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2018:00133 - Unrestricted

Report

EXT4-T3-D1

Biodegradation of Naturally Occurring Substances in Produced Water

Revision of data for the DREAM model

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2018-02-26

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REPORT NO.	PROJECT NO.	VERSION	DATE
2018:00133	302003686-3	1.0	2018-02-26

KEYWORDS:
Produced Water
Primary Biodegradation
Ultimate Biodegradation
Biotransformation
Biomineralization
DREAM Model
Q10

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CLIENT'S REF.
Cecilie F. Nygaard

NUMBER OF PAGES/APPENDICES:
26 + Appendices

CLASSIFICATION	CLASSIFICATION THIS PAGE	ISBN
Unrestricted	Unrestricted	978-82-14-06645-6

ABSTRACT

A literature review was conducted to obtain more reliable primary (biotransformation) and ultimate (biomineralization) biodegradation rates for compounds in produced water for the DREAM model, than the current biodegradation data. During the literature review, it became apparent that many compounds lacked quality ultimate biodegradation rates, which is preferred in the model. Therefore, ultimate biodegradation rates for these compounds were estimated based on their primary biodegradation rates and a FACTOR. These data and calculations are described in the report below. Calculated ultimate biodegradation rates are compared to rates found in the literature. This report also includes two separate Excel spreadsheets that summarize the primary and ultimate biodegradation data obtained during the literature review and their corresponding experimental details. A Q10 approach was applied to calculated ultimate biodegradation rates to display rates at three relevant temperatures (5, 13, and 20°C). The ultimate biodegradation rates included in this report will substantially improve the DREAM model, but the majority of these rates are extrapolated estimates. Additional biodegradation tests are recommended to correlate these calculations with laboratory experiments.

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Document History

VERSION	DATE	VERSION DESCRIPTION
Version 1.0	2018-01-30	Draft version for comments

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APPENDICES

1 List of Tables

2 Introduction

Produced water (PW) from offshore oil and gas production is a mixture of formation water and re-injected water produced alongside oil and gas. The composition of PW can be complex and varies significantly between different oil fields and throughout the lifetime of the well (Rye and Ditlevesen, 2014; Røe Utvik, 1999; Neff et al., 2011). Before discharge, free oil and larger oil droplets are separated from the waste stream by oil/water separation processes. This process lowers the average concentration of dispersed and dissolved oil to a level permitted by the appropriate regulating authority. In 2015, the average oil concentration in PW released from activities on the Norwegian Continental Shelf (NCS) was 12.3 mg/ L (NOROG, 2016), compared to the discharge limit of 30 mg/L set by the OSPAR Convention for the Protection of the Marine Environment of the North-East Atlantic (OSPAR, 2001). Once discharged, PW rapidly mixes with natural seawater and undergoes biodegradation, reducing the levels of organic components, thereby also reducing potential exposure levels (Neff et al., 2011; Bakke et al., 2013). Natural biodegradation is therefore a very important process for the reduction of the potential effects of PW compounds in the seawater column. The oil fraction of PW is often referred to as "naturally occurring substances" (OSPAR, 2014), and consists of dispersed oil containing aromatic compounds of environmental concern (particularly polycyclic aromatic hydrocarbons (PAHs) and alkylated phenols (APs)), and metals. To understand the effect of these compounds on the environment, predicted no-effect concentrations (PNECs) were established for compounds in PW (OSPAR, 2014).

Natural biodegradation is an attenuation process in which organic compounds are subject to oxidation processes. For hydrocarbons (HCs) with moderate or low water-solubility, this results in increased polarity of the compounds, and subsequently increased water-solubility. Bioaccumulation is associated with water-solubility by the octanol-water partition coefficient (logPow), and biodegradation of HCs with low water solubilities therefore results in reduced logPow. The relation between acute toxicity (LC_{50}) and logPow has also been established, with reduced logPow resulting in lower acute toxicity reduced acute toxicity (French-McCay, 2002). Biodegradation may therefore result in reduced acute toxicity during the biodegradation period, and this has also been shown in laboratory studies (Brakstad et al., submitted).

Biodegradation is the only process except combustion that completely mineralizes organic compounds to carbon dioxide and water. Degradation can be separated between *primary* and *ultimate biodegradation* (OECD, 2006). Primary biodegradation is measured by specific analyses and may also be equivalent to biotransformation, which describes the first biochemical bond-breakage during the biodegradation process. Ultimate biodegradation refers to the final biomineralization of the tested substance(s) and is commonly measured with respiration analyses (oxygen consumption and CO_2-evolution); however, it can also be measured with non-specific analyses of total organic material.

During the period between primary and ultimate biodegradation a cascade of reactions occurs, resulting often in the generation of numerous oxidized products, but they all eventually lead to mineralization (conversion of organic matter to CO_2). A typical partial degradation pathway is shown in Appendix 1 for 2-methylnaphthalene with a strain of *Pseudomonas putida* (Mahajan et al., 1994), resulting in the 4-hydroxymethyl catechol. The catechol product may subsequently be subject to ring-fission (Seo et al., 2009).

3 Objectives of the Study

The objectives of the current study were to:

- Review recent database and literature data on naturally occurring compounds in PW, with emphasis on the comparison of ultimate and primary biodegradation data. Data was collected in a comprehensive manor, describing experimental conditions, rates and half-lives and citations.
- Determine quantitative relationships between primary and ultimate biodegradation where possible. Since more data exist on primary than ultimate biodegradation, an extrapolation factor may aid in the estimation of ultimate biodegradation when experimental data are inadequate or are lacking.
- Determine Q10-rates from experimental data, if possible. This is of importance since experimental data may be generated at different temperatures.

4 Produced Water Composition

PW is the largest wastewater stream in the oil exploration and production process. Between 2003 and 2014, annual discharges of PW have varied between 130 and 160 million standard m^3, while injected PW have been around 20 % of the total PW (NOROG, 2017). The composition of PW varies considerably between different fields, but consists in general of dispersed oil, inorganic salts, heavy metals, organic compounds and natural radioactive substances. In addition, PW contains large concentrations of dissolved gases and small organic acids (Neff et al., 2011). Gases like methane may be biogenically generated in formation waters from oil and gas fields (Gray et al., 2009). Small organic acids <C6 (formic to pentanoic acids) may be present in concentrations of up to 1000 mg/L (Røe Utvik, 1999). These acids do not represent any environmental risk in the environment and will be rapidly biodegraded after discharge.

Naturally occurring substances associated with environmental impacts include aromatic oil compounds and heavy metals. The aromatic compounds include mono- and polyaromatic HCs (BTEX, naphthalenes, 3- to 6-ring PAH and alkylphenols). However, non-aromatic HCs associated with the dispersed oil may also be of environmental significance, especially since some of these may be associated with chronic effects (Scarlett et al., 2007). Six years ago, the average levels of natural compounds in produced water were averaged from 11 different fields on the Norwegian Continental Shelf. These averages are provided in Table 1. Neff et al. (2011) also reported BTEX concentrations measured from four platforms in the US Gulf of Mexico and from three offshore production facilities in Indonesia, these concentrations ranged from 0.96-5.33 mg/L and 0.33-3.64 mg/L, respectively. In a more recent study, we analysed PW from a North Sea oil reservoir in the NCS and compared the compound concentrations to their PNEC values, as shown in Table 2 (Lofthus et al., *submitted*).

A typical feature in most PWs is the high content of C1-C3 alkylphenols, as observed from the data in Table 1 and Table 2. In Table 2, we have also reported whether the substances are categorized as PBT (persistent, bioaccumulating and toxic) and/or vPvB (very persistent and very bioaccumulating). The criteria for these designations are defined by the European Chemical Agency (ECHA) and described in the Technical Guidance Document (TGD, 2003). These criteria are described in Appendix 2. Contrary to crude oil, alkylphenol concentrations are usually higher than naphthalene and PAH concentrations in PW (Neff et al., 2011). Therefore, considerable attention has therefore been on the potential environmental impacts of these compounds (Bakke et al., 2013; Beyer et al., 2012; Meier et al., 2011; Tollefsen et al., 2007).

In addition to naturally occurring substances, PW also contains production chemicals, including scale inhibitors, anti-foam agents, emulsion breakers, corrosion inhibitors, biocides and H2S-scavengers (NOROG, 2003). These are subject to a number of standardized environmental tests before approved for use in the North Sea oil and gas industry. These tests include three or four acute toxicity tests to marine organisms (different trophic levels), one ultimate marine biodegradation test (biochemical oxygen demand; BOD), and a bioaccumulation test describing the partition between octanol and water (HOCNF, 2013).

Table 1. Average levels of natural compounds in produced water and associated PNEC's from 11 fields on the Norwegian Continental Shelf (NCS), 2012. Data was provided by Statoil and is also located in Rye & Ditlevsen (2014).

Component Group	Concentration in Release (mg/L)	PNEC (ug/L)
Dispersed oil	17.9153	40.4
BTEX	15.8695	17
Napthalenes	1.4194	2.1
PAH 2-3 ring	0.1691	0.15
PAH 4-ring +	0.0022	0.05
Phenols C0-C3	7.3408	10
Phenols C4-C5	0.1053	0.36
Phenols C6+	0.0009	0.04
Zinc (Zn)	0.0145	0.46
Copper (Cu)	0.0010	0.02
Nickel (Ni)	0.0036	1.22
Cadmium (Cd)	0.0001	0.028
Lead (Pb)	0.0021	0.182
Mercury (Hg)	0.0004	0.008

Table 2. Concentrations of naturally occurring substances in a North Sea PW recently analysed (Lofthus et al., *submitted*), and compared to reported PNEC values (OSPAR, 2014). The experimental conditions of Lofthus et al. (submitted) are provided in Table 6.

