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A unified approach to SimpleTreat input and settings for wastewater treatment removal predictions

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Abstract

SimpleTreat has become a common tool used in ecological risk assessments to estimate the removal efficiency of a chemical from a secondary wastewater treatment plant and hence inform on release to the environment. Organization A, Organization B, and Organization C performed a comparative study of SimpleTreat predictions and parameter selection methodologies across the three organizations. SimpleTreat versions 3.1 and 4.1 were run for a set of 10 chemicals using different settings and different approaches to obtain the inputs needed to run the tool. The impacts of these differences on removal predictions for the set of chemicals were explored, and a unified framework was proposed to guide users in the effective use of SimpleTreat.

Keywords: ecological risk assessment, wastewater treatment plant, chemical assessment, in silico modeling, SimpleTreat

Introduction

The goal of this work was to compare different methods of running SimpleTreat v3.1 and 4.1 (Lautz et al., 2017) for a set of 10 chemicals by three independent organizations. Notable differences were observed for some substances when different methods were used for selecting the Henry's Law Constant (H), the biodegradation rate constant, the representation of ionizable chemicals, and the settings for the modeled wastewater treatment plant (WWTP).

Understanding the behavior of a chemical in a WWTP is important in assessing potential impacts on environmental and human health. Removal efficiency from a WWTP is a key parameter in the estimation of the amount of a chemical that will enter the environment.

Since measured pre- and post-treatment concentrations of chemicals in WWTPs are rarely available, removal efficiencies in WWTPs are often predicted. A popular tool for this is SimpleTreat (Struijs, 1996, 2014), a mechanistic model that simulates the removal of chemicals from a secondary WWTP. The model is incorporated in the European substance evaluation tool EUSES (European Chemical Bureau, 2019), the evaluation tool Chesar (CHEmical Safety Assessment and Reporting Tool [CHESAR], 2023) developed by the European Chemicals Agency (ECHA) for chemical safety assessments under the European Union REACH Regulation, and also used within the EAS-E suite by ARC (Arnot Research and Consulting Inc., 2023). The SimpleTreat tool can be operated with refined input on chemical properties such as the measured partition coefficient between water and sewage sludge and the biodegradation rate constant. Since this information is frequently unavailable, SimpleTreat can also be run with basic inputs. In this instance, the model requires the user to provide the chemical's Henry's Law Constant (Pa m^3 mol^{-1} at 25°C), the octanol–water partition coefficient, the acid dissociation constant (pK_a), and the outcome of OECD screening tests for biodegradation (OECD 301, 302, or 310). Using a set of parameters designed to simulate a generic secondary WWTP, SimpleTreat then calculates the removal of the chemical in the primary settler, aerator, and secondary clarifier to produce a final removal prediction (Figure 1).

SimpleTreat requires high-quality chemical property inputs to generate reliable results. Variability in input selection, as well as model execution, may cause discrepancies in outputs across different users (Comber et al., 2019; Kah & Brown, 2011; Zhang et al., 2021). Kah and Brown (2011) performed a sensitivity analysis on the input parameters used in SimpleTreat 3.1 and determined that the model output was most sensitive to sewage flow and degradation rates. A separate study found that the modeling of WWTP outputs using SimpleTreat 4.0 is highly sensitive to predicted carbon–water partition coefficients (K_{oc}; Zhang et al., 2021). Furthermore, there is currently no standardized practice of data selection, WWTP parameter selection, and data reporting. In collaborative meetings between the three organizations involved in this work, it was apparent that different approaches to

