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Simulating behavior of petroleum compounds during refinery effluent treatment using the SimpleTreat model

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HIGHLIGHTS

- Dissolved air flotation (DAF) was included in multimedia model SimpleTreat.
- Predicted removal with DAF was on average 17% larger than removal with primary sedimentation.
- More removal via air was predicted with DAF due to injected gas bubbles.
- The improved model supports reliable risk assessment of petroleum products.

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ABSTRACT

Distribution and elimination of petroleum products can be predicted in aerobic wastewater treatment plants (WWTPs) using models such as multimedia fate model SimpleTreat. An advantage of the SimpleTreat model is that it only requires a few basic properties of a chemical in wastewater to calculate partitioning, biodegradation and ultimately emissions to air, surface water and produced sludge. The SimpleTreat model structure reflects a WWTP scheme. However, refinery WWTPs typically incorporate more advanced treatment processes such as dissolved air flotation (DAF), a process that clarifies wastewaters by the removal of suspended matter such as oil or solids. The objective of this work was to develop a WWTP removal model that includes DAF treatment. To understand how including a DAF in the model affects the predicted concentrations of petroleum constituents in effluent, we replaced the primary sedimentation module in SimpleTreat with a module simulating DAF. Subsequently, we compared results from the WWTP-DAF model with results obtained with the original SimpleTreat model for a library of over 1500 representative hydrocarbon constituents. The increased air-water exchange in a WWTP-DAF unit resulted in higher predicted removal of volatile constituents. Predicted removal with DAF was on average 17% larger than removal with primary sedimentation. We compared modelled results with measured removal data from the literature, which supported that this model refinement continues to improve the technical basis of assessment of petroleum products.

1. Introduction

Contamination of the aquatic environment can occur via many routes such as sewage disposal, run-off from agricultural land, atmospheric fallout and waste management activities, including discharge of effluents associated with oil refining (Wake, 2005). The composition of refinery wastewater varies greatly depending on wastewater treatment plant configuration, operation procedures and type of oil being processed (Saien and Nejati, 2007). Thus, refinery effluents contain many different chemicals at different concentrations (Wake, 2005). The removal of hydrocarbon compounds by refinery wastewater treatment plants (WWTPs) is an important part of the refining process and various technologies are used to

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achieve acceptable effluent quality. The physical-chemical properties of these compounds vary widely and as a result, the substances will behave differently upon release to the environment (van de Meent et al., 2010). In recognition of the hydrophobic nature and content of petroleum compounds, more advanced treatment processes have been implemented in refinery WWTPs compared to e.g. municipal WWTPs. Some technologies are based on separation processes such as flotation and membrane separation (Yu et al., 2017), while others are based on hydrocarbon degradation by biological (Scholz and Fuchs, 2000) or chemical (Ma and Wang, 2006; Santos et al., 2006) processes. A typical refinery WWTP consists of an oil-water-solid gravity separation system and a gas flotation system to remove insoluble substances, and a biological treatment system plus a clarification system to remove soluble substances (Barthe et al., 2015).

An example of such a separation process is dissolved air flotation (DAF), which is a technique to remove suspended matter (i.e. suspended solids, oils, grease and metals) from the aqueous phase by bringing the particles to the surface for removal by skimming (Al-Shamrani et al., 2002). Flotation units such as a DAF do not rely on gravity forces to separate the oil droplets. Instead, large quantities of small-diameter gas bubbles are injected into the water stream. Oil droplets and suspended particles attach to the bubbles, causing them to rise to the water surface and form a froth layer; i.e. a foam layer consisting of oily droplets and gas bubbles. This oily sludge (froth) can then be skimmed off, resulting in oil removal percentages of >90% (Bennett and Shammas, 2010). Advantages of DAF compared to sedimentation, which is generally used in WWTPs, are compact designs, short retention times and ability to cope with high hydraulic loads (Crossley and Valade, 2006; Haarhoff, 2008; Rybachuk and Jodlowski, 2019). Disadvantages, however, are the relatively complex plant needed, and operating costs associated with water recirculation (Rybachuk and Jodlowski, 2019).