Component	**Effluent conc. (µg/L)**	**PNEC (µg/L)**	**PBT[A] substances?**
THC	24 400	70.5	No
BTEX			
Benzene	na	8	No
Toluene	na	7.4	No
Ethylbenzene	na	10	No
Naphthalenes			
Naphthalenes and alkyl homologues	357	2	No
2- to 3-ring PAH			
Acenaphthene	0.95	0.38	No
Acenaphtylene	0.11	0.13	No
Fluorene	9.46	0.25	No
Anthracene and dibenzothiophenes	26.7	0.1	PBT and vPvB
Phenanthrene and alkyl homologues	53.0	1.3	vPvB
4-ring PAH			
Fluoranthene	0.11	0.0063	PBT and vPvB
Pyrene	0.63	0.023	PBT and vPvB
Benz(a)anthracene	0.076	0.0012	PBT and vPvB
Chrysene	0.53	0.007	PBT and vPvB
5- to 6-ring PAH			
Dibenzo(a,h)anthracene	0.010	0.00014	No
Benzo(a)pyrene (and benzo(g,h,i)perylene, benzo(b)fluoranthene, benzo(k)fluoranthene and indeno(1,2,3-cd)pyrene)	0.112	0.00017	PBT and vPvB (benzo(a)pyrene, benzo(g,h,i)perylene, benzo(k)fluoranthene)
Alkylphenols			
Phenol and C1- to C3-alkylphenols	1106	7.7	No
Butylphenol and other C4-alkylphenols	13.0	0.64	No
Pentylphenol and other C5-alkylphenols	0.16	0.2	No
Octylphenols and C6- to C8-alkylphenols	0.423	0.01	No
Nonylphenol and other C9-alkylphenols	0.041	0.3	No

[A] PBT, persistent, bioaccumulating and toxic; vPvB, very persistent and very bioaccumulative (OSPAR, 2014; TGD, 2003). These criteria are described in Appendix 2.

5 Current Biodegradation Data in the DREAM Model

In 2003, biodegradation rates for naturally occurring substances in PW were established as input into the DREAM model for substances which were defined to be included in the environmental impact factor (EIF) (NOROG, 2003). The biodegradation data used in EIF calculations were based on ultimate biodegradation and reported as half-lives and first-order rate constants. Different produced water compound groups were selected to represent naturally occurring components in PW. Since limited biodegradation data were available, one substance was selected from each group (defined with similar chemical/physical properties) to represent biodegradation properties for all substances in that same group. For example, chrysene was selected as the representitive compound for PAHs with 4-5 rings (Table 3). For naturally occurring compounds in PW, biodegradation was estimated based on these representitive compounds and was determined using standardized tests at 13°C. For non-naturally occurring production chemicals, biodegradation was determined by a standard screening seawater test as reported in the Harmonized Offshore Chemical Notification Format (HOCNF) for evaluation of persistence in the marine environment (OSPAR, 2010). These tests are based upon ultimate biodegradation by measurement of biochemical oxygen demand (BOD) after 28 days with marine bacteria at 20°C (OECD 203). The biodegradation rate coefficients (k-values) and half-lives for PW compounds were estimated by following Equation 1, where time is usually 28 days:

$$k = -\left(\frac{1}{time}\right) * \ln\left(\frac{100-\%BOD}{100}\right) \qquad \text{(Equation 1)}$$

The biodegradation rates, *k*, and half-lives are shown for the defined groups of naturally occurring substances in Table 3, as described in the EIF computational guideline (NOROG, 2003).

Table 3. Standard biodegradation rates for PW compound groups at 13°C (NOROG, 2003).

Group	Main group	Repr. compound	Half-life (days)	*k*-value
1	EIF-BTEX	Ethyl benzene	0.5	1.39
2	EIF-Naphthalenes	Naphthalene	1.5	0.462
3	EIF-PAH 2-3 ring	Phenanthrene	17	0.041
4	EIF PAH 4-5 ring	Chrysene	350	0.002
5	EIF-Phenol C0-C3	p-Cresol	1.2	0.578
6	EIF-Phenol C4-C5	Pentylphenol	10	0.069
7	EIF-Phenol C6-C9	Nonylphenol	350	0.002
8	EIF-Heptane*	Heptane	60	0.012
9	EIF-Copper (Cu)	Field-specific	No degradation	0.0000001
10	EIF-Zink (Zn)	Field-specific	No degradation	0.0000001
11	EIF-Nickel (Ni)	Field-specific	No degradation	0.0000001
12	EIF-Lead (Pb)	Field-specific	No degradation	0.0000001
13	EIF-Cadmium (Cd)	Field-specific	No degradation	0.0000001
14	EIF-Mercury (Hg)	Field-specific	No degradation	0.0000001
11-n	Production chemicals		HOCNF (BOD_{28})	

*Aliphatic hydrocarbons (oil in water)

Over time, uncertainty pertaining to the ultimate biodegradation half-lives reported by NOROG (2003) and used in the DREAM model increased. The original data provided by NOROG (2003) were based on quality standardized tests, but these tests did not represent the conditions experienced in the Norwegian offshore environment. In addition, the short half-lives of some compounds made some wonder if primary biodegradation was used as input instead of ultimate biodegradation. Furthermore, since many rates were unknown, many biodegradation rates were estimates based on a representitive compound. For example, dispersed oil biodegradation rates are represented by Heptane in the DREAM model, and currently we do not consider this compound to be representative of the biodegradation of dispersed oil as a whole. In 2012, OSPA adopted a risk-based approach (RBA) and guidelines to manage PW and created a list of PNEC

(predicted no effect concentrations) for naturally occurring substances in PW (OSPAR 2014). The PNEC list included additional compounds for which biodegradation data was either not available or known. Therefore, there has been an interest to expand the list of PW compounds within DREAM to represent the complex nature of PW based on the established PNECs (OSPAR 2014) and provide accurate environmentally relevant ultimate biodegradation rates.

6 Biodegradation Tests Included in Study

In order to update the biodegradation data included in the DREAM model, we have conducted a thorough literature review of individual PW compounds as identified in OSPAR (2014) and focused on studies that mimicked experimental conditions relevant to Norwegian offshore marine environments. The literature review included peer-reviewed scientific literature and internal SINTEF reports. Scientific literature was freely available and obtained by searching key-words and authors on Google Scholar. Data from relevant scientific literature is summarized in Table 5 and includes reports of primary biodegradation and ultimate biodegradation, with primary biodegradation on the left of the table and ultimate biodegradation on the right. As mentioned above, biodegradation tests may be separated in primary and ultimate tests. In primary tests, complex mixtures like crude oil and PW can be tested as one substance, and degradation data can be resolved for individual compounds, or for compound groups, depending of the resolution of the analytical method. Typical analytical methods include gas chromatographic methods like GC-FID and GC-MS. Usually, GC-FID analyses are used for determination of primarily saturates, while GC-MS analyses are used for analyses of monoaromatic and polyaromatic hydrocarbons, decalines and phenols. For volatiles, direct injection of samples in a Purge & Trap unit are performed as part of the GC-MS analyses, while for larger analytes (phenols, decalins, naphthalenes, and 2- to 6-ring PAH) the samples are extracted in a solvent (e.g. dichloromethane) before analyses. Primary biodegradation was reported as half-lives (days), percent losses, and/or first order rate coefficients (k) in reference to starting concentrations determined by gas chromatographic analysis. Therefore, only studies that proved chemical loss with gas chromatographic analysis were included in our list of primary biodegradation rates.

Compared to primary biodegradation, the data reported for ultimate biodegradation were analysed with different methods, as this is a measure of the final biomineralization of the test compound. For ultimate biodegradation tests, respirometric analyses are mostly used, but analyses of total organic materials may also be an option. Typically, respirometer tests are performed as CO_2-evolution tests, measuring the CO_2 increase in the headspace above the water containing the substrate. Ultimate biodegradation can also be analyzed using radiolabeled compounds (e.g. ^{14}C-labelled), by determining the labelled CO_2 trapped in a CO_2-trap of KOH. As an alternative to CO_2-evolution tests, biochemical oxygen demand (BOD) analysis can also be used to determine oxygen consumption. The level of ultimate biodegradation is then determined by comparison of the BOD concentrations to the theoretical oxygen consumption (ThOD) needed for complete mineralization of the substrate to CO_2 and water. Based on the data from primary or ultimate biodegradation tests, the biodegradation rates and half-lives may be determined.

Table 5 includes ultimate biodegradation analyses such as oxygen consumption (% BOD), and/or the loss and recovery of radioactive isotopes. Data reported using standardized testing, such as OECD 301 or OECD 306, were also reported for ultimate biodegradation and are labelled as standardized tests in Table 5. Ultimate biodegradation data reported using methods that reported CO_2-evolution or oxygen consumption were given priority over ultimate biodegradation measured using radioisotopes, and radioisotope data were given priority over standardized tests (i.e. OECD) (see Section 6.1 Quality Assurance of Data for further explanation). All data contributed to the calculation of rate coefficients and half-lives and these calculations are shown in the attached spreadsheet (Table 5).

6.1 Quality Assurance of Data

The quality of each cited reference varied with respect to experimental methods, test substance, and the environmental relevance for Norwegian waters (e.g. temperature). Therefore, it was necessary to rank the data based on environmental relevance to the Norwegian offshore marine environment as well as the reported analysis method. As mentioned above (Section 5), ultimate biodegradation data was collected from different analysis methods: %BOD, loss of radioactive

isotopes, and standardized OECD testing. When reviewing the data, a quality score was assigned to each reported biodegradation rate that accounted for the analysis method and test conditions.

Biodegradation studies can be performed in natural water, water fortified with extra microbial inocula, with enrichment cultures, or with single isolated bacterial cultures. SINTEF usually performs biodegradation tests in natural seawater, as we consider this to be the most environmentally relevant approach. Although, sometimes it is necessary to enrich the natural seawater with mineral nutrients or oxygen if these variables become limiting factors, which usually occurs when high concentrations of carbon substrates are added to closed laboratory experiments. To limit the addition of nutrients and oxygen, and thus risk creating an experiment that does not mimic environmental conditions, we usually perform oil and biodegradation experiments at low substrate concentrations. A study conducted with natural seawater, at Norwegian offshore seawater temperatures (~13°C), at low substrate concentrations, and with minimal nutrients (or excess carbon) added would be considered a high-quality study.

Ultimate biodegradation rates measured using respirometry or BOD methods were considered the highest-quality data. If ultimate biodegradation rates were reported using radioisotopes, the quality score of the data decreased since radioactivity was reported instead of oxygen consumption or carbon dioxide production. In addition, relatively smaller substrate concentrations are normally utilized in radioisotope experiments, which can create artificial rates. Therefore, priority was given to respirometry/BOD methods. Furthermore, oxygen consumption and radioisotope methods usually produced higher-quality data than standardized tests, because standardized tests were often conducted at conditions that did not represent Norwegian offshore conditions. Experimental details pertaining to the quality of the data and its relevance to Norwegian waters are mainly included in Table 6, but some experimental data are also included in Table 5 next to each individual rate.

