

Application of the target lipid and equilibrium partitioning models to non-polar organic chemicals in soils and sediments



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ABSTRACT

The Target Lipid Model (TLM) provides a framework for deriving predicted no effect concentrations (PNEC) for nonpolar organic chemicals to organisms in the environment. This approach has been used to perform environmental risk assessment of individual hydrocarbons as well as complex petroleum substances. The TLM is based primarily on data for aquatic test organisms and this work evaluates the potential for extending the TLM to soil and sediment using Equilibrium Partitioning (EqP) theory.

Literature data for other nonpolar organics were compiled for acute and chronic exposures to invertebrates in soils and sediments. New data were generated according to OECD guidelines (CONCAWE, 2011 and 2012) to evaluate soil and sediment dwelling organisms and to test potential toxicity cut-offs for high log K_{ow} compounds. The default TLM was applied to these data using EqP to develop critical target lipid body burdens (CTLBB) including associated uncertainty in the model application.

Comparison of the CTLBBs for soil and sediment species to CTLBBs from the larger TLM database for aquatic organisms showed little difference in the relative sensitivity between these two groups of species within the uncertainty of the model and experimental data. Furthermore, the acute to chronic ratios (ACRs) for soil and sediment tests were within the range of ACRs for aquatic organisms exposed to nonpolar organic chemicals.

The TLM-derived PNEC applied to these data, also, demonstrated sufficient level of protection approximately 95% of data above PNEC, even for chemicals up to log K_{ow} 6. For chemicals with log K_{ow} >6 an increasing incidence of no observed toxicity consistent with the dataset for aquatic organisms was observed. The duration of the pre-equilibration step was important for some chemicals. For example, toxicity was observed for these chemicals following short pre-equilibration times (<2 days), whereas no toxicity was observed for spiked soils that had been aged up to 7 weeks prior to exposure.

In conclusion, the work shows that the TLM can be extended to the soil and sediment compartments using the EqP for the purposes of a tier 1 risk assessment.

KEYWORDS

Target Lipid Model, Equilibrium Partitioning Model, Soil and Sediment PNECs

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SUMMARY

In environmental risk assessments Equilibrium partitioning (EqP) approach is often used to extrapolate environmental quality benchmarks derived from aquatic test data to soils and sediments and can be used in REACH (ECHA, 2008 and 2012). A literature review has been conducted to compile available soil and sediment toxicity data for petroleum hydrocarbons and other non-polar organic chemicals. This information was used to validate the combination of the EqP-theory and the Target Lipid Model (TLM) for its application to soils and sediments (Di Toro et al, 2000; Di Toro and McGrath, 2000). The TLM is a Quantitative Structure-Activity Relationship (QSAR) model that relates chemical structures to their toxicity using critical target lipid body burdens for chemicals with a narcotic or base-line mode of action. This framework uses toxicity data developed using standard methods to derive environmental quality guidelines based on species sensitivity distribution. The EqP model has been used with success to extrapolate water-based screening values to soils and sediments (Di Toro and McGrath, 2008 and 2012).

The advantage of this approach is that it makes use of the rigorously developed modelling framework of the TLM. Furthermore, the TLM has been used to derive environment quality guidelines using a statistical extrapolation approach. This results in a predicted hazardous concentration that affects 5% of exposed organisms (HC5), or alternatively is protective of 95% of organisms. This report provides technical validation for the application of the HC5 as the PNEC in the risk assessments for emissions of petroleum substances to soils and sediments performed under REACH using PETRORISK (Redman et al, 2013).

A database of critical target lipid body burdens (CTLBB) was used to develop a database for sediment- and soil-dwelling organisms for comparison to the species sensitivity distribution (SSD) for aquatic organisms (e.g. fish, daphnids, algae, etc.). It is assumed that the SSD for aquatic organisms can be used derive Tier 1 screening levels for soil and sediment environments. There is some inherent uncertainty in this assumption, since there are few comparisons of soil/sediment and aquatic species on a CTLBB-basis. This study evaluated this assumption by comparing the SSD for soil and sediment species to that of aquatic species to validate the combination TLM-EqP framework.

The results showed that the distribution of CTLBBs from the two datasets overlapped with similar range in observed sensitivity and support the general conclusion that the relative sensitivity of the two groups of species is similar. Factors such as test duration and data availability explain some of the variability between the two datasets (aquatic vs. soil and sediment).

Importantly, this study demonstrated that the HC5-EqP framework can be applied to soil and sediments to derive reasonably protective Soil (Sediments) Quality Guidelines (SQGs) or Risk Based Screening Levels (RBSLs). The available chronic No Observed Effects Concentrations (NOECs) were consistent with the EqP-HC5 (e.g. 95% of data above HC5) indicating that the TLM-derived HC5 is a suitable benchmark for assessing risk of petroleum substances in sediment and soil media. Therefore, extension of the TLM using EqP provides a technically sound and consistent basis for extrapolating the HC5 that was derived from aquatic organisms.

It is noted that additional data would be helpful to reduce the uncertainty for some of the endpoints and CTLBBs derived in the present study. In particular, the uncertainty

around *Chironomus riparius* and *Eisenia andrei* could limit the use and interpretation of data for these test species for further hazard assessments.

Further study on the fate and effects of high log K_{ow} chemicals may be justified to better understand processes that control the bioavailability hydrophobic chemicals in soils and sediments. While this is relevant for interpreting toxicity data from soil or sediments exposures of poorly water soluble chemicals at high concentrations (e.g. >500 ppm) since, in some case, the likely presence of free product phases could influence the results of those tests, in the context of risk assessment this is not necessary. Environmental quality standards should be protective of physical oiling (Verbruggen, 2004) however this mechanism of toxicity (e.g. suffocation, etc.) is outside the scope of the TLM-EqP. A TLM-EqP framework that accounts for aging, i.e. the reduction of the bioavailable fraction of the contaminants, could help interpret those results (e.g. degradation, adsorption and absorption, kinetics of equilibration, effect levels vs. solubility limits).

Lastly, several test species evaluated here are commonly used in water only tests (e.g. *Chironomus riparius, Hyalella azteca*). Furthermore, several studies report effect levels in terms of pore water concentration data. Analysis of these data could provide more direct comparison of TLM-derived CTLBBs to the aquatic dataset since it avoids potential uncertainty related to application of the EqP model. These data may also help resolve discrepancies in the reported effects data discussed above by providing another line of evidence for evaluating soil and sediment effects data.

1. INTRODUCTION

The Target Lipid Model (TLM) is a QSAR model that relates chemical structure to toxicity using critical target lipid body burdens (CTLBBs) for chemicals with a narcotic mode of action. This framework uses toxicity data developed using standard methods to derive environmental quality guidelines based on species sensitivity distribution. The Equilibrium Partitioning theory (EqP) model has been used with success to extrapolate water-based screening values to soils and sediments (Redman and McGrath, 2006; Di Toro and McGrath, 2000; US EPA, 2003; ECHA, 2012).

In order to address the extrapolation of the TLM to the soils and sediment compartments, for the purposes of risk assessment of Petroleum Products a series of experimental studies were commissioned by CONCAWE to assess the effects of specific hydrocarbons to soil and sediment organisms (CONCAWE, 2011 and 2012).

Subsequently, the CONCAWE Ecology Group requested HydroQual to conduct a literature review to assess the potential for extrapolating the TLM to soil and sediment organisms utilizing the new data and any data that may be present in the open literature. HydroQual have subsequently conducted a literature review and compiled available soil and sediment toxicity data for petroleum hydrocarbons and other non-polar organic chemicals.

This information was then used to validate the combination of the EqP and the Target Lipid Model (TLM) for its application to soils and sediments (Di Toro et al, 2000; Di Toro and McGrath, 2000; HydroQual, 2010). The advantage of this approach is that it makes use of the rigorously developed modelling framework of the TLM. Furthermore, the TLM has been used to derive environment quality guidelines using a statistical extrapolation approach. This results in a predicted hazardous concentration that affects 5% of exposed organisms (HC5), or alternatively is protective of 95% of organisms. The full report is given in **Appendix 1**.

2. RESULTS

The goal of this work was to develop a database of critical target lipid body burdens (CTLBB) for sediment- and soil-dwelling organisms and to compare the resultant species sensitivity distribution (SSD) to that for aquatic organisms (e.g. fish, daphnids, algae, etc.).

As described in HydroQual, 2013 (**Appendix 1**), a literature search was conducted to compile available soil and sediment toxicity data. The search covered petroleum hydrocarbons and other non-polar organic chemicals. The data were evaluated for reliability and acceptable test/exposure concentrations and are included in the report. The results were used to generate SSDs for soil and sediment combines, which could then be compared to that for the aquatic compartment. It was necessary to do this as the data for sediment was limited, however, the key assumption of Equilibrium Partitioning is that all phases are in equilibrium, i.e. soil (sediment), organism and water, and therefore effects may be described by the pore water concentration to which the test species is exposed.

The modelling approach adopted, was to use the EqP with the existing aquatic HC5 to derive a soil/sediment quality guideline. By combining the EqP, the TLM and the data obtained for soil and sediment organisms, a CTLBB database could be compiled.

Using this approach, a CTLBB database was generated covering 26 species, including plants, earthworms, and springtails, as well as, other terrestrial and benthic invertebrates. However, seven of these are based on only one data point and a further six are based on two to four data points. In general the toxicity data were within a factor 4 of the TLM predictions, consistent with the variability in the aquatic TLM database (Di Toro et al, 2000; McGrath and Di Toro, 2009).

2.1. MORTALITY

Specific points noted were;

- *Hyalella azteca* the data were showed a large variation, which may be explained by the two different data sources, one of which included a 60 day equilibration period.
- *Eisenia andrei* these data fell into two groups, suggesting two different populations and sensitivities, which may make interpretation difficult.
- Chironomus riparius toxicity data for this organism are variable and conflicting. Analysis of water only data suggest that this species has average sensitivity, while the chronic toxicity data in sediment range from insensitive to very sensitive with NOECs that span over two orders of magnitude with no discernible trend between endpoint or chemical properties. Additional experimental work would be required to reconcile these differences.

2.2. CRITICAL TARGET LIPID BODY BURDEN

The report notes that within the limitations of the datasets, i.e. some with as few as one data point, the variability of tests and the model, the soil/sediment CTLBB database demonstrates to be of a similar order of magnitude and consistent with the comparisons for aquatic organisms (Di Toro et al, 2000).

The median CTLBB for the soil/sediment species was 59 μ mol/g lipid versus 119 μ mol/g lipid for the aquatic database. This difference may be partly due to the longer-term nature of soil/sediment studies and possible variability in the experimental data or modeling assumptions.

In general the report shows that the two datasets, aquatic and soil/sediment are similar in terms of distribution, range of the datasets and the general shape of the SSD curves.