Several tools are available to model the behavior of chemicals during wastewater treatment. Activated sludge models (ASM) are generally regarded as the state of the art for modelling WWTP (Henze et al., 2000). Alternatives are generalized fate models such as those described by Byrns (2001). WATER9 (USEPA, 2001) and TOXCHEM (ENVIROMEGA, 2003) are the most widely applied empirical mass balance models for the estimation of odorous emissions, and consider the characteristics of effluent and gaseous phases. By contrast, SimpleTreat is a 'first–principles' model, requiring only a few basic properties of a chemical to simulate its fate in a standard activated sludge facility for treatment of municipal wastewater (Struijs, 1996). SimpleTreat 4.0 (Struijs, 2014) is currently prescribed by the European Commission to simulate the fate processes in a municipal WWTP in chemical safety assessment under the EU Registration, Evaluation, Authorization and Restriction of Chemicals Directive (EU-REACH) (ECHA, 2019). SimpleTreat is also used in PETRORISK, a tool that applies the hydrocarbon block method (HBM) to allow for an appropriate environmental exposure and risk assessment of petroleum substances (Redman et al., 2014). The HBM allows for the extrapolation of petroleum substance compositional information (such as 2-dimensional gas chromatography data) to hypothetical concentrations of up to more than 1500 representative petroleum constituents (King et al., 1996). Each representative constituent is subsequently subjected to an exposure and risk assessment according to REACH technical guidance, and finally the obtained constituent risk quotients are summed up to represent the risks related to the entire petroleum substance.

The latest SimpleTreat, version 4.0 (Struijs, 2014), and I-SimpleTreat, which simulates behavior of chemicals in industrial WWTPs (Struijs et al., 2016) allow for a wider choice of input options to define wastewater properties to simulate the fate of chemicals in industrial wastewater. Also, the formulation of the partitioning of chemicals between environmental compartments is improved compared to SimpleTreat 3.1, and some fixed and default parameters were revised.

However, despite the use of advanced treatment processes in refinery WWTPs, SimpleTreat does not include an oil-separation step in the treatment process. Therefore, the objective of this study was to develop a multimedia fate model including realistic simulation of DAF treatment. For this, we replaced the primary sedimentation module with a DAF unit in the I-SimpleTreat model. Subsequently, we compared the obtained WWTP fate modelling for 1518 representative hydrocarbon constituents obtained from Redman et al. (2014), subdivided over several hydrocarbon blocks (HCBs), with results obtained with the I-SimpleTreat model with primary sedimentation. We illustrated the performance of the upgraded SimpleTreat by calculating WWTP fate results for these representative structures. Finally, we compared modelled removal efficiencies of 14 hydrocarbon constituents with measured removal efficiencies in actual refinery WWTPs.

2. Materials and methods

2.1. SimpleTreat model

For our study, we built on I-SimpleTreat, which simulates a primary sedimentation tank, an aeration tank and a solids liquid separation (Struijs et al., 2016). I-SimpleTreat is a steady state non-equilibrium model. Chemical elimination through biodegradation and chemical concentrations are determined in four distinct phases that leave the WWTP, i.e. air, water, primary sludge, and surplus sludge. From these outputs, the release of pollutants into the environment is derived (Struijs, 2014).

I-SimpleTreat determines the fraction (unit-less) of a chemical volatized during sewage treatment (f_{air}), the fraction of a chemical discharged with effluent (f_{water}), the fractions transferred to primary sludge ($f_{primarysludge}$) and surplus sludge ($f_{surplussludge}$), and the fraction degraded during sewage treatment (f_{degr}). Input parameters for chemicals are equilibrium partition coefficients between two adjacent media at each treatment step and first order degradation rate constants inside each medium. The modelling approach assumes that partitioning processes are independent of concentration and that there is no interaction between the constituents.

2.2. Inclusion of DAF

We modelled simulation of the DAF process in I-SimpleTreat, made operational as a replacement for the primary sedimentation process (Fig. 1). The primary treatment step of wastewater of the oil industry involving a primary bulk oil water separator unit (e.g. an American Petroleum Institute (API) or Corrugated Plate Interceptor (CPI) unit) was not considered in this study. All default DAF process settings used are shown in Table 1 and are averages based on Concawe survey data and earlier versions of SimpleTreat. Concawe is the scientific division of the European Refining Association representing petrochemical companies in the EU. They obtain survey data via those petrochemical companies and experts on refinery. Concawe survey data can be found in the Supporting Information (Tabel A2). Temperature was based on previous work and communication with experts (Struijs et al., 2016). As illustrated in Fig. 1b, the raw wastewater flow enters the tank at the inlet panel. A minor part of the water flow (in this study a fraction of 0.3) is recycled. This water is pressurized (5.5 bar) before released into the DAF tank. The pressurized water enters the DAF unit from the bottom of the tank where initially tiny bubbles evolve. The small bubbles manipulate particles and oily droplets upwards to the

