raw sewage (Kps)		3,886565E+00	l/kg
Partition coefficient in activated sludge (Kpas)		4,793431E+00	l/kg
Mode of operation			
Facility type	**Municipal**	Municipal	-
Operation mode	**Primary solids removal**	Primary solids removal	-
Sewage flow (Q)	**0,2**	0,2	m3/d PE
Mass of sewage solids (SO)	**0,09**	0,09	kg/d PE
Mass of O2 binding material in sewage (BOD)	**60**	60	g O2/d PE
Fraction of BOD in sewage solids (FB)	**0,5417**	0,5417	-
Fraction of sewage solids removed by primary sedimentation (FS)	**0,67**	0,67	-
Sludge loading rate (kslr)	**0,1**	0,1	-
pH	**7**	7	-
Surface or bubble aeration	**surface**	surface	-
Biodegradation			
Biodegradation method selected	**OECD 301 series, 310, 302 series**		-
Biodegradation constant	**1**		hr-1
Biodegradation constant used (temp. corrected)			hr-1
Temperature for determining biodegradation constant			Kelvin
Biodegradation applies to	**Aqueous phase**		-
Emission scenario			
Temperature environment	**288,15**	288,15	Kelvin
Wind speed	**3**	3	m/s
Number of inhabitants	**10000**	10000	Person
Emission rate chemical	**1**	1	kg/d

Output		
Elimination percentages	**Value**	**Unit**
Elimination in the primary settler		
Volatilization	4,40	%
Via primary sludge	0,12	%
Total	4,52	%
Elimination in the aerator		
Stripping	23,90	%
Biodegradation	65,84	%
Total	89,74	%
Elimination in the solids liquid separator		
Volatilization	0,89	%
Via surplus sludge	0,00	%
Total	0,90	%
Total elimination from waste water	**95,15**	%
Total emission via effluent	**4,85**	%
Balance	**100,00**	%
Concentrations		
Air	4,91E-06	g/m3
Combined sludge	1,38E+00	mg/kg
Primary sludge	1,91E+00	mg/kg
Surplus sludge	1,38E-01	mg/kg
Raw sewage	5,00E-01	mg/l
Dissolved	4,99E-01	mg/l
Associated	8,61E-04	mg/l
Settled sewage	4,77E-01	mg/l
Dissolved	4,77E-01	mg/l
Associated	2,84E-04	mg/l
Mixed liquor	2,93E-02	mg/l
Dissolved	2,87E-02	mg/l
Associated	5,54E-04	mg/l
Effluent	2,42E-02	mg/l
Dissolved	2,42E-02	mg/l
Associated	1,04E-06	mg/l
In solids effluent	1,38E-01	mg/kg

Pentachlorophenol (PCP), EC No 201-778-6, CAS No 87-86-5

SimpleTreat 4.0 Export file			
Calculation mode:	**SimpleTreat 4.0**		
Version:	**4.0.9**		
Date:	Thursday, December 12, 2019		

Input			
Substance	**User value**	Default value	Unit
Chemical class	**Neutral**		-
Molecular weight	**266**		g/mole
Octanol-water particion coefficient (Kow)	**131825,7**		-
Aparent Kow at actual pH (Dow)			-
Vapour pressure	**0,02**		Pa
Vapour pressure used (temp. corrected)	**1,401006E-02**		Pa
Temperature for determining vapour pressure	**293,15**	293,15	Kelvin
Solubility (S)	**20**		mg/l
Solubility used (temp. corrected)	**1,862567E+01**		mg/l
Temperature for determining solubility	**293,15**	293,15	Kelvin
pKa			-
Henry coefficient (H)		2,000828E-01	Pam3/mole
Henry coefficient used (temp. corrected - only for user value)			Pam3/mole
Temperature for determining Henry coefficient (only for user value)	**293,15**	2,931500E+02	Kelvin
Organic carbon partition coefficient (Koc)		1,766852E+04	l/kg
Partition coefficient in raw sewage (Kps)		5,300555E+03	l/kg
Partition coefficient in activated sludge (Kpas)		6,537351E+03	l/kg
Mode of operation			
Facility type	**Municipal**	Municipal	-
Operation mode	**Primary solids removal**	Primary solids removal	-
Sewage flow (Q)	**0,2**	0,2	m3/d PE
Mass of sewage solids (SO)	**0,09**	0,09	kg/d PE
Mass of O2 binding material in sewage (BOD)	**60**	60	g O2/d PE
Fraction of BOD in sewage solids (FB)	**0,5417**	0,5417	-
Fraction of sewage solids removed by primary sedimentation (FS)	**0,67**	0,67	-
Sludge loading rate (kslr)	**0,1**	0,1	-
pH	**7**	7	-
Surface or bubble aeration	**surface**	surface	-
Biodegradation			
Biodegradation method selected	**OECD 301 series, 310, 302 series**		-
Biodegradation constant	**0**		hr-1
Biodegradation constant used (temp. corrected)			hr-1
Temperature for determining biodegradation constant			Kelvin
Biodegradation applies to	**Aqueous phase**		-
Emission scenario			
Temperature environment	**288,15**	288,15	Kelvin
Wind speed	**3**	3	m/s
Number of inhabitants	**10000**	10000	Person
Emission rate chemical	**1**	1	kg/d

Output		
Elimination percentages	**Value**	**Unit**
Elimination in the primary settler		
Volatilization	0,01	%
Via primary sludge	47,21	%
Total	47,22	%
Elimination in the aerator		
Stripping	0,09	%
Biodegradation	0,00	%
Total	0,09	%
Elimination in the solids liquid separator		
Volatilization	0,05	%
Via surplus sludge	23,41	%
Total	23,45	%
Total elimination from waste water	**70,76**	%
Total emission via effluent	**29,24**	%
Balance	**100,00**	%
Concentrations		
Air	2,47E-08	g/m3
Combined sludge	8,21E+02	mg/kg
Primary sludge	7,83E+02	mg/kg
Surplus sludge	9,12E+02	mg/kg
Raw sewage	5,00E-01	mg/l
Dissolved	1,48E-01	mg/l
Associated	3,52E-01	mg/l
Settled sewage	2,64E-01	mg/l
Dissolved	1,48E-01	mg/l
Associated	1,16E-01	mg/l
Mixed liquor	3,79E+00	mg/l
Dissolved	1,40E-01	mg/l
Associated	3,65E+00	mg/l
Effluent	1,46E-01	mg/l
Dissolved	1,39E-01	mg/l
Associated	6,84E-03	mg/l
In solids effluent	9,12E+02	mg/kg

SimpleTreat 4.0 Export file			
Calculation mode:	**SimpleTreat 4.0**		
Version:	**4.0.9**		
Date:	Thursday, December 12, 2019		

Input			
Substance	**User value**	Default value	Unit
Chemical class	**Neutral**		-
Molecular weight	**163**		g/mole
Octanol-water partition coefficient (Kow)	**1148,1**		-
Aparent Kow at actual pH (Dow)			-
Vapour pressure	**7,49**		Pa
Vapour pressure used (temp. corrected)	**5,246769E+00**		Pa
Temperature for determining vapour pressure	**293,15**	293,15	Kelvin
Solubility (S)	**2000**		mg/l
Solubility used (temp. corrected)	**1,862567E+03**		mg/l
Temperature for determining solubility	**293,15**	293,15	Kelvin
pKa			-
Henry coefficient (H)		4,591637E-01	Pam3/mole
Henry coefficient used (temp. corrected - only for user value)			Pam3/mole
Temperature for determining Henry coefficient (only for user value)	**293,15**	2,931500E+02	Kelvin
Organic carbon partition coefficient (Koc)		3,789514E+02	l/kg
Partition coefficient in raw sewage (Kps)		1,136854E+02	l/kg
Partition coefficient in activated sludge (Kpas)		1,402120E+02	l/kg
Mode of operation			
Facility type	**Municipal**	Municipal	-
Operation mode	**Primary solids removal**	Primary solids removal	-
Sewage flow (Q)	**0,2**	0,2	m3/d PE
Mass of sewage solids (SO)	**0,09**	0,09	kg/d PE
Mass of O2 binding material in sewage (BOD)	**60**	60	g O2/d PE
Fraction of BOD in sewage solids (FB)	**0,5417**	0,5417	-
Fraction of sewage solids removed by primary sedimentation (FS)	**0,67**	0,67	-
Sludge loading rate (kslr)	**0,1**	0,1	-
pH	**7**	7	-
Surface or bubble aeration	**surface**	surface	-
Biodegradation			
Biodegradation method selected	**OECD 301 series, 310, 302 series**		-
Biodegradation constant	**0**		hr-1
Biodegradation constant used (temp. corrected)			hr-1
Temperature for determining biodegradation constant			Kelvin
Biodegradation applies to	**Aqueous phase**		-
Emission scenario			
Temperature environment	**288,15**	288,15	Kelvin
Wind speed	**3**	3	m/s
Number of inhabitants	**10000**	10000	Person
Emission rate chemical	**1**	1	kg/d

Output		
Elimination percentages	**Value**	**Unit**
Elimination in the primary settler		
Volatilization	0,09	%
Via primary sludge	3,26	%
Total	3,35	%
Elimination in the aerator		
Stripping	0,68	%
Biodegradation	0,00	%
Total	0,68	%
Elimination in the solids liquid separator		
Volatilization	0,35	%
Via surplus sludge	1,69	%
Total	2,05	%
Total elimination from waste water	**6,08**	%
Total emission via effluent	**93,92**	%
Balance	**100,00**	%
Concentrations		
Air	1,89E-07	g/m3
Combined sludge	5,76E+01	mg/kg
Primary sludge	5,41E+01	mg/kg
Surplus sludge	6,60E+01	mg/kg
Raw sewage	5,00E-01	mg/l
Dissolved	4,76E-01	mg/l
Associated	2,43E-02	mg/l
Settled sewage	4,83E-01	mg/l
Dissolved	4,75E-01	mg/l
Associated	8,03E-03	mg/l
Mixed liquor	7,35E-01	mg/l
Dissolved	4,71E-01	mg/l
Associated	2,64E-01	mg/l
Effluent	4,70E-01	mg/l
Dissolved	4,69E-01	mg/l
Associated	4,95E-04	mg/l
In solids effluent	6,60E+01	mg/kg

N-dimethylacetamide, EC No: 204-826-4, CAS No: 127-19-5

SimpleTreat 4.0 Export file			
Calculation mode:	**SimpleTreat 4.0**		
Version:	**4.0.9**		
Date:	Monday, May 13, 2019		