2.3. ACUTE TO CHRONIC RATIOS

Where paired data of e.g. LC50 and NOECs were available ACRs were calculated. It appeared possible to establish 62 ACRs, covering 21 chemicals and 11 different species. The report notes that the range and distribution of the ACRs is similar between the two datasets (aquatic and soil/sediment), which demonstrates a similar toxic mechanism is occurring.

The median ACR obtained from the soil/sediment database was 3.7, compared to 4.5 for the aquatic database. This difference may be due to the longer term nature of the tests conducted, but may also be due to uncertainties in the experimental and modelling methods.

2.4. CHRONIC TOXICITY AND HC5

The chronic data for 33 organisms, covering plants, invertebrates and microorganisms were compiled and compared to the HC5-EqP derived value. The chronic data compared favourably to the HC5-EqP with 10 of the NOECs out of a total of 188 being below the HC5-EqP. As this is 5.3%, this is consistent with the target of 5%, of which the HC5 is protective.

2.5. PRE-EQUILIBRATION

It is noted in the report that the toxicity of chemicals may reduce over time due to a number of factors, including diffusion into the soil matrix, equilibration with voids and degradative processes, all of which are referred to as aging. In the data sets examined, a reduction in toxicity was observed for aliphatics but not for the PAHs tested. However, the conclusions should be treated with some caution as the impact of soil/sediment chemistry, pre-equilibration and the log K_{ow} of the chemicals tested, plus that some of the data were based on nominal concentrations, will all impact these findings.

3. DISCUSSION AND CONCLUSIONS

The work reported derives soil/sediment quality guidelines based on the aquatic effects database using the EqP. The application of the TLM and EqP led to the generation of 26 new CTLBBs for plants and invertebrates. Although the ACR for the soil/sediment data set was slightly lower than that for the aquatic database (3.7 and 4.5 respectively), the two SSDs are sufficiently similar to conclude that the two datasets have similar levels of sensitivity.

The available chronic data from soil/sediment organisms are shown to be consistent with the EqP-TLM, confirming that extending the TLM using the EqP for soil/sediment risk assessments is sound and provides a level of protection that is conservative enough for a Tier 1 risk assessment.

4. GLOSSARY OF TERMS

Acute to Chronic Ratio (ACR)	The ratio of the concentrations of an acute effect (e.g. LC50) to that of a chronic effect (e.g. NOEC), always in the same species.
Bioconcentration Factor (BCF)	The ratio of the concentration of a substance in an aquatic organism to that in the water to which the organism is exposed.
Critical Target Lipid Body Burdens (CTLBB)	The concentration of a substance in an organism at which effects are expected, usually expressed in molar terms.
Dissolved Organic Carbon (DOC)	The concentration of dissolved organic carbon in soil, sediment or water.
Effect Concentration 10 (EC10)	The concentration of a substance at which it is calculated that 10% of the animals will be affected, based on the observed results in a study.
Equilibrium Partitioning theory (EqP)	Is a model that has been used with success to extrapolate water-based screening values to soils and sediments (Redman and McGrath, 2006, Di Toro and McGrath 2000; US EPA, 2003; ECHA, 2012).
HC5	A predicted hazardous concentration that affects 5% of exposed organisms or alternatively is protective of 95% of organisms.
L(E)C50	The lethal (effect) concentration of a substance at which 50% of the organisms exposed to that substance are killed (effected).
Lowest Observed Effect Concentration (LOEC)	The lowest concentration in a study at which effects were observed.
Octanol-Water Partition Coefficient	The ratio of the concentration of a substance in octanol to that in water, when the two are in equilibrium with each other. Often expressed as log K_{ow} or P_{ow} .
No Observed Effect Concentration (NOEC)	The concentration of a substance below which no effects to an exposed organism were observed in a study.
PETRORISK	A model, coded in Excel [®] which conducts the environmental risk assessment of petroleum products using the principles outlined in REACH guidance.
Predicted No Effect Concentration (PNEC)	This is the predicted concentration in the environment below which effects to organisms would not be expected.
Risk Based Screening Levels (RBSLs)	Indicative concentrations, designed to protect the organisms of concern, which could also be humans.

Standard Error (SE)	The standard deviation of the sampling distribution involved in assessing a sub-group of a population.
Soil (or sediment) Organic Carbon (SOC)	The concentration of organic matter in the soil (or sediment).
Soil (or sediment) Quality Guideline (SQG)	A concentration, derived from e.g. the HC5 that is considered to be equivalent to the PNEC.
Species Sensitivity Distribution (SSD)	In the context of the TLM, this is a plot of the CTLBBs against the species for which these CTLBBs exist.
Soil (Sediments) Quality Guidelines (SQGs)	Are a series of measurements and values used by regulators to measure contamination of the soil and designed to indicate whether the soil/sediment is contaminated.
Target Lipid Model (TLM)	Is a QSAR model that relates chemical structure to toxicity using critical target lipid body burdens for chemicals with a narcotic mode of action.

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APPENDIX I HYDROQUAL PROJECT REPORT TO CONCAWE

CONCAWE

Application of the Target Lipid and Equilibrium Partitioning Models to Non-Polar Organic Chemicals in Soils and Sediments

July 2013



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INTRODUCTION

A literature review has been conducted to compile available soil and sediment toxicity data for petroleum hydrocarbons and other non-polar organic chemicals. This information was used to validate the combination of the Equilibrium Partitioning theory (EqP) and the Target Lipid Model (TLM) for its application to soils and sediments (Di Toro et al., 2000a and 2000b; Redman et al., 2009). The TLM is a QSAR model that relates chemical structure to toxicity using critical target lipid body burdens for chemicals with a narcotic mode of action. This framework uses toxicity data developed using standard methods to derive environmental quality guidelines based on species sensitivity distribution. The EqP model has been used with success to extrapolate water-based screening values to soils and sediments (Redman and McGrath 2006, Di Toro and McGrath 2000; EPA 2008; ECHA 2012). The advantage of this approach is that it makes use of the rigorously developed modeling framework of the TLM. Furthermore, the TLM has been used to derive environment quality guidelines using a statistical extrapolation approach. This results in a predicted hazardous concentration that affects 5% of exposed organisms (HC5), or alternatively is protective of 95% of organisms. This report provides technical validation for the application of the HC5 as the PNEC in the risk assessments for emissions of petroleum substances to soils and sediments performed under REACH using PETRORISK (CONCAWE 2011).

The goal of this work was to develop a database of critical target lipid body burdens (CTLBB) for sediment- and soil-dwelling organisms for comparison to the species sensitivity distribution (SSD) for aquatic organisms (e.g., fish, daphnids, algae, etc.). It is often assumed that the SSD for aquatic organisms is applicable to soil and sediment environments for derivation of soil and sediment screening guidelines (Redman and McGrath 2006). There is some uncertainty inherent in this assumption since there are few comparisons of soil/sediment and aquatic species on a CTLBB-basis. Further, most generic risk assessments use some form of EqP to estimate soil/sediment quality guidelines from water-based guidelines. This study evaluates this assumption by comparing a modeled species sensitivity distribution for soil and sediment species to the relative sensitivity of aquatic species to validate the combination TLM-EqP framework.

METHODS

2.1 LITERATURE SEARCH

Existing databases (Versonnen et al., 2007; Redman and McGrath, 2006; McGrath and Di Toro 2006) were used as the starting point of the literature search but extended to include literature sources identified from the peer-reviewed literature. As an example, these additional searches focused on search terms that included "hydrocarbon," "sediment," "Equilibrium Partitioning," "toxicity" and others, which resulted in hundreds of hits. A full list of the articles reviewed as part of this study are given in the Appendix 1 bibliography, though many were not included in this analysis due to their use of complex mixtures, incomplete chemistry or reliance on nominal concentrations, poor data quality, or lack of soil or sediment organic carbon (SOC) measurements. Available reports from petroleum trade associations and government agencies were also used as part of this compilation.

The initial focus of the literature search was solely on petroleum hydrocarbons (alkanes, PAH, BTEX, etc.). However, this resulted in partial datasets where only a few toxicity data were identified for any given organism being evaluated. In an effort to fill out these datasets, the literature search was expanded to include all non-polar organic chemicals (e.g., halogenated hydrocarbons) similar to other similar efforts with aquatic species (Di Toro et al 2000; Redman et al 2007; McGrath et al 2004).

The data were evaluated for reliability and acceptable test/exposure conditions. The criteria for inclusion in the dataset included measured concentrations, reporting of clear endpoints, acceptable controls, less than the theoretical solubility limit, and reported SOC concentrations. Toxicity data for a variety of soil and sediment dwelling organisms including invertebrates (e.g., earth worms, springtails, midges, amphipods), plants and microbial endpoints (e.g., soil nitrification) were compiled in Table 3.

The results from data analysis of soil and sediment exposures were used together for comparing relative species sensitivity between compartments (e.g., aquatic vs. soil and sediment). This, in part, is due to the lower number of toxicity data for sediment organisms but due to the EqP assumption that all phases are in equilibrium with the porewater in sediment or aqueous soil solution phase, the modeling assumptions and data analysis follow the same pattern, so it is appropriate to combine the results from soil and sediment compartments. Soil and sediment results will be identified in figures and tables for comparisons. For chronic toxicity data, preference was given to NOEC data though LOECs and EC10 data were used where NOECs had not been reported. Endpoints with direct ecological relevance were included (e.g., mortality, reproduction, growth). The lowest effect level was used for comparison to the HC5 in studies where multiple NOECs were reported for different endpoints. For computing acute to chronic ratios, preference was given to data from the same study to maintain consistency in the experimental methods.

2.2 MODELING APPROACH

The objective of this analysis was to evaluate the use of the published TLM (McGrath and Di Toro 2009) and EqP models (Di Toro 1991) for application to soil- and sedimentdwelling organisms. These models were used here to derive critical target lipid body burdens (CTLBBs) based on the acute soil and sediment toxicity data for comparison to CTLBBs derived for aquatic organisms. This was done by solving for the CTLBB using the standard aquatic TLM and the EqP models. One objective of this work is to evaluate the potential for using previously established models for setting environmental quality criteria.

All physico-chemical properties, including $\log K_{\text{OW}}$, for the compounds in this analysis were derived from SPARC for consistency with the initial development of the TLM for aquatic species. The mortality data used to calculate a CTLBB for a given organism were restricted to similar exposure durations to maintain internal consistency within the database.

The aquatic TLM is a quantitative structure activity model (QSAR) that is based on the chemical nature of a compound (e.g., BCF $\sim K_{ow}$) and the individual sensitivity of the organism being evaluated. It has the following generic form

$$\log C_{W}^{*} = -0.936 \log K_{OW} + \Delta c + \log C_{L}^{*}$$
(1)

where C_w^* is a critical aqueous effects concentration (e.g., LC50, mmol/L), -0.936 is the universal narcosis slope and octanol-water partition coefficient (log K_{OW}) are used for estimate the lipid-water partitioning of a chemical. The Δc is a chemical class correction factor applied to mono- and poly-aromatic hydrocarbons (MAH and PAH) and chlorinated compounds and C_L^* is the CTLBB. Development of the TLM for aquatic species is documented elsewhere (McGrath and Di Toro 2009; McGrath et al 2004; Di Toro et al 2000).