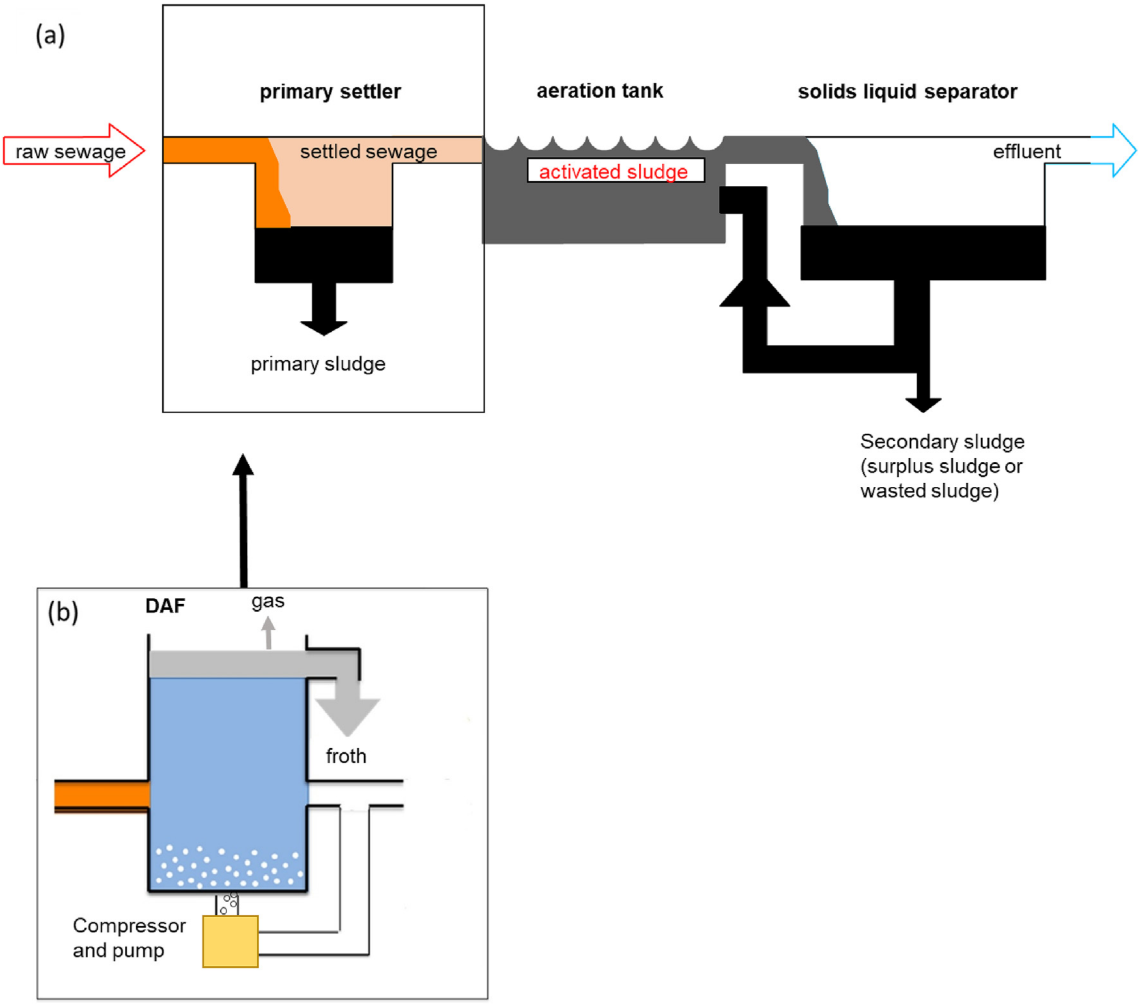

Fig. 1. Scheme of a refinery effluent WWTP with (a) a primary settler and (b) primary settler replaced by a DAF unit (with raw refinery effluent (orange), effluent water of DAF unit (white), water, suspended solids and gas (blue), and froth (grey) adapted from Struijs (2014). (For interpretation of the references to colour in this figure legend, the reader is referred to the Web version of this article.)

Table 1
Default input parameters for the DAF unit in SimpleTreat based on Concawe survey data (Table A2) and earlier versions of SimpleTreat.

Input parameter of a DAF unit	Units	Default
Fraction high pressure water flow	–	0.3
Hydraulic retention time	hr	1
Pressure side stream	bar	5.5
Fraction removal Froth	–	0.9
Density of the non-aqueous phase liquids in raw sewage	kg m^{-3}	850
Temperature	°C	15

surface of the tank forming a blanket (froth) which is removed by a skimmer. Treated water by the DAF unit flows out of the tank into the aeration tank minus 30% which is recycled back - under pressure - into the DAF unit. 90% of the froth was considered to be removed by DAF as default value, based on Concawe survey data and the papers of Galil and Wolf (2001) and Dlangamandla et al. (2018). The default value of hydraulic retention time (HRT) of DAF was considered 1 h on average. Removal efficiencies by DAF (RE_{solids} and $RE_{volatilization}$) were obtained according to Eq. (1) and Eq. (2) and Table 2:

$$RE_{solids} = \frac{C_{solids} * fraction\ removal\ solids\ by\ DAF * V_s}{E * \frac{HRT}{24}}. \tag{1}$$

$$RE_{volatilization} = \frac{C_g * V_g}{E * \frac{HRT}{24}}. \tag{2}$$

with:

RE_{solids} = Removal efficiency through solids
$RE_{volatilization}$ = Removal efficiency through volatilization
HRT = Hydraulic retention time (hr)
C_{solids} = Concentration of chemical in solids (kg m^{-3})
C_g = Concentration of chemical in gas (air) (kg m^{-3})
V_g = Volume of gas (m^3)
V_s = Volume of solids (m^3)
E = Emission rate of the chemical (kg d^{-1})

2.3. Petroleum compounds library

A dataset with over 1500 unique hydrocarbon structures and associated estimated physical-chemical properties was extracted from PETRORISK v7.04, downloaded from https://www.concawe.