Input			
Substance	**User value**	Default value	Unit
Chemical class	**Neutral**		-
Molecular weight	**87,12**		g/mole
Octanol-water particion coefficient (Kow)	**0,17**		-
Aparent Kow at actual pH (Dow)			-
Vapour pressure	**0,02**		Pa
Vapour pressure used (temp. corrected)	**1,401006E-02**		Pa
Temperature for determining vapour pressure	**293,15**	293,15	Kelvin
Solubility (S)	**1000000**		mg/l
Solubility used (temp. corrected)	**9,312837E+05**		mg/l
Temperature for determining solubility	**293,15**	293,15	Kelvin
pKa			-
Henry coefficient (H)	**0,001**	1,310617E-06	Pam3/mole
Henry coefficient used (temp. corrected - only for user value)	**0,000931284**		Pam3/mole
Temperature for determining Henry coefficient (only for user value)	**293,15**	2,931500E+02	Kelvin
Organic carbon partition coefficient (Koc)	**9,31**	2,996840E-01	l/kg
Partition coefficient in raw sewage (Kps)		2,793000E+00	l/kg
Partition coefficient in activated sludge (Kpas)		3,444700E+00	l/kg
Mode of operation			
Facility type	**Municipal**	Municipal	-
Operation mode	**Primary solids removal**	Primary solids removal	-
Sewage flow (Q)	**0,2**	0,2	m3/d PE
Mass of sewage solids (SO)	**0,09**	0,09	kg/d PE
Mass of O2 binding material in sewage (BOD)	**60**	60	g O2/d PE
Fraction of BOD in sewage solids (FB)	**0,5417**	0,5417	-
Fraction of sewage solids removed by primary sedimentation (FS)	**0,67**	0,67	-
Sludge loading rate (kslr)	**0,1**	0,1	-
pH	**7**	7	-
Surface or bubble aeration	**surface**	surface	-
Biodegradation			
Biodegradation method selected	**OECD 301 series, 310, 302 series**		-
Biodegradation constant	**0,3**		hr-1
Biodegradation constant used (temp. corrected)			hr-1
Temperature for determining biodegradation constant			Kelvin
Biodegradation applies to	**Aqueous phase**		-
Emission scenario			
Temperature environment	**288,15**	288,15	Kelvin
Wind speed	**3**	3	m/s
Number of inhabitants	**10000**	10000	Person
Emission rate chemical	**1**	1	kg/d

Output		
Elimination percentages	**Value**	**Unit**
Elimination in the primary settler		
Volatilization	0,00	%
Via primary sludge	0,08	%
Total	0,08	%
Elimination in the aerator		
Stripping	0,00	%
Biodegradation	77,40	%
Total	77,40	%
Elimination in the solids liquid separator		
Volatilization	0,00	%
Via surplus sludge	0,01	%
Total	0,01	%
Total elimination from waste water	**77,50**	%
Total emission via effluent	**22,50**	%
Balance	**100,00**	%
Concentrations		
Air	1,18E-10	g/m3
Combined sludge	1,09E+00	mg/kg
Primary sludge	1,39E+00	mg/kg
Surplus sludge	3,88E-01	mg/kg
Raw sewage	5,00E-01	mg/l
Dissolved	4,99E-01	mg/l
Associated	6,28E-04	mg/l
Settled sewage	5,00E-01	mg/l
Dissolved	4,99E-01	mg/l
Associated	2,07E-04	mg/l
Mixed liquor	1,14E-01	mg/l
Dissolved	1,13E-01	mg/l
Associated	1,55E-03	mg/l
Effluent	1,13E-01	mg/l
Dissolved	1,13E-01	mg/l
Associated	2,91E-06	mg/l
In solids effluent	3,88E-01	mg/kg

SimpleTreat 4.0 Export file			
Calculation mode:	**SimpleTreat 4.0**		
Version:	**4.0.9**		
Date:	Monday, May 13, 2019		

Input			
Substance	**User value**	Default value	Unit
Chemical class	**Neutral**		-
Molecular weight	**282,29**		g/mole
Octanol-water particion coefficient (Kow)	**12,88**		-
Aparent Kow at actual pH (Dow)			-
Vapour pressure	**0,037**		Pa
Vapour pressure used (temp. corrected)	**2,591862E-02**		Pa
Temperature for determining vapour pressure	**293,15**	293,15	Kelvin
Solubility (S)	**8500**		mg/l
Solubility used (temp. corrected)	**7,915912E+03**		mg/l
Temperature for determining solubility	**293,15**	293,15	Kelvin
pKa			-
Henry coefficient (H)		9,242860E-04	Pam3/mole
Henry coefficient used (temp. corrected - only for user value)			Pam3/mole
Temperature for determining Henry coefficient (only for user value)	**293,15**	2,931500E+02	Kelvin
Organic carbon partition coefficient (Koc)		9,977732E+00	l/kg
Partition coefficient in raw sewage (Kps)		2,993320E+00	l/kg
Partition coefficient in activated sludge (Kpas)		3,691761E+00	l/kg
Mode of operation			
Facility type	**Municipal**	Municipal	-
Operation mode	**Primary solids removal**	Primary solids removal	-
Sewage flow (Q)	**0,2**	0,2	m3/d PE
Mass of sewage solids (SO)	**0,09**	0,09	kg/d PE
Mass of O2 binding material in sewage (BOD)	**60**	60	g O2/d PE
Fraction of BOD in sewage solids (FB)	**0,5417**	0,5417	-
Fraction of sewage solids removed by primary sedimentation (FS)	**0,67**	0,67	-
Sludge loading rate (kslr)	**0,1**	0,1	-
pH	**7**	7	-
Surface or bubble aeration	**surface**	surface	-
Biodegradation			
Biodegradation method selected	**OECD 301 series, 310, 302 series**		-
Biodegradation constant	**1**		hr-1
Biodegradation constant used (temp. corrected)			hr-1
Temperature for determining biodegradation constant			Kelvin
Biodegradation applies to	**Aqueous phase**		-
Emission scenario			
Temperature environment	**288,15**	288,15	Kelvin
Wind speed	**3**	3	m/s
Number of inhabitants	**10000**	10000	Person
Emission rate chemical	**1**	1	kg/d

Output		
Elimination percentages	**Value**	**Unit**
Elimination in the primary settler		
Volatilization	0,00	%
Via primary sludge	0,09	%
Total	0,09	%
Elimination in the aerator		
Stripping	0,00	%
Biodegradation	91,89	%
Total	91,89	%
Elimination in the solids liquid separator		
Volatilization	0,00	%
Via surplus sludge	0,00	%
Total	0,00	%
Total elimination from waste water	**91,99**	%
Total emission via effluent	**8,01**	%
Balance	**100,00**	%
Concentrations		
Air	6,25E-11	g/m3
Combined sludge	1,09E+00	mg/kg
Primary sludge	1,49E+00	mg/kg
Surplus sludge	1,49E-01	mg/kg
Raw sewage	5,00E-01	mg/l
Dissolved	4,99E-01	mg/l
Associated	6,73E-04	mg/l
Settled sewage	5,00E-01	mg/l
Dissolved	4,99E-01	mg/l
Associated	2,22E-04	mg/l
Mixed liquor	4,07E-02	mg/l
Dissolved	4,01E-02	mg/l
Associated	5,94E-04	mg/l
Effluent	4,01E-02	mg/l
Dissolved	4,01E-02	mg/l
Associated	1,11E-06	mg/l
In solids effluent	1,49E-01	mg/kg

SimpleTreat 4.0 Export file			
Calculation mode:	**SimpleTreat 4.0**		
Version:	**4.0.9**		
Date:	Thursday, December 12, 2019		

Input			
Substance	**User value**	Default value	Unit
Chemical class	**Neutral**		-
Molecular weight	**390,6**		g/mole
Octanol-water particion coefficient (Kow)	**31622776,6**		-
Aparent Kow at actual pH (Dow)			-
Vapour pressure	**0,000018**		Pa
Vapour pressure used (temp. corrected)	**1,260906E-05**		Pa
Temperature for determining vapour pressure	**293,15**	293,15	Kelvin
Solubility (S)	**0,086**		mg/l
Solubility used (temp. corrected)	**8,009040E-02**		mg/l
Temperature for determining solubility	**293,15**	293,15	Kelvin
pKa			-
Henry coefficient (H)		6,149423E-02	Pam3/mole
Henry coefficient used (temp. corrected - only for user value)			Pam3/mole
Temperature for determining Henry coefficient (only for user value)	**293,15**	2,931500E+02	Kelvin
Organic carbon partition coefficient (Koc)	**165000**	1,496236E+06	l/kg
Partition coefficient in raw sewage (Kps)		4,950000E+04	l/kg
Partition coefficient in activated sludge (Kpas)		6,105000E+04	l/kg
Mode of operation			
Facility type	**Municipal**	Municipal	-
Operation mode	**Primary solids removal**	Primary solids removal	-
Sewage flow (Q)	**0,2**	0,2	m3/d PE
Mass of sewage solids (SO)	**0,09**	0,09	kg/d PE
Mass of O2 binding material in sewage (BOD)	**60**	60	g O2/d PE
Fraction of BOD in sewage solids (FB)	**0,5417**	0,5417	-
Fraction of sewage solids removed by primary sedimentation (FS)	**0,67**	0,67	-
Sludge loading rate (kslr)	**0,1**	0,1	-
pH	**7**	7	-
Surface or bubble aeration	**surface**	surface	-
Biodegradation			
Biodegradation method selected	**OECD 301 series, 310, 302 series**		-
Biodegradation constant	**1**		hr-1
Biodegradation constant used (temp. corrected)			hr-1
Temperature for determining biodegradation constant			Kelvin
Biodegradation applies to	**Aqueous phase**		-
Emission scenario			
Temperature environment	**288,15**	288,15	Kelvin
Wind speed	**3**	3	m/s
Number of inhabitants	**10000**	10000	Person
Emission rate chemical	**1**	1	kg/d

Output	**Output**	**Output**	
Elimination percentages		**Value**	**Unit**
Elimination in the primary settler			
Volatilization		0,00	%
Via primary sludge		64,12	%
Total		64,12	%
Elimination in the aerator			
Stripping		0,00	%
Biodegradation		18,82	%
Total		18,82	%
Elimination in the solids liquid separator			
Volatilization		0,00	%
Via surplus sludge		14,46	%
Total		14,46	%
Total elimination from waste water		**97,40**	%
Total emission via effluent		**2,60**	%
Balance		**100,00**	%
Concentrations			
Air		5,13E-10	g/m3
Combined sludge		9,14E+02	mg/kg
Primary sludge		1,06E+03	mg/kg
Surplus sludge		5,63E+02	mg/kg
Raw sewage		5,00E-01	mg/l
Dissolved		2,15E-02	mg/l
Associated		4,79E-01	mg/l
Settled sewage		1,79E-01	mg/l
Dissolved		2,15E-02	mg/l
Associated		1,58E-01	mg/l
Mixed liquor		2,26E+00	mg/l
Dissolved		8,21E-03	mg/l
Associated		2,25E+00	mg/l
Effluent		1,30E-02	mg/l
Dissolved		8,78E-03	mg/l
Associated		4,22E-03	mg/l
In solids effluent		5,63E+02	mg/kg

SimpleTreat 4.0 Export file			
Calculation mode:	**SimpleTreat 4.0**		
Version:	**4.0.9**		
Date:	Thursday, December 12, 2019		