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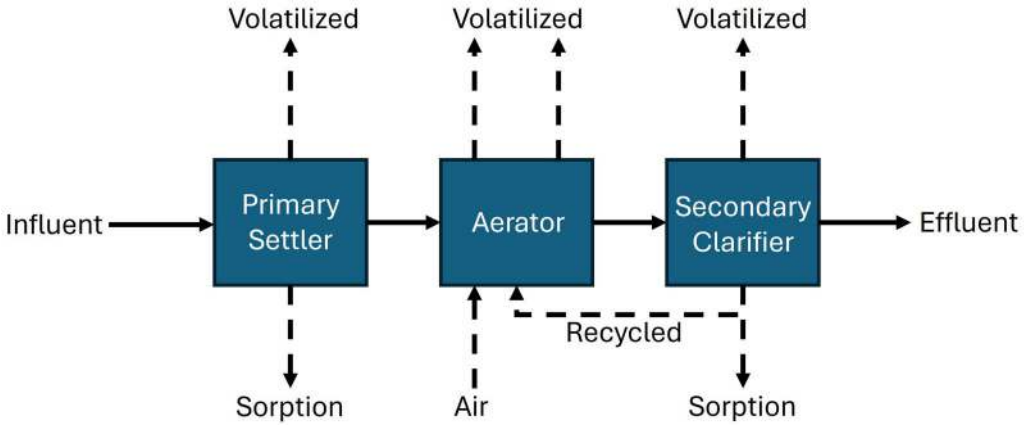


Figure 1. Schematic diagram of a typical activated sludge wastewater treatment plant (WWTP), which includes the primary settler, aerator, and secondary clarifier. The solid black lines denote the flow of the chemical through the WWTP from the influent stream through the three main sections of the WWTP into the effluent stream, while the dashed lines denote the loss of the chemical to volatilization, sorption, and the input of air into the aerator as well as the recycling of activate sludge back into the aeration tank.

running SimpleTreat were being employed, resulting in inconsistent removal efficiency predictions across organizations. Since the removal efficiency may have consequences on risk assessment decisions, the source of these discrepancies and their impacts was investigated.

In this work, different methodologies were used to determine the Henry's Law Constants and octanol–water partition coefficients and to translate the outputs from OECD biodegradation screening tests into biodegradation rate constants. The impact of these differing methodologies, as well as tool parameters such as the aeration method, on the SimpleTreat prediction of removal efficiency was explored and a general unified framework to run SimpleTreat with basic input information was developed.

There are two versions of SimpleTreat: 3.1 (Struijs, 1996) and 4.1 (Struijs, 2014) considered in this work. These versions differ in the handling key wastewater treatment parameters: effluent suspended solids and bioreactor hydraulic retention times. SimpleTreat 4.1 was parameterized to be more representative of wastewater treatment facilities in the European Union (Struijs, 2014). Meanwhile, the values for the hydraulic retention time and suspended solid concentrations in SimpleTreat 3.1 better represent wastewater facilities in Canada (Government of Canada, 2012; Kim et al., 2013). This version is therefore still actively in use in Canada, and the results of the comparative analysis of both versions of SimpleTreat are of interest and included in this study.

In this work, different methodologies were used to determine the Henry's Law Constants and octanol–water partition coefficients, and to translate the outputs from OECD biodegradation screening tests into biodegradation rate constants. The impact of these differing methodologies, as well as tool parameters such as the aeration method, on the SimpleTreat prediction of removal efficiency was explored, and a general unified framework to run SimpleTreat with basic input information was developed.

Methods

Modeled chemicals

To study the difference in SimpleTreat procedures, a test set of 10 chemicals was curated. These chemicals were selected to represent a broad variety of chemical moieties, physicochemical and biodegradation properties, and removal efficiencies predicted using modeled inputs. The Chemical Abstracts Service registry numbers, names, and structures of the 10 chemicals selected for this work are presented in Table 1. The USEPA Estimation Programs Interface (EPI) Suite (USEPA, 2012) was used to estimate chemical properties for first-pass SimpleTreat calculations. The EPI Suite v4.11 predictions and first-pass SimpleTreat calculations for the 10 test chemicals are presented in online supplementary material, Table S1.

SimpleTreat calculations

The SimpleTreat output of interest for this work is the total removal of a chemical from wastewater by the WWTP. The measurable equivalent to this removal value is known as the removal efficiency and is defined as the percent change of the effluent and influent concentrations for a chemical, shown in *Equation* 1, where C is the concentration in the influent and effluent streams.