Table 2
Derived variable for aqueous, non-aqueous and gaseous phases in equilibrium in DAF unit. Parameters are explained in Table A3.

Derived parameter of a DAF unit	Symbol	Units	Equation
Concentration of chemical in water	C_w	kg m^{-3}	$\frac{\text{Emission rate of chemical}}{24}*\frac{HRT}{K_p*V_s*\text{density of solids}+V_w+K_w*V_g}$
Concentration of chemical in solids	C_s	kg m^{-3}	$C_w*K_p*\text{density of solids}$
Concentration of chemical in gas	C_g	kg m^{-3}	C_w*K_w
Volume of water	V_w	m^3	$\frac{HRT}{24}*\text{Sewage flow}$
Volume of solids	V_s	m^3	$\frac{HRT*\text{Sewage flow}}{24}*\frac{[\text{solids in wastewater}]}{\text{Density of solids}}$
Volume of gas	V_g	m^3	$(\text{pressure side stream}-1)*\left(\frac{[N_2]}{MW\ N_2}+\frac{[O_2]}{MW\ O_2}\right)*\frac{\text{Molar volume of gas}*\text{fraction of high pressure water}*\text{sewage flow}}{24/HRT}$
Mass of chemical in water	M_w	kg	C_w*V_w
Mass of chemical in solids	M_s	kg	C_s*V_s
Mass of chemical in gas	M_g	kg	C_g*V_g

eu/reach/petrorisk/(Redman et al., 2014). The fraction removal in WWTP was calculated with our model for each of the library structures. Library structures were binned according to their carbon number (C#), making a distinction between aromatics (AR) and aliphatics (AL) to increase readability (Table A1). Most oil products lay between C_8 and C_{30}.

To understand the chemical distribution under steady state conditions, a chemical space plot was created, following Gouin et al. (2000). Chemical partitioning between environmental media (air, water, and solids) was described using a fugacity model based on air-water partition coefficients (K_{AW}) and solids-water partition coefficients (K_{SW}). By using this method, the removal mechanism of a chemical can be predicted.

2.4. Scenario analyses

To determine the impact of the variety in WWTP conditions on chemical removal, results were determined for different temperature and HRT settings. Removal fractions were calculated for the default temperature of 15 °C and for 35 °C, as a maximum known to occur in some refineries (Struijs et al., 2016). Furthermore, the HRT of the DAF unit was varied from 0.5 to 1 and 1.5 h.

2.5. Comparison with measurements

To determine the impact of the inclusion of a DAF unit in SimpleTreat, the output of I-SimpleTreat with primary sedimentation (without DAF) was compared with I-SimpleTreat with DAF (but primary sedimentation switched off). The SimpleTreat default values fraction high pressure water flow, hydraulic retention time, pressure side stream and fraction removal froth were adapted based on Concawe survey data (see Table 1). A dataset of petroleum compounds from measurements of influent and effluent concentrations of refinery WWTPs' DAF units as well as final WWTP effluents ($n = 5$) was compiled by Concawe (Table A7 and A8). Samples for these measurements were taken in 2015 and 2016, using the Concawe sampling protocol developed for a previous Concawe project, the effluent speciation project (Concawe, 2010). Samples were single spot samples taken during stable running conditions. Therefore, the results cannot illustrate any variations in the influent concentration nor the effluent concentration, which both could vary in time. Nevertheless, a snapshot of refinery WWTP DAF operation is obtained. From the samples, the dissolved fraction of PAHs was analyzed by Biochemical Institute for Environmental Carcinogens (BIU; Grosshansdorf, Germany) for the presence of the EU 32 priority PAHs (Lerda, 2011), according to the BIU's protocols based upon Grimmer et al. (1997). In addition, benzene, toluene, ethylbenzene, and xylenes (BTEX) analyses were based on NEN-EN-ISO 15680. Information about limit of detection can be found in the supporting information (Table A9).

In this comparison, the predicted volatilization during DAF was included in the removal fraction by DAF, as this resembles the measurements where only the concentration before and after DAF is known. Data below the detection limit or with negative removal efficiencies were excluded. Data showing negative removals were found for constituents with measurements near the detection limit and are assumed measurement errors and not representative of actual removal potential by DAF. This resulted in removal efficiencies for 14 compounds measured in up to four WWTPs that were compared with our modelled data.