The EqP model (Di Toro 1991) is another $\log K_{OW}$ -based QSAR that has been used successfully to convert water quality standards to sediment quality guidelines (Di Toro and McGrath 2000; US EPA 2008).

$$\log K_{OC} = 0.983 \log K_{OW} + 0.000283 \tag{2}$$

where the organic carbon-water partition coefficient (K_{OC} , L/kg OC) is related to the log K_{OW} of a given compound. This relationship was used to convert critical water concentrations, C_w^* (mmol/L), to critical sediment (or soil) effect concentrations, C_s^* (mmol/kg OC) to that are used to calculate the CTLBB.

$$\log C_s^* = \log C_w^* + \log K_{OC} \tag{3}$$

The log C_L^* , or CTLBB, was calculated for each valid data entry by combining equations 1, 2, 3 and solving for log C_L^* . The average log C_L^* for all of the valid data with log K_{OW} > 3 were used to establish the CTLBB for an organism. Chemicals with log K_{OW} < 3 were subject to losses through volatilization or degradation and resulted in a strong bias in the results, see figures and text below.

$$\log C_L^* = \log C_S^* - 0.047 \log K_{OW} - \Delta c - 0.000283 \tag{4}$$

The uncertainty in the model estimates of the CTLBB were evaluated using estimated 95% confidence intervals (i.e., 1.96 * SE) of the regression (eq 4). The uncertainties were compared to the CTLBBs and SEs for the aquatic dataset to identify possible trends and similarities.

An adjustment was used to correct for the solid and moisture content of the sediments and soils consistent with Fuchsman (1996). This adjustment is meant to account for highly soluble chemicals (e.g., benzene and lighter) when calculating bulk sediment concentrations (e.g., porewater + solids). There were no chemicals in this range for validation but it is presented for reference.

Previous work with complex mixtures suggests that the bioavailability of very high $\log K_{OW}$ compounds (Redman et al 2012) is limited possibly due to the presence of DOC or other phases that bind very hydrophobic compounds or slow the kinetics of uptake and hence limit the ability of very large compounds to partition into target lipid of an aquatic organism. This is modeled by setting an upper limit on the log lipid-water partition coefficient of 6. This

relationship was evaluated for application to the soil and sediment toxicity data be replacing $\log K_{OW}$ in Eq. 1 with $\log K_{LW}$ that is described here.

$$\log K_{LW} = \langle \frac{\log K_{OW}, for \log K_{OW} < 6}{6, for \log K_{OW} > = 6}$$
(5)

Chronic toxicity data were evaluated with the HC5, which is a statistical extrapolation that is used as a conservative guideline for evaluating water, sediment and soil quality. The HC5 accounts for variability in the CTLBB database, the acute-to-chronic ratios that are used for chronic predictions and in the universal narcosis slope. This approach provides a rigorous and defensible method for establishing protective water quality guidelines that can be extrapolated to sediment quality guidelines using the EqP framework in Eq. 2 and 3. The HC5 that was derived with the aquatic dataset was converted into a sediment quality guideline for this work using the standard EqP relationship, Eqn 3.

$$\log HC5 = -0.936 \log K_{OW} - \log ACR + \Delta c + \log CTLBB - k_Z \sqrt{V_{slope} \log K_{OW}^2 + V_{\log CTLBB} + V_{\log ACR}}$$
(6)

Where the HC5 is calculated using the median slope (-0.936), ACR (3.83) and CTLBB (119), which is further modified by the sample size extrapolation factor (k_Z ; 2.3) and the variance ($V_{logCTLBB}$ 0.105, V_{logACR} 0.112 of these parameters. Additional details on the derivation of the HC5 extrapolation are found elsewhere (McGrath et al 2004; McGrath and Di Toro 2009). In this study we applied the HC5 parameterized by McGrath et al 2009 to be consistent with the present risk assessment in PETRORISK (Redman et al 2013). We acknowledge that this is a slight inconsistency since the ACRs used in that derivation is based on hydrocarbons whereas this study used data for all nonpolar organics, consistent with the McGrath et al 2004 derivation. However, the 2009 and 2004 derivations provide nearly identical predictions so this discrepancy is not expected to introduce significant error to the results and conclusions.

RESULTS AND DISCUSSION

3.1 MORTALITY

Mortality data were compiled for various soil- and sediment-dwelling organisms to derive a database of CTLBBs. This initial compilation was limited in the number of data available for each of the species identified in the literature search (Figure 1, Table 1), which affects the confidence in the CTLBB estimate. For consistency with the aquatic datasets, only mortality data were used to derive CTLBBs for invertebrates and growth data were used for plant species. Other endpoints (e.g., reproduction, growth) were considered for chronic toxicity comparisons to the HC5.

The mortality dataset resulted in 26 new CTLBBs for plants, earthworms, springtails and other terrestrial and benthic invertebrates but 13 of those are based on less than four LC50s and 7 of those were based on only one entry (Table 1). Of the remaining CTLBBs, some show consistent behavior between the model and data (e.g., *L. rubellus, F. fimetaria, R. abronius, T. pratense, E. fetida, E. veneta*) even between studies and soil/sediment types (Table 2). However, data for other organisms varied by several orders of magnitude and show inconsistent results (e.g., *E. andrei, E. crypticus, F. candida, H. azteca*). However, most toxicity data are within a factor of 4 of the TLM predictions, consistent with the variability in the aquatic TLM database (Di Toro et al 2000; McGrath and Di Toro 2009).

The measured data are generally consistent with the model predictions (Figure 1a-c) in that the slope of the acute toxicity data vs. $\log K_{OW}$ is generally very shallow, consistent with TLM-EqP predictions (Eq 4). The mortality data ranged from 0.7 to >2500 mmol/kg OC with typical LC50s near 35 mmol/kg OC (Table 2) over a relatively narrow range in logKow (3-7). The duration of the exposures varied from 10 days to more than 40 days but typical exposure times were between 14 and 28 days depending on the organism and endpoint. Mortality data were available for natural and artificial soils/sediments but no apparent systematic differences can be noted since there are not many chemicals or species that were tested in both media.

There were few data available (n=4) for *H. azteca*, which had a large degree of variation (SE of logCBB = 0.93, highest of other entries). The effect data are derived from two primary studies; Suedel et al (1993) and Driscoll and Landrum (1997), both of which used Fluoranthene in 10 day exposures. The Suedel et al 1993 LC50 data from three sediments center around 5 mmol/kg OC whereas the LC50 from Driscoll and Landrum (1997) is 311 mmol/kg OC. This difference is possibly due to the use of an extended pre-equilibration period of 60 days for the Driscoll and Landrum (1997) LC50 compared to a <1 day pre-equilibration period for

the Suedel et al (1993) data. Since this species is commonly used a monitoring programs additional toxicity data for a wider variety of chemicals spanning $\log K_{OW}$ 3-8 would be helpful to establish a CTLBB with more confidence for this species and endpoint.

The LC50 data for *E. andrei* are fall into two general groupings based on study and author. For example, Hudrzan and Lanno 2009 report LC50s for a series of chlorinated benzenes that range from ~1 to 7 mmol/kg oc. Other datasets from Belfroid et al 1993; 1994; and van Gestel and Ma 1993; 1990 report LC50s that range from ~20 to 300 mmol/kg OC. It appears that there might be two populations of *E. andrei* with different sensitivities. Each population was generally consistent with the TLM-EqP predictions and exhibit the same trend of increasing LC50s at log K_{OW} <4 that was observed in other datasets. The Belfroid et al 1993; 1994 and van Gestel and Ma 1990; 1993 datasets were used to derive a CBB since there are more data across several studies, which provide a well behaved dataset for modeling CBBs.

There is one LC50 for tetrachlorobenzene from Hurdzan and Lanno (2009) that is approximately an order of magnitude lower than the LC50s for other chlorinated benzenes in that study as well as the other studies. Hurdzan and Lanno (2009) do not discuss this discrepancy and instead focus on results for tissue residues and passive sampling devices, which do not show this degree of variability. The available data for this endpoint are mainly chlorinated benzenes, which resulted in some uncertainty regarding species sensitivity between studies. Therefore, additional toxicity data with hydrocarbons, including PAH, would be needed to characterize the sensitivity of this species for hazard assessment screening

The logCTLBB (1.17) for *C. riparius* is the lowest value in the dataset for mortality measured after 28 days of exposure (Table 1) but is similar in sensitivity (e.g., with factor of 2 of other sensitive endpoints) to several other CTLBBs in the database and so does not appear to be an outlier. This endpoint is based on three LC50s for anthracene and phenanthrene (Paumen et al 2008; Marinkovic et al 2012), which despite having similar log K_{OW} (4.55 and 4.58, respectively) have LC50s that vary by a factor of nearly 5. While this is within the expected level of uncertainty for toxicity tests, there are few data to judge the robustness of this endpoint. However, an analysis of an aquatic exposure of hydrocarbons to *C. riparius* (Roghair et al 1994) resulted in a logCTLBB nearer to 2.4 based on 2-day exposures to a series of alcohols, chlorinated benzenes and toluene (Figure 4). This is quite different than the CTLBB derived from sediment exposures. Additional validation work is needed to reconcile available water-only and soil/sediment tests.

Despite these sources of uncertainty and variability in the TLM-EqP model application appeared to provide reasonably good descriptions of the mortality dataset. The extension of the TLM to soils and sediments using EqP provides a method for quantitatively comparing the relative sensitivity of these species with aquatic species using CTLBBs.

3.2 CRITICAL TARGET LIPID BODY BURDEN

The mortality data were used to calculate CTLBBs using the TLM and EqP approach (Eq. 4). Since the default TLM and EqP models were used in this analysis it was possible to derive a CTLBB for organism-specific datasets with as few as one toxicity data point. This results in a CTLBB estimate of unknown variability. The variability in the CTLBBs was evaluated using the standard errors to estimate 95% confidence intervals (e.g., ~1.96 * SE). The CTLBB_{soil/sediment} ranged from 12 to 402 μ mol/g lipid overlapping the range of CTLBB_{aquatic} (Figure 2). Within the variability of the model and measurements and within the limitations of this comparison the model and measured CTLBBs are of a similar order of magnitude and consistent with the comparisons for aquatic organisms (Di Toro et al 2000).

The CTLBB_{aquatic} database is data-rich and the variability displayed in Figure 2 is assumed to be close to the actual underlying variability in ecotoxicity data. However, there are several CTLBB in the soil/sediment database (Table 1) that were derived for species using only one LC50 so it is not possible to evaluate the variability in these CTLBB estimates.