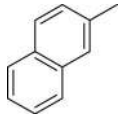
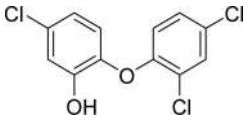
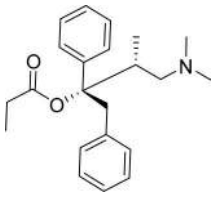
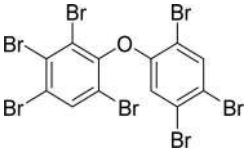
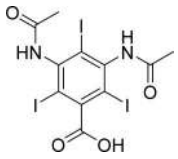
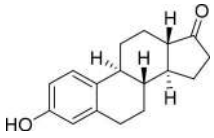
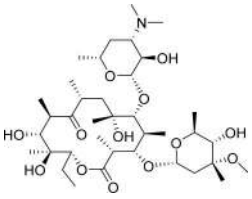
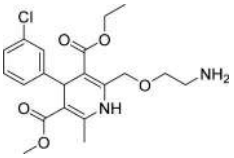
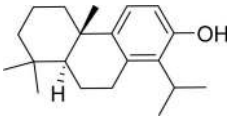
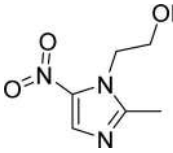
$$\text{Removal efficiency } [\%] = 100\% \frac{C_{\text{influent}} - C_{\text{effluent}}}{C_{\text{influent}}} \quad (1)$$

Data gathering: physicochemical properties

When gathering the physicochemical properties necessary for running SimpleTreat, a search was performed for experimental data available in the literature or accessible in online databases such as the ECHA's Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH) dossiers (European Chemical Agency's [ECHA] Registration, Evaluation, Authorization and Restriction of Chemicals [REACH] Dossiers, 2024).

In the absence of experimental data for a given chemical, QSAR models were used to generate estimates of the necessary values. Different software models were used to calculate pKa: ACD Percepta (Advanced Chemistry Development Inc., 2014) MarvinSketch (ChemAxon Ltd., 2016), and Bio-Loom (BioByte, 2023). The USEPA EPI Suite v4.11 (USEPA, 2012) program was used to generate the Henry's Law Constant (H) and EPI Suite v4.11 or Bio-Loom were used to estimate the octanol–water partition coefficients (K_{ow}). When an experimental value for H was not available, but reliable experimental values for the vapor pressure (VP in Pa) *and* water solubility (WS in g/m^3) could be found under similar conditions (corrected to 293.15 K/20 °C), H was calculated within SimpleTreat using *Equation* 2 (Boethling & Mackay, 2000; Boethling et al., 1995) where MW is the molar mass (g/mol).

Table 1. A list of the CAS registry numbers and common chemical names of the 10 test chemicals used in this work to study SimpleTreat methodologies.

Chemical ID	CAS	Chemical name	Structure
1	**91-57-6**	2-Methylnaphthalene	
2	**3380-34-5**	Triclosan	
3	**469-62-5**	Propoxyphene	
4	**207122-16-5**	2,2′,3,4,4′,5′,6-Heptabromodiphenyl ether	
5	**117-96-4**	Diatrizoate	
6	**53-16-7**	Estrone (E1)	
7	**114-07-8**	Erythromycin-H_2O	
8	**88150-42-9**	Amlodipine	
9	**511-15-9**	Totarol	
10	**443-48-1**	Metronidazole	

Note. Each numerical chemical ID is included to aid in referencing the chemicals in the text.

$$\text{Henry's Law Constant } [\text{Pa m}^3\text{mol}^{-1}] = \frac{VP \times MW}{WS} \quad (2)$$

For substances suspected of being nonvolatile (e.g., H < 0.1 Pa m^3 mol^{-1}), the H was set to 10^{-6} Pa m^3 mol^{-1} as an alternative to this calculation. Since the substances in question were nonvolatile, this difference yielded no significant impact on the predicted removal efficiency.