3. Results

3.1. Inclusion of DAF

Estimated removal of petroleum by DAF was on average 17% larger than via primary sludge (Fig. 2; Table A4). According to the results, the fraction of removal differed between aliphatics and aromatics. This variation can also be seen throughout the different carbon numbers. Elimination through sludge withdrawal and volatilization were the most important processes for the aliphatic compounds (Fig. 2a). Degradation was less important for the removal of aliphatic compounds (20%), particularly for carbon numbers above 10. For the aromatic compounds, the fraction removal by degradation was dominant for compounds with carbon numbers below 11 (Fig. 2b). With increasing carbon number, elimination through sludge removal increased for the aromatics. The fraction removal via surplus sludge was overall less than 50% and less than 10% was discharged with effluent.

Fig. 3 illustrates the environmental space occupied by the library substances when there is an equilibrium. The lines in Fig. 3 corresponding to one-third in each compartment converge at the point where solids-water partition coefficient (log K_{sw}) is 2.3 and air-water partition coefficient (log K_{aw}) is −0.7 and V_w, $K_{aw}V_a$ and $K_{sw}V_s$ are equal (Gouin et al., 2000). Based on their partitioning coefficients, the aliphatics prefer the air and solids compartment, whereas aromatics prefer mostly the solids compartment. This means that aromatics are mainly predicted to be removed by froth of DAF and aliphatics will be predicted to be removed by froth of DAF and are released towards air in the DAF compartment.