Quality scores were developed to rank the data based on analysis method and its environmental relevance to the Norwegian offshore marine environment. Quality scores (QS) ranged from 1 to 4 (with 1 being the best) and are defined below:

1. **BEST:** Data are reliable. Experimental conditions are relevant to Norwegian offshore produced water.
2. **GOOD**: Data are somewhat reliable. One environmental condition is not consistent with Norwegian offshore produced water, but the data are a good comparison.
3. **OK**: Data are not likely to be reliable. More than one environmental condition is not consistent with Norwegian offshore produced water.
4. **POOR**: Data are not reliable. Data are likely based on reproducible and sound scientific methods, but details concerning the experiment may be missing; or the experimental conditions created a system that will not mimic that of the Norwegian marine environment.

Quality scores are located adjacent to the rate constants in Tables 5, 7 and 8.

When scoring the biodegradation rates, all data started with a QS of 1. Specific questions were then asked pertaining to the study and the answers to these questions dictated the quality score. Table 4 includes the list of questions asked about each study and how the answers dictated the QS.

Table 4. Questions asked about experimental data to determine quality score.

Questions	**No**	**Yes**
Was the experiment conducted using radiorespirometry?	QS stayed the same	QS increased by 1
Was natural seawater used in the experiment?	QS increased by 1	QS stayed the same
Were bacteria added to the experiment?	QS stayed the same	QS increased by 1
Was the temperature environmentally relevant (-1 – 13°C)?	QS increased by 1	QS stayed the same
Was the added carbon substrate representitive of PW?	QS increased by 1	QS stayed the same
Were excess nutrients added?	QS stayed the same	QS increased by 1

7 Data Calculations

The following sub-sections detail the different calculations that were necessary to conduct on the collected data (scientific literature and databases).

7.1 Half-Lives

If half-lives were not reported in the literature cited, they were calculated from the first-order rate constants using the following equation:

$$t_{1/2} = \frac{0.693}{k} \quad \text{(Equation 2)}$$

7.2 Rate Constants

Rate constants were calculated using first-order reaction kinetics and the exact calculation depended upon the given data. If half-lives were reported ($t_{½}$) but rate constants were not reported, then Equation 2 was rearranged to solve for the rate constant (*k*). For ultimate biodegradation rate coefficients, if % loss (i.e. % BOD) was reported, then Equation 1 was used to calculate the rate (NOROG, 2003). Equation 1 is described in Section 5. For primary biodegradation rate coefficients, if the percent loss was given together with an initial concentration, then the integrated from of the first-order rate law was used to calculate the rate (Equation 3):

$$[C] = [C_O]e^{-kt} \quad \text{(Equation 3)}$$

Where [C] is the concentration at the time *t* (days), [C_O] is the initial concentration, and *k* is the rate constant.

In reference to the raw data in Table 5, if the rate coefficient was calculated then a description of the exact calculation was provided in a 'cell note'.

7.3 Correction Factor and Extrapolated Ultimate Biodegradation Rate

Compounds that contained quality primary and ultimate biodegradation data were used to calculate a correction factor, which was applied to compounds that lacked quality ultimate biodegradation rates. This correction factor estimated an ultimate biodegradation rate based on the compound's primary biodegradation rate and is identified as the BIO/MIN FACTOR. Three compounds (toluene, naphthalene, and phenanthrene) had both primary and ultimate biodegradation rates with quality scores of 1, so these three compounds were used to generate the BIO/MIN FACTOR. A BIO/MIN FACTOR was first calculated for these three compounds by dividing their primary biodegradation rate by their ultimate biodegradation rate. Then the three FACTORS from these three compounds (that had primary and ultimate biodegradation quality scores of 1) were averaged to calculate a general BIO/MIN FACTOR for the remaining compounds (Equation 4).

$$\frac{BIO}{MIN}FACTOR = \frac{\left(\frac{Primary\ Biodeg.\ Rate}{Ultimate\ Biodeg.\ Rate}\right)_{toluene} + \left(\frac{Primary\ Biodeg.\ Rate}{Ultimate\ Biodeg.\ Rate}\right)_{naphthalene} + \left(\frac{Primary\ Biodeg.\ Rate}{Ultimate\ Biodeg.\ Rate}\right)_{phenanthrene}}{3} = 6.30$$

(Equation 4)

The calculated FACTOR from toluene, naphthalene and phenanthrene was 6.30 and was applied to the remaining compounds to extrapolate an ultimate biodegradation rate using Equation 5. Dispersed oil was not included in the determination of the correction factor, as the factor is only applicable to single compounds and not mixtures.

The extrapolated ultimate biodegradation rate was determined by multiplying the primary biodegradation rate (from the literature) by the BIO/MIN FACTOR. For example:

$$Primary\ Biodegradation\ Rate\ (k) \times \frac{BIO}{MIN} FACTOR\ = Extrapolated\ Ultimate\ Biodegradation\ Rate$$

(Equation 5)

It's important to note that the quality of each extrapolated ultimate biodegradation rate is dependent upon two variables: (1) the quality of the primary biodegradation rate for each compound and (2) the accuracy of the rates for the three reference compounds that were used to create the BIO/MIN FACTOR (toluene, naphthalene, and phenanthrene). The rates reported in Table 8 are calculated from a variety of temperatures, but the primary and ultimate biodegradation rates for the reference compounds were measured at approximately the same temperature.

The extrapolated ultimate biodegradation rates for dispersed oil, toluene, naphthalene, and phenanthrene are the same as their raw data ultimate biodegradation rates, since these compounds were the only compounds that had high-quality raw ultimate biodegradation rates (QS = 1).

7.4 Temperature Correction, Q10

A Q10 approach was applied to the calculated ultimate biodegradation rates (Bagi, 2014). As mentioned, raw data obtained from the literature on primary and ultimate biodegradation was reported at different temperatures. The Q10 approach is used to estimate biodegradation rate coefficients at different temperatures. Equation 6 was used to calculate biodegradation rates at different temperatures from what was reported in the literature. We have used a Q10 factor that corresponds to a Q10 value of 2, which doubles the rate for every 10°C temperature increase. The OSCAR model also adopts a Q10 = 2 and this value is also commonly accepted in the scientific literature (Bagi, 2014).

$$k_{water\ temp} = k_{reference\ temp} * 10^{Q10\ factor*(water\ temp - reference\ temp)}$$

(Equation 6)

(where Q10 factor = 0.0301029995 and corresponds to a Q10 = 2)

For example, if the ultimate biodegradation rate was reported at a temperature of 5°C and we wanted to calculate the rate at 13°C; then the reference temperature would be 5°C, the water temperature would be 13°C and the $k_{\text{reference temp}}$ would be the reported raw data (ultimate biodegradation rate) at 5°C.

8 Calculated and Extrapolated Biodegradation Data

8.1 Data Collection

Five tables were generated with the collected data (Tables 5-9). The tables include primary and/or ultimate biodegradation of the most common naturally occurring substances in produced water as identified by the OSPAR RBA Guidelines (OSPAR, 2014b). Data in bold represents raw data from the cited source. For example, if the half-live and the rate constant are reported for a compound and only the half-life is bold then the half-life was reported in the reference (raw data) and the rate constant was calculated using Equation 2. Table 5 includes data collected from the scientific literature and Table 6 describes the experimental conditions of the literature cited. It was determined to share Tables 5 & 6 in an electronic format due to their size. Therefore, Tables 5 & 6 are provided as an Excel workbook attachment. Scaled-down copies of Tables 5 & 6 are provided below for reference. To illustrate differences between rates, some details pertaining to the experimental conditions of the data are located next the rate constants in Table 5, such as temperature, oil type, and the citation. As noted, Table 6 includes a comprehensive list of the experimental conditions and should, therefore, be used as a guide for the given quality scores identified in Tables 5 & 8.

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Table 5. Primary and Ultimate Biodegradation - Raw Data, Half-lives and Rate Coefficients.
(located in attached Excel spreadsheet; cropped version shown below for reference)