The CTLBBs for the soil/sediment database were in the same range as those from the aquatic database. The median CTLBB_{soil/sediment} is 59 μ mol/g lipid compared to 119 umol/g lipid for the aquatic dataset. The CTLBB_{soil/sediment} were derived using toxicity data from longer durations than the data used to derive CTLBB_{aquatic}, which resulted in systematically lower CTLBB_{soil/sediment}. In this sense the CTLBB_{soil/sediment} are more similar to chronic endpoints than the short-term acute aquatic endpoints. More quantitative or statistical comparisons between the two datasets were not attempted given the uncertainties and the paucity soil/sediment datasets discussed above.

This analysis shows that the two SSDs compare favorably in terms of the distribution, range of the datasets, general shape of the SSD curves and that the variability for sufficiently large subsets of data for soil and sediment species are similar to aquatic species. This suggests that the sensitivity of soil and sediment species are similar to that of aquatic species. The generally lower SSD for soil and sediment endpoints does not necessarily mean that these endpoints are inherently more sensitive given the typically longer test durations. An analysis of chronic data and acute-to-chronic ratios is provided below to evaluate the protectiveness of the aquatic-derived HC5 to soil and sediment compartments using EqP.

Reported critical tissue concentrations were similar to the TLM-derived CTLBBs using the modeling framework described above (Figure 3). This is a qualitative check on the TLMderived CTLBBs since factors such as metabolism, growth dilution, extraction efficiencies can affect the comparison.

Due to the relatively low sensitivity of *C. riparius* mortality and relatively sparse dataset additional aquatic datasets were analyzed to provide some basis for comparison of this endpoint (Figure 3). These data appear to be entirely consistent with the aquatic TLM in that there are linear relationships between logLC50 and log K_{OW} that results in a logCTLBB of 2.4. This is similar in sensitivity to *D.magna* but approximately an order of magnitude less sensitive than the CTLBB derived from sediment exposure data for a similar exposure duration (10 days). There is a need to further reconcile CTLBBs derived for water-only and soil/sediment exposures to establish consistency between the datasets for species that have been tested in water and soil or sediment media.

3.3 ACUTE-TO-CHRONIC RATIOS

Acute-to-chronic ratios were calculated with paired mortality (i.e., LC50) and chronic (i.e., EC10, NOECs) endpoints for a given chemical and organism (Figure 5, Table 2). There are 62 ACR entries that represent 21 chemicals, including aliphatic, aromatic and chlorinated chemicals, and 11 different species including invertebrates and plants exposed to mono- and polycyclic aromatics, and chlorinated chemicals. The range and distribution of ACRs are similar between the two datasets (i.e., aquatic vs. soil/sediment) suggesting similar toxic mechanisms are occurring in aquatic, benthic and terrestrial organisms (Figure 5).

The median ACR for soils and sediments (i.e., 3.7) is somewhat lower than the median ACR for the aquatic database for nonpolar organic chemicals (i.e., 4.5, McGrath et al 2004), which is due in part to the typically longer duration of the endpoints used in the ACR derivation. Also, many of the NOECs are based on the same long-term dose responses that were used to determine the LC50. ACRs based on the same response curve are an indication of the slope of the dose-response endpoint rather than a comparison of short term acute toxicity to long term chronic toxicity. This discrepancy is manifest in the slightly higher ACR in the aquatic database as well as the higher median CTLBB_{Aquatic}.

The ACRs were compared to the $\log K_{OW}$ for the individual chemicals in the database to evaluate possible impacts of chemical speciation or route of exposure, such as increasing dietary exposure for high $\log K_{OW}$ chemicals (Figure 6). There are more aquatic ACRs for chemicals $\log K_{OW} < 3$ relative to the soil/sediment database but there are no discernible trends on the comparison. This suggests that the variability in the ACRs, and by extension the mortality and chronic toxicity datasets, is probably due to uncertainties in the experimental and modeling methods and that this approach is not consistently biased or missing major processes that could affect toxicity.

3.4 CHRONIC TOXICITY AND HC5

Chronic toxicity data were compiled for comparison to the HC5 to evaluate the potential of the TLM and EqP models for establishing protective soil and sediment quality guidelines. The chronic effects data were compiled for 33 organisms including invertebrates, plants and microbial endpoints, (Table 3). The chronic data range from 0.2 to >3,000

mmol/kg OC and appear to be consistent with the slope of the TLM-EqP derivation (e.g., essentially flat, Eq 4). Chronic data compared favorably to the HC5-EqP (Figure 7) with 5.3% of the NOECs in the database below the HC5 (i.e. 10 outliers out of 188 datapoints), which is consistent with the target of 5%.

Several of those outliers (n=4) are for *C. riparius* and include several data for high $\log K_{OW}$ substances, where test results are affected by pre-equilibration times. The other outliers are distributed among 6 other species including midges, plants and oligochaetes. All of the outliers are within a factor of 5 of the HC5 and 6 are within a factor of 2. The incidence of the observations that are less than the HC5 does not have a strong pattern with respect to $\log K_{OW}$ and appear to be evenly distributed among the range of chemicals in this analysis (Figure 8). This suggests that the performance of the TLM-derived HC5 is consistent across the range of chemicals analyzed in the present study and that no additional assessment factors were required to establish a protective PNEC.

It is noted that there are several NOECs that did not result in toxicity (Figure 7) even at elevated concentrations greater than 100 mmol/kg oc. For some chemicals this is greater than the theoretical solubility limit in soil or sediment based on EqP and the solubility relationship developed by McGrath et al., (2004). Between $\log K_{OW}$ 4-6 the theoretical solubility limit is around 900-300 mmol/kg OC, however at $\log K_{OW} > 6$ the solubility limit ranges from 150-30 mmol/kg OC (between $\log K_{OW}$ 7 to 9). This means that several of the reported NOECs are near or above the estimated solubility limit at high $\log K_{OW}$ and suggests that free product might be present at higher testing concentrations, but since many of these observations are not toxic possible physical effects seems to be limited.

Previous work has suggested that the bioavailability of high log K_{OW} compounds (i.e., >6) may be limited (Redman et al 2012a; Staples et al 1997; Schafer et al 2009; Verbruggen 2004). Factors that influence the bioavailability of these very hydrophobic compounds include binding to dissolved organic carbon, kinetic limitations on the ability of these compounds to partition into target lipid of aquatic organisms or solubility limitations. These processes are described generically in Eq. 5 and the membrane-water partition coefficient. When this parameter is substituted for log K_{OW} in Eq 1 or 6 it results in a soil HC5 (see also Eq 3) that increases proportionally with log K_{OW} (diagonal line in Figure 7) instead of the generally shallow slope given in Eq 4 (flat line in Figure 1 and 7). This is due to the differences in the log K_{OW} -related slopes in the toxicity and K_{OC} relationships.

There is a marked increase in the fraction of observations that resulted in no toxicity at the maximum tested concentration (Figure 9) at $\log K_{OW} > 6$. It is possible that some of these observations were due to short pre-equilibration times but the few available chronic toxicity data are consistent with the application of the K_{LW} . However, it is not possible to draw substantive conclusions due to the uncertainty introduced by the chironomid dataset and the role that pre-equilibration has on the results.

3.5 PRE-EQUILIBRATION

The toxicity of chemicals is related to a large degree on the speciation and bioavailability of the test material in a given exposure environment. This can change over time as various weathering processes occur such as sorption to/from solid phases (e.g., soil organic carbon), diffusion within the soil matrix, dissolution from oil phases, equilibration with void spaces (e.g., headspace or porespace), and as a result of biodegradation. These processes can influence the result of toxicity tests used to develop regulatory benchmarks and must be taken into consideration when developing toxicity assays.

Pre-equilibration, or aging can impact the results of toxicity testing on soils and sediment (Sverdrup et al 2002). It is assumed that this process is generally more important for higher logKow substances due to their typically lower mass transfer rates (Chapra 1997). It was observed that the toxicity of high $\log K_{OW}$ chemicals varied with the duration of pre-equilibration times, meaning that the amount of time between initial mixing of the chemicals and the addition of test organisms can be important.

Available toxicity data from internally consistent studies (e.g., consistent soils, researchers, methods) were compared to the duration of the pre-equilibration step in Figure 10. The pre-equilibration times varied from 1, 10, 28, 40 to 120 days for several chemicals including PAH and >C10 aliphatic hydrocarbons. In some cases, the toxicity did not change appreciably with longer durations (e.g., phenanthrene and pyrene exposures to *F. fimetaria*). However, for aliphatic chemicals tested the effect of pre-equilibration time appears to result in an increase in the effect level (e.g., less toxic) by a factor of 5 to more than 10. In some cases a limit test was performed under short duration periods resulted in significant effects (e.g., '<' symbol) that disappeared (e.g., not toxicity, '>' symbol) or became less toxic with longer pre-equilibration times.

The time to reach a steady state with respect to the effect levels and pre-equilibration duration seems to be loosely correlated with $\log K_{OW}$ of the test chemical. The ratio of the effect levels from the shortest (~1 d) and the longest duration was plotted against $\log K_{OW}$ as an indication of the time to reach steady state, Figure 11. Tests with definitive effect levels (e.g., LC50 or NOECs) at short and longer durations are plotted as circles. There is one test with a definitive short-term LC50 of 14 mmol/kg OC for Phenanthrene and a long-term LC50 of >14 mmol/kg OC. This was plotted as '>' at a value to 1 to indicate that this ratio could be higher with a definitive LC50 at the longer duration. However, the source of these data (Sverdrup et al 2002) suggested that while a 50% mortality threshold was not reached in the tests, suggesting declining bioavailability / potential biodegradation, the EC10 and EC50

values were similar to the results at shorter aging times suggesting a ratio of <2, which would be consistent with this evaluation.

The other data with results plotted as '<' symbols are based on definitive long-term NOECs and a short-term LOEC as determined by a single-dose limit test. The actual short-term NOEC is expected to be lower, which would result in a lower ratio. The ratios suggest that compounds with higher $\log K_{OW}$ may require longer to reach a steady state with respect to toxicity than lower $\log K_{OW}$ compounds. These data do not show a consistent trend with increasing $\log K_{OW}$ so it is difficult to identify physico-chemical properties that control this process. For example, the NOECs for *F. candida* reproduction for pentadecane show that aging increases toxicity, whereas the NOECs for mortality in those same tests show a strong effect of aging. Further, this subset of data is based on nominal concentrations due to the highly variable measurements that complicates interpretation of the observed effect of aging but analysis based on measured data (not shown) supports principle that aging limits bioavailbility.

The effect of aging, also, appears to diminish between pre-equilibration periods of 7-28 days. Toxicity tests with chemicals with $\log K_{OW} > 6$ should consider a pre-equilibration step to introduce realistic exposure scenarios such as might be encountered in the field. The concept that aging affects bioavailability is widely recognized within the field of metals ecotoxicology and has been used to recommend soil quality standards (Smolders et al 2009) where aging of up to 120 d is common.