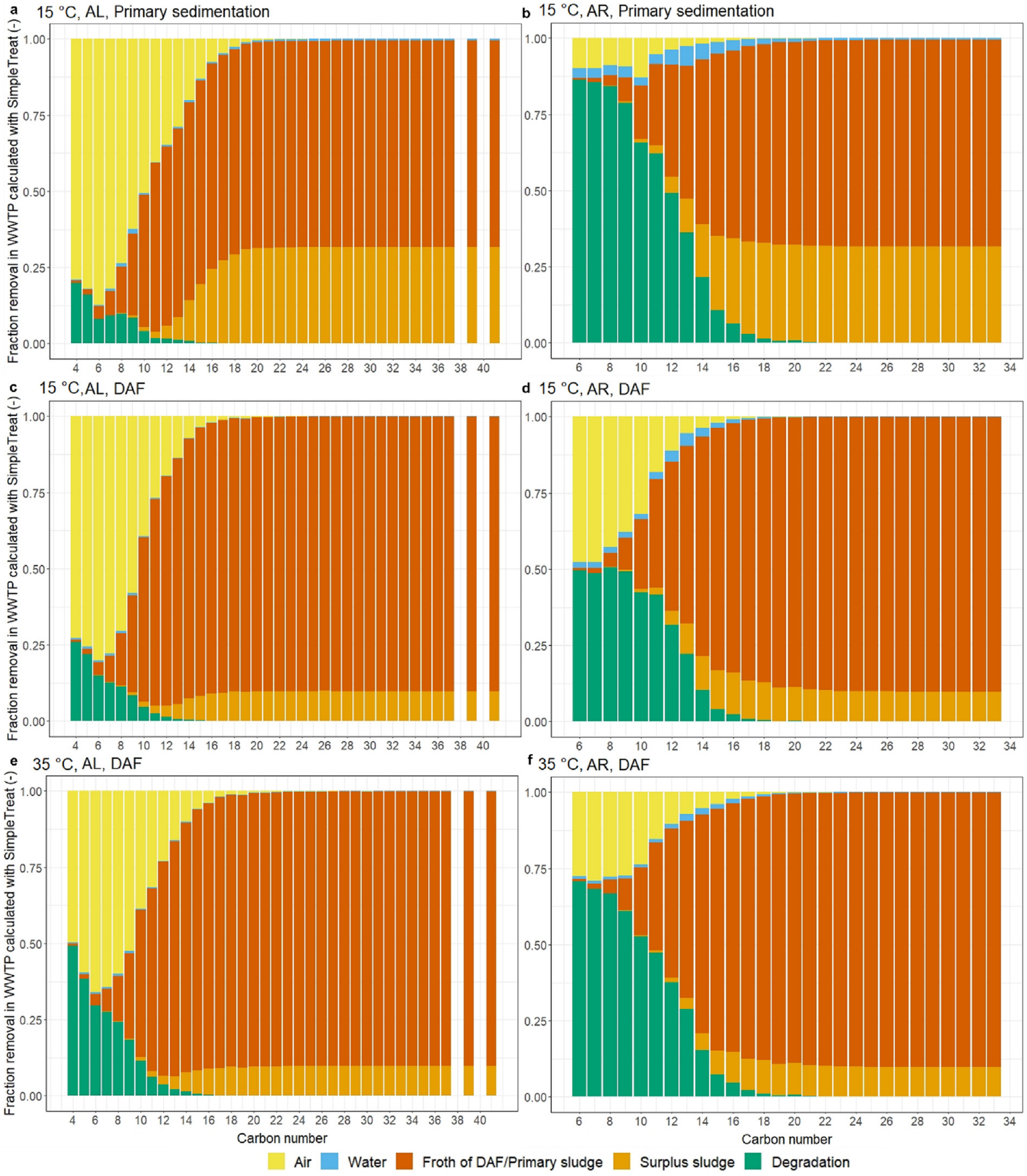

Fig. 2. Fraction removal of petroleum compounds when calculated with SimpleTreat with primary sedimentation (a, b), DAF at 15 °C (c, d) and DAF at 35 °C (e, f) for aliphatics (AL) (a, c, e) and aromatics (AR) (b, d, f).

3.2. *Scenario analyses*

In the first scenario, predicted removal fractions were calculated with the model including DAF at 35 °C instead of 15 °C (Fig. 2c–f; Table A5). Predicted removal by froth of DAF was up to 8% larger for the aliphatic compounds at 15 °C compared to 35 °C (Fig. 2c and e). For the aromatic compounds, the predicted removal fractions of froth of DAF did not differ between the two different temperatures. Predicted removal fractions of surplus sludge of the aromatic compounds were up to 6.3% smaller when calculated at 35 °C when compared to 15 °C (Fig. 2d and f). The aliphatic compounds demonstrated a difference of removal fraction of surplus sludge up to 1%. Overall, degradation increased with increasing temperature up to a relative difference of 23%, whereas emission towards air decreased with increasing temperature up to a relative difference of 23% (Fig. 2c and e). The observed differences in the predicted fate patterns can be explained by the fact that the SimpleTreat model employs temperature dependent volatilization and biodegradation (e.g., Arrhenius-like behavior).

In a second scenario, the model was simulated with two

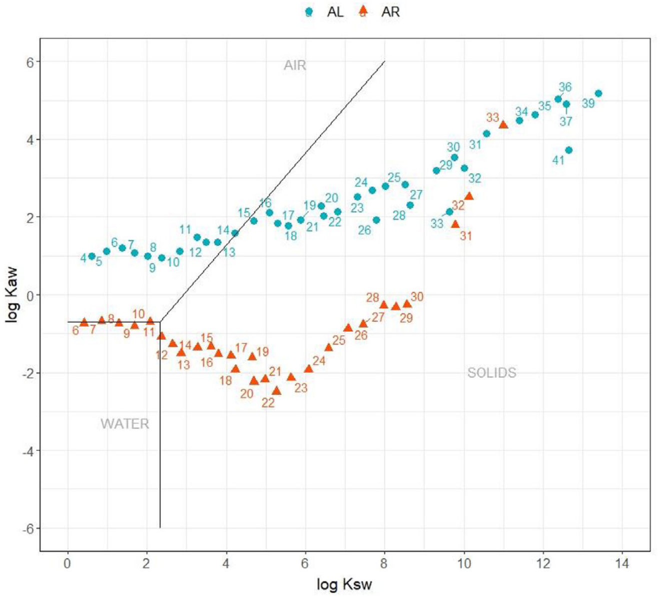

Fig. 3. Chemical space plot of air-water partition (log K_{aw}) and solids-water partition (log K_{sw}) showing the distribution of the chemicals from the Concawe library based on carbon numbers where a distinction was made between aliphatics (in blue) and aromatics (in red). This plot is based on the method of Gouin et al. (2000). The region to the upper left, where more than 99% is in air, shows that fate is controlled by the half-life of a chemical in air. Similarly, the region to the lower left, where more than 99% is in water, shows that fate is controlled by the half-life in water; the region to the lower right, where more than 99% is in solids, shows that fate is controlled by the half-life in solids. The lines corresponding to one-third in each compartment converge at the single point where log K_{sw} is 2.3 and log K_{aw} is −0.6. (For interpretation of the references to colour in this figure legend, the reader is referred to the Web version of this article.)

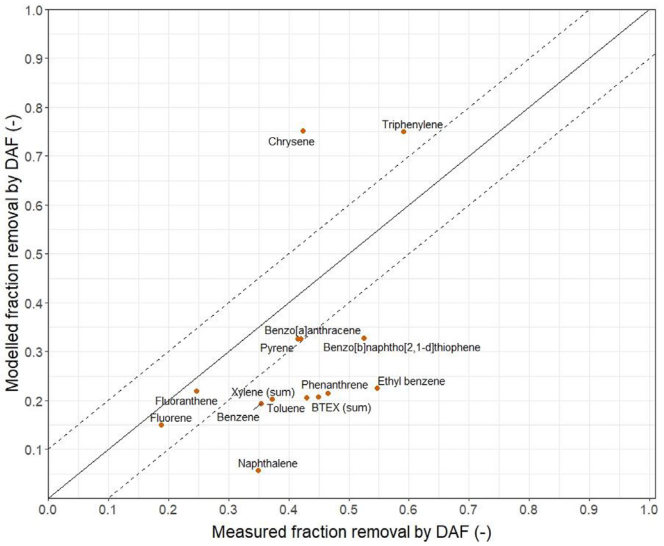

Fig. 4. Modelled versus measured average fraction of removal of a chemical via DAF. The solid 1:1 line indicates perfect model fit. The dashed lines represent a fraction of 0.1 under- and overestimation by SimpleTreat.