Experimental			Primary Biodegradation (Transformation)							Ultimate Biodegradation (Mineralization)													
			Half-life (days)			Rate Coefficient, *k*	Quality	Temp	Reference		Isotope Data: rates, % loss, % recovery (time)			Oxygen Consumption Data: % BOD (time)			Half-life (days)			Rate Coefficient, *k*	Quality	Temp.	Reference	
Compound	PW Substance Group	CAS	fresh water	marine	soil	(day^{-1})	Score	(°C)	Oil Type	Citation	fresh water	marine	soil	fresh water	marine	soil	fresh water	marine	soil	(day^{-1})	Score	(°C)	Oil Type and Relevant Media	Citation
			52.1			0.0133	1	-1	weathered ANS crude	McFarlin et al. (2014)					**11% (60 d)**			357		0.0019	1	-1	weathered ANS crude	McFarlin et al. (2014)
			20.7			**0.0336**	1	5	fresh macondo oil (10 um droplets)	Brakstad et al. (2015)					**27% (64 d)**			138		0.0050	2	0-1	fresh Troll crude (15-17 um droplets)	Brakstad et al. *submitted*
			34.4			**0.0202**	1	5	fresh macondo oil (30 um droplets)	Brakstad et al. (2015)					**38% (64 d)**			91.9		0.0075	2	0-1	fresh Troll crude (15-17 um droplets)	Brakstad et al. *submitted*
			44.4			0.0156	1	5	fresh Statfjord crude (10 um droplets)	Ribicic et al. *accepted*														
			72.9			0.0095		5	fresh Grane (25 um droplets)	Ribicic et al. *submitted*					**14% (64 d)**			295		0.0024	2	5	fresh Grane (25 um droplets)	Brakstad et al. *submitted*
Dispersed Oil	Dispersed Oil	na	61.3			0.0113	2	13	fresh Grane (25 um droplets)	Ribicic et al. *submitted*					**41% (64 d)**			84.5		0.0082	2	13	fresh Grane (25 um droplets)	Brakstad et al. *submitted*
			45.9			0.0151	2	13	weathered Statfjord crude (25 um droplets)	Brakstad et al. (2018)					**44% (64 d)**			75.9		0.0091	2	13	weathered Statfjord crude (25 um droplets)	Brakstad et al. *submitted*
			23.7			0.0293	1	13	fresh Statfjord crude (10-13 um droplets)	Brakstad et al. (2018)					**58% (64 d)**			51.3		0.0135	2	13	fresh Statfjord crude (10-13 um droplets)	Brakstad et al. *submitted*
			41.5			0.0167	1	13	fresh Troll crude (10-13 um droplets)	Brakstad et al. (2018)					**40% (64 d)**			86.2		0.0080	2	13	fresh Troll crude (10-13 um droplets)	Brakstad et al. *submitted*
			32.8			0.0211	1	13	fresh Balder crude (10-13 um droplets)	Brakstad et al. (2018)					**41% (64 d)**			83.9		0.0083	2	13	fresh Balder crude (10-13 um droplets)	Brakstad et al. *submitted*
			23.1			0.0300	1	13	Produced Water	Lofthus et al. *submitted*														
			12.9			0.0537	1	5	fresh macondo oil (10 um droplets)	Brakstad et al. (2015)	**0.1-0.5 mg/L*d**						17.3			0.0400	3	5	single compound + spilled oil in GW	Braddock and McCarthy (1996)
			16.5			0.0420	2	5	fresh macondo oil (30 um droplets)	Brakstad et al. (2015)		**k = 1.66/d**						0.42		**1.66**	4	18-21	single compound	Wakeham et al. (1986)
			24.7			0.0280	1	5	fresh Statfjord crude (WAF)	Brakstad et al. (2017)		**66% loss (52 d)**						33.4		0.0207	3	21	single compound	Chung and King (1999)
			18.8			0.0369	1	5	fresh Statfjord crude (10 um droplets)	Ribicic et al. *accepted*														
Benzene	BTEX	71-43-2	**16.7**			0.0415	1	5	fresh Troll crude (14 um droplets)	Ribicic et al. *submitted*														
			17.8			0.0389	1	5	frest Grane (25 um droplets)	Ribicic et al. *submitted*														
			9.9			**0.07**	3	21	tar mixture	Liou et al. (2008)			**14% loss (2.5 d)**						11.5	0.0603	3	21	single compound + coal tar mixture	Liou et al. (2008)
			10.6			**0.0656**	3	23	gasoline spill in groundwater	Lahvis et al. (1999)							3.8			**0.183**	4	24	single compound	Kelly et al. (1996)
			9.9			0.0700	1	5	fresh macondo oil (10 um droplets)	Brakstad et al. (2015)		**48% loss (47 d)**						**50**		0.0139	1	2-10	single compound	Wakeham et al. (1985)
			11.6			0.0597	2	5	fresh macondo oil (30 um droplets)	Brakstad et al. (2015)			**16.3% loss (1 d)**						3.89	0.1779	2	5	single compound + spilled oil in GW	Bradley and Chapelle (1995)
			14.9			0.0466	1	5	fresh Statfjord crude (WAF)	Brakstad et al. (2017)		**0.12 ng/L (11 hr)**			0.16% (11 hr)			198		0.0035	1	6	single compound	Button et al. (1981)
			17.0			0.0407	1	5	fresh Statfjord crude (10 um droplets)	Ribicic et al. *accepted*		**91% loss (18 d)**						0.63		**1.1**	4	16-18	single compound	Wakeham et al. (1985)
			16.4			0.0423	1	5	fresh Troll crude (14 um droplets)	Ribicic et al. *submitted*		**k = 0.50/d**						1.39		**0.50**	4	18-19	single compound	Wakeham et al. (1986)
			16.3			0.0425	1	5	frest Grane (25 um droplets)	Ribicic et al. *submitted*							1.9			**0.3720**	4	24	single compound	Kelly et al. (1996)
Toluene	BTEX	108-88-3	8.11			**0.0855**	3	23	gasoline in groundwater	Lahvis et al. (1999)	**15% loss (72 hr)**						12.8			0.0542	3	25	single compound + contaminated GW	Armstrong et al. (1991)
			9.7			0.0714	1	5	fresh macondo oil (10 um droplets)	Brakstad et al. (2015)				**79% (28 d)**			12.4			0.0557	3	20	Standard Test: OECD 301B	ECHA, ethylbenzene
			10.7			0.0648	2	5	fresh macondo oil (30 um droplets)	Brakstad et al. (2015)														
			12.5			0.0554	1	5	fresh Statfjord crude (WAF)	Brakstad et al. (2017)														
Ethylbenzene	BTEX	100-41-4	8.52			0.0813	1	5	fresh Statfjord crude (10 um droplets)	Ribicic et al. *accepted*														
			16.2			0.0428	1	5	fresh Troll crude (14 um droplets)	Ribicic et al. *submitted*														
			16.1			0.0430	1	5	frest Grane (25 um droplets)	Ribicic et al. *submitted*														
			6.79			**0.102**	3	23	gasoline in groundwater	Lahvis et al. (1999)														
Xylene	BTEX	1330-20-7	15.9			0.0437	1	5	fresh Statfjord crude (10 um droplets)	Ribicic et al. *accepted*							2.9			**0.2350**	4	24	single compound	Kelly et al. (1996)
														87.8% (28 d)			12.4			0.0557	3	20	Standard Test: OECD 301F	ECHA, xylene
			9.0			0.0770	1	5	fresh macondo oil (10 um droplets)	Brakstad et al. (2015)					**19% (56 d)**			184		0.0038	1	0	single compound + Statfjord crude	Brakstad and Bonaunet (2006)
			9.6			0.0722	2	5	fresh macondo oil (30 um droplets)	Brakstad et al. (2015)					**60% (56 d)**			42.4		0.0164	1	5	single compound + Statfjord crude	Brakstad and Bonaunet (2006)
			14.9			0.0464	1	5	fresh Statfjord crude (10 um droplets)	Ribicic et al. *accepted*		**9.0±0.1ugC/d**						7.35		0.0943	3	8	single compound + ANS crude	Lindstrom and Braddock (2002)
			13.4			0.0517	1	5	fresh Troll crude (14 um droplets)	Ribicic et al. *submitted*								10.2		**0.068**	1	0.5-15	single compound + Arctic seawater	Bagi et al. (2014)
Naphthalene	Naphthalenes	91-20-3	**13.0**			0.0533	1	5	frest Grane (25 um droplets)	Ribicic et al. *submitted*								14.4		**0.048**	1	0.5-15	single compound + Temperate seawater	Bagi et al. (2014)
			2.3			0.3013	1	8	fresh ANS crude	Prince et al. (2013)					**66% (5 d)**			3.21		0.2158	1	10	Standard Test: OECD 306	Brakstad et al. (1996)
			8.4			0.0825	1	13	Produced Water	Lofthus et al. *submitted*	**59.5% loss (14 d)**						10.7			0.0646	3	24	single compound	Heitkamp and Cerniglia (1988)
			4.8			0.1444	2	13	4 different oils (mean value, <30 um droplets)	Brakstad et al. (2018)														

Table 6. Experimental Details of Literature Cited in Table 5.
(located in attached Excel spreadsheet; smaller version shown below for reference)