Data gathering: biodegradation

The biodegradation rate constant (k, in $hours^{-1}$) was determined differently under three scenarios. In Scenario 1, it was assumed that all 10 chemicals were persistent and did not biodegrade in the WWTP. In Scenario 2, experimental results based on the OECD 301 (OECD, 1992a), 302 (OECD, 1981, 1992b, 2009), or 310 (OECD, 2014) test guidelines were used, which include: not biodegradable, readily biodegradable, or inherently biodegradable. The presets of SimpleTreat, based on REACH guidance (Guidance on Information Requirements and Chemical Safety Assessment Chapter R.16: Environmental Exposure Estimation. Version 3.0, 2016) along with the corresponding rate constants as shown in Table 2 were used. In the absence of experimental results for a chemical, the "*not biodegradable*" option was conservatively used.

In Scenario 3, the predicted biodegradation half-life of the substance in activated sludge was used. When experimental biodegradation data were available, Table 3 was used to determine the half-life in activated sludge following the guidelines proposed by the U.S. Environmental Protection Agency (USEPA, 2023). When no biodegradation data were available, the BIOWIN program in EPI Suite v4.11 (USEPA, 2012) was used to predict the approximate rates of biodegradation in activated sludge, followed by the method outlined in Table 4 to select a corresponding half-life. Once the half-life had been determined, the rate constant in activated sludge was calculated assuming first-order kinetics (*Equation 3*), where k is the biodegradation rate constant and $t_{1/2,a}$ is the half-life in activated sludge.

$$k = \frac{\ln(2)}{t_{1/2,a}} \quad (3)$$

Data gathering: sorption

The outcome of SimpleTreat simulations can also be influenced by sorption of the chemical onto suspended solids in the WWTP. SimpleTreat allows for entry of an organic carbon–water partition coefficient (K_{oc}), but if this parameter is not available, it can be calculated from K_{ow} using built in QSARs (Struijs, 2014), which include models for mono-protic acids and bases. SimpleTreat calculates a nonnormalized solid–water equilibrium partition coefficient (K_p) in raw sewage and activated sludge from K_{oc}, but K_p values can be entered manually if available. Since both the sewage and sludge matrices show different sorption characteristics as compared to soil, entry of experimentally determined sorption parameters in activated sludge and/or sewage, when available, is expected to improve removal efficiency estimates when available. Scientific literature can be used as a source for some groups of substances (e.g., pharmaceuticals; Andersen et al., 2005; Berthod et al., 2016; Carballa et al., 2008; Hyland et al., 2012).

Tool parameters: aeration methods

To simulate the WWTP, two aeration methods were used: (1) surface aeration (the default settings in SimpleTreat v4.1) and (2) bubble aeration. The different methods can have a drastic impact on the predicted removal efficiency of volatile chemicals, so the most appropriate type of aeration needs to be selected to ensure predictions are relevant.

Three scenarios for input values and settings

To illustrate the impact in selecting different SimpleTreat input values and settings, the three scenarios presented in Table 5 were run. Although the scenarios presented in Table 5 represent the parameterization methodology used in this work, it should be noted that the approaches to running SimpleTreat are not limited to these three scenarios.

Results and discussion

Comparative study

To compare the methodologies for the different scenarios, 10 organic chemicals were selected to cover a range of removal efficiencies, properties, and chemical types. The chemicals selected for this test are presented along with the predicted SimpleTreat v4.1 removal efficiency values calculated for the three scenarios in Table 6. The full details of these calculations, along with the input parameters used, can be found in online supplementary material, Table S2.

The results from this comparative study show noticeable differences in the removal efficiency predictions across scenarios. For example, the test substance with chemical ID **1** (Chemical Abstracts Service 91-57-6, 2-methylnaphthalene) shows poor agreement in all three scenarios. The results from running SimpleTreat v3.1 were consistent with those shown in Table 6, in terms of differences observed in the removal efficiency predictions across scenarios and are presented in online supplementary material, Table S3.