Input			
Substance	**User value**	Default value	Unit
Chemical class	**Neutral**		-
Molecular weight	**278**		g/mole
Octanol-water particion coefficient (Kow)	**12882,5**		-
Aparent Kow at actual pH (Dow)			-
Vapour pressure	**11,2**		Pa
Vapour pressure used (temp. corrected)	**7,845635E+00**		Pa
Temperature for determining vapour pressure	**293,15**	293,15	Kelvin
Solubility (S)	**20,3**		mg/l
Solubility used (temp. corrected)	**1,890506E+01**		mg/l
Temperature for determining solubility	**293,15**	293,15	Kelvin
pKa			-
Henry coefficient (H)		1,153705E+02	Pam3/mole
Henry coefficient used (temp. corrected - only for user value)			Pam3/mole
Temperature for determining Henry coefficient (only for user value)	**293,15**	2,931500E+02	Kelvin
Organic carbon partition coefficient (Koc)	**1148**	2,685964E+03	l/kg
Partition coefficient in raw sewage (Kps)		3,444000E+02	l/kg
Partition coefficient in activated sludge (Kpas)		4,247600E+02	l/kg
Mode of operation			
Facility type	**Municipal**	Municipal	-
Operation mode	**Primary solids removal**	Primary solids removal	-
Sewage flow (Q)	**0,2**	0,2	m3/d PE
Mass of sewage solids (SO)	**0,09**	0,09	kg/d PE
Mass of O2 binding material in sewage (BOD)	**60**	60	g O2/d PE
Fraction of BOD in sewage solids (FB)	**0,5417**	0,5417	-
Fraction of sewage solids removed by primary sedimentation (FS)	**0,67**	0,67	-
Sludge loading rate (kslr)	**0,1**	0,1	-
pH	**7**	7	-
Surface or bubble aeration	**surface**	surface	-
Biodegradation			
Biodegradation method selected	**OECD 301 series, 310, 302 series**		-
Biodegradation constant	**1**		hr-1
Biodegradation constant used (temp. corrected)			hr-1
Temperature for determining biodegradation constant			Kelvin
Biodegradation applies to	**Aqueous phase**		-
Emission scenario			
Temperature environment	**288,15**	288,15	Kelvin
Wind speed	**3**	3	m/s
Number of inhabitants	**10000**	10000	Person
Emission rate chemical	**1**	1	kg/d

Output	**Output**	**Output**	
Elimination percentages		**Value**	**Unit**
Elimination in the primary settler			
Volatilization		3,45	%
Via primary sludge		8,89	%
Total		12,34	%
Elimination in the aerator			
Stripping		11,04	%
Biodegradation		70,14	%
Total		81,18	%
Elimination in the solids liquid separator			
Volatilization		0,87	%
Via surplus sludge		0,34	%
Total		1,21	%
Total elimination from waste water		**94,72**	%
Total emission via effluent		**5,28**	%
Balance		**100,00**	%
Concentrations			
Air		2,58E-06	g/m3
Combined sludge		1,07E+02	mg/kg
Primary sludge		1,47E+02	mg/kg
Surplus sludge		1,31E+01	mg/kg
Raw sewage		5,00E-01	mg/l
Dissolved		4,33E-01	mg/l
Associated		6,63E-02	mg/l
Settled sewage		4,38E-01	mg/l
Dissolved		4,16E-01	mg/l
Associated		2,19E-02	mg/l
Mixed liquor		8,32E-02	mg/l
Dissolved		3,06E-02	mg/l
Associated		5,26E-02	mg/l
Effluent		2,64E-02	mg/l
Dissolved		2,63E-02	mg/l
Associated		9,86E-05	mg/l
In solids effluent		1,31E+01	mg/kg

P-nonylphenol, EC No: 203-199-4, CAS No: 104-40-5

SimpleTreat 4.0 Export file			
Calculation mode:	**SimpleTreat 4.0**		
Version:	**4.0.9**		
Date:	Thursday, December 12, 2019		

Input			
Substance	**User value**	Default value	Unit
Chemical class	**Neutral**		-
Molecular weight	**250,3**		g/mole
Octanol-water particion coefficient (Kow)	**575439,9**		-
Aparent Kow at actual pH (Dow)			-
Vapour pressure	**0,109**		Pa
Vapour pressure used (temp. corrected)	**7,635484E-02**		Pa
Temperature for determining vapour pressure	**293,15**	293,15	Kelvin
Solubility (S)	**7**		mg/l
Solubility used (temp. corrected)	**6,518986E+00**		mg/l
Temperature for determining solubility	**293,15**	293,15	Kelvin
pKa			-
Henry coefficient (H)		2,931686E+00	Pam3/mole
Henry coefficient used (temp. corrected - only for user value)			Pam3/mole
Temperature for determining Henry coefficient (only for user value)	**293,15**	2,931500E+02	Kelvin
Organic carbon partition coefficient (Koc)	**38260**	5,829079E+04	l/kg
Partition coefficient in raw sewage (Kps)		1,147800E+04	l/kg
Partition coefficient in activated sludge (Kpas)		1,415620E+04	l/kg
Mode of operation			
Facility type	**Municipal**	Municipal	-
Operation mode	**Primary solids removal**	Primary solids removal	-
Sewage flow (Q)	**0,2**	0,2	m3/d PE
Mass of sewage solids (SO)	**0,09**	0,09	kg/d PE
Mass of O2 binding material in sewage (BOD)	**60**	60	g O2/d PE
Fraction of BOD in sewage solids (FB)	**0,5417**	0,5417	-
Fraction of sewage solids removed by primary sedimentation (FS)	**0,67**	0,67	-
Sludge loading rate (kslr)	**0,1**	0,1	-
pH	**7**	7	-
Surface or bubble aeration	**surface**	surface	-
Biodegradation			
Biodegradation method selected	**OECD 301 series, 310, 302 series**		-
Biodegradation constant	**1**		hr-1
Biodegradation constant used (temp. corrected)			hr-1
Temperature for determining biodegradation constant			Kelvin
Biodegradation applies to	**Aqueous phase**		-
Emission scenario			
Temperature environment	**288,15**	288,15	Kelvin
Wind speed	**3**	3	m/s
Number of inhabitants	**10000**	10000	Person
Emission rate chemical	**1**	1	kg/d

Output		
Elimination percentages	**Value**	**Unit**
Elimination in the primary settler		
Volatilization	0,09	%
Via primary sludge	56,11	%
Total	56,20	%
Elimination in the aerator		
Stripping	0,13	%
Biodegradation	34,31	%
Total	34,44	%
Elimination in the solids liquid separator		
Volatilization	0,07	%
Via surplus sludge	5,93	%
Total	5,99	%
Total elimination from waste water	**96,63**	%
Total emission via effluent	**3,37**	%
Balance	**100,00**	%
Concentrations		
Air	4,84E-08	g/m3
Combined sludge	7,22E+02	mg/kg
Primary sludge	9,30E+02	mg/kg
Surplus sludge	2,31E+02	mg/kg
Raw sewage	5,00E-01	mg/l
Dissolved	8,11E-02	mg/l
Associated	4,19E-01	mg/l
Settled sewage	2,19E-01	mg/l
Dissolved	8,08E-02	mg/l
Associated	1,38E-01	mg/l
Mixed liquor	9,39E-01	mg/l
Dissolved	1,50E-02	mg/l
Associated	9,24E-01	mg/l
Effluent	1,68E-02	mg/l
Dissolved	1,51E-02	mg/l
Associated	1,73E-03	mg/l
In solids effluent	2,31E+02	mg/kg

SimpleTreat 4.0 Export file			
Calculation mode:	**SimpleTreat 4.0**		
Version:	**4.0.9**		
Date:	Friday, May 10, 2019		

Input			
Substance	**User value**	Default value	Unit
Chemical class	**Neutral**		-
Molecular weight	**296,6**		g/mole
Octanol-water particion coefficient (Kow)	**3090295**		-
Aparent Kow at actual pH (Dow)			-
Vapour pressure	**132**		Pa
Vapour pressure used (temp. corrected)	**9,246642E+01**		Pa
Temperature for determining vapour pressure	**293,15**	293,15	Kelvin
Solubility (S)	**0,056**		mg/l
Solubility used (temp. corrected)	**5,215189E-02**		mg/l
Temperature for determining solubility	**293,15**	293,15	Kelvin
pKa			-
Henry coefficient (H)	**1195640**	5,258782E+05	Pam3/mole
Henry coefficient used (temp. corrected - only for user value)	**1113480,089**		Pam3/mole
Temperature for determining Henry coefficient (only for user value)	**293,15**	2,931500E+02	Kelvin
Organic carbon partition coefficient (Koc)	**16596**	2,274573E+05	l/kg
Partition coefficient in raw sewage (Kps)		4,978800E+03	l/kg
Partition coefficient in activated sludge (Kpas)		6,140520E+03	l/kg
Mode of operation			
Facility type	**Municipal**	Municipal	-
Operation mode	**Primary solids removal**	Primary solids removal	-
Sewage flow (Q)	**0,2**	0,2	m3/d PE
Mass of sewage solids (SO)	**0,09**	0,09	kg/d PE
Mass of O2 binding material in sewage (BOD)	**60**	60	g O2/d PE
Fraction of BOD in sewage solids (FB)	**0,5417**	0,5417	-
Fraction of sewage solids removed by primary sedimentation (FS)	**0,67**	0,67	-
Sludge loading rate (kslr)	**0,1**	0,1	-
pH	**7**	7	-
Surface or bubble aeration	**surface**	surface	-
Biodegradation			
Biodegradation method selected	**OECD 301 series, 310, 302 series**		-
Biodegradation constant	**0**		hr-1
Biodegradation constant used (temp. corrected)			hr-1
Temperature for determining biodegradation constant			Kelvin
Biodegradation applies to	**Aqueous phase**		-
Emission scenario			
Temperature environment	**288,15**	288,15	Kelvin
Wind speed	**3**	3	m/s
Number of inhabitants	**10000**	10000	Person
Emission rate chemical	**1**	1	kg/d

Output		
Elimination percentages	**Value**	**Unit**
Elimination in the primary settler		
Volatilization	1,49	%
Via primary sludge	46,01	%
Total	47,50	%
Elimination in the aerator		
Stripping	47,02	%
Biodegradation	0,00	%
Total	47,02	%
Elimination in the solids liquid separator		
Volatilization	0,49	%
Via surplus sludge	2,42	%
Total	2,90	%
Total elimination from waste water	**97,42**	%
Total emission via effluent	**2,58**	%
Balance	**100,00**	%
Concentrations		
Air	8,24E-06	g/m3
Combined sludge	5,63E+02	mg/kg
Primary sludge	7,63E+02	mg/kg
Surplus sludge	9,41E+01	mg/kg
Raw sewage	5,00E-01	mg/l
Dissolved	1,54E-01	mg/l
Associated	3,43E-01	mg/l
Settled sewage	2,63E-01	mg/l
Dissolved	1,49E-01	mg/l
Associated	1,13E-01	mg/l
Mixed liquor	3,91E-01	mg/l
Dissolved	1,40E-02	mg/l
Associated	3,77E-01	mg/l
Effluent	1,29E-02	mg/l
Dissolved	1,22E-02	mg/l
Associated	7,06E-04	mg/l
In solids effluent	9,41E+01	mg/kg