Citation	Water Type	Additional Bacteria Added?	Type of Oil or Compound Added	Temperature	Dispersant (type)	Droplet Size	Incubation Duration	Nutrients Added	Notes
Armstrong et al. (1991)	ground water (aerobic) at hazardous waste site (B,T,X)	no	14C-toluene (20 to 40 ug/L) in 50 mL of ground water	25°C	no	no droplets	72 hr	yes	Treatmen
Bagi et al. (2014)	seawater	no	single compound - naphthalene (10 mg/L)	0.5, 4,8,15°C	no	no droplets	28 days and 48 days	yes	oxygen co
Bauer and Capone (1985)	enriched intertidal marine sediments + filtered seawater	no	soil enriched with PAH solution + 14C labeled naphthalene, anthracene	20°C	no	no droplets	14 days	yes	Sediment
Bogan and Lamar (1995)	nutrient medium	yes	single compounds and creosote from rail-road ties	room temp	no	no droplets	7 d	yes	Liquid cul
Boonchan et al. (2000)	PAH contaminated soil (65% moisture)	yes	14C labeled benzo[a]pyrene (50 mg/kg) in PAH-contaminated soil (100g)	25°C	no	no droplets	100 days	yes	PAH mine
Braddock and McCarthy (1996)	groundwater- aerobic	no	contaminated ground water (25,000 ug/L BTEX)	5°C	no	no droplets	10 days	no	$^{14}CO2$ fron
Bradley and Chapelle (1995)	groundwater- aerobic	no	aquifer sediments + 14C-labeled toluene (9.7 mCi/mmol)	5°C	no	no droplets	25 hr	no	Aerobic, p
Brakstad and Bonaunet (2006)	seawater (80m, NF w/ enriched culture)	oil-enriched culture from seawater	50ug Statfjord oil + 14C labeled naphthalene, phenanthrene, n-hexadecane	0°C and 5°C	no	no droplets	56 days	Yes (PO_4, NO_3, Fe)	Mesocosm
Brakstad et al. (1996)	seawater (80 m, NF)	no	naphthalene or phenanthrene	10°C	no	no droplets	5 days	no	Biochemic
Brakstad (2004)	seawater (80 m, NF)	no	WAFS of Statfjord and Oseberg, and produced water in different experiments	10°C	no	no droplets	21	yes	Experime
Brakstad et al. (2015)	seawater (80m, NF, pre-adapted 5 days)	no	2 mg/L unweathered macondo oil	5°C	Corexit 1:100	10 um and 30 um	64 days	No	Seawater
Brakstad et al. (2017)	seawater (80 m, NF, pre-adapted 5 days)	no	Statfjord crude blend paraffinic oil	5°C	no	na	64 days	No	A low-ene
Brakstad et al. (2018)	seawater (80 m, NF)	no	4 different oils: Statjford crude, Troll, Grane, and Balder (2.5 - 2.8 mg/L)	13°C	yes (Corexit, Slickgone, and Finasol)	mean < 30 µm	64 days	no	Dispersibi
Brakstad et al. *submitted*	seawater (80m, pre-adapted)	no	2 mg/L individual substrates	5°C	no	no droplets	63 days	yes (conc ?)	Mineraliz
Button et al. (1981)	seawater	no	14C-toluene (0.4 ug/L seawater)	6°C	no	no droplets	11 hr	no	See Figure
Carmichael et al. (1997)	oil-contamined soil (superfund site in MN and FL, USA)	no	single compound in contaminated soil/water slurry. (1.6, 1.7, and 2.8 ug/L of 14C chrysene)	20°C	no	no droplets	10 hr	no	Mineraliz
Chung and King (1999)	articifcial seawater and intertidal sediments	no	2.4 nmol/cm3 of ^{14}C-hexadecane or ^{14}C-benzene	room temp	no	no droplets	52 days	no	$^{14}CO2$ was
CONCAWE, 2012	seawater	no	single compounds	20°C				yes	Measured
Dean-Ross et al. (2002)	mineral salts medium	yes	single compound (50 ppm) anthracene	24°C	no	no droplets	10 days	yes	Flasks wer
Deeb and Alvarez-Cohen (1999)	mineral salts medium	tolune-enriched culture from aquifer soil	pure phase BTEX compounds (80 mg/L)	20 and 35°C	no	no droplets	4-15 hours	yes	batch reac
ECHA, 4-tert-butylphenol	fresh (OECD 301F): measures oxygen consumption	activated sludge	5 mg/L and 25 mg/L ptBP	20°C (?)	no	no droplets	28 days	yes	Manometr
ECHA, ethylbenzene	fresh (OECD 301B): measures production of CO2	yes - unknown origin	ethylbenzene	(?)	no	no droplets	28	yes	Ethylbenz
ECHA, pentylphenol	fresh (OECD 301B): measures production of CO2	activated sludge	p-tert.-amylphenol	(?)	no	no droplets	28 days	yes	Conducte
Eriksson et al. (1999)	Bushnell Haas medium and distilled water	yes	contaminated soil	20°C	no	no droplets	30 d	yes	Duplicate
Grosser et al. (1991)	soil from coal gasification plat	no	^{14}C labeled pyrene (8.5 ng/g) and benz[a]pyrene (84 ng/g)	22°C	no	no droplets	62	yes	Mineraliz
Heitkamp and Cerniglia (1987)	estuary sediment and water	no	single PAH compounds	22°C	no	no droplets	8 weeks	no	Estuarine
Heitkamp and Cerniglia (1988)	basal salts medium (BSM, 0.3g NaCl)	yes	individual labeled PAHs (0.92uCi) and an unlabelled PAH mixture (50 ug)	24°C	no	no droplets	14	yes	A PAH-deg
Juhasz et al. (1997)	basal salts medium (BSM, 0.3g NaCl)	pyrene-enriched PAH contaminated soil	fluorene, phenanthrene, fluoranthene, pyrene and benz[a]anthracene (10 mg/L); dibenz[a,h]	30°C	no	no droplets	7-28 days	yes	Pyrene de
Kanaly et al. (2000)	nutrient medium	benzo[a]pyrene and jet fuel-enriched soil	[7-^{14}C]benzo[a]pyrene, benzo[a]pyrene (10 mg/L) and jet fuel (0.1% wt/vol)	28°C	no	no droplets	21 days	yes	Incubation
Kelly et al. (1996)	groundwater-aquifer simulation in flow-through columns	yes	single substrate (0.06 - 0.38 mmol/L) and mixture of benzene, toluene, and xylene	24°C	no	no droplets		yes	Steady-sta
Kincannon and Lin (1985)	?	no	acenapthene and acenaphthalene (no concentration given)	(?)	no	no droplets	?	?	Reference
Lahvis et al. (1999)	groundwater- aerobic	no	gasoline sill in groundwater	23	no	na	in situ	No	By modell
Lindstrom and Braddock (2002)	articifcial seawater	oil-enriched culture from intertidal sediment	1400 mg/L fresh ANS crude + 100 ug/10 L ^{14}C labeled naphthalene, phenanthrene	8°C	Corexit (1:10 or 1:20)	nm	96 hr (respirometry)	No	No differe
Liou et al. (2008)	water-saturated sediment	no	5g coal-tar waste-contaminated sediment + 36 ppm ^{13}C-benzene	room temp (?)	no	no droplets	2.5 day (60 hours)	no	Benzene r
Lofthus et al. (2017)	seawater (80 m, NF)	no	Produced Water (1 PW: 3.5 Seawater)	13°C	no	na	62 days	No	Incubation
Mackay et al. (1992)	various media	yes	test included a variety of inputs	wide range	no	no droplets	wide range	yes	Estimation
Maeda et al. (2013)	Stanier's basal medium	yes	single compound	30°C	no	no droplets	10	yes	Biotransfo
McFarlin et al. (2014)	seawater	no	weathered Alaska North Slope crude oil with and without dispersant (Corexit 9500)	-1°C	Corexit 9500	no droplets	56 days	no	Oxygen co
Mihelcic and Luthy (1988)	soil/water mixture	no	single compound in soil-water system (1:50 g/ml; denitrification conditons, no oxygen!)	21°C	no	no droplets	70 days	yes	Experime
Montgomery et al. (2008)	sediment cores from San Diego Bay and filtered seawater	no	14C labeled naphthalene, fluoranthene, and phenanthrene (0.2 ug/g)	in situ on seabed	no	no droplets	2h h	no	Evolved 1
Pillis and Davis (1985)	industrial wastewater	single strain	350 mg/L phenol	11-13°C	no	no droplets	5 days	yes (PO_4, SO_4)	Respirom
Prince et al. (2013)	seawater (surface, New Jersey)	no	2.5 mg/L Alaska North Slope (ANS) crude	8°C	Corexit 1:20	nm	60-88 days	No	Surface se
Rentz et al. (2007)	fresh	single strain	14C labeled benzo[a]pyrene (1.2 ug/L)	30°C	no	no droplets	20 h & 7 days	yes	Radio-labe
Ribicic et al. *accepted*	seawater (80 m, NF)	no	Statfjord crude blend paraffinic oil	5°C	slickgone (DOR 1:100)	10 um	64 days	no	Microcosm
Ribicic et al. *submitted*	seawater (80 m, NF)	no	fresh Troll (naphthenic, 14 um droplets) and Grane (asphaltenic, 25 um droplets) at 2 mg/L	5 and 13°C	Corexit 9500 (1:100)	14 & 25 um	64 days	no	Two fresh
Rubin and Alexander (1983)	fresh water	no	single (200 ng) phenol	29°C	no	no droplets	?	no	Mineraliz
Staples et al. (2001)	fresh (OECD 301B): measures production of CO2	activated sludge	octylphenol and nonylphenol	22°C	no	no droplets	35 days	yes	activated
Subba-Rao et al. (1982)	fresh water	no	single compound: phenol	29°C	no	no droplets	5	no	This study
Urano and Kato (1986)	fresh (OECD 301C)	activated sludge	100 mg/L phenol	20°C	no	no droplets	100 hours (4.2 days)	yes	Oxygen co
Wakeham et al. (1985)	seawater (1 m depth), Rhode Island, USA	no	14C labeled toluene (250 uCi)	2-10°C & 18-19°C	no	no droplets	47 days & 18 days	no	The Marin
Wakeham et al. (1986)	seawater (1 m depth), Rhode Island, USA	no	14C labeled benzene (240 uCi), toluene (230 uCi), and naphthalene (400 uCi)	13-20°C	no	no droplets	2-9	no	Mineraliz
Walter et al. (1991)	mineral salts medium	yes	single compound	room temp	no	no droplets	14 days	yes	Mineraliz
Wild and Jones (1993)	soils	yes	PAH mixture	20	no	no droplets	205 days	yes	Sewage sl
Ya-lei et al. (2005)	Bushnell Haas medium and distilled water	yes	single compound: 2,6-di-tert-butylphenol	37°C	no	no droplets	11 days	yes	Flasks con
Yuan et al. (2002)	nutrient medium	yes	PAH mixture of phenantrene, acenaphthene, anthracene, fluorene, and pyrene (5ug/g each)	20°C	no	no droplets	40 days	yes	Soil sampl

Table 7 includes data collected from two databases, the PBT Profiler (PBT Profiler, 2016) and the ECETOC (ECETOC, 2009) biodegradation databases. The PBT Profiler provides ultimate biodegradation data from the BIOWIN estimation program using the expert survey module (Boethling et al., 1994). The ECETOC database provides both primary and ultimate biodegradation data, but only ultimate biodegradation data are presented in this report (Table 7). The PBT Profiler and ECETOC databases were utilized to report the half-lives of ultimate biodegradation for individual compounds in both marine and fresh water, with a preference for marine when available.

Several databases exist where biodegradation data may be collected. Some of biodegradation databases are based on structure-activity relationship (SAR) models. Generation of SAR biodegradation data are derived from the combination of data from standard methods (e.g. from data provided by the OECD 301 method - biodegradation in freshwater at 20°C; OECD, 1992) and the chemical structures/active molecular sites. Examples of such databases are the BIOWIN module in the Estimation Programs Interface (EPI) Suite™, which was developed by the US EPA. Biodegradability estimates in the BIOWIN module are based upon fragment constants that were developed using multiple linear or non-linear regression analyses (Howard et al. 1992). The models are based upon data from testing of several hundreds of chemicals, with test results and methods judged by experts. Data from the BIOWIN module are transformed into half-lives by US EPA, assuming first-order rate kinetics, and are available in the PBT (persistent, bioaccumulative, and toxic) profiler (http://www.pbtprofiler.net/). Therefore, the PBT profilers is based on the BIOWIN module and includes biodegradation half-lives of numerous persistent, bioaccumulative, and toxic compounds. The BIOWIN model includes both primary and ultimate biodegradation, as well as anaerobic estimations, but the PBT profiler uses the ultimate biodegradation data for calculation of half-lives. The half-lives and first-order rate constants of PW components in the PBT profiler are reported in Table 7. The PBT profiler reports ultimate biodegradation in fresh water at 20°C and therefore does not rank high in our quality index. We have ranked the PBT profiler data with a QS of 4, which represents data that will not mimic that of Norwegian marine environments. It must be noted that during the writing of this report, the US EPA ceased access to the online PBT Profiler but we were able to collect the majority of the data prior to the shutdown (February 8, 2018). Unfortunately, the shutdown occurred prior to our search for xylene and 4-methylphenol (p-Cresol), so ultimate biodegradation rates are not included for these compounds with the PBT Profiler. In addition, the half-live and rate coefficient of dispersed oil are also absent from Table 7 since mixtures were not represented in the PBT Profiler.