Differences in biodegradation rate constant

Scenario 1 assumes no biodegradation, providing a worst-case scenario for the removal efficiency. The methods used in Scenarios 2 and 3 for determining the biodegradation rate constant, although similar, are not identical and may lead to variations in the SimpleTreat results. The values of half-life in activated sludge with the corresponding rate constant are

Table 2. Classification table provided by SimpleTreat used to determine the degradation rate constant based on OECD 301 (OECD, 1992a), 302 (OECD, 1981, 1992b, 2009), or 310 (OECD, 2014) test guidelines.

OECD guideline	Result	Half-life in activated sludge (hours)	Rate constant (k) ($hours^{-1}$)
301, 310	Readily biodegradable	0.69	1
301, 310	Readily biodegradable, failing 10-day window	0.23	0.3
302	Inherently biodegradable, fulfilling specific criteria	0.069	0.1
302	Inherently biodegradable, not fulfilling specific criteria	–	0
302	Not biodegradable	–	0

Table 3. Results from OECD 301 (OECD, 1992a) or 302B (OECD, 1992b) biodegradation tests used to estimate the biodegradation half-life in activated sludge.

OECD 301 Ready biodegradability	OECD 302B Inherent biodegradability	Half-life in activated sludge (hours)	Rate constant (k) ($hours^{-1}$)
Pass (≥ 70% or 60%)		1	0.69
≥ 40% but not pass		3	0.23
20%-40%	≥ 70%	10	0.069
	20%–70%	30	0.023
≤ 20%	≤ 20%	10,000	6.9×10^{-5}

Table 4. Results from BIOWIN program in EPI Suite v4.11 (USEPA, 2012) used to estimate the biodegradation half-life in activated sludge.

BIOWIN 3 Numerical value	BIOWIN3 Timeframe	BIOWIN5 Numerical value	Half-life in activated sludge (hours)	Rate constant (k) ($hours^{-1}$)
2.75–5	≤ Weeks	>0.5	1	0.69
2.75–5	≤ Weeks	<0.5	3	0.23
0–2.75	> Weeks	>0.5	10	0.069
2.25–2.75	Weeks to months	<0.5	30	0.023
1.75–2.25	Months	<0.5	100	6.9×10^{-3}
0–1.75	Recalcitrant	<0.5	10,000	6.9×10^{-5}

Table 5. The three scenarios explored in this study demonstrating the different approaches to running SimpleTreat.

Scenario	pKa	K_{ow}/H	Biodeg	Aeration method
1	Literature	QSAR predictions	No degradation	Surface aeration
2	Bio-Loom MarvinSketch	Exp. data when available if not QSAR prediction	Exp. data when available using SimpleTreat preset rate constant, if not no degradation assumed	Surface aeration
3	ACD Percepta	Exp. data when available if not QSAR prediction	Exp. data when available using EPA guideline to calculate rate constant, if not degradation predicted using BIOWIN	Bubble aeration

Table 6. Comparison of the removal efficiency values calculated using SimpleTreat v4.1 using the three scenarios described in Table 5.

Chemical ID	Scenario 1 removal efficiency (%)	Scenario 2 removal efficiency (%)	Scenario 3 removal efficiency (%)
1	96	58	81
2	55	86	65
3	29	21	46
4	97	98	98
5	0	1	8
6	4	36	47
7	5	5	21
8	2	17	25
9	97	93	89
10	0	64	27

presented in Tables 2–4. The difference these methods have on the rate constant can be demonstrated when considering a chemical that underwent an OECD 302 biodegradation (OECD, 1981, 2009) test, which produced the result "inherently biodegradable." In this example, Scenario 3 would assign a value of 10 hr for the biodegradation half-life based on Table 3 (which, from *Equation* 3, corresponds to a rate constant of $0.07\,hr^{-1}$), while Scenario 2 would assign a rate constant of $0.1\,hr^{-1}$ based on Table 2 (which has a corresponding half-life of 6.9 hr). Since the default hydraulic retention times used in SimpleTreat are 6.9 hr and 11.5 hr for versions 3.1 and 4.1, respectively, the difference in such biodegradation half-lives (6.9 and 10 hr) is likely to have an impact on the removal efficiency. For further details on the impacts of the biodegradation rate constant on the removal efficiency covering a wide range of adsorption coefficient and H values, see online supplementary material, Figure S2.