SimpleTreat 4.0 Export file			
Calculation mode:	**SimpleTreat 4.0**		
Version:	**4.0.9**		
Date:	Monday, May 13, 2019		

Input			
Substance	**User value**	Default value	Unit
Chemical class	**Neutral**		-
Molecular weight	**370,77**		g/mole
Octanol-water partition coefficient (Kow)	**105438689,6**		-
Aparent Kow at actual pH (Dow)			-
Vapour pressure	**33,2**		Pa
Vapour pressure used (temp. corrected)	**2,325670E+01**		Pa
Temperature for determining vapour pressure	**293,15**	293,15	Kelvin
Solubility (S)	**0,017**		mg/l
Solubility used (temp. corrected)	**1,583182E-02**		mg/l
Temperature for determining solubility	**293,15**	293,15	Kelvin
pKa			-
Henry coefficient (H)	**3343725**	5,446554E+05	Pam3/mole
Henry coefficient used (temp. corrected - only for user value)	**3113956,718**		Pam3/mole
Temperature for determining Henry coefficient (only for user value)	**293,15**	2,931500E+02	Kelvin
Organic carbon partition coefficient (Koc)	**147910,8**	3,968533E+06	l/kg
Partition coefficient in raw sewage (Kps)		4,437324E+04	l/kg
Partition coefficient in activated sludge (Kpas)		5,472700E+04	l/kg
Mode of operation			
Facility type	**Municipal**	Municipal	-
Operation mode	**Primary solids removal**	Primary solids removal	-
Sewage flow (Q)	**0,2**	0,2	m3/d PE
Mass of sewage solids (SO)	**0,09**	0,09	kg/d PE
Mass of O2 binding material in sewage (BOD)	**60**	60	g O2/d PE
Fraction of BOD in sewage solids (FB)	**0,5417**	0,5417	-
Fraction of sewage solids removed by primary sedimentation (FS)	**0,67**	0,67	-
Sludge loading rate (kslr)	**0,1**	0,1	-
pH	**7**	7	-
Surface or bubble aeration	**surface**	surface	-
Biodegradation			
Biodegradation method selected	**OECD 301 series, 310, 302 series**		-
Biodegradation constant	**0**		hr-1
Biodegradation constant used (temp. corrected)			hr-1
Temperature for determining biodegradation constant			Kelvin
Biodegradation applies to	**Aqueous phase**		-
Emission scenario			
Temperature environment	**288,15**	288,15	Kelvin
Wind speed	**3**	3	m/s
Number of inhabitants	**10000**	10000	Person
Emission rate chemical	**1**	1	kg/d

Output		
Elimination percentages	**Value**	**Unit**
Elimination in the primary settler		
Volatilization	0,23	%
Via primary sludge	63,72	%
Total	63,95	%
Elimination in the aerator		
Stripping	22,59	%
Biodegradation	0,00	%
Total	22,59	%
Elimination in the solids liquid separator		
Volatilization	0,27	%
Via surplus sludge	11,17	%
Total	11,44	%
Total elimination from waste water	**97,99**	%
Total emission via effluent	**2,01**	%
Balance	**100,00**	%
Concentrations		
Air	3,88E-06	g/m3
Combined sludge	8,71E+02	mg/kg
Primary sludge	1,06E+03	mg/kg
Surplus sludge	4,35E+02	mg/kg
Raw sewage	5,00E-01	mg/l
Dissolved	2,38E-02	mg/l
Associated	4,76E-01	mg/l
Settled sewage	1,80E-01	mg/l
Dissolved	2,33E-02	mg/l
Associated	1,57E-01	mg/l
Mixed liquor	1,75E+00	mg/l
Dissolved	6,74E-03	mg/l
Associated	1,74E+00	mg/l
Effluent	1,01E-02	mg/l
Dissolved	6,79E-03	mg/l
Associated	3,26E-03	mg/l
In solids effluent	4,35E+02	mg/kg

SimpleTreat 4.0 Export file			
Calculation mode:	**SimpleTreat 4.0**		
Version:	**4.0.9**		
Date:	Tuesday, May 14, 2019		

Input			
Substance	**User value**	Default value	Unit
Chemical class	**Neutral**		-
Molecular weight	**444,924**		g/mole
Octanol-water partition coefficient (Kow)	**100000000**		-
Aparent Kow at actual pH (Dow)			-
Vapour pressure	**4,7**		Pa
Vapour pressure used (temp. corrected)	**3,292365E+00**		Pa
Temperature for determining vapour pressure	**293,15**	293,15	Kelvin
Solubility (S)	**0,0051**		mg/l
Solubility used (temp. corrected)	**4,749547E-03**		mg/l
Temperature for determining solubility	**293,15**	293,15	Kelvin
pKa			-
Henry coefficient (H)	**2520000**	3,084193E+05	Pam3/mole
Henry coefficient used (temp. corrected - only for user value)	**2346835,021**		Pam3/mole
Temperature for determining Henry coefficient (only for user value)	**293,15**	2,931500E+02	Kelvin
Organic carbon partition coefficient (Koc)	**790000**	3,801894E+06	l/kg
Partition coefficient in raw sewage (Kps)		2,370000E+05	l/kg
Partition coefficient in activated sludge (Kpas)		2,923000E+05	l/kg
Mode of operation			
Facility type	**Municipal**	Municipal	-
Operation mode	**Primary solids removal**	Primary solids removal	-
Sewage flow (Q)	**0,2**	0,2	m3/d PE
Mass of sewage solids (SO)	**0,09**	0,09	kg/d PE
Mass of O2 binding material in sewage (BOD)	**60**	60	g O2/d PE
Fraction of BOD in sewage solids (FB)	**0,5417**	0,5417	-
Fraction of sewage solids removed by primary sedimentation (FS)	**0,67**	0,67	-
Sludge loading rate (kslr)	**0,1**	0,1	-
pH	**7**	7	-
Surface or bubble aeration	**surface**	surface	-
Biodegradation			
Biodegradation method selected	**OECD 301 series, 310, 302 series**		-
Biodegradation constant	**0**		hr-1
Biodegradation constant used (temp. corrected)			hr-1
Temperature for determining biodegradation constant			Kelvin
Biodegradation applies to	**Aqueous phase**		-
Emission scenario			
Temperature environment	**288,15**	288,15	Kelvin
Wind speed	**3**	3	m/s
Number of inhabitants	**10000**	10000	Person
Emission rate chemical	**1**	1	kg/d

Output		
Elimination percentages	**Value**	**Unit**
Elimination in the primary settler		
Volatilization	0,05	%
Via primary sludge	66,36	%
Total	66,41	%
Elimination in the aerator		
Stripping	8,56	%
Biodegradation	0,00	%
Total	8,56	%
Elimination in the solids liquid separator		
Volatilization	0,11	%
Via surplus sludge	23,02	%
Total	23,13	%
Total elimination from waste water	**98,10**	%
Total emission via effluent	**1,90**	%
Balance	**100,00**	%
Concentrations		
Air	1,47E-06	g/m3
Combined sludge	1,04E+03	mg/kg
Primary sludge	1,10E+03	mg/kg
Surplus sludge	8,97E+02	mg/kg
Raw sewage	5,00E-01	mg/l
Dissolved	4,64E-03	mg/l
Associated	4,95E-01	mg/l
Settled sewage	1,68E-01	mg/l
Dissolved	4,55E-03	mg/l
Associated	1,63E-01	mg/l
Mixed liquor	3,59E+00	mg/l
Dissolved	2,55E-03	mg/l
Associated	3,59E+00	mg/l
Effluent	9,51E-03	mg/l
Dissolved	2,79E-03	mg/l
Associated	6,72E-03	mg/l
In solids effluent	8,97E+02	mg/kg

Cobalt(II) sulphate

The substance is not suitable to be run in SimpleTreat. Data on partition coefficient (Kow) is lacking. Such a study technically not feasible. The substance is inorganic and the study was waived in the ECHA registration dossier.

Strontium chromate EC No: 232-142-6, CAS: 7789-06-2

Inorganic, partition coefficient not available. Substance not modelled in SimpleTreat

SimpleTreat 4.0 Export file			
Calculation mode:	**SimpleTreat 4.0**		
Version:	**4.0.9**		
Date:	Monday, May 13, 2019		

Input			
Substance	**User value**	Default value	Unit
Chemical class	**Neutral**		-
Molecular weight	**381,37**		g/mole
Octanol-water particion coefficient (Kow)	**0,03**		-
Aparent Kow at actual pH (Dow)			-
Vapour pressure	**213**		Pa
Vapour pressure used (temp. corrected)	**1,492072E+02**		Pa
Temperature for determining vapour pressure	**293,15**	293,15	Kelvin
Solubility (S)	**49740**		mg/l
Solubility used (temp. corrected)	**4,632205E+04**		mg/l
Temperature for determining solubility	**293,15**	293,15	Kelvin
pKa			-
Henry coefficient (H)		1,228424E+00	Pam3/mole
Henry coefficient used (temp. corrected - only for user value)			Pam3/mole
Temperature for determining Henry coefficient (only for user value)	**293,15**	2,931500E+02	Kelvin
Organic carbon partition coefficient (Koc)		7,353062E-02	l/kg
Partition coefficient in raw sewage (Kps)		2,205919E-02	l/kg
Partition coefficient in activated sludge (Kpas)		2,720633E-02	l/kg
Mode of operation			
Facility type	**Municipal**	Municipal	-
Operation mode	**Primary solids removal**	Primary solids removal	-
Sewage flow (Q)	**0,2**	0,2	m3/d PE
Mass of sewage solids (SO)	**0,09**	0,09	kg/d PE
Mass of O2 binding material in sewage (BOD)	**60**	60	g O2/d PE
Fraction of BOD in sewage solids (FB)	**0,5417**	0,5417	-
Fraction of sewage solids removed by primary sedimentation (FS)	**0,67**	0,67	-
Sludge loading rate (kslr)	**0,1**	0,1	-
pH	**7**	7	-
Surface or bubble aeration	**surface**	surface	-
Biodegradation			
Biodegradation method selected	**OECD 301 series, 310, 302 series**		-
Biodegradation constant	**1**		hr-1
Biodegradation constant used (temp. corrected)			hr-1
Temperature for determining biodegradation constant			Kelvin
Biodegradation applies to	**Aqueous phase**		-
Emission scenario			
Temperature environment	**288,15**	288,15	Kelvin
Wind speed	**3**	3	m/s
Number of inhabitants	**10000**	10000	Person
Emission rate chemical	**1**	1	kg/d