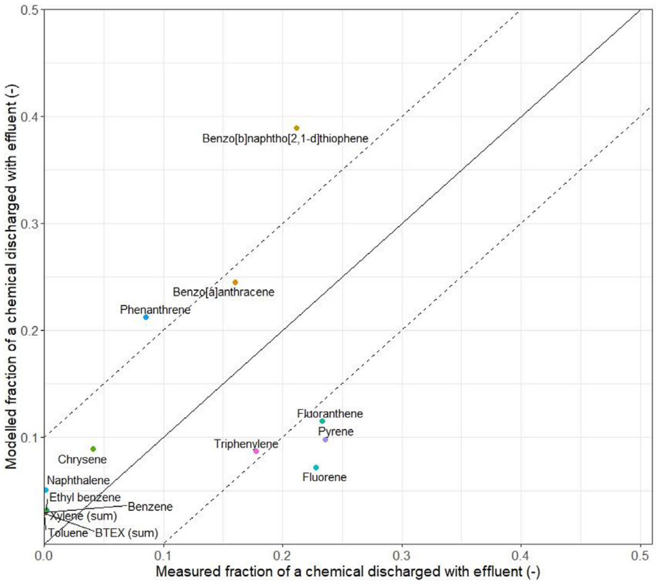

Fig. 5. Modelled versus measured fraction of a chemical in the final effluent. The solid 1:1 line indicates perfect model fit. The dashed lines represent a fraction of 0.1 under- and overestimation by SimpleTreat.

different HRTs of DAF. Emission to air of the aliphatic compounds decreased with up to 8% increasing HRT from 0.5 to 1.5 h (see Table A6). The predicted removal fractions of froth increased up to 7% and degradation increased up to 5% with increasing HRT of 0.5–1.5 h. Predicted removal fractions of surplus sludge and water of the aliphatic compounds did not differ. Overall, the removal fractions of the different treatments of aromatic compounds did not differ between different HRTs.

3.3. Comparison with WWTP measurements

Measured dissolved concentration in four different WWTPs with DAF were retrieved for 14 petroleum compounds. Overall, modelled fractions of total compound removal by DAF were lower than measured, except for chrysene and triphenylene (Fig. 4). Model estimates differed by less than a factor 10 from the measured data for 4 petroleum compounds. Fig. 5 shows modelled versus measured fraction of chemical in the final WWTP effluent. Model estimates for the fraction in the final effluent were within a factor 10 of the measured fractions in the final effluent for 9 petroleum compounds.

4. Discussions and conclusions

4.1. Reliability of the adapted model

We have developed, implemented and tested a DAF module for the wastewater treatment simulation model SimpleTreat, to replace the currently used primary settler module. Settling and flotation are essentially similar in the general model framework in that for both processes a non-aqueous phase (e.g. solids and oil) is separated from an aqueous phase. Predicted overall removal by DAF was slightly (~17%) more effective than removal by means of primary settling, mainly due to a greater extent of volatilization, predicted in the DAF system. Significant transport to air has been reported in several studies (Al-Muzaini et al., 1994; Hamoda, 2006), and is explained by escape of gas bubbles from the froth layer, which is described mechanistically in the new SimpleTreat DAF module. The DAF model used in this study assumes complete thermodynamic equilibrium between the rising gas bubbles and the water phase. This is different from the SimpleTreat primary settling module, where hindered; steady-state transport across the air-water interface is modelled, which explains the greater predicted removal of aromatics by DAF.

Through this steady-state transport route, chemicals are released into the atmosphere upon dissolved air flotation. Increased removal of lighter aromatics from DAF to air partly comes at the expense of less degradation in the aerobic treatment system. The difference between DAF-operated waste treatment systems and settler-operated systems thus seems to be that with DAF, more (aromatic) petroleum chemicals are emitted to air, whereas with primary settling, more are mineralized to CO_2 and H_2O, according to the model.

For the SimpleTreat model with DAF, default values for parameters were obtained from Concawe survey data. By default, the DAF model uses a constant fraction for removal of the froth layer, while instead this may depend on the wastewater, operation parameters such as flow rate, HRT and SRT and the shape of the tanks (Aslam, 2013).