Scenario 3 aims to calculate the removal efficiency by filling experimental data gaps via in silico modeling, whereas Scenarios 1 and 2 take a more conservative approach and will reliably yield lower removal predictions compared to Scenario 3. All three approaches have merit and should be well documented and justified when reporting SimpleTreat removal efficiency results.

Unified methodology: hierarchy of data

Based on this exercise, a general unified approach to data gathering and running of SimpleTreat is proposed. This approach is based on the premise that better SimpleTreat predictions can be achieved by more accurate determinations for three removal-governing parameters (H, equilibrium sorption coefficient, and biodegradation rate constant). For selecting the most appropriate value for the needed inputs, the following hierarchy of data sources is recommended to guide users:

1. Experimental data of high quality, with the test report;
2. Experimental data found in literature or a REACH dossier;
3. Experimental data of a valid structural analogue;
4. Modeled data.

Although this hierarchy appears self-evident, it is important to consider the source of each input and assess the reliability of

the data prior to running any SimpleTreat calculations. This step is likely to have the largest impact on the predicted removal efficiencies for a chemical. While this does not prescribe which models to use when experimental data are not available, each user should select and document their modeling approach.

Unified methodology: acidic, basic, and neutral chemicals

The ionic/acid dissociation state of a chemical is also likely to have an impact on the WWTP removal efficiency and is therefore an important consideration when running SimpleTreat calculations (see online supplementary material, Figure S3). SimpleTreat relies on the user providing a pKa for monoprotic acids and bases to determine the degree of ionization via the Henderson–Hasselbalch equation. If experimental pKa values are not available for a substance, the user should consult their standard method of predicting pKa values. If acidic or basic functional groups are identified by the user in the chemical, the setting "Acid" or "Base" chemical class should be selected in the SimpleTreat options, accordingly. If a chemical is determined to be predominantly neutral around the pH in SimpleTreat (default pH = 7), this step may not be necessary. Importantly, SimpleTreat is not equipped to handle molecules containing multiple acidic protons or basic functional groups, and therefore may not provide accurate estimates for the sorption contribution to an estimated removal efficiency.

Unified methodology: Henry's Law Constant

There are several ways to source the H for SimpleTreat calculations. When experimentally derived H are available, these should take priority. In the absence of quality H studies and when high-quality experimental VP and WS values are available, the H should be calculated using *Equation 2*, applying appropriate corrections for temperature when needed. It is therefore recommended that when experimental H values are not available for a substance, the user should consult their organization's standard method of predicting H.

Unified methodology: partition coefficients

The partition coefficients K_{ow} and K_{oc} will impact the removal efficiency of a chemical by determining the amount of sorption onto the solids within the WWTP. The differences in methods used in the selection K_{ow}/K_{oc} across scenarios, however, did not appear to have a significant impact on the predicted removal efficiency. Chemical **5** had the greatest variation across the three scenarios, which resulted in a difference of 7% total removal when comparing calculations run with Log K_{ow} of 0.76 (Scenario 2) and 3.3 (Scenario 3). It is therefore recommended that when experimental partition coefficient values are not available for a substance, the user should consult their organization's standard method of predicting K_{ow} or K_{oc}. For further details on the sensitivity of SimpleTreat predictions to the partition coefficients, see online supplementary material, Figure S2.