Output		
Elimination percentages	**Value**	**Unit**
Elimination in the primary settler		
Volatilization	0,24	%
Via primary sludge	0,00	%
Total	0,24	%
Elimination in the aerator		
Stripping	0,15	%
Biodegradation	91,61	%
Total	91,77	%
Elimination in the solids liquid separator		
Volatilization	0,08	%
Via surplus sludge	0,00	%
Total	0,08	%
Total elimination from waste water	**92,09**	%
Total emission via effluent	**7,91**	%
Balance	**100,00**	%
Concentrations		
Air	7,95E-08	g/m3
Combined sludge	8,06E-03	mg/kg
Primary sludge	1,10E-02	mg/kg
Surplus sludge	1,09E-03	mg/kg
Raw sewage	5,00E-01	mg/l
Dissolved	5,00E-01	mg/l
Associated	4,96E-06	mg/l
Settled sewage	4,99E-01	mg/l
Dissolved	4,99E-01	mg/l
Associated	1,64E-06	mg/l
Mixed liquor	4,00E-02	mg/l
Dissolved	3,99E-02	mg/l
Associated	4,37E-06	mg/l
Effluent	3,96E-02	mg/l
Dissolved	3,96E-02	mg/l
Associated	8,19E-09	mg/l
In solids effluent	1,09E-03	mg/kg

SimpleTreat 4.0 Export file			
Calculation mode:	**SimpleTreat 4.0**		
Version:	**4.0.9**		
Date:	Friday, May 10, 2019		

Input			
Substance	**User value**	Default value	Unit
Chemical class	**Neutral**		-
Molecular weight	**71,08**		g/mole
Octanol-water partition coefficient (Kow)	**0,126**		-
Aparent Kow at actual pH (Dow)			-
Vapour pressure	**2500**		Pa
Vapour pressure used (temp. corrected)	**1,751258E+03**		Pa
Temperature for determining vapour pressure	**293,15**	293,15	Kelvin
Solubility (S)	**2155000**		mg/l
Solubility used (temp. corrected)	**2,006916E+06**		mg/l
Temperature for determining solubility	**293,15**	293,15	Kelvin
pKa			-
Henry coefficient (H)		6,202521E-02	Pam3/mole
Henry coefficient used (temp. corrected - only for user value)			Pam3/mole
Temperature for determining Henry coefficient (only for user value)	**293,15**	2,931500E+02	Kelvin
Organic carbon partition coefficient (Koc)		2,351257E-01	l/kg
Partition coefficient in raw sewage (Kps)		7,053772E-02	l/kg
Partition coefficient in activated sludge (Kpas)		8,699652E-02	l/kg
Mode of operation			
Facility type	**Municipal**	Municipal	-
Operation mode	**Primary solids removal**	Primary solids removal	-
Sewage flow (Q)	**0,2**	0,2	m3/d PE
Mass of sewage solids (SO)	**0,09**	0,09	kg/d PE
Mass of O2 binding material in sewage (BOD)	**60**	60	g O2/d PE
Fraction of BOD in sewage solids (FB)	**0,5417**	0,5417	-
Fraction of sewage solids removed by primary sedimentation (FS)	**0,67**	0,67	-
Sludge loading rate (kslr)	**0,1**	0,1	-
pH	**7**	7	-
Surface or bubble aeration	**surface**	surface	-
Biodegradation			
Biodegradation method selected	**OECD 301 series, 310, 302 series**		-
Biodegradation constant	**0,3**		hr-1
Biodegradation constant used (temp. corrected)			hr-1
Temperature for determining biodegradation constant			Kelvin
Biodegradation applies to	**Aqueous phase**		-
Emission scenario			
Temperature environment	**288,15**	288,15	Kelvin
Wind speed	**3**	3	m/s
Number of inhabitants	**10000**	10000	Person
Emission rate chemical	**1**	1	kg/d

Output		
Elimination percentages	**Value**	**Unit**
Elimination in the primary settler		
Volatilization	0,01	%
Via primary sludge	0,00	%
Total	0,02	%
Elimination in the aerator		
Stripping	0,02	%
Biodegradation	77,45	%
Total	77,47	%
Elimination in the solids liquid separator		
Volatilization	0,01	%
Via surplus sludge	0,00	%
Total	0,01	%
Total elimination from waste water	**77,50**	%
Total emission via effluent	**22,50**	%
Balance	**100,00**	%
Concentrations		
Air	7,85E-09	g/m3
Combined sludge	2,77E-02	mg/kg
Primary sludge	3,53E-02	mg/kg
Surplus sludge	9,81E-03	mg/kg
Raw sewage	5,00E-01	mg/l
Dissolved	5,00E-01	mg/l
Associated	1,59E-05	mg/l
Settled sewage	5,00E-01	mg/l
Dissolved	5,00E-01	mg/l
Associated	5,24E-06	mg/l
Mixed liquor	1,13E-01	mg/l
Dissolved	1,13E-01	mg/l
Associated	3,92E-05	mg/l
Effluent	1,13E-01	mg/l
Dissolved	1,13E-01	mg/l
Associated	7,35E-08	mg/l
In solids effluent	9,81E-03	mg/kg

4,4'-isopropylidenediphenol (Bisphenol, BPA), EC No 201-245-8. CAS No 80-05-7,

SimpleTreat 4.0 Export file			
Calculation mode:	**SimpleTreat 4.0**		
Version:	**4.0.9**		
Date:	Thursday, May 9, 2019		

Input			
Substance	**User value**	Default value	Unit
Chemical class	**Neutral**		-
Molecular weight	**228,3**		g/mole
Octanol-water partition coefficient (Kow)	**3,4**		-
Aparent Kow at actual pH (Dow)			-
Vapour pressure	**4,12E-09**		Pa
Vapour pressure used (temp. corrected)	**2,886073E-09**		Pa
Temperature for determining vapour pressure	**293,15**	293,15	Kelvin
Solubility (S)	**300**		mg/l
Solubility used (temp. corrected)	**2,793851E+02**		mg/l
Temperature for determining solubility	**293,15**	293,15	Kelvin
pKa			-
Henry coefficient (H)	**0,000000312**	2,358359E-09	Pam3/mole
Henry coefficient used (temp. corrected - only for user value)	**2,90561E-07**		Pam3/mole
Temperature for determining Henry coefficient (only for user value)	**293,15**	2,931500E+02	Kelvin
Organic carbon partition coefficient (Koc)	**750**	3,392329E+00	l/kg
Partition coefficient in raw sewage (Kps)		2,250000E+02	l/kg
Partition coefficient in activated sludge (Kpas)		2,775000E+02	l/kg
Mode of operation			
Facility type	**Municipal**	Municipal	-
Operation mode	**Primary solids removal**	Primary solids removal	-
Sewage flow (Q)	**0,2**	0,2	m3/d PE
Mass of sewage solids (SO)	**0,09**	0,09	kg/d PE
Mass of O2 binding material in sewage (BOD)	**60**	60	g O2/d PE
Fraction of BOD in sewage solids (FB)	**0,5417**	0,5417	-
Fraction of sewage solids removed by primary sedimentation (FS)	**0,67**	0,67	-
Sludge loading rate (kslr)	**0,1**	0,1	-
pH	**7**	7	-
Surface or bubble aeration	**surface**	surface	-
Biodegradation			
Biodegradation method selected	**OECD 301 series, 310, 302 series**		-
Biodegradation constant	**1**		hr-1
Biodegradation constant used (temp. corrected)			hr-1
Temperature for determining biodegradation constant			Kelvin
Biodegradation applies to	**Aqueous phase**		-
Emission scenario			
Temperature environment	**288,15**	288,15	Kelvin
Wind speed	**3**	3	m/s
Number of inhabitants	**10000**	10000	Person
Emission rate chemical	**1**	1	kg/d

Output		
Elimination percentages	**Value**	**Unit**
Elimination in the primary settler		
Volatilization	0,00	%
Via primary sludge	6,16	%
Total	6,16	%
Elimination in the aerator		
Stripping	0,00	%
Biodegradation	86,05	%
Total	86,05	%
Elimination in the solids liquid separator		
Volatilization	0,00	%
Via surplus sludge	0,27	%
Total	0,27	%
Total elimination from waste water	**92,48**	%
Total emission via effluent	**7,52**	%
Balance	**100,00**	%
Concentrations		
Air	1,81E-14	g/m3
Combined sludge	7,48E+01	mg/kg
Primary sludge	1,02E+02	mg/kg
Surplus sludge	1,05E+01	mg/kg
Raw sewage	5,00E-01	mg/l
Dissolved	4,54E-01	mg/l
Associated	4,60E-02	mg/l
Settled sewage	4,69E-01	mg/l
Dissolved	4,54E-01	mg/l
Associated	1,52E-02	mg/l
Mixed liquor	7,95E-02	mg/l
Dissolved	3,75E-02	mg/l
Associated	4,20E-02	mg/l
Effluent	3,76E-02	mg/l
Dissolved	3,75E-02	mg/l
Associated	7,88E-05	mg/l
In solids effluent	1,05E+01	mg/kg

SimpleTreat 4.0 Export file			
Calculation mode:	**SimpleTreat 4.0**		
Version:	**4.0.9**		
Date:	Friday, May 10, 2019		

Input			
Substance	**User value**	Default value	Unit
Chemical class	**Neutral**		-
Molecular weight	**58,08**		g/mole
Octanol-water particion coefficient (Kow)	**1,14**		-
Aparent Kow at actual pH (Dow)			-
Vapour pressure	**74000**		Pa
Vapour pressure used (temp. corrected)	**5,183723E+04**		Pa
Temperature for determining vapour pressure	**293,15**	293,15	Kelvin
Solubility (S)	**425**		mg/l
Solubility used (temp. corrected)	**3,957956E+02**		mg/l
Temperature for determining solubility	**293,15**	293,15	Kelvin
pKa			-
Henry coefficient (H)		7,606721E+03	Pam3/mole
Henry coefficient used (temp. corrected - only for user value)			Pam3/mole
Temperature for determining Henry coefficient (only for user value)	**293,15**	2,931500E+02	Kelvin
Organic carbon partition coefficient (Koc)		1,399887E+00	l/kg
Partition coefficient in raw sewage (Kps)		4,199661E-01	l/kg
Partition coefficient in activated sludge (Kpas)		5,179581E-01	l/kg
Mode of operation			
Facility type	**Municipal**	Municipal	-
Operation mode	**Primary solids removal**	Primary solids removal	-
Sewage flow (Q)	**0,2**	0,2	m3/d PE
Mass of sewage solids (SO)	**0,09**	0,09	kg/d PE
Mass of O2 binding material in sewage (BOD)	**60**	60	g O2/d PE
Fraction of BOD in sewage solids (FB)	**0,5417**	0,5417	-
Fraction of sewage solids removed by primary sedimentation (FS)	**0,67**	0,67	-
Sludge loading rate (kslr)	**0,1**	0,1	-
pH	**7**	7	-
Surface or bubble aeration	**surface**	surface	-
Biodegradation			
Biodegradation method selected	**OECD 301 series, 310, 302 series**		-
Biodegradation constant	**0,3**		hr-1
Biodegradation constant used (temp. corrected)			hr-1
Temperature for determining biodegradation constant			Kelvin
Biodegradation applies to	**Aqueous phase**		-
Emission scenario			
Temperature environment	**288,15**	288,15	Kelvin
Wind speed	**3**	3	m/s
Number of inhabitants	**10000**	10000	Person
Emission rate chemical	**1**	1	kg/d