SUMMARY AND CONCLUSIONS

The goal of this study was to demonstrate that the HC5-EqP framework can be applied to soil and sediments to derive reasonably protective SQGs. Generally, SQGs are derived using effects data for aquatic organisms using EqP. It is assumed that the SSD and variability in the acute and chronic (and ACR) datasets derived for the aquatic datasets are similar to soiland sediment-dwelling organisms. This is an important assumption in applying the TLMderived HC5 to sediments and soils since it is based on the toxicity characteristics of the aquatic database (Eq 6).

The application of TLM derived HC5 to soils and sediments using EqP resulted in 26 new CTLBBs for plants and invertebrates that were similar to the aquatic TLM database of CTLBBs, indicating that benthic and terrestrial invertebrates have similar levels of sensitivity as the aquatic organisms. The ACRs for the soil and sediment organisms slightly lower than the ACRs for aquatic tests due to differences in the duration of the exposure used to calculate these values. However, the difference between the two distributions is slight, further confirming this conclusion that these two groups of organisms have similar levels of sensitivity. Finally, the available chronic NOECs were consistent with the EqP-HC5 (e.g., 95% of data above HC5) indicating that the TLM-derived HC5 is a suitable benchmark for assessing risk of petroleum substances in sediment and soil media.

Extension of the TLM using EqP provides a technically sound and consistent basis for extrapolating the HC5 that was derived from aquatic organisms. This analysis confirms the similarity in the distribution of species sensitivity between these two general environmental compartments and documents an important consideration related to aging of test substances prior to testing.

RECOMMENDATIONS

Recommendations for additional work as discussed above are summarized here. There is a general lack of data for a range of chemicals (logK_{ow} 3-8) for most soil and sediment species. Additional data, particularly for PAHs would be helpful to establish more confidence for the endpoints and CTLBBs derived in the present study. In particular, the uncertainty around *C.riparious* and *E.andrei* could limit the use and interpretation of these test species for further hazard assessments.

Further study on the fate and effects of high $\log K_{OW}$ chemicals may be warranted to better understand processes that control the bioavailability hydrophobic chemicals in soils and sediments. This is relevant for interpreting toxicity data from elevated soil or sediments exposures of poorly water soluble chemicals since, in some case, the likely presence of free product phases could influence the results of those tests. Environmental quality standards should be protective of physical oiling (Verbruggen 2004) but this mechanism of toxicity (e.g., suffocation, etc.) is outside the scope of the TLM-EqP. A TLM-EqP framework that accounts for aging could help interpret those results (e.g., kinetics of equilibration, effect levels vs. solubility limits).

Lastly, several test species evaluated here are commonly used in water only tests (e.g., *C.riparious, H.azteca*). Further, several studies report effect levels in terms of pore water concentration data. Analysis of these data could provide more direct comparison of TLM-derived CTLBBs to the aquatic dataset since it avoids potential uncertainty related to application of the EqP model. These data may also help resolve discrepancies in the reported effects data discussed above by providing another line of evidence for evaluating soil and sediment effects data. Plus, analysis of these data could help make more definitive comparisons of SSDs between the aquatic and soil and sediment compartments.

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SECTION 7

TABLES

Species	Duration (d)	Endpoint	Ν	logCTLBB	SE
B. rapa	14	Mortality	1	1.41	NA
A. sativa	14	Emergence	2	2.03	0.28
L. perenne	14	Seed growth	7	2.61	0.05
S. alba	14	Seed growth	6	2.15	0.18
T. pratense	14	Seed growth	6	2.02	0.14
A. tuberculata	14	Mortality	1	1.76	NA
E. eugeniae	14 and 28	Mortality	2	1.47	0.00
E. fetida	7 and 14	Mortality	5	1.50	0.11
E. veneta	21	Survival	6	1.80	0.09
L. rubellus	14 and 42	Survival	17	1.72	0.04
P. excavatus	14 and 28	Mortality	2	1.52	0.10
E. andrei	3, 5, 8, 10 and 14	Mortality	23	1.74	0.06
E. crypticus	21 and 28	Survival	15	2.54	0.10
F. candida	21 and 28	Mortality	38	1.44	0.05
F. fimetaria	21	Survival	27	1.43	0.05
C. riparius	28	Survival	3	1.17	0.07
C. spinicorne	10	Survival	1	1.25	NA
R. abronius	10	Survival	18	1.38	0.08
Coullana sp.	10	Survival	1	1.75	NA
N. lacustris	10	Survival	1	1.55	NA
S. knabeni	10	Survival	2	2.10	0.15
L. hoffmeisteri	3 and 10	Survival	2	2.51	NA
B. caribaeum	10	Mortality	2	2.50	0.05
C. tentans	10	Mortality	7	1.44	0.23
Diporeia	8	Survival	1	2.31	NA
H. azteca	10 and 16	Mortality	8	1.24	0.33

Table 1. Organisms, Endpoints and Critical Target Lipid Body Burdens in Soil/Sediment Effects Database

Compound	Log Kow	Species	Endpoint		Matrix	NOEC (mmol / kg OC)	Duration (d)	L/EC50 (mmol/kg OC)	ACR		Reference
Styrene	2.93	E. fetida	Survival	NOEC	Soil OECD	16.3	7 vs 14	59.4	3.6	Survival	Cushman et al. (1997)
1,4-dichlorobenzene	3.09	F. candida	reproduction	EC10	LUFA soil	22.6	28	15.9	0.7	Survival	Geisen et al 2012
1,4-dichlorobenzene	3.09	F. candida	reproduction	EC10	OECD	11.4	28	18.6	1.6	Survival	Geisen et al 2012
Naphthalene	3.30	E. fetida	Mortality	NOEC	Soil	20.6	7	35.1	1.7	Mortality	Canada-Wide Standard for PHC
Naphthalene	3.30	F. fimetaria	Reproduction	EC10	Soil	9.8	21	81.4	8.4	Survival	Sverdrup et al. (2002c)
Acenaphthylene	3.44	F. fimetaria	Reproduction	EC10	Soil	9.4	21	59.5	6.3	Survival	Sverdrup et al. (2002c)
1,2,4-Trichlorobenzene	3.72	B. caribaeum	Mortality	NOEC	Sediment	95.0	10	190.1	2.0	Survival	Clark et al. (1987)
1,2,4-trichlorobenzene	3.72	F. candida	reproduction	EC10	LUFA soil	9.5	28	19.8	2.1	Survival	Geisen et al 2012
1,2,4-trichlorobenzene	3.72	F. candida	reproduction	EC10	OECD	5.1	28	9.0	1.8	Survival	Geisen et al 2012
1,2,3-trichlorobenzene	3.74	F. candida	reproduction	EC10	LUFA soil	10.6	28	15.5	1.5	Survival	Geisen et al 2012
1,2,3-trichlorobenzene	3.74	F. candida	reproduction	EC10	OECD	4.2	28	14.0	3.3	Survival	Geisen et al 2012
1,3,5-trichlorobenzene	3.76	F. candida	reproduction	EC10	LUFA soil	10.2	28	15.7	1.5	Survival	Geisen et al 2012
1,3,5-trichlorobenzene	3.76	F. candida	reproduction	EC10	OECD	4.6	28	13.6	3.0	Survival	Geisen et al 2012
Acenaphthene	3.88	F. fimetaria	Reproduction	EC10	Soil	12.6	21	43.4	3.5	Survival	Sverdrup et al. (2002c)
Fluorene	3.93	L. perenne	Seed growth	EC20	Soil	142.9	14	357.2	2.5	Seed growth	Sverdrup et al. (2003)

Table 2 Acute-to-Chronic Ratios

Compound	Log Kow	Species	Endpoint		Matrix	NOEC (mmol / kg OC)	Duration (d)	L/EC50 (mmol/kg OC)	ACR		Reference
Fluorene	3.93	T. pratense	Seed growth	EC20	Soil	20.7	14	135.4	6.5	Seed growth	Sverdrup et al. (2003)
Fluorene	3.93	E. veneta	Reproduction	NOEC	Soil	10.5	21	25.9	2.5	Survival	Sverdrup et al. (2002d)
Fluorene	3.93	E. crypticus	Reproduction	NOEC	Soil	10.2	21	676.8	66.7	Mortality	Sverdrup et al. 2002a
Fluorene	3.93	F. candida	Reproduction and survival	NOEC	Soil	12.0	21	46.6	3.9	Survival	Sorensen TS and Holmstrup M (2005)
Fluorene	3.93	F. fimetaria	Reproduction	EC10	Soil	2.9	21	14.7	5.1	Survival	Sverdrup et al. (2002c)
Dibenzofuran	3.95	L. perenne	Seed growth	EC20	Soil	34.6	14	341.9	9.9	Seed emergence	Sverdrup et al. (2003)
Dibenzofuran	3.95	S. alba	Seed growth	EC20	Soil	30.5	14	185.8	6.1	Seed growth	Sverdrup et al. (2003)
Dibenzofuran	3.95	T. pratense	Seed growth	EC20	Soil	16.0	14	59.5	3.7	Seed growth	Sverdrup et al. (2003)
Dibenzofuran	3.95	E. veneta	Reproduction	NOEC	Soil	11.1	21	29.0	2.6	Survival	Sverdrup et al. (2002d)
Dibenzofuran	3.95	E. crypticus	Reproduction	NOEC	Soil	23.0	21	144.9	6.3	Mortality	Sverdrup et al. (2002a)
Dibenzofuran	3.95	F. fimetaria	Reproduction	NOEC	Soil	5.2	21	18.6	3.6	Survival	Sverdrup et al. (2001)
Dibenzothiophene	4.37	L. perenne	Seed growth	EC20	Soil	37.3	14	301.9	8.1	Seed growth	Sverdrup et al. (2003)
Dibenzothiophene	4.37	S. alba	Seed growth	EC20	Soil	12.6	14	31.5	2.5	Seed growth	Sverdrup et al. (2003)
Dibenzothiophene	4.37	T. pratense	Seed growth	EC20	Soil	12.9	14	31.9	2.5	Seed growth	Sverdrup et al. (2003)
Dibenzothiophene	4.37	E. veneta	Reproduction	NOEC	Soil	9.8	21	45.1	4.6	Survival	Sverdrup et al. (2002d)