Additional consideration: aeration settings

The difference in aeration settings used across scenarios only influences the predicted removal efficiency for volatile chemicals. The impact of the chosen aeration settings on a volatile chemical was explored using Chemical **1** and with the results shown in Figure 2. Using the Log K_{ow} and biodegradation settings curated in Scenario 2 for **1**, the total removal was calculated using SimpleTreat v4.1 for a range of H values. This allowed for the comparison between the two aeration methods over a wide range of possible volatilities. The results of the comparison in Figure 2 demonstrate the impact of volatility on total removal, with the bubble aeration yielding more conservative estimates for the range of H from ~4 to ~2,000 Pa m^3 mol^{-1}. Interestingly, this behavior is reversed when the H of the chemical exceeds ~2,000 Pa m^3 mol^{-1}, with the surface aeration acting as the more conservative estimate. Although these results are specific to a chemical with a Log K_{ow} and biodegradation rate constants comparable to **1**, the impacts of the aeration settings are only dependent on a chemical's volatility potential and is therefore applicable to all volatile substances. An analysis performed using SimpleTreat v3.1 yielded similar results, shown in online supplementary material, Figure S1. Similarly, a sensitivity analysis of the remaining inputs performed in SimpleTreat v3.1 for neutral substances is presented in online supplementary material, Figure S2. These results reinforce the need for users to carefully consider the settings selected when running SimpleTreat to ensure the results are applicable to the WWTPs common in their jurisdictions.

Unified approach: summary

The unified approach proposed in this article suggests that SimpleTreat users consider the following when simulating the removal of a chemical in a WWTP:

1. Data source and quality: The user should search for the highest quality input data, following the proposed hierarchy.
2. Ionic/dissociation state of chemical: When potentially acidic or basic functional groups are present, it is recommended to run SimpleTreat with the appropriate chemical class selected.
3. Henry's Law Constant: Use experimental H when available. When experimental H is not available, but high-quality experimental vapor pressure *and* water solubility are available, calculate H using *Equation 2*. Otherwise, use a modeled value for H.
4. K_{ow} and K_{oc}: When high-quality experimental partition coefficient values are not available for a substance, the user should consult their organization's standard method of predicting K_{ow} or K_{oc}.
5. Biodegradation rate constant: The approach to determining the biodegradation rate constant depends on the goals of the user. In Scenario 3, the user attempts to refine the calculated removal efficiency using in silico modeling to address absent data. Conversely, Scenario 2 favored a conservative approach to be used as a "worst-case scenario." Both approaches have merit and should be well documented and justified when reporting SimpleTreat removal efficiency results.
6. Aeration settings: Use the aeration setting (bubble vs. surface) most appropriate to the WWTPs of interest. Aeration setting only impacts volatile chemicals.

This proposed approach aims to unify the use of SimpleTreat to produce consistent predictions across jurisdictions. Despite this proposed approach, it is likely that variation across jurisdictions will persist due to differences in WWTP configurations and the availability of quality data. The most important recommendation for the use of SimpleTreat is therefore proper documentation and reporting of the data sources and inputs. This will increase confidence and reproducibility of SimpleTreat removal predictions.

Future developments

The observed sensitivity to user-specific decisions and input parameters discussed herein demonstrates the need for a consistent methodology for running SimpleTreat with some flexibility when modeling local WWTPs. When reporting results, the input