Output		
Elimination percentages	**Value**	**Unit**
Elimination in the primary settler		
Volatilization	4,75	%
Via primary sludge	0,01	%
Total	4,76	%
Elimination in the aerator		
Stripping	73,74	%
Biodegradation	16,66	%
Total	90,39	%
Elimination in the solids liquid separator		
Volatilization	0,81	%
Via surplus sludge	0,00	%
Total	0,81	%
Total elimination from waste water	**95,96**	%
Total emission via effluent	**4,04**	%
Balance	**100,00**	%
Concentrations		
Air	1,33E-05	g/m3
Combined sludge	1,49E-01	mg/kg
Primary sludge	2,07E-01	mg/kg
Surplus sludge	1,26E-02	mg/kg
Raw sewage	5,00E-01	mg/l
Dissolved	5,00E-01	mg/l
Associated	9,31E-05	mg/l
Settled sewage	4,76E-01	mg/l
Dissolved	4,76E-01	mg/l
Associated	3,07E-05	mg/l
Mixed liquor	2,43E-02	mg/l
Dissolved	2,42E-02	mg/l
Associated	5,05E-05	mg/l
Effluent	2,02E-02	mg/l
Dissolved	2,02E-02	mg/l
Associated	9,46E-08	mg/l
In solids effluent	1,26E-02	mg/kg

SimpleTreat 4.0 Export file			
Calculation mode:	**SimpleTreat 4.0**		
Version:	**4.0.9**		
Date:	Monday, May 13, 2019		

Input			
Substance	**User value**	Default value	Unit
Chemical class	**Neutral**		-
Molecular weight	**233,1**		g/mole
Octanol-water partition coefficient (Kow)	**776**		-
Aparent Kow at actual pH (Dow)			-
Vapour pressure	**0,00000076**		Pa
Vapour pressure used (temp. corrected)	**5,323824E-07**		Pa
Temperature for determining vapour pressure	**293,15**	293,15	Kelvin
Solubility (S)	**28,8**		mg/l
Solubility used (temp. corrected)	**2,682097E+01**		mg/l
Temperature for determining solubility	**293,15**	293,15	Kelvin
pKa			-
Henry coefficient (H)		4,626914E-06	Pam3/mole
Henry coefficient used (temp. corrected - only for user value)			Pam3/mole
Temperature for determining Henry coefficient (only for user value)	**293,15**	2,931500E+02	Kelvin
Organic carbon partition coefficient (Koc)	**395**	2,759231E+02	l/kg
Partition coefficient in raw sewage (Kps)		1,185000E+02	l/kg
Partition coefficient in activated sludge (Kpas)		1,461500E+02	l/kg
Mode of operation			
Facility type	**Municipal**	Municipal	-
Operation mode	**Primary solids removal**	Primary solids removal	-
Sewage flow (Q)	**0,2**	0,2	m3/d PE
Mass of sewage solids (SO)	**0,09**	0,09	kg/d PE
Mass of O2 binding material in sewage (BOD)	**60**	60	g O2/d PE
Fraction of BOD in sewage solids (FB)	**0,5417**	0,5417	-
Fraction of sewage solids removed by primary sedimentation (FS)	**0,67**	0,67	-
Sludge loading rate (kslr)	**0,1**	0,1	-
pH	**7**	7	-
Surface or bubble aeration	**surface**	surface	-
Biodegradation			
Biodegradation method selected	**OECD 301 series, 310, 302 series**		-
Biodegradation constant	**0**		hr-1
Biodegradation constant used (temp. corrected)			hr-1
Temperature for determining biodegradation constant			Kelvin
Biodegradation applies to	**Aqueous phase**		-
Emission scenario			
Temperature environment	**288,15**	288,15	Kelvin
Wind speed	**3**	3	m/s
Number of inhabitants	**10000**	10000	Person
Emission rate chemical	**1**	1	kg/d

Output		
Elimination percentages	**Value**	**Unit**
Elimination in the primary settler		
Volatilization	0,00	%
Via primary sludge	3,39	%
Total	3,39	%
Elimination in the aerator		
Stripping	0,00	%
Biodegradation	0,00	%
Total	0,00	%
Elimination in the solids liquid separator		
Volatilization	0,00	%
Via surplus sludge	1,78	%
Total	1,78	%
Total elimination from waste water	**5,17**	%
Total emission via effluent	**94,83**	%
Balance	**100,00**	%
Concentrations		
Air	1,94E-12	g/m3
Combined sludge	6,01E+01	mg/kg
Primary sludge	5,63E+01	mg/kg
Surplus sludge	6,92E+01	mg/kg
Raw sewage	5,00E-01	mg/l
Dissolved	4,75E-01	mg/l
Associated	2,53E-02	mg/l
Settled sewage	4,83E-01	mg/l
Dissolved	4,75E-01	mg/l
Associated	8,35E-03	mg/l
Mixed liquor	7,51E-01	mg/l
Dissolved	4,74E-01	mg/l
Associated	2,77E-01	mg/l
Effluent	4,74E-01	mg/l
Dissolved	4,74E-01	mg/l
Associated	5,19E-04	mg/l
In solids effluent	6,92E+01	mg/kg

SimpleTreat 4.0 Export file			
Calculation mode:	**SimpleTreat 4.0**		
Version:	**4.0.9**		
Date:	Monday, May 13, 2019		

Input			
Substance	**User value**	Default value	Unit
Chemical class	**Neutral**		-
Molecular weight	**241,36**		g/mole
Octanol-water partition coefficient (Kow)	**3020**		-
Aparent Kow at actual pH (Dow)			-
Vapour pressure	**0,00013**		Pa
Vapour pressure used (temp. corrected)	**9,106541E-05**		Pa
Temperature for determining vapour pressure	**293,15**	293,15	Kelvin
Solubility (S)	**22**		mg/l
Solubility used (temp. corrected)	**2,048824E+01**		mg/l
Temperature for determining solubility	**293,15**	293,15	Kelvin
pKa			-
Henry coefficient (H)	**0,0013**	1,072788E-03	Pam3/mole
Henry coefficient used (temp. corrected - only for user value)	**0,001210669**		Pam3/mole
Temperature for determining Henry coefficient (only for user value)	**293,15**	2,931500E+02	Kelvin
Organic carbon partition coefficient (Koc)		8,294794E+02	l/kg
Partition coefficient in raw sewage (Kps)		2,488438E+02	l/kg
Partition coefficient in activated sludge (Kpas)		3,069074E+02	l/kg
Mode of operation			
Facility type	**Municipal**	Municipal	-
Operation mode	**Primary solids removal**	Primary solids removal	-
Sewage flow (Q)	**0,2**	0,2	m3/d PE
Mass of sewage solids (SO)	**0,09**	0,09	kg/d PE
Mass of O2 binding material in sewage (BOD)	**60**	60	g O2/d PE
Fraction of BOD in sewage solids (FB)	**0,5417**	0,5417	-
Fraction of sewage solids removed by primary sedimentation (FS)	**0,67**	0,67	-
Sludge loading rate (kslr)	**0,1**	0,1	-
pH	**7**	7	-
Surface or bubble aeration	**surface**	surface	-
Biodegradation			
Biodegradation method selected	**OECD 301 series, 310, 302 series**		-
Biodegradation constant	**0**		hr-1
Biodegradation constant used (temp. corrected)			hr-1
Temperature for determining biodegradation constant			Kelvin
Biodegradation applies to	**Aqueous phase**		-
Emission scenario			
Temperature environment	**288,15**	288,15	Kelvin
Wind speed	**3**	3	m/s
Number of inhabitants	**10000**	10000	Person
Emission rate chemical	**1**	1	kg/d

Output		
Elimination percentages	**Value**	**Unit**
Elimination in the primary settler		
Volatilization	0,00	%
Via primary sludge	6,75	%
Total	6,75	%
Elimination in the aerator		
Stripping	0,00	%
Biodegradation	0,00	%
Total	0,00	%
Elimination in the solids liquid separator		
Volatilization	0,00	%
Via surplus sludge	3,53	%
Total	3,53	%
Total elimination from waste water	**10,28**	%
Total emission via effluent	**89,72**	%
Balance	**100,00**	%
Concentrations		
Air	4,80E-10	g/m3
Combined sludge	1,19E+02	mg/kg
Primary sludge	1,12E+02	mg/kg
Surplus sludge	1,37E+02	mg/kg
Raw sewage	5,00E-01	mg/l
Dissolved	4,50E-01	mg/l
Associated	5,04E-02	mg/l
Settled sewage	4,66E-01	mg/l
Dissolved	4,50E-01	mg/l
Associated	1,66E-02	mg/l
Mixed liquor	9,97E-01	mg/l
Dissolved	4,48E-01	mg/l
Associated	5,49E-01	mg/l
Effluent	4,49E-01	mg/l
Dissolved	4,48E-01	mg/l
Associated	1,03E-03	mg/l
In solids effluent	1,37E+02	mg/kg

SimpleTreat 4.0 Export file			
Calculation mode:	**SimpleTreat 4.0**		
Version:	**4.0.9**		
Date:	Tuesday, May 14, 2019		

Input			
Substance	**User value**	Default value	Unit
Chemical class	**Neutral**		-
Molecular weight	**102,15**		g/mole
Octanol-water partition coefficient (Kow)	**0,21**		-
Aparent Kow at actual pH (Dow)			-
Vapour pressure	**0,00027**		Pa
Vapour pressure used (temp. corrected)	**1,891359E-04**		Pa
Temperature for determining vapour pressure	**293,15**	293,15	Kelvin
Solubility (S)	**27400**		mg/l
Solubility used (temp. corrected)	**2,551717E+04**		mg/l
Temperature for determining solubility	**293,15**	293,15	Kelvin
pKa			-
Henry coefficient (H)	**0,04**	7,571460E-07	Pam3/mole
Henry coefficient used (temp. corrected - only for user value)	**0,03725135**		Pam3/mole
Temperature for determining Henry coefficient (only for user value)	**293,15**	2,931500E+02	Kelvin
Organic carbon partition coefficient (Koc)		3,556294E-01	l/kg
Partition coefficient in raw sewage (Kps)		1,066888E-01	l/kg
Partition coefficient in activated sludge (Kpas)		1,315829E-01	l/kg
Mode of operation			
Facility type	**Municipal**	Municipal	-
Operation mode	**Primary solids removal**	Primary solids removal	-
Sewage flow (Q)	**0,2**	0,2	m3/d PE
Mass of sewage solids (SO)	**0,09**	0,09	kg/d PE
Mass of O2 binding material in sewage (BOD)	**60**	60	g O2/d PE
Fraction of BOD in sewage solids (FB)	**0,5417**	0,5417	-
Fraction of sewage solids removed by primary sedimentation (FS)	**0,67**	0,67	-
Sludge loading rate (kslr)	**0,1**	0,1	-
pH	**7**	7	-
Surface or bubble aeration	**surface**	surface	-
Biodegradation			
Biodegradation method selected	**OECD 301 series, 310, 302 series**		-
Biodegradation constant	**0**		hr-1
Biodegradation constant used (temp. corrected)			hr-1
Temperature for determining biodegradation constant			Kelvin
Biodegradation applies to	**Aqueous phase**		-
Emission scenario			
Temperature environment	**288,15**	288,15	Kelvin
Wind speed	**3**	3	m/s
Number of inhabitants	**10000**	10000	Person
Emission rate chemical	**1**	1	kg/d