In addition to the PBT profiler, biodegradation data were also collected from the ECETOC (European Centre for Ecotoxicology and Toxicology of Chemicals) database (ECETOC, 2009). While the data collected from the PBT profiler were based on the BIOWIN module and represented biodegradation in fresh water, the ECETOC database is based on experimental data from marine biodegradation experimental tests. Relevant ultimate biodegradation data for the PW compounds included in the DREAM model are located in Table 7. As shown, the ECETOC dataset lacked information on more than half of the substances.

The rate coefficients in Table 7 are calculated from the half-lives assuming a first-order relationship (Equation 2) and the half-lives include the lag phase, as with all half-lives reported in this report. While the PBT Profiler reports a single half-life for each compound, the ECETOC biodegradation database is a compilation of data published in peer-reviewed journals between 1976 and 2005 and therefore reports a median value based on a range of half-lives. The number of studies included in each median value calculation is shown in a separate column in Table 7 next to the corresponding rate. The rates reported with the PBT Profiler do not report the number of studies because these rates are based on estimations within the BIOWIN module. Unlike the PBT Profiler, which reported data at a given temperature of 20°C, the ECETOC biodegradation database reported data at various incubation temperatures, these temperatures are identified in Table 7. Quality scores have been added to the ultimate biodegradation rates obtained from the PBT Profiler and ECETOC databases to identify how representative these data are to environmental conditions experienced in Norwegian offshore seawater. Quality scores are described in Section 6.1.

Table 7. Predicted Ultimate Biodegradation Half-lives and Rates in Freshwater Based on the PBT Profiler and ECETOC Databases (10-24 °C).

			PBT Profiler				ECETOC				
Compound	PW Substance Group	CAS	Half-life (days)	Rate Coefficient, *k* (day^{-1})	Temp. (°C)	Quality Score	Half-life (days)	Rate Coefficient, *k* (day^{-1})	Temp. (°C)	# of studies	Quality Score
Dispersed Oil	Dispersed Oil	--	--	--		--	--	--			--
Benzene	BTEX	71-43-2	**38**	0.0182	20	4	**72**	0.0096	24	*n* = 1	4
Toluene	BTEX	108-88-3	**15**	0.0462	20	4	**79**	0.0088	10	*n* = 3	4
Ethylbenzene	BTEX	100-41-4	**15**	0.0462	20	4	--	--			--
Xylene	BTEX	1330-20-7	--	--		--	--	--			--
Naphthalene	Naphthalenes	91-20-3	**38**	0.0182	20	4	**28**	0.02	10	*n* = 23	4
Acenaphthene	PAH 2-3 ring	83-32-9	**38**	0.0182	20	4	--	--			--
Acenaphthylene	PAH 2-3 ring	208-96-8	**15**	0.0462	20	4	--	--			--
Fluorene	PAH 2-3 ring	86-73-7	**15**	0.0462	20	4	**> 150**	< 0.0046	24	*n* = 1	4
Anthracene	PAH 2-3 ring	120-12-7	**60**	0.0116	20	4	--	--			--
Dibenzothiophene	PAH 2-3 ring	132-65-0	**15**	0.0462	20	4	**7.0**	0.099	20	*n* = 1	4
Phenanthrene	PAH 2-3 ring	85-01-8	**60**	0.0116	20	4					
Fluoranthene	PAH 4 ring	206-44-0	**60**	0.0116	20	4	--	--			--
Pyrene	PAH 4 ring	129-00-0	**60**	0.0116	20	4	**24**	0.0289	22	*n* = 1	4
Benz[a]anthracene	PAH 4 ring	56-55-3	**60**	0.0116	20	4	--	--			--
Chrysene	PAH 4 ring	218-01-9	**60**	0.0116	20	4	--	--			--
Dibenzo[a,h]anthracene	PAH 5-6 ring	53-70-3	**60**	0.0116	20	4	**16**	0.0433	22	*n* = 1	4
Benzo[a]pyrene	PAH 5-6 ring	50-32-8	**60**	0.0116	20	4	**179**	0.0039	10	*n* = 2	2
Benzo(k)fluoranthene	PAH 5-6 ring	207-08-9	**60**	0.0116	20	4	--	--			--
Benzo(g,h,i)perylene	PAH 5-6 ring	191-24-2	**60**	0.0116	20	4	--	--			--
Benzo[b]fluoranthene	PAH 5-6 ring	205-99-2	**60**	0.0116	20	4	--	--			--
indeno(1,2,3-cd)pyrene	PAH 5-6 ring	19339-5	**60**	0.0116	20	4	--	--			--
Phenol	C_0-C_3 alkyl phenols	108-95-2	**15**	0.0462	20	4	**14.2**	0.0488	16	*n* = 1	4
4-methylphenol (p-Cresol)	methyl phenol	106-44-5	--	--		--	--	--			--
4-tert-butylphenol	C_4 alkyl phenols	98-54-4	**38**	0.0182	20	4	--	--			--
Pentylphenol	C_5 alkyl phenols	80-46-6	**38**	0.0182	20	4	--	--			--
4-tert-octylphenol	C_6-C_8 alkyl phenols	140-66-9	**38**	0.0182	20	4	**60**	0.0116	20	*n* = 1	4
Nonylphenol	C_9 alkyl phenols	25154-52-3	**15**	0.0462	20	4	--	--			--

8.2 Summary of Calculated and Extrapolated Ultimate Biodegradation Rates

The best data for each PW compound are summarized in Table 8. The table includes the highest-quality raw data found in literature or databases (from Tables 5 & 7). These data are presented as individual biodegradation rates or average rates if multiple data were present for a compound with a quality score of 1, and within the same temperature range. For example, if a compound only had one rate with a quality score (QS) of 1, and two rates with a QS of 3, then only the rate with the QS = 1 is included in the summary table. If a compound had more than one rate with a QS = 1, than the average rate was included in the summary table. Rates were only averaged within similar temperature ranges. If a compound had high quality data (QS = 1) spanning different temperatures, then the rate(s) within the most relevant temperature to Norwegian seawater was(were) reported in the summary table, with preference given to 5°C. Many compounds only had rates reported at 20°C in the literature. The temperature at which the rate was measured is also shown in Table 8.

In Table 8, data with QS = 1 are the most reliable and are shown in blue, while data that are not as relevant to Norwegian seawater are shown in dark red (QS = 2, 3, or 4). The primary or ultimate biodegradation rate of many compounds shown in Table 8 were obtained from one experiment, but as mentioned, the rates of some compounds were averages of data within the same quality score and temperature range. The number of studies (n) used to determine the rate in Table 8 are shown next to each corresponding rate. For example, n = 3 indicates that three different studies reported data for that compound at the reported quality score (QS) and temperature. The rates from studies with n > 1 were then averaged to calculate the primary or ultimate biodegradation rate shown in Table 8. Some compounds did not have rate data available in the literature, but have rates identified in the summary table (Table 8). Due to lack of data, the rates for these compounds were estimated from similar compounds and the number of studies (n) is shown as 0. Compounds with estimated rates (n = 0) are identified with superscripts and rate estimates are explained in notes under Table 8.

Table 8 also helps to illustrate how the BIO/MIN factor was calculated (Equation 4) and compares the corresponding extrapolated ultimate biodegradation rate to the experimental ultimate biodegradation rate. The extrapolated ultimate biodegradation rates are recommended for incorporation into the DREAM model. The BIO/MIN factor was based on compounds that had ultimate biodegradation rates with quality scores of 1 within the same temperature range. Only three individual compounds had ultimate and primary biodegradation rates with quality scores of 1 (toluene, naphthalene and phenanthrene), and the ultimate biodegradation rates reported for these compounds are recommended to be used directly. In contrast, twenty individual compounds had ultimate biodegradation rates with quality scores above 1 (ranging from 2-4), but had primary biodegradation rates with quality scores of 1. Since biodegradation is a factor of primary and ultimate biodegradation, an equation was developed that illustrated a mathematical relationship between primary biodegradation and ultimate biodegradation. By using the primary and ultimate biodegradation data for toluene, naphthalene and phenanthrene, an average BIO/MIN correction factor was calculated (Equation 4). The three BIO/MIN FACTORS are highlighted in green, and the calculated FACTOR from these three compounds (which was applied to the remaining compounds) was 6.30 (Equation 5). This BIO/MIN factor was used in the calculation of ultimate biodegradation rates for compounds that lacked data on ultimate biodegradation and is described in more detail in Section 7.3. For these compounds, extrapolated ultimate degradation rates were calculated by dividing the primary biodegradation rate with the general BIO/MIN factor (6.30) for each substance (Table 8).

Dispersed oil was not included in the determination of the correction factor, as the factor is only applicable to single compounds and not mixtures. Finalized primary and ultimate biodegradation rates with corresponding quality scores from Table 5 are also included in Table 8 for comparison to the extrapolated ultimate biodegradation rate.

Table 8. Summary of Highest-Quality Primary and Ultimate Biodegradation Rates with Calculated Ultimate Biodegradation Rates for Incorporation into the DREAM Model. Dispersed oil was not included in the BIO/MIN FACTOR because it is a mixutre and the FACTOR is only relevant to individual compounds. Data with quality scores (QS) = 1 are shown in blue, data with QS > 1 are shown in dark red. QS = 1 indicates the best available data, while QS = 2 indicates good data, QS = 3 indicates OK data, and QS = 4 indicates poor data (see Section 6.1 for details). The number of studies (*n*) used to summarize the rates in are shown next to each corresponding rate. Some rates are based on data obtained from one study, while other rates are averages from different high-quality studies. If *n* = 0, then the rate is estimated from a different compound (or from a database) and is explained in a superscript below the table.