Table 2 Acute-to-Chronic Ratios

Compound	LogKow	Species	Endpoint		Matrix	NOEC (mmol / kg OC)	Duration (d)	L/EC50 (mmol/kg OC)	ACR		Reference
Dibenzothiophene	4.37	F. fimetaria	Reproduction	NOEC	Soil	2.9	21	7.1	2.4	Survival	Sverdrup et al. (2001)
1,2,3,4- tetrachlorobenzene	4.43	F. candida	reproduction	EC10	LUFA soil	5.6	28	14.7	2.6	Survival	Geisen et al 2012
1,2,3,4- tetrachlorobenzene	4.43	F. candida	reproduction	EC10	OECD	2.0	28	16.6	8.4	Survival	Geisen et al 2012
1,2,3,5- tetrachlorobenzene	4.47	F. candida	reproduction	EC10	LUFA soil	2.7	28	17.9	6.6	Survival	Geisen et al 2012
1,2,3,5- tetrachlorobenzene	4.47	F. candida	reproduction	EC10	OECD	1.8	28	12.5	7.1	Survival	Geisen et al 2012
Anthracene	4.55	F. fimetaria	Reproduction	EC10	Soil	1.8	21	23.5	13.4	Survival	Sverdrup et al. (2002c)
Phenanthrene	4.58	L. perenne	Seed growth	EC20	Soil	105.2	14	266.5	2.5	Seed growth	Sverdrup et al. (2003)
Phenanthrene	4.58	S. alba	Seed growth	EC20	Soil	27.0	14	168.3	6.2	Seed growth	Sverdrup et al. (2003)
Phenanthrene	4.58	T. pratense	Seed growth	EC20	Soil	13.0	14	27.7	2.1	Seed growth	Sverdrup et al. (2003)
Phenanthrene	4.58	E. veneta	Reproduction	NOEC	Soil	10.9	21	47.0	4.3	Survival	Sverdrup et al. (2002d)
Phenanthrene	4.58	E. crypticus	Reproduction	EC10	Soil	16.1	28	91.7	5.7	Survival	Droge et al. (2006)
Phenanthrene	4.58	F. candida	Reproduction	NOEC	Soil	7.3	28	14.0	1.9	Mortality	Bowmer et al. (1993)
Phenanthrene	4.58	F. candida	Reproduction	EC10	Soil	6.1	28	15.9	2.6	Survival	Droge et al. (2006)
Phenanthrene	4.58	F. fimetaria	Reproduction	NOEC	Soil	7.4	21	14.4	2.0	Survival	Sverdrup et al. (2002c)
Phenanthrene	4.58	F. fimetaria	Reproduction	NOEC	Askov Soil	7.4	21	14.4	2.0	Survival	Sverdrup et al. (2002b)
Phenanthrene	4.58	L. hoffmeisteri	Egestion	EC20	Sediment	19.6	10	238.4	12.1	Survival	Lotufo GR and Fleeger JW (1996)

Table 2 Acute-to-Chronic Ratios

Compound	Log K _{ow}	Species	Endpoint		Matrix	NOEC (mmol / kg OC)	Duration (d)	L/EC50 (mmol/kg OC)	ACR		Reference
Pyrene	5.13	T. pratense	Seed growth	EC20	Soil	15.1	14	117.4	7.8	Seed growth	Sverdrup et al. (2003)
Pyrene	5.13	E. veneta	Reproduction	NOEC	Soil	9.0	21	47.9	5.3	Survival	Sverdrup et al. (2002d)
Pyrene	5.13	F. candida	Reproduction	NOEC	Soil	0.4	28	1.8	4.3	Survival	Herbert et al. (2004)
Pyrene	5.13	F. candida	Reproduction	EC10	Soil	2.4	28	32.2	13.2	Survival	Droge et al. (2006)
Pyrene	5.13	F. fimetaria	Reproduction	EC10	Soil	3.1	21	16.4	5.3	Survival	Sverdrup et al. (2002c)
Pyrene	5.13	F. fimetaria	Reproduction	NOEC	Soil	4.6	21	22.9	4.9	Survival	Jensen J and Sverdrup LE (2002c)
Pyrene	5.13	F. fimetaria	Reproduction	NOEC	Askov Soil	4.0	21	13.6	3.4	Survival	Sverdrup et al. (2002b)
Pentachlorobenzene	5.14	F. candida	reproduction	EC10	LUFA soil	6.5	28	16.1	2.5	Survival	Geisen et al 2012
Pentachlorobenzene	5.14	F. candida	reproduction	EC10	OECD	2.7	28	18.0	6.7	Survival	Geisen et al 2012
Fluoranthene	5.19	T. pratense	Seed growth	EC20	Soil	43.3	14	219.4	5.1	Seed growth	Sverdrup et al. (2003)
Fluoranthene	5.19	E. veneta	Reproduction	NOEC	Soil	30.3	21	128.5	4.2	Survival	Sverdrup et al. (2002d)
Fluoranthene	5.19	F. fimetaria	Reproduction	EC10	Soil	11.4	21	25.0	2.2	Survival	Sverdrup et al. (2002c)
Phenanthrene	4.58	C.riparius	Emergence	LOEC	artificial	79.9	28	119.5	1.5	Emergence	soil
Pentadecane (28 d)	8.68	F. candida	survival	LOEC	Artificial soil	15.3	28	320.8	21.0	LC50	CONCAWE (2011a)
n-Octylcyclohexane (28 d)	7.80	F. candida	survival	NOEC	Artificial soil	16.5	28	136.5	8.3	LC50	CONCAWE (2011a)
1-Phenylnonane (28 d)	6.81	F. candida	survival	NOEC	Artificial soil	45.3	28	74.8	1.7	LC50	CONCAWE (2011a)

Table 2 Acute-to-Chronic Ratios

Compound	Species	Endpoint	Matrix	Duration	Effect (mmol / kg OC)	ENDPOINT	LogKow	FLAG	Reference
Phenanthrene	H. assimilis	growth	Soil	0	14.2	NOEC	4.58	>	Cortet et al. 2006
Phenanthrene	I. prasinus	growth	Soil	0	14.2	NOEC	4.58	<	Cortet et al. 2006
Phenanthrene	M. macrochaeta	growth	Soil	0	14.2	NOEC	4.58	<	Cortet et al. 2006
Phenanthrene	P. armata	growth	Soil	0	14.2	NOEC	4.58	>	Cortet et al. 2006
Pyrene	B. rapa	growth	Soil	0	1373.4	NOEC	5.13	>	Kalsch et al. 2006
Benzo[a]pyrene	microbes	Nitrification	Soil	28	72.6	NOEC	6.41		Sverdrup et al. (2007)
Dibenzofuran	microbes	Nitrification	Soil	28	27.9	NOEC	3.95		Sverdrup et al. (2002e)
Dibenzothiophene	microbes	Nitrification	Soil	28	7.5	NOEC	4.37		Sverdrup et al. (2002e)
Fluoranthene	microbes	Nitrification	Soil	28	7.4	NOEC	5.19		Sverdrup et al. (2002e)
Fluorene	microbes	Nitrification	Soil	28	27.1	NOEC	3.93		Sverdrup et al. (2002e)
Phenanthrene	microbes	Nitrification	Soil	28	9.1	NOEC	4.58		Sverdrup et al. (2002e)
Pyrene	microbes	Nitrification	Soil	28	24.4	NOEC	5.13		Sverdrup et al. (2002e)
Benzo[a]pyrene	B. alba	Growth	Soil	14	21.3	NOEC	6.41		Sverdrup et al. (2007)

Table 3. Compiled Effects Data

Compound	Species	Endpoint	Matrix	Duration	Effect (mmol / kg OC)	ENDPOINT	LogKow	FLAG	Reference
Benzo[a]pyrene	L. perenne	Growth	Soil	14	116.4	NOEC	6.41	>	Sverdrup et al. (2007)
Dibenzofuran	L. perenne	Seed growth	Soil	14	34.6	EC20	3.95		Sverdrup et al. (2003)
Dibenzothiophene	L. perenne	Seed growth	Soil	14	37.3	EC20	4.37		Sverdrup et al. (2003)
Fluoranthene	L. perenne	Seed growth	Soil	14	151.4	EC20	5.19		Sverdrup et al. (2003)
Fluorene	L. perenne	Seed growth	Soil	14	142.9	EC20	3.93		Sverdrup et al. (2003)
Pyrene	L. perenne	Seed growth	Soil	14	309.0	EC20	5.13	>	Sverdrup et al. (2003)
Phenanthrene	L. perenne	Seed growth	Soil	14	105.2	EC20	4.58		Sverdrup et al. (2003)
Benzo[a]pyrene	L. sativa	Seed emergence	Soil	14	2947.6	LOEC	6.41		Sverdrup, 2007
Naphthalene	L. sativa	Seedling emergence	Soil	5	1.2	NOEC	3.30		Canada-Wide Standard for PHC
Dibenzofuran	S. alba	Seed growth	Soil	14	30.5	EC20	3.95		Sverdrup et al. (2003)
Dibenzothiophene	S. alba	Seed growth	Soil	14	12.6	EC20	4.37		Sverdrup et al. (2003)
Fluoranthene	S. alba	Seed growth	Soil	14	200.9	EC20	5.19		Sverdrup et al. (2003)
Fluorene	S. alba	Seed growth	Soil	14	45.1	EC20	3.93		Sverdrup et al. (2003)

Table 3. Compiled Effects Data

Compound	Species	Endpoint	Matrix	Duration	Effect (mmol / kg OC)	ENDPOINT	LogKow	FLAG	Reference
Phenanthrene	S. alba	Seed growth	Soil	14	27.0	EC20	4.58		Sverdrup et al. (2003)
Pyrene	S. alba	Seed growth	Soil	14	37.1	EC20	5.13		Sverdrup et al. (2003)
Benzo[a]pyrene	S. cereale	Emergence/growth	Soil	0	0.8	LOEC	6.41	>	Do"rr (1970
Benzo[a]pyrene	T. pratense	Growth	Soil	14	116.4	NOEC	6.41	>	Sverdrup et al. (2007)
Dibenzofuran	T. pratense	Seed growth	Soil	14	16.0	EC20	3.95		Sverdrup et al. (2003)
Dibenzothiophene	T. pratense	Seed growth	Soil	14	12.9	EC20	4.37		Sverdrup et al. (2003)
Fluoranthene	T. pratense	Seed growth	Soil	14	43.3	EC20	5.19		Sverdrup et al. (2003)
Fluorene	T. pratense	Seed growth	Soil	14	20.7	EC20	3.93		Sverdrup et al. (2003)
Phenanthrene	T. pratense	Seed growth	Soil	14	13.0	EC20	4.58		Sverdrup et al. (2003)
Pyrene	T. pratense	Seed growth	Soil	14	15.1	EC20	5.13		Sverdrup et al. (2003)
Benzo[a]pyrene	H. aculeifer	Reproduction	Soil	21	234.6	NOEC	6.41	>	Sverdrup et al. (2007)
Phenanthrene	H. aculeifer	growth	Soil	0	14.2	NOEC	4.58	>	Cortet et al. 2006
Anthracene	E. fetida	growth	Soil	0	222.5	NOEC	4.55	>	Contreras-Ramon et al. 2006