Output		
Elimination percentages	**Value**	**Unit**
Elimination in the primary settler		
Volatilization	0,01	%
Via primary sludge	0,00	%
Total	0,01	%
Elimination in the aerator		
Stripping	0,06	%
Biodegradation	0,00	%
Total	0,06	%
Elimination in the solids liquid separator		
Volatilization	0,03	%
Via surplus sludge	0,00	%
Total	0,03	%
Total elimination from waste water	**0,10**	%
Total emission via effluent	**99,90**	%
Balance	**100,00**	%
Concentrations		
Air	1,65E-08	g/m3
Combined sludge	5,70E-02	mg/kg
Primary sludge	5,33E-02	mg/kg
Surplus sludge	6,57E-02	mg/kg
Raw sewage	5,00E-01	mg/l
Dissolved	5,00E-01	mg/l
Associated	2,40E-05	mg/l
Settled sewage	5,00E-01	mg/l
Dissolved	5,00E-01	mg/l
Associated	7,92E-06	mg/l
Mixed liquor	5,00E-01	mg/l
Dissolved	5,00E-01	mg/l
Associated	2,63E-04	mg/l
Effluent	4,99E-01	mg/l
Dissolved	4,99E-01	mg/l
Associated	4,93E-07	mg/l
In solids effluent	6,57E-02	mg/kg

Nitrobenzene, EC No: 202-716-0, CAS 98-95-3,

SimpleTreat 4.0 Export file			
Calculation mode:	**SimpleTreat 4.0**		
Version:	**4.0.9**		
Date:	Tuesday, May 14, 2019		

Input			
Substance	**User value**	Default value	Unit
Chemical class	**Neutral**		-
Molecular weight	**123,06**		g/mole
Octanol-water partition coefficient (Kow)	**72,4**		-
Aparent Kow at actual pH (Dow)			-
Vapour pressure	**20**		Pa
Vapour pressure used (temp. corrected)	**1,401006E+01**		Pa
Temperature for determining vapour pressure	**293,15**	293,15	Kelvin
Solubility (S)	**1900**		mg/l
Solubility used (temp. corrected)	**1,769439E+03**		mg/l
Temperature for determining solubility	**293,15**	293,15	Kelvin
pKa			-
Henry coefficient (H)	**1,296**	9,743643E-01	Pam3/mole
Henry coefficient used (temp. corrected - only for user value)	**1,206943725**		Pam3/mole
Temperature for determining Henry coefficient (only for user value)	**293,15**	2,931500E+02	Kelvin
Organic carbon partition coefficient (Koc)	**118**	4,040064E+01	l/kg
Partition coefficient in raw sewage (Kps)		3,540000E+01	l/kg
Partition coefficient in activated sludge (Kpas)		4,366000E+01	l/kg
Mode of operation			
Facility type	**Municipal**	Municipal	-
Operation mode	**Primary solids removal**	Primary solids removal	-
Sewage flow (Q)	**0,2**	0,2	m3/d PE
Mass of sewage solids (SO)	**0,09**	0,09	kg/d PE
Mass of O2 binding material in sewage (BOD)	**60**	60	g O2/d PE
Fraction of BOD in sewage solids (FB)	**0,5417**	0,5417	-
Fraction of sewage solids removed by primary sedimentation (FS)	**0,67**	0,67	-
Sludge loading rate (kslr)	**0,1**	0,1	-
pH	**7**	7	-
Surface or bubble aeration	**surface**	surface	-
Biodegradation			
Biodegradation method selected	**OECD 301 series, 310, 302 series**		-
Biodegradation constant	**1**		hr-1
Biodegradation constant used (temp. corrected)			hr-1
Temperature for determining biodegradation constant			Kelvin
Biodegradation applies to	**Aqueous phase**		-
Emission scenario			
Temperature environment	**288,15**	288,15	Kelvin
Wind speed	**3**	3	m/s
Number of inhabitants	**10000**	10000	Person
Emission rate chemical	**1**	1	kg/d

Output		
Elimination percentages	**Value**	**Unit**
Elimination in the primary settler		
Volatilization	0,24	%
Via primary sludge	1,05	%
Total	1,29	%
Elimination in the aerator		
Stripping	0,15	%
Biodegradation	90,62	%
Total	90,77	%
Elimination in the solids liquid separator		
Volatilization	0,07	%
Via surplus sludge	0,04	%
Total	0,12	%
Total elimination from waste water	**92,17**	%
Total emission via effluent	**7,83**	%
Balance	**100,00**	%
Concentrations		
Air	7,72E-08	g/m3
Combined sludge	1,27E+01	mg/kg
Primary sludge	1,74E+01	mg/kg
Surplus sludge	1,73E+00	mg/kg
Raw sewage	5,00E-01	mg/l
Dissolved	4,92E-01	mg/l
Associated	7,83E-03	mg/l
Settled sewage	4,94E-01	mg/l
Dissolved	4,91E-01	mg/l
Associated	2,59E-03	mg/l
Mixed liquor	4,64E-02	mg/l
Dissolved	3,95E-02	mg/l
Associated	6,93E-03	mg/l
Effluent	3,92E-02	mg/l
Dissolved	3,91E-02	mg/l
Associated	1,30E-05	mg/l
In solids effluent	1,73E+00	mg/kg

4,4'-methylenedianiline, EC No: 202-974-4, CAS No: 101-77-9

SimpleTreat 4.0 Export file			
Calculation mode:	**SimpleTreat 4.0**		
Version:	**4.0.9**		
Date:	Thursday, December 12, 2019		

Input			
Substance	**User value**	Default value	Unit
Chemical class	**Neutral**		-
Molecular weight	**198,3**		g/mole
Octanol-water particion coefficient (Kow)	**35,5**		-
Aparent Kow at actual pH (Dow)			-
Vapour pressure	**0,00025**		Pa
Vapour pressure used (temp. corrected)	**1,751258E-04**		Pa
Temperature for determining vapour pressure	**293,15**	293,15	Kelvin
Solubility (S)	**1010**		mg/l
Solubility used (temp. corrected)	**9,405966E+02**		mg/l
Temperature for determining solubility	**293,15**	293,15	Kelvin
pKa			-
Henry coefficient (H)		3,692066E-05	Pam3/mole
Henry coefficient used (temp. corrected - only for user value)			Pam3/mole
Temperature for determining Henry coefficient (only for user value)	**293,15**	2,931500E+02	Kelvin
Organic carbon partition coefficient (Koc)	**7041**	2,268219E+01	l/kg
Partition coefficient in raw sewage (Kps)		2,112300E+03	l/kg
Partition coefficient in activated sludge (Kpas)		2,605170E+03	l/kg
Mode of operation			
Facility type	**Municipal**	Municipal	-
Operation mode	**Primary solids removal**	Primary solids removal	-
Sewage flow (Q)	**0,2**	0,2	m3/d PE
Mass of sewage solids (SO)	**0,09**	0,09	kg/d PE
Mass of O2 binding material in sewage (BOD)	**60**	60	g O2/d PE
Fraction of BOD in sewage solids (FB)	**0,5417**	0,5417	-
Fraction of sewage solids removed by primary sedimentation (FS)	**0,67**	0,67	-
Sludge loading rate (kslr)	**0,1**	0,1	-
pH	**7**	7	-
Surface or bubble aeration	**surface**	surface	-
Biodegradation			
Biodegradation method selected	**OECD 301 series, 310, 302 series**		-
Biodegradation constant	**0**		hr-1
Biodegradation constant used (temp. corrected)			hr-1
Temperature for determining biodegradation constant			Kelvin
Biodegradation applies to	**Aqueous phase**		-
Emission scenario			
Temperature environment	**288,15**	288,15	Kelvin
Wind speed	**3**	3	m/s
Number of inhabitants	**10000**	10000	Person
Emission rate chemical	**1**	1	kg/d

Output		
Elimination percentages	**Value**	**Unit**
Elimination in the primary settler		
Volatilization	0,00	%
Via primary sludge	32,65	%
Total	32,65	%
Elimination in the aerator		
Stripping	0,00	%
Biodegradation	0,00	%
Total	0,00	%
Elimination in the solids liquid separator		
Volatilization	0,00	%
Via surplus sludge	16,63	%
Total	16,63	%
Total elimination from waste water	**49,28**	%
Total emission via effluent	**50,72**	%
Balance	**100,00**	%
Concentrations		
Air	8,16E-12	g/m3
Combined sludge	5,73E+02	mg/kg
Primary sludge	5,41E+02	mg/kg
Surplus sludge	6,48E+02	mg/kg
Raw sewage	5,00E-01	mg/l
Dissolved	2,56E-01	mg/l
Associated	2,44E-01	mg/l
Settled sewage	3,37E-01	mg/l
Dissolved	2,56E-01	mg/l
Associated	8,04E-02	mg/l
Mixed liquor	2,84E+00	mg/l
Dissolved	2,49E-01	mg/l
Associated	2,59E+00	mg/l
Effluent	2,54E-01	mg/l
Dissolved	2,49E-01	mg/l
Associated	4,86E-03	mg/l
In solids effluent	6,48E+02	mg/kg

SimpleTreat 4.0 Export file			
Calculation mode:	**SimpleTreat 4.0**		
Version:	**4.0.9**		
Date:	Wednesday, May 8, 2019		