Compound	Substance Group	Primary Biodegradation				Ultimate Biodegradation				BIO/MIN	**Ultimate Biodegradation Rate**	
		Rate (*k*)	(QS)	Temp.	# of studies	Rate (*k*)	(QS)	Temp.	# of studies	FACTOR	**Extrapolated (*k*)**	**Temp.**
Dispersed Oil	Dispersed Oil	0.0225	(1)	-1-13°C	*n* = 8	0.0024	(1)	5°C	*n* = 1	na	**0.0024**	5°C
Benzene	BTEX	0.0398	(1)	5°C	*n* = 5	0.0400	(3)	5°C	*n* = 1	6.30	**0.0063**	5°C
Toluene	BTEX	0.0484	(1)	5°C	*n* = 5	0.0087	(1)	2-10°C	*n* = 2	5.58	**0.0087**	2-10°C
Ethylbenzene	BTEX	0.0588	(1)	5°C	*n* = 5	0.0557	(3)	20°C	*n* = 1	6.30	**0.0093**	5°C
Xylene	BTEX	0.0437	(1)	5°C	*n* = 1	0.0557	(3)	20°C	*n* = 1	6.30	**0.0069**	5°C
Naphthalene	Naphthalenes	0.1059	(1)	5-8°C	*n* = 5	0.0164	(1)	5°C	*n* = 1	6.47	**0.0164**	5°C
C1-naphthalene	Naphthalenes	0.0924	(1)	13°C	*n* = 1	0.0164[2]	(2)	5°C	*n* = 0	6.30	**0.0147**	13°C
C2-naphthalene	Naphthalenes	0.0485	(1)	13°C	*n* = 1	0.0164[2]	(2)	5°C	*n* = 0	6.30	**0.0077**	13°C
C3-naphthalene	Naphthalenes	0.0444	(1)	13°C	*n* = 1	0.0164[2]	(2)	5°C	*n* = 0	6.30	**0.0070**	13°C
Acenaphthene	PAH 2-3 ring	0.0603	(1)	13°C	*n* = 1	0.0049	(4)	21°C	*n* = 1	6.30	**0.0096**	13°C
Acenaphthylene	PAH 2-3 ring	0.0312	(1)	13°C	*n* = 1	0.0462[3]	(4)	20°C	*n* = 0	6.30	**0.0050**	13°C
Fluorene	PAH 2-3 ring	0.0845	(1)	5-8°C	*n* = 5	0.0462[3]	(4)	20°C	*n* = 0	6.30	**0.0134**	5-8°C
Anthracene	PAH 2-3 ring	0.0976	(3)	20-24°C	*n* = 4	0.0042	(3)	20°C	*n* = 1	6.30	**0.0155**	20-24°C
Dibenzothiophene	PAH 2-3 ring	0.0502	(1)	5°C	*n* = 3	0.0462[3]	(4)	20°C	*n* = 0	6.30	**0.0080**	5°C
C1-dibenzothiophene	PAH 2-3 ring	0.0385	(1)	13°C	*n* = 1	0.0462[2]	(4)	20°C	*n* = 0	6.30	**0.0061**	13°C
C2-dibenzothiophene	PAH 2-3 ring	0.0305	(1)	13°C	*n* = 1	0.0462[2]	(4)	20°C	*n* = 0	6.30	**0.0048**	13°C
C3-dibenzothiophene	PAH 2-3 ring	0.0244	(1)	13°C	*n* = 1	0.0462[2]	(4)	20°C	*n* = 0	6.30	**0.0039**	13°C
Phenanthrene	PAH 2-3 ring	0.0549	(1)	5°C	*n* = 5	0.0080	(1)	5°C	*n* = 2	6.85	**0.0080**	5°C
C1-phenanthrene	PAH 2-3 ring	0.0433	(1)	13°C	*n* = 1	0.0080[2]	(2)	5°C	*n* = 0	6.30	**0.0069**	13°C
C2-phenanthrene	PAH 2-3 ring	0.0354	(1)	13°C	*n* = 1	0.0080[2]	(2)	5°C	*n* = 0	6.30	**0.0056**	13°C
C3-phenanthrene	PAH 2-3 ring	0.0218	(1)	13°C	*n* = 1	0.0080[2]	(2)	5°C	*n* = 0	6.30	**0.0035**	13°C
Fluoranthene	PAH 4 ring	0.0316	(1)	5°C	n = 4	0.0026	(3)	20°C	*n* = 1	6.30	**0.0050**	5°C

Pyrene	PAH 4 ring	0.0342	(1)	5°C	n = 3	0.0029	(2)	22°C	*n* = 1	6.30	**0.0054**	5°C
Benz[a]anthracene	PAH 4 ring	0.0261	(1)	8°C	n = 1	0.3153	(4)	20°C	*n* = 1	6.30	**0.0041**	8°C
Chrysene	PAH 4 ring	0.0182	(1)	5-8°C	n = 5	0.3591	(4)	20°C	*n* = 2	6.30	**0.0029**	5-8°C
Dibenzo[a,h]anthracene	PAH 5-6 ring	0.0053	(3)	20°C	n = 1	0.0116[3]	(3)	20°C	*n* = 0	6.30	**0.0008**	20°C
Benzo[a]pyrene	PAH 5-6 ring	0.0245	(1)	13°C	n = 1	0.0041	(3)	22-28°C	*n* = 3	6.30	**0.0039**	13°C
Benzo(k)fluoranthene	PAH 5-6 ring	0.0044	(3)	20°C	n = 2	0.1382	(4)	20°C	*n* = 1	6.30	**0.0007**	20°C
Benzo(g,h,i)perylene	PAH 5-6 ring	0.0015	(3)	20°C	n = 1	0.1109	(4)	20°C	*n* = 1	6.30	**0.0002**	20°C
Benzo[b]fluoranthene	PAH 5-6 ring	0.0189	(1)	13°C	n = 1	0.0907	(4)	20°C	*n* = 1	6.30	**0.0030**	13°C
indeno(1,2,3-cd)pyrene	PAH 5-6 ring	0.0245[1]	(2)	13°C	n = 0	0.0116[3]	(4)	20°C	*n* = 0	6.30	**0.0039**	13°C
Phenol	alkyl phenols	0.1023	(1)	10-13°C	n = 5	0.0145	(2)	29°C	*n* = 2	6.30	**0.0162**	10-13°C
C1-phenol	alkyl phenols	0.0573	(1)	13°C	n = 1	0.0145[2]	(3)	29°C	*n* = 0	6.30	**0.0091**	13°C
C2-phenol	alkyl phenols	0.0529	(1)	13°C	n = 1	0.0145[2]	(3)	29°C	*n* = 0	6.30	**0.0084**	13°C
C3-phenol	alkyl phenols	0.0459	(1)	13°C	n = 1	0.0145[2]	(3)	29°C	*n* = 0	6.30	**0.0073**	13°C
C4-phenol	alkyl phenols	0.0413	(1)	13°C	n = 1	0.0145[2]	(3)	29°C	*n* = 0	6.30	**0.0065**	13°C
4-methylphenol (p-Cresol)	alkyl phenols	0.0866	(1)	13°C	n = 1	0.1808	(2)	10°C	*n* = 1	6.30	**0.0137**	13°C
4-tert-butylphenol	alkyl phenols	0.0673	(1)	13°C	n = 1	0.0261	(3)	20°C	*n* = 2	6.30	**0.0107**	13°C
Pentylphenol	alkyl phenols	0.0224	(1)	13°C	n = 1	0.0206	(2)	10°C	*n* = 1	6.30	**0.0035**	13°C
4-tert-octylphenol	alkyl phenols	0.0207	(1)	13°C	n = 1	0.0343	(3)	22°C	*n* = 1	6.30	**0.0033**	13°C
Nonylphenol	alkyl phenols	0.0377	(1)	13°C	*n* = 1	0.0188	(3)	22°C	*n* = 1	6.30	**0.0060**	13°C

[1)]: No primary biodegradation rate for indeno(1,2,3-cd)pyrene was found in the literature. Therefore, the primary biodegradation rate for indeno(1,2,3-cd)pyrene is assumed to be equal to the rate of benzo[a]pyrene. The quality score for indeno(1,2,3-cd)pyrene is increased to reflect this estimation.

[2)]: No ultimate biodegradation was found in literature or databases. Therefore, the ultimate biodegradation rate shown is that of the parent compound. The quality score was increased to reflect this estimation.

[3)]: No ultimate biodegradation data was found in the literature. Therefore, the ultimate biodegradation rate shown is from the PBT Profiler database, which is also shown in Table 7.

Table 9 includes ultimate biodegradation rates at various temperatures. Bold data are rates from the extrapolated ultimate biodegradation rates (shown as bold in Table 8 as well). The majority of primary and ultimate biodegradation data was either reported at 5 °C, 13 °C, or 20 °C. Although, data for two compounds, benz[a]anthracene and dibenzo[a,h]anthracene, were not reported at these temperatures. Instead, ultimate biodegradation rate coefficients for these compounds were reported at 8 °C and 30 °C, respectively (as noted in Table 9). Ultimate biodegradation rates for temperatures not shown in bold have been calculated by a temperature correction (Q10) using Equation 6 described in Section 7.4 (Bagi et al., 2014). For dispersed oil, which was not extrapolated with the BIO/MIN FACTOR, high-quality (QS = 1) experimental data was provided at both 5°C and 13°C, so the Q10 equation (Equation 6) was only used to calculate the ultimate biodegradation at 20°C.

Table 9. Ultimate biodegradation Rates with Temperature Correction (Q10), shown as ultimate biodegradation rates (*k*). Bold data are extrapolated rates based on the BIO/MIN FACTOR (Equation 6).