Table 3. Compiled Effects Data

Compound	Species	Endpoint	Matrix	Duration	Effect (mmol / kg OC)	ENDPOINT	LogKow	FLAG	Reference
Benzo[a]pyrene	E. fetida	NRR'	Soil	28	9.0	LOEC	6.41		Eason et al. (1999)
Benzo[a]pyrene	E. fetida	growth	Soil	0	31.7	NOEC	6.41	>	Contreras-Ramon et al. 2006
Chrysene	E. fetida	Reproduction	Soil	21	75.5	NOEC	5.78	>	Bowmer et al. (1993)
Chrysene	E. fetida	Reproduction	Soil	0	66.9	NOEC	5.78	>	Bowmer et al. 1993
Phenanthrene	E. fetida	Reproduction	Soil	21	31.9	LOEC	4.58		Bowmer et al. (1993)
Phenanthrene	E. fetida	growth	Soil	0	26.2	EC10	4.58		Contreras-Ramon et al. 2006
Naphthalene	E. fetida	Mortality	Soil	7	20.6	NOEC	3.30		Canada-Wide Standard for PHC
Dibenzofuran	E. veneta	Reproduction	Soil	21	11.1	NOEC	3.95		Sverdrup et al. (2002d)
Dibenzothiophene	E. veneta	Reproduction	Soil	21	9.8	NOEC	4.37		Sverdrup et al. (2002d)
Fluoranthene	E. veneta	Reproduction	Soil	21	30.3	NOEC	5.19		Sverdrup et al. (2002d)
Fluorene	E. veneta	Reproduction	Soil	21	10.5	NOEC	3.93		Sverdrup et al. (2002d)
Phenanthrene	E. veneta	Reproduction	Soil	21	10.9	NOEC	4.58		Sverdrup et al. (2002d)
Pyrene	E. veneta	Reproduction	Soil	21	9.0	NOEC	5.13		Sverdrup et al. (2002d)

Table 3. Compiled Effects Data

Compound	Species	Endpoint	Matrix	Duration	Effect (mmol / kg OC)	ENDPOINT	LogKow	FLAG	Reference
Benzo[a]pyrene	E. crypticus	Reproduction	Soil	30	17.5	LOEC	6.41		Achazi et al. (1995b)
Benzo[a]pyrene	E. crypticus	Reproduction	Soil	28	276.6	LOEC	6.41	>	Bleeker et al. (2003)
Benzo[a]pyrene	E. crypticus	Reproduction	Soil	21	234.6	NOEC	6.41	>	Sverdrup et al. (2007)
Dibenzofuran	E. crypticus	Reproduction	Soil	21	23.0	NOEC	3.95		Sverdrup et al. 2002a
Dibenzothiophene	E. crypticus	Reproduction	Soil	21	21.7	NOEC	4.37		Sverdrup et al. 2002a
Fluoranthene	E. crypticus	Reproduction	Soil	21	11.7	NOEC	5.19		Sverdrup et al. 2002a
Fluoranthene	E. crypticus	Reproduction	Soil	30	262.3	LOEC	5.19		Achazi et al. (1995a)
Fluorene	E. crypticus	Reproduction	Soil	21	10.2	NOEC	3.93		Sverdrup et al. 2002a
Phenanthrene	E. crypticus	Reproduction	Soil	21	11.9	NOEC	4.58		Sverdrup et al. 2002a
Phenanthrene	E. crypticus	Reproduction	Soil	28	16.1	EC10	4.58		Droge et al. (2006)
Phenanthrene	E. crypticus	growth	Soil	0	14.2	NOEC	4.58	>	Cortet et al. 2006
Pyrene	E. crypticus	Reproduction	Soil	21	5.6	NOEC	5.13		Sverdrup et al. 2002a
Benzo[a]pyrene	F. candida	Reproduction	Soil	28	276.6	LOEC	6.41	>	Bleeker et al. (2003)
Fluorene	F. candida	Reproduction and survival	Soil	21	12.0	NOEC	3.93		Sorensen TS and Holmstrup M (2005)

Table 3. Compiled Effects Data

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Compound	Species	Endpoint	Matrix	Duration	Effect (mmol / kg OC)	ENDPOINT	LogKow	FLAG	Reference
Naphthalene	F. candida	Reproduction and Survival	Soil	28	3.8	NOEC	3.30		Droge et al. (2006)
Phenanthrene	F. candida	Reproduction	Soil	28	7.3	NOEC	4.58		Bowmer et al. (1993)
Phenanthrene	F. candida	Reproduction	Soil	33	21.3	LOEC	4.58		Crouau et al. (1999)
Phenanthrene	F. candida	Reproduction	Soil	28	6.1	EC10	4.58		Droge et al. (2006)
Pyrene	F. candida	Reproduction	Soil	28	0.4	NOEC	5.13		Herbert et al. (2004)
Pyrene	F. candida	Reproduction	Soil	28	2.4	EC10	5.13		Droge et al. (2006)
Pyrene	F. candida	Reproduction	Soil	21	15.5	LOEC	5.13		Sorensen TS and Holmstrup M (2005)
Pyrene	F. candida	Survival	Soil	21	61.8	NOEC	5.13		Sorensen TS and Holmstrup M (2005)
Acenaphthene	F. fimetaria	Reproduction	Soil	21	12.6	EC10	3.88		Sverdrup et al. (2002c)
Acenaphthylene	F. fimetaria	Reproduction	Soil	21	9.4	EC10	3.44		Sverdrup et al. (2002c)
Anthracene	F. fimetaria	Reproduction	Soil	21	1.8	EC10	4.55		Sverdrup et al. (2002c)
Benz[a]anthracene	F. fimetaria	Reproduction	Soil	21	268.3	EC10	5.74	>	Sverdrup et al. (2002c)
Benzo[a]pyrene	F. fimetaria	Reproduction	Soil	21	208.1	LOEC	6.41	>	Sverdrup et al. (2002c)

Table 3. Compiled Effects Data

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Compound	Species	Endpoint	Matrix	Duration	Effect (mmol / kg OC)	ENDPOINT	LogKow	FLAG	Reference
Benzo[b]fluoranthene	F. fimetaria	Reproduction	Soil	21	89.2	EC10	6.43	>	Sverdrup et al. (2002c)
Benzo[k]fluoranthene	F. fimetaria	Reproduction	Soil	21	138.7	EC10	6.40	>	Sverdrup et al. (2002c)
Chrysene	F. fimetaria	Reproduction	Soil	21	282.0	EC10	5.78	>	Sverdrup et al. (2002c)
Dibenz[a,h]anthracene	F. fimetaria	Reproduction	Soil	21	175.1	EC10	7.13	>	Sverdrup et al. (2002c)
Dibenzofuran	F. fimetaria	Reproduction	Soil	21	5.2	NOEC	3.95		Sverdrup et al. (2001)
Dibenzothiophene	F. fimetaria	Reproduction	Soil	21	2.9	NOEC	4.37		Sverdrup et al. (2001)
Fluoranthene	F. fimetaria	Reproduction	Soil	21	11.4	EC10	5.19		Sverdrup et al. (2002c)
Fluorene	F. fimetaria	Reproduction	Soil	21	2.9	EC10	3.93		Sverdrup et al. (2002c)
Indeno[1,2,3-cd]pyrene	F. fimetaria	Reproduction	Soil	21	205.8	EC10	6.99	>	Sverdrup et al. (2002c)
Naphthalene	F. fimetaria	Reproduction	Soil	21	9.8	EC10	3.30		Sverdrup et al. (2002c)
Perylene	F. fimetaria	Reproduction	Soil	21	138.7	EC10	6.45	>	Sverdrup et al. (2002c)
Phenanthrene	F. fimetaria	Reproduction	Soil	21	7.4	NOEC	4.58		Sverdrup et al. (2002c)
Phenanthrene	F. fimetaria	0	Soil	0	14.2	NOEC	4.58	>	Cortet et al. 2006

Table 3. Compiled Effects Data

Compound	Species	Endpoint	Matrix	Duration	Effect (mmol / kg OC)	ENDPOINT	LogKow	FLAG	Reference
Pyrene	F. fimetaria	Reproduction	Soil	21	3.1	EC10	5.13		Sverdrup et al. (2002c)
Pyrene	F. fimetaria	Reproduction	Soil	21	4.6	NOEC	5.13		Jensen and Sverdrup, 2001
Pyrene	F. fimetaria	Reproduction	Soil	21	4.6	NOEC	5.13		Jensen J and Sverdrup LE (2002)
Fluoranthene	H. aspersa	Growth	Soil	28	865.2	EC10	5.19	>	Sverdrup et al. (2006)
Fluorene	H. aspersa	Growth	Soil	28	1052.8	EC10	3.93	>	Sverdrup et al. (2006)
Phenanthrene	H. aspersa	Growth	Soil	28	981.8	EC10	4.58	>	Sverdrup et al. (2006)
Pyrene	H. aspersa	Growth	Soil	28	865.2	EC10	5.13	>	Sverdrup et al. (2006)
Fluoranthene	Coullana sp.	Grazing	Sediment	10	5.9	NOEC	5.19		Lotufo GR (1998)
Fluoranthene	S. knabeni	Grazing	Sediment	10	1.6	NOEC	5.19		Lotufo GR (1998)
Phenanthrene	L. hoffmeisteri	Egestion	Sediment	10	19.6	EC20	4.58		Lotufo GR and Fleeger JW (1996)
Pyrene	L. hoffmeisteri	Egestion	Sediment	10	36.4	EC20	5.13		Lotufo GR and Fleeger JW (1996)
1,2,4-Trichlorobenzene	P. pugio	Mortality	Sediment	10	12.7	NOEC	3.72		van Wijk D et al. (2006)
1,2,4-Trichlorobenzene	B. caribaeum	Mortality	Sediment	10	95.0	NOEC	3.72		van Wijk D et al. (2006)

Table 3. Compiled Effects Data

Compound	Species	Endpoint	Matrix	Duration	Effect (mmol / kg OC)	ENDPOINT	LogKow	FLAG	Reference
Hexachlorobenzene	C. elegans	Mortality	Soil	2	119.5	LC10	6.02		Sochova I et al. (2007)
Pyrene	F. fimetaria	Reproduction	Askov Soil	21	4.0	NOEC	5.13		Sverdrup et al. (2002b)
Phenanthrene	F. fimetaria	Reproduction	Askov Soil	21	7.4	NOEC	4.58		Sverdrup et al. (2002b)
Hexachlorocyclohexane (Lindane)	T. tubifex	Reworking activity	Sediment	3	2.4	NOEC	3.39		Meller et al. (1998)
Hexachlorocyclohexane (Lindane)	L. hoffmeisteri	Reworking activity	Sediment	3	0.5	NOEC	3.39		Meller et al. (1998)
Hexachlorobenzene	H. azteca	Growth and survival	Sediment	14	25.4	NOEC	6.02		Barber et al. (1997)
Hexachlorobenzene	C. tentans	Growth and survival	Sediment	14	25.4	NOEC	6.02		Barber et al. (1997)
1,2,4-Trichlorobenzene	G. max	Root Growth	Soil	2	26.2	EC10	3.72		Liu et al. (2004)
Phenanthrene	E. fetida	Reproduction	Soil	21	9.7	NOEC	4.58		Bowmer et al. (1993)
Styrene	E. fetida	Survival	Soil OECD	14	16.3	NOEC	2.93		Cushman et al. (1997)
3,3',4,4'- Tetrachlorobiphenyl	L. variegatus	Reproduction	Sediment	10	34.2	NOEC	6.28		Fuchsman et al. (2006)
Pyrene	F. fimetaria	Survival Drought tolerance	Soil	21	4.0	NOEC	5.13		Sjursen et al. (2001)
Fluoranthene	F. fimetaria	Survival Drought tolerance	Soil	21	14.5	NOEC	5.19		Sjursen et al. (2001)