Input			
Substance	**User value**	Default value	Unit
Chemical class	**Neutral**		-
Molecular weight	**99,13**		g/mole
Octanol-water particion coefficient (Kow)	**0,46**		-
Aparent Kow at actual pH (Dow)			-
Vapour pressure	**0,0032**		Pa
Vapour pressure used (temp. corrected)	**2,241610E-03**		Pa
Temperature for determining vapour pressure	**293,15**	293,15	Kelvin
Solubility (S)	**1000000**		mg/l
Solubility used (temp. corrected)	**9,312837E+05**		mg/l
Temperature for determining solubility	**293,15**	293,15	Kelvin
pKa			-
Henry coefficient (H)	**0,000324**	2,386070E-07	Pam3/mole
Henry coefficient used (temp. corrected - only for user value)	**0,000301736**		Pam3/mole
Temperature for determining Henry coefficient (only for user value)	**293,15**	2,931500E+02	Kelvin
Organic carbon partition coefficient (Koc)		6,711720E-01	l/kg
Partition coefficient in raw sewage (Kps)		2,013516E-01	l/kg
Partition coefficient in activated sludge (Kpas)		2,483336E-01	l/kg
Mode of operation			
Facility type	**Municipal**	Municipal	-
Operation mode	**Primary solids removal**	Primary solids removal	-
Sewage flow (Q)	**0,2**	0,2	m3/d PE
Mass of sewage solids (SO)	**0,09**	0,09	kg/d PE
Mass of O2 binding material in sewage (BOD)	**60**	60	g O2/d PE
Fraction of BOD in sewage solids (FB)	**0,5417**	0,5417	-
Fraction of sewage solids removed by primary sedimentation (FS)	**0,67**	0,67	-
Sludge loading rate (kslr)	**0,1**	0,1	-
pH	**7**	7	-
Surface or bubble aeration	**surface**	surface	-
Biodegradation			
Biodegradation method selected	**OECD 301 series, 310, 302 series**		-
Biodegradation constant	**1**		hr-1
Biodegradation constant used (temp. corrected)			hr-1
Temperature for determining biodegradation constant			Kelvin
Biodegradation applies to	**Aqueous phase**		-
Emission scenario			
Temperature environment	**288,15**	288,15	Kelvin
Wind speed	**3**	3	m/s
Number of inhabitants	**10000**	10000	Person
Emission rate chemical	**1**	1	kg/d

Output		
Elimination percentages	**Value**	**Unit**
Elimination in the primary settler		
Volatilization	0,00	%
Via primary sludge	0,01	%
Total	0,01	%
Elimination in the aerator		
Stripping	0,00	%
Biodegradation	91,97	%
Total	91,97	%
Elimination in the solids liquid separator		
Volatilization	0,00	%
Via surplus sludge	0,00	%
Total	0,00	%
Total elimination from waste water	**91,98**	%
Total emission via effluent	**8,02**	%
Balance	**100,00**	%
Concentrations		
Air	2,04E-11	g/m3
Combined sludge	7,36E-02	mg/kg
Primary sludge	1,01E-01	mg/kg
Surplus sludge	1,00E-02	mg/kg
Raw sewage	5,00E-01	mg/l
Dissolved	5,00E-01	mg/l
Associated	4,53E-05	mg/l
Settled sewage	5,00E-01	mg/l
Dissolved	5,00E-01	mg/l
Associated	1,49E-05	mg/l
Mixed liquor	4,01E-02	mg/l
Dissolved	4,01E-02	mg/l
Associated	4,00E-05	mg/l
Effluent	4,01E-02	mg/l
Dissolved	4,01E-02	mg/l
Associated	7,50E-08	mg/l
In solids effluent	1,00E-02	mg/kg

SimpleTreat 4.0 Export file			
Calculation mode:	**SimpleTreat 4.0**		
Version:	**4.0.9**		
Date:	Tuesday, May 14, 2019		

Input			
Substance	**User value**	Default value	Unit
Chemical class	**Neutral**		-
Molecular weight	**116,08**		g/mole
Octanol-water partition coefficient (Kow)	**7,94**		-
Aparent Kow at actual pH (Dow)			-
Vapour pressure	**0,00000002**		Pa
Vapour pressure used (temp. corrected)	**1,401006E-08**		Pa
Temperature for determining vapour pressure	**293,15**	293,15	Kelvin
Solubility (S)	**33**		mg/l
Solubility used (temp. corrected)	**3,073236E+01**		mg/l
Temperature for determining solubility	**293,15**	293,15	Kelvin
pKa			-
Henry coefficient (H)		5,291777E-08	Pam3/mole
Henry coefficient used (temp. corrected - only for user value)			Pam3/mole
Temperature for determining Henry coefficient (only for user value)	**293,15**	2,931500E+02	Kelvin
Organic carbon partition coefficient (Koc)	**13**	6,743022E+00	l/kg
Partition coefficient in raw sewage (Kps)		3,900000E+00	l/kg
Partition coefficient in activated sludge (Kpas)		4,810000E+00	l/kg
Mode of operation			
Facility type	**Municipal**	Municipal	-
Operation mode	**Primary solids removal**	Primary solids removal	-
Sewage flow (Q)	**0,2**	0,2	m3/d PE
Mass of sewage solids (SO)	**0,09**	0,09	kg/d PE
Mass of O2 binding material in sewage (BOD)	**60**	60	g O2/d PE
Fraction of BOD in sewage solids (FB)	**0,5417**	0,5417	-
Fraction of sewage solids removed by primary sedimentation (FS)	**0,67**	0,67	-
Sludge loading rate (kslr)	**0,1**	0,1	-
pH	**7**	7	-
Surface or bubble aeration	**surface**	surface	-
Biodegradation			
Biodegradation method selected	**OECD 301 series, 310, 302 series**		-
Biodegradation constant	**0**		hr-1
Biodegradation constant used (temp. corrected)			hr-1
Temperature for determining biodegradation constant			Kelvin
Biodegradation applies to	**Aqueous phase**		-
Emission scenario			
Temperature environment	**288,15**	288,15	Kelvin
Wind speed	**3**	3	m/s
Number of inhabitants	**10000**	10000	Person
Emission rate chemical	**1**	1	kg/d

Output		
Elimination percentages	**Value**	**Unit**
Elimination in the primary settler		
Volatilization	0,00	%
Via primary sludge	0,12	%
Total	0,12	%
Elimination in the aerator		
Stripping	0,00	%
Biodegradation	0,00	%
Total	0,00	%
Elimination in the solids liquid separator		
Volatilization	0,00	%
Via surplus sludge	0,06	%
Total	0,06	%
Total elimination from waste water	**0,18**	%
Total emission via effluent	**99,82**	%
Balance	**100,00**	%
Concentrations		
Air	2,34E-14	g/m3
Combined sludge	2,08E+00	mg/kg
Primary sludge	1,95E+00	mg/kg
Surplus sludge	2,40E+00	mg/kg
Raw sewage	5,00E-01	mg/l
Dissolved	4,99E-01	mg/l
Associated	8,76E-04	mg/l
Settled sewage	4,99E-01	mg/l
Dissolved	4,99E-01	mg/l
Associated	2,89E-04	mg/l
Mixed liquor	5,09E-01	mg/l
Dissolved	4,99E-01	mg/l
Associated	9,60E-03	mg/l
Effluent	4,99E-01	mg/l
Dissolved	4,99E-01	mg/l
Associated	1,80E-05	mg/l
In solids effluent	2,40E+00	mg/kg

2-Methyl-1,2-thiazol-3(2H)-one - 5-chloro-2-methyl-1,2-thiazol-3(2H)-one, Polyacrylate,
EC No: 911-418-6, CAS number: 55965-84-9

SimpleTreat 4.0 Export file			
Calculation mode:	**SimpleTreat 4.0**		
Version:	**4.0.9**		
Date:	Monday, May 13, 2019		

Input			
Substance	**User value**	Default value	Unit
Chemical class	**Neutral**		-
Molecular weight	**264,7**		g/mole
Octanol-water partition coefficient (Kow)	**5,6**		-
Aparent Kow at actual pH (Dow)			-
Vapour pressure	**2,2**		Pa
Vapour pressure used (temp. corrected)	**1,541107E+00**		Pa
Temperature for determining vapour pressure	**293,15**	293,15	Kelvin
Solubility (S)	**3000000**		mg/l
Solubility used (temp. corrected)	**2,793851E+06**		mg/l
Temperature for determining solubility	**293,15**	293,15	Kelvin
pKa			-
Henry coefficient (H)	**0,005**	1,460103E-04	Pam3/mole
Henry coefficient used (temp. corrected - only for user value)	**0,004656419**		Pam3/mole
Temperature for determining Henry coefficient (only for user value)	**293,15**	2,931500E+02	Kelvin
Organic carbon partition coefficient (Koc)		5,081972E+00	l/kg
Partition coefficient in raw sewage (Kps)		1,524592E+00	l/kg
Partition coefficient in activated sludge (Kpas)		1,880330E+00	l/kg
Mode of operation			
Facility type	**Municipal**	Municipal	-
Operation mode	**Primary solids removal**	Primary solids removal	-
Sewage flow (Q)	**0,2**	0,2	m3/d PE
Mass of sewage solids (SO)	**0,09**	0,09	kg/d PE
Mass of O2 binding material in sewage (BOD)	**60**	60	g O2/d PE
Fraction of BOD in sewage solids (FB)	**0,5417**	0,5417	-
Fraction of sewage solids removed by primary sedimentation (FS)	**0,67**	0,67	-
Sludge loading rate (kslr)	**0,1**	0,1	-
pH	**7**	7	-
Surface or bubble aeration	**surface**	surface	-
Biodegradation			
Biodegradation method selected	**OECD 301 series, 310, 302 series**		-
Biodegradation constant	**0,1**		hr-1
Biodegradation constant used (temp. corrected)			hr-1
Temperature for determining biodegradation constant			Kelvin
Biodegradation applies to	**Aqueous phase**		-
Emission scenario			
Temperature environment	**288,15**	288,15	Kelvin
Wind speed	**3**	3	m/s
Number of inhabitants	**10000**	10000	Person
Emission rate chemical	**1**	1	kg/d

Output		
Elimination percentages	**Value**	**Unit**
Elimination in the primary settler		
Volatilization	0,00	%
Via primary sludge	0,05	%
Total	0,05	%
Elimination in the aerator		
Stripping	0,00	%
Biodegradation	53,38	%
Total	53,39	%
Elimination in the solids liquid separator		
Volatilization	0,00	%
Via surplus sludge	0,01	%
Total	0,01	%
Total elimination from waste water	**53,45**	%
Total emission via effluent	**46,55**	%
Balance	**100,00**	%
Concentrations		
Air	1,05E-09	g/m3
Combined sludge	6,65E-01	mg/kg
Primary sludge	7,62E-01	mg/kg
Surplus sludge	4,38E-01	mg/kg
Raw sewage	5,00E-01	mg/l
Dissolved	5,00E-01	mg/l
Associated	3,43E-04	mg/l
Settled sewage	5,00E-01	mg/l
Dissolved	5,00E-01	mg/l
Associated	1,13E-04	mg/l
Mixed liquor	2,35E-01	mg/l
Dissolved	2,33E-01	mg/l
Associated	1,75E-03	mg/l
Effluent	2,33E-01	mg/l
Dissolved	2,33E-01	mg/l
Associated	3,28E-06	mg/l
In solids effluent	4,38E-01	mg/kg

Annex II: Annex II: SimpleTreat Modelling – results and input data

Published as separate excel-file: Substances_SimpleTreat effluent and properties.xlsx