Compound	Substance Group	Ultimate Biodegradation Rates		
		5°C	13°C	20°C
Dispersed Oil	Dispersed Oil	0.0024[1]	0.0094[1]	0.0153
Benzene	BTEX	**0.0063**	0.0110	0.0179
Toluene	BTEX	**0.0087**[2]	0.0152	0.0247
Ethylbenzene	BTEX	**0.0093**	0.0162	0.0264
Xylene	BTEX	**0.0069**	0.0121	0.0196
Naphthalene	Naphthalenes	**0.0164**	0.0285	0.0463
C1-naphthalene	Naphthalenes	0.0084	**0.0147**	0.0238
C2-naphthalene	Naphthalenes	0.0044	**0.0077**	0.0125
C3-naphthalene	Naphthalenes	0.0040	**0.0070**	0.0115
Acenaphthene	PAH 2-3 ring	0.0055	**0.0096**	0.0155
Acenaphthylene	PAH 2-3 ring	0.0028	**0.0050**	0.0080
Fluorene	PAH 2-3 ring	**0.0134**	0.0233	0.0379
Anthracene	PAH 2-3 ring	0.0055	0.0095	**0.0155**
Dibenzothiophene	PAH 2-3 ring	**0.0080**	0.0139	0.0225
C1-dibenzothiophene	PAH 2-3 ring	0.0035	**0.0061**	0.0099
C2-dibenzothiophene	PAH 2-3 ring	0.0028	**0.0048**	0.0079
C3-dibenzothiophene	PAH 2-3 ring	0.0022	**0.0039**	0.0063
Phenanthrene	PAH 2-3 ring	**0.0080**	0.0140	0.0227
C1-phenanthrene	PAH 2-3 ring	0.0039	**0.0069**	0.0112
C2-phenanthrene	PAH 2-3 ring	0.0032	**0.0056**	0.0091
C3-phenanthrene	PAH 2-3 ring	0.0020	**0.0035**	0.0056
Fluoranthene	PAH 4 ring	**0.0050**	0.0087	0.0142
Pyrene	PAH 4 ring	**0.0054**	0.0095	0.0154
Benz[a]anthracene	PAH 4 ring	**0.0041**[3]	0.0058	0.0095
Chrysene	PAH 4 ring	**0.0029**	0.0050	0.0082
Dibenzo[a,h]anthracene	PAH 5-6 ring	0.0001	0.0003	**0.0008**[4]
Benzo[a]pyrene	PAH 5-6 ring	0.0022	**0.0039**	0.0063
Benzo(k)fluoranthene	PAH 5-6 ring	0.0002	0.0004	**0.0007**
Benzo(g,h,i)perylene	PAH 5-6 ring	0.0001	0.0002	**0.0002**
Benzo[b]fluoranthene	PAH 5-6 ring	0.0017	**0.0030**	0.0049
Indeno(1,2,3-cd)pyrene[5]	PAH 5-6 ring	0.0022	**0.0039**	0.0063
Phenol	alkyl phenols	0.0093	**0.0162**	0.0264
C1-phenol	alkyl phenols	0.0052	**0.0091**	0.0148
C2-phenol	alkyl phenols	0.0048	**0.0084**	0.0136

C3-phenol	alkyl phenols	0.0042	**0.0073**	0.0118
C4-phenol	alkyl phenols	0.0038	**0.0065**	0.0106
4-methylphenol (p-Cresol)	alkyl phenols	0.0079	**0.0137**	0.0223
4-tert-butylphenol	alkyl phenols	0.0061	**0.0107**	0.0173
Pentylphenol	alkyl phenols	0.0020	**0.0035**	0.0058
4-tert-octylphenol	alkyl phenols	0.0019	**0.0033**	0.0053
Nonylphenol	alkyl phenols	0.0034	**0.0060**	0.0097

[1)]: Ultimate biodegradation rate for dispersed oil at 5 & 13°C was calculated from experimental data.
[2)]: Ultimate biodegradation rate for toluene was calcuated at temperatures 2-10°C.
[3)]: Ultimate biodegradation rate for benz[a]anthracene was calcuated at 8°C.
[4)]: Ultimate biodegradation rate for dibenzo[a,h]anthracene was calculated at 30°C.
[5)]: Ultimate biodegradation rates for indeno(1,2,3-cd)pyrene are based on benzo(k)fluoranthene.

9 Conclusion

The objective of our review and subsequent calculations were to enhance our knowledge of relevant ultimate biodegradation rates for the DREAM model. Finalized data are included in Tables 8 and 9. The best available data to date on primary and ultimate biodegradation rates are included in these tables. Therefore, Tables 8 and 9 are intended to be utilized as a source for input into the DREAM model.

The ultimate biodegradation rates provided in this report were found to vary considerably from the previously published rates by NOROG (2003). As mentioned previously, the data presented in NOROG (2003) utilized a single compound to represent a whole substance group. When we compare the ultimate biodegradation rates between the representative compounds in NOROG (2003) to the new rates provided in this report, we note that some rates are slower while some rates are faster. Table 10 compares the ultimate biodegradation rates between the data provided in NOROG (2003) to the data provided in this report, at the same temperature (13°C). The ultimate biodegradation half-lives calculated in this report for ethylbenzene, naphthalene, phenanthrene, p-Cresol, and pentylphenol were substantially higher, while the half-lives for chrysene and nonylphenol were lower.

Table 10. Comparison between previously reported ultimate biodegradation rates from NOROG (2003) and the finalized data provided in this report (taken from Table 9; 13°C). Both data sets report ultimate biodegradation rates at 13°C.

		Previous Data (NOROG, 2003)		New Data (this report)	
Compound	Substance Group	Half-life (days)	k-value	Half-life (days)	k-value
Ethylbenzene	BTEX	0.5	1.39	43	0.016
Naphthalene	Naphthalenes	1.5	0.462	24	0.028
Phenanthrene	PAH 2-3 ring	17	0.041	50	0.014
Chrysene	PAH 4-5 ring	350	0.002	138	0.005
p-Cresol	Phenol C0-C3	1.2	0.578	50	0.014
Pentylphenol	Phenol C4-C5	10	0.069	195	0.004
Nonylphenol	Phenol C6-C9	350	0.002	116	0.006

The majority of PW compounds did not have reliable ultimate biodegradation rates reported in the literature. Therefore, we estimated a compound's ultimate biodegradation rate from its primary biodegradation rate. While we are confident in our analysis, most of the data presented in Tables 8 and 9 are estimates and we therefore recommend for ultimate biodegradation experiments to be conducted for the majority of these compounds. Priority should be given to indeno(1,2,3-cd)pyrene, which (to our knowledge) had no primary or ultimate biodegradation data reported in the literature. In addition

to indeno(1,2,3-cd)pyrene, four other compounds did not have quality primary biodegradation data reported in the literature: anthracene, dibenzo[a,h]anthracene, benzo(k)fluoranthene, and benzo(g,h,i)perylene. Since the calculated ultimate biodegradation rates are dependent upon the quality of the primary biodegradation data, we recommend for primary biodegradation experiments to be conducted on these compounds as well.

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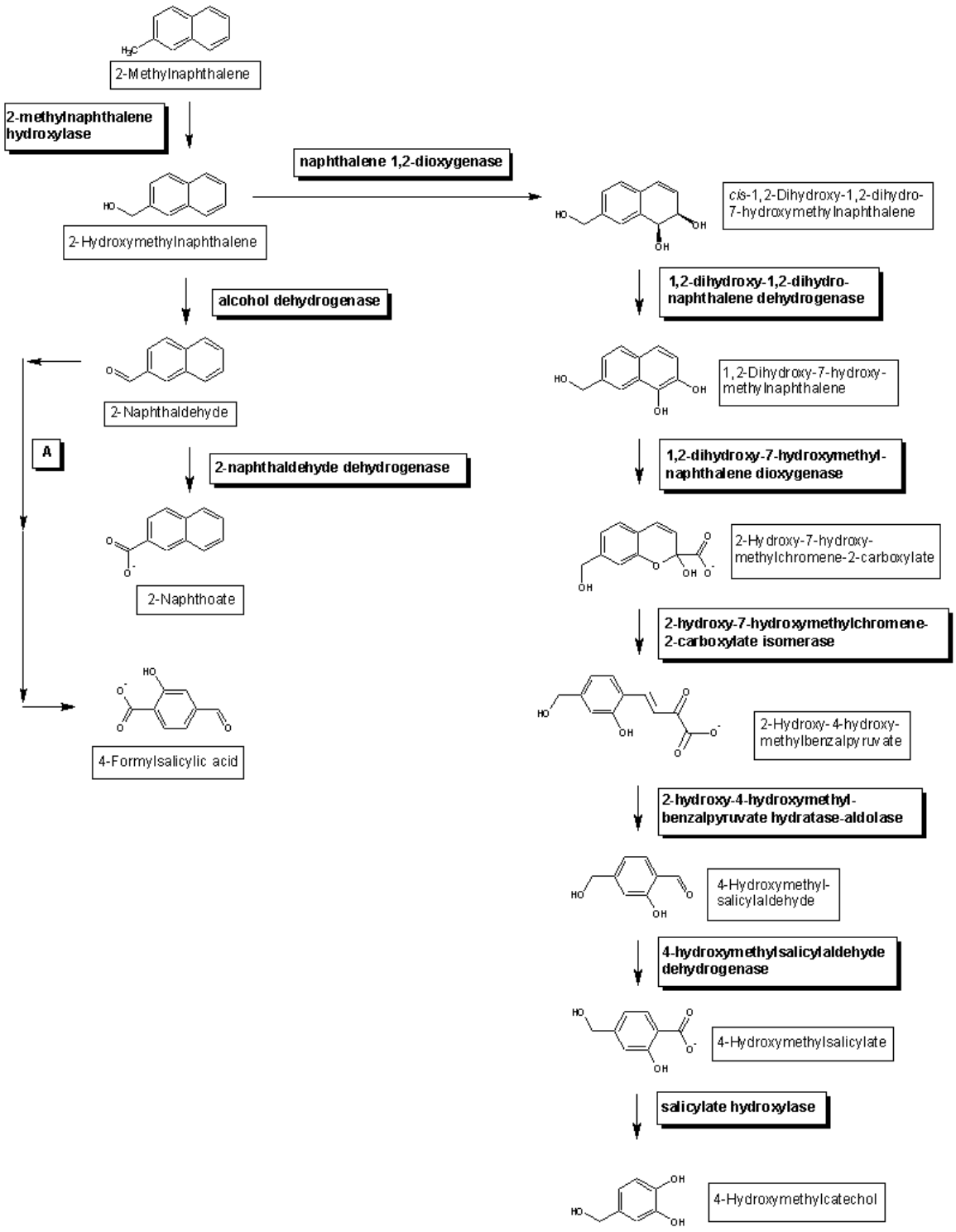
Appendix 1. Biodegradation of 2-methylnaphthalene to 4-hydroxymethylcatechol by *Pseudomonas putida* CSV86 (Mahajan et al., 1994), as described in the EAWAG Biocatalysis and Biodegradation Database (http://eawag-bbd.ethz.ch/index.html)



Appendix 2. Criteria for classification of substances as persistent, bioaccumulating and toxic (PBT), and for classifying them as very persistent, very bioaccumulating (vPvB), as described in the Technical Guidance Document (TGD, 2003).

Criterion	PBT criteria	vPvB
P	Half-life > 60 d in marine water or > 40 d in freshwater* or half-life > 180 d in marine sediment or > 120 d in freshwater sediment[A)]	Half-life > 60 d in marine- or freshwater or >180 d in marine or freshwater sediment
B	BCF > 2 000	BCF > 5 000
T	Chronic NOEC < 0.01 mg/l or CMR or endocrine disrupting effects	Not applicable

[A)] For the purpose of marine environmental risk assessment half-life data in freshwater and freshwater sediment can be overruled by data obtained under marine conditions.