Table 3. Compiled Effects Data

Compound	Species	Endpoint	Matrix	Duration	Effect (mmol /	ENDPOINT	LogKow	FLAG	Reference
					kg OC)				
Fluorene	F. fimetaria	Survival Drought tolerance	Soil	21	5.3	NOEC	3.93		Sjursen et al. (2001)
Dibenzothiophene	F. fimetaria	Survival Drought tolerance	Soil	21	2.9	NOEC	4.37	>	Sjursen et al. (2001)
Dibenzofuran	F. fimetaria	Survival Drought tolerance	Soil	21	24.2	NOEC	3.95	>	Sjursen et al. (2001)
Decane	E. fetida	Reproduction, growth, mortality	Artificial soil	28	325.4	NOEC	5.86	>	CONCAWE (2011a)
Pentadecane	E. fetida	Reproduction, growth, mortality	Artificial soil	28	217.9	NOEC	8.68	>	CONCAWE (2011a)
1-Phenylnonane	E. fetida	Reproduction, growth, mortality	Artificial soil	28	226.5	NOEC	6.81	>	CONCAWE (2011a)
o-Terphenyl	E. fetida	Reproduction, growth, mortality	Artificial soil	28	201.0	LOEC	6.22	<	CONCAWE (2011a)
Amylcyclohexane	E. fetida	Reproduction, growth, mortality	Artificial soil	28	300.0	NOEC	6.08	>	CONCAWE (2011a)
n-Octylcyclohexane	E. fetida	Reproduction, growth, mortality	Artificial soil	28	235.7	NOEC	7.80	>	CONCAWE (2011a)
Decane	F. candida	survival	Artificial soil	28	325.4	NOEC	5.86	<	CONCAWE (2011a)
o-Terphenyl	F. candida	survival	Artificial soil	28	201.0	NOEC	6.22	<	CONCAWE (2011a)
Amylcyclohexane	F. candida	survival	Artificial soil	28	300.0	NOEC	6.08	<	CONCAWE (2011a)

Table 3. Compiled Effects Data

Compound	Species	Endpoint	Matrix	Duration	Effect (mmol / kg OC)	ENDPOINT	LogKow	FLAG	Reference
Pentadecane (28 d)	F. candida	survival	Artificial soil	28	15.3	LOEC	8.68		CONCAWE (2011a)
n-Octylcyclohexane (28 d)	F. candida	survival	Artificial soil	28	16.5	NOEC	7.80		CONCAWE (2011a)
1-Phenylnonane (28 d)	F. candida	survival	Artificial soil	28	45.3	NOEC	6.81		CONCAWE (2011a)
Decane	A. sativa	growth	Artificial soil	21	325.4	NOEC	5.86	>	CONCAWE (2011a)
Pentadecane	A. sativa	growth	Artificial soil	21	217.9	LOEC	8.68	<	CONCAWE (2011a)
1-Phenylnonane	A. sativa	growth	Artificial soil	21	226.5	LOEC	6.81	<	CONCAWE (2011a)
o-Terphenyl	A. sativa	growth	Artificial soil	21	201.0	LOEC	6.22	<	CONCAWE (2011a)
Amylcyclohexane	A. sativa	growth	Artificial soil	21	300.0	NOEC	6.08	>	CONCAWE (2011a)
n-Octylcyclohexane	A. sativa	growth	Artificial soil	21	235.7	LOEC	7.80	<	CONCAWE (2011a)
1,3,5-trimethylbenzene	A. sativa	growth	Artificial soil	21	271.8	NOEC	6.96	>	CONCAWE (2011a)
2,2,4,6,6- pentamethylheptane	A. sativa	growth	Artificial soil	21	271.9	NOEC	7.18	>	CONCAWE (2011a)
Decane	G. max	growth	Artificial soil	21	325.4	NOEC	5.86	>	CONCAWE (2011a)

Table 3. Compiled Effects Data

Compound	Species	Endpoint	Matrix	Duration	Effect (mmol / kg OC)	ENDPOINT	LogKow	FLAG	Reference
Pentadecane	G. max	growth	Artificial soil	21	217.9	NOEC	8.68	>	CONCAWE (2011a)
1-Phenylnonane	G. max	growth	Artificial soil	21	226.5	NOEC	6.81	>	CONCAWE (2011a)
o-Terphenyl	G. max	growth	Artificial soil	21	201.0	NOEC	6.22	>	CONCAWE (2011a)
Amylcyclohexane	G. max	growth	Artificial soil	21	300.0	NOEC	6.08	>	CONCAWE (2011a)
n-Octylcyclohexane	G. max	growth	Artificial soil	21	235.7	LOEC	7.80	<	CONCAWE (2011a)
1,3,5-trimethylbenzene	G. max	growth	Artificial soil	21	271.8	NOEC	6.96	>	CONCAWE (2011a)
2,2,4,6,6- pentamethylheptane	G. max	growth	Artificial soil	21	271.9	NOEC	7.18	>	CONCAWE (2011a)
Decane	B. napus	growth	Artificial soil	21	325.4	NOEC	5.86	>	CONCAWE (2011a)
Pentadecane	B. napus	growth	Artificial soil	21	217.9	LOEC	8.68	<	CONCAWE (2011a)
1-Phenylnonane	B. napus	growth	Artificial soil	21	226.5	LOEC	6.81	<	CONCAWE (2011a)
o-Terphenyl	B. napus	growth	Artificial soil	21	201.0	LOEC	6.22	<	CONCAWE (2011a)
Amylcyclohexane	B. napus	growth	Artificial soil	21	300.0	NOEC	6.08	>	CONCAWE (2011a)

Table 3. Compiled Effects Data

Compound	Species	Endpoint	Matrix	Duration	Effect (mmol / kg OC)	ENDPOINT	LogKow	FLAG	Reference
n-Octylcyclohexane	B. napus	growth	Artificial soil	21	235.7	NOEC	7.80	>	CONCAWE (2011a)
1,3,5-trimethylbenzene	B. napus	growth	Artificial soil	21	271.8	NOEC	6.96	>	CONCAWE (2011a)
2,2,4,6,6- pentamethylheptane	B. napus	growth	Artificial soil	21	271.9	NOEC	7.18	>	CONCAWE (2011a)
2,2,4,4,6,8,8-heptamethyl nonane (28d)	C. riparius	emergence	Artificial sediment	28	184.0	NOEC	9.12	<	CONCAWE (2011b)
bicyclohexyl (2d)	C. riparius	emergence	Artificial sediment	28	5.7	NOEC	6.07		CONCAWE (2011b)
decane (2d)	C. riparius	emergence	Artificial sediment	28	4.2	NOEC	5.86	<	CONCAWE (2011b)
pentadecane (28d)	C. riparius	emergence	Artificial sediment	28	605.3	NOEC	8.68		CONCAWE (2011b)
trans-decalin (2d)	C. riparius	emergence	Artificial sediment	28	15.9	NOEC	4.90		CONCAWE (2011b)
1,3,5-trimethylcyclohexane (7d)	C. riparius	emergence	Artificial sediment	28	4.3	NOEC	6.96		CONCAWE (2011b)
pentylcyclohexane (2d)	C. riparius	emergence	Artificial sediment	28	2.0	NOEC	5.30		CONCAWE (2011b)
2,3-dimethylheptane (2d)	C. riparius	emergence	Artificial sediment	28	10.5	NOEC	5.25		CONCAWE (2011b)
propyldecalin (7d)	C. riparius	emergence	Artificial sediment	28	9.2	NOEC	6.59	<	CONCAWE (2011b)

Table 3. Compiled Effects Data

Compound	Species	Endpoint	Matrix	Duration	Effect (mmol / kg OC)	ENDPOINT	LogKow	FLAG	Reference
2,2,4,4,6,8,8-heptamethyl nonane (2d)	L. variegatus	Growth and survival	Artificial sediment	28	220.8	NOEC	9.12	>	CONCAWE (2011b)
bicyclohexyl (2d)	L. variegatus	Growth and survival	Artificial sediment	28	1.7	NOEC	6.07	<	CONCAWE (2011b)
pentadecane (2d)	L. variegatus	Growth and survival	Artificial sediment	28	235.4	NOEC	8.68	>	CONCAWE (2011b)
pentylcyclohexane (2d)	L. variegatus	Growth and survival	Artificial sediment	28	35.6	NOEC	5.30	>	CONCAWE (2011b)
1,4-dichlorobenzene	F. candida	reproduction	LUFA soil	28	22.6	EC10	3.09		Geisen et al 2012
1,2,3-trichlorobenzene	F. candida	reproduction	LUFA soil	28	10.6	EC10	3.74		Geisen et al 2012
1,2,4-trichlorobenzene	F. candida	reproduction	LUFA soil	28	9.5	EC10	3.72		Geisen et al 2012
1,3,5-trichlorobenzene	F. candida	reproduction	LUFA soil	28	10.2	EC10	3.76		Geisen et al 2012
1,2,3,4-tetrachlorobenzene	F. candida	reproduction	LUFA soil	28	5.6	EC10	4.43		Geisen et al 2012
1,2,3,5-tetrachlorobenzene	F. candida	reproduction	LUFA soil	28	2.7	EC10	4.47		Geisen et al 2012
1,2,4,5-tetrachlorobenzene	F. candida	reproduction	LUFA soil	28	7.7	EC10	4.43		Geisen et al 2012
Pentachlorobenzene	F. candida	reproduction	LUFA soil	28	6.5	EC10	5.14		Geisen et al 2012
1,4-dichlorobenzene	F. candida	reproduction	OECD	28	11.4	EC10	3.09		Geisen et al 2012
1,2,3-trichlorobenzene	F. candida	reproduction	OECD	28	4.2	EC10	3.74		Geisen et al 2012
1,2,4-trichlorobenzene	F. candida	reproduction	OECD	28	5.1	EC10	3.72		Geisen et al 2012
1,3,5-trichlorobenzene	F. candida	reproduction	OECD	28	4.6	EC10	3.76		Geisen et al 2012

Table 3. Compiled Effects Data

Compound	Species	Endpoint	