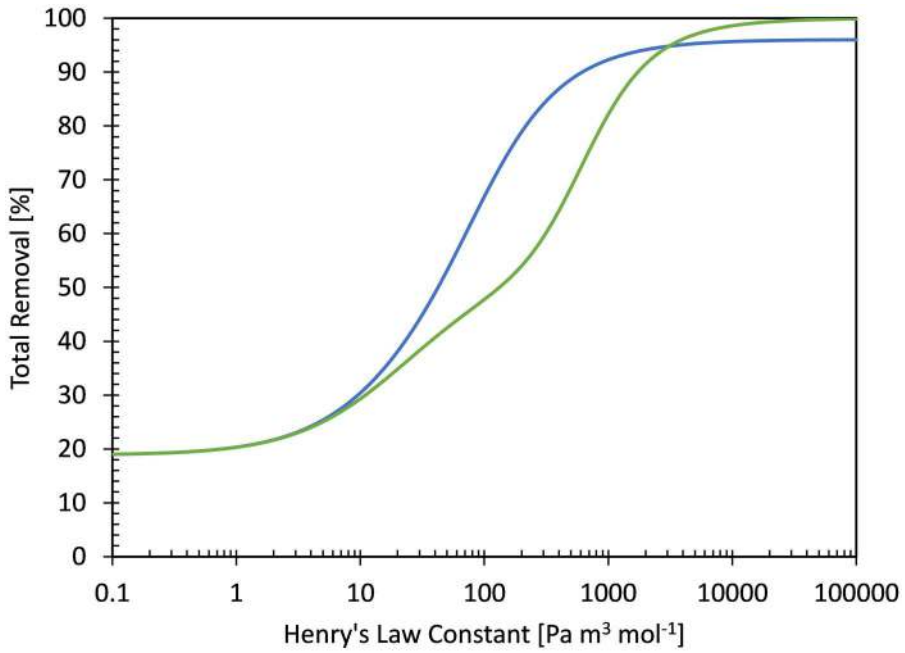


Figure 2. Removal efficiency for CAS 91-57-6 (**1**) as a function of H using the surface aerator (blue line) and the bubble aerator (green line). For this figure, the removal efficiencies were calculated using SimpleTreat v4.1 and the phys-chem and biodegradation properties used in Scenario 2.

values, biodegradation rate constant methodology, and aeration settings used should be reported to allow for an understanding of the calculated removal efficiencies and how they were obtained.

Organization A is involved with several projects aimed at improving predictions of WWTP removal efficiencies. These projects include ongoing attempts to improve in silico biodegradation modeling techniques to better predict the biodegradation rate constants in WWTPs and the development of an AI model to predict removal rates for a generalized WWTP. This AI model is designed to solely use chemical structure and does not need physicochemical or biodegradation inputs, as molecular descriptors are themselves correlated with those properties. This may be particularly valuable when dealing with chemicals where important property information is not available and where specific operating conditions of WWTPs of interest are not known.

Conclusion

A comparative study on the use of SimpleTreat across three different organizations was performed on 10 chemicals for different scenarios illustrating the impact of different inputs, such as the biodegradation rate constant, Henry's Law Constant, and plant aeration settings. Based on the results, a framework for a unified approach to running SimpleTreat was developed and presented. This recommended framework is meant to guide users and is not meant to be a rigid set of rules for running SimpleTreat. Instead, this work emphasizes the importance of documenting and reporting the inputs and settings used whenever SimpleTreat is used to support chemical risk assessments.

Supplementary material

Supplementary material is available online at *Integrated Environmental Assessment and Management*.

Data availability

Supplemental details and data are available in the Supporting Information.

Author contributions

Thomas D. Burns (Conceptualization, Data curation, Formal analysis, Investigation, Methodology, Software, Validation, Visualization, Writing—original draft, Writing—review & editing), Michael Beking (Conceptualization, Methodology, Writing—review & editing), Jesse Shen (Conceptualization, Methodology, Writing—review & editing), Joop de Knecht (Conceptualization, Data curation, Investigation, Methodology, Validation, Writing—review & editing), Joost Bakker (Conceptualization, Data curation, Investigation, Methodology, Validation, Writing—review & editing), Peter van Vlaardingen (Conceptualization, Data curation, Investigation, Methodology, Validation, Writing—review & editing), Johannes Tolls (Conceptualization, Data curation, Investigation, Methodology, Validation, Writing—review & editing), and Todd Gouin (Conceptualization, Data curation, Investigation, Methodology, Validation, Visualization, Writing—review & editing)

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Conflicts of interest

The authors declare no conflicts of interest.

Disclaimer

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