Although the removal efficiency of the froth layer in the DAF unit was set at a default of 90% (Table 1), most of the compounds were not removed for 90% by the DAF according to the model results. The amount of chemicals that will go to the froth layer depends on their hydrophobicy and carbon number. A DAF unit tends to be more efficient for more hydrophobic and larger compounds (Gochin and Solari, 1983; Schneider et al., 1995). According to Schneider et al. (1995), the DAF process removes compounds more rapidly than a primary sedimentation, if the substance is sufficiently hydrophobic and air-solid ratio adequate.

According to the model predictions, removal fractions via froth of DAF decreased with increasing temperature for the aliphatic compounds. No difference was found for the aromatic compounds. However, Edzwald (1995) stated that flotation is improved at 20 °C in comparison with 4 °C. At cold-water temperatures, the displacement or thinning of water is hindered by the hydrophilic effect of the bonded water. For particle-bubble attachment to occur, water must be displaced between the particle and the bubble as they approach (Edzwald, 1995). Since the DAF model assumes instantaneous equilibrium between gas phase and water, simulated results are not dependent on the HRT of the water.

The model showed that with a higher temperature the emission fraction towards air decreased (Fig. 2). In the aeration tank volatilization competes with biodegradation. If, due rising temperatures, the increase of biodegradation is greater than the increase of volatilization, less of the chemical will be available for volatilization with increasing temperature because more rapid biodegradation does not allow the chemical to volatilize. This explains why the contribution of volatilization the overall removal from DAF and aeration tank decreased with increasing temperature.

4.2. Comparison with measurements

The comparison of the removal in the full WWTP (DAF + secondary treatment) with measurement data on removal illustrated that the prediction of the fraction of the final effluent was more in line with these measurements than the prediction of the fraction of removal by DAF alone. In SimpleTreat, the emission to air is separated from the removal of froth from the DAF. The data used for the comparison only included aqueous concentrations before and after DAF and therefore chemicals attached to suspended matter are assumed to be removed, which could cause the underestimation of prediction of the removal via DAF. Furthermore, some petroleum products included in the dataset of Concawe (Table A7) showed negative removal rates. This could be due to measurement uncertainty or it could reflect that the effluent entering the treatment system varies in concentration over time, so if different locations are measured at different times you see variation in concentrations. Alternatively, another explanation could be found in sampling protocols, because the measurements were done by different people or because of spot sampling. To minimize uncertainty, the sampling periods should be related to the HRT or residence time of distribution (Majewsky et al., 2011). Therefore, 24-h composite samples, which are commonly used, may be insufficient to determine removal of petroleum products in WWTPs (Ort, 2010). To confirm this, additional data are needed for further comparison.

Although limited measurement data were available, SimpleTreat with DAF predictions are within a factor of 10 of the measured fractions in the final effluent. The factor 10 is in agreement with known variations in emissions resulting from different emission scenarios and spatio-temporal scales (van de Meent et al., 2010) and the sensitivity of input parameters that are driving uncertainty (Bonin, 2012).

A thorough literature survey did not reveal any papers that describe removal efficiencies of individual oil compounds in WWTPs. Most papers focus on COD, BOD and oil removal, without providing details on oil type and individual compounds that this oil contained. We therefore recommend that future surveys focus more on the collection of data on individual (oil) compounds to enable validation of models like SimpleTreat. Such validation exercises should preferably include a comparison of ranges of measured removal fractions for different oil compounds with modelled ranges based on variability and uncertainty in model parameters.

4.3. Practical implications

A DAF unit is a compact and faster alternative for settlement tanks. According to the predictions in this study, air emissions are higher in a WWTP equipped with a DAF unit than in a WWTP with a primary sedimentation tank. Emissions to air are followed by rapid degradation by photochemical processes, which mitigate exposures as well. However, a detailed evaluation of these processes is beyond the scope of this paper. Further implementation of the model by implementing a primary separator (e.g. an API or CPI unit) is recommended, as this is often used in refinery WWTPs (Hu et al., 2013).

With our work, we showed the possibility to adapt SimpleTreat to generate predictions for a different WWTP system. The model appears conservative, but generally consistent with available measured data. Further refinement would be possible with focused monitoring datasets.

Credit author statement

N.W. Thunnissen: data collection, data treatment, modelling, writing. D. van de Meent: data collection, data treatment, modelling, writing/editing, reviewing. J. Struijs: data collection, data treatment, modelling, writing/editing, reviewing. M. Hjort: data collection, data treatment, writing/editing, reviewing. A.D. Redman: data collection, data treatment, writing/editing, reviewing. M.G.D. Smit: writing/editing, reviewing, A.J. Hendriks: conceptualisation, writing/editing, reviewing. R. van Zelm: conceptualisation, writing/editing, reviewing.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.chemosphere.2020.128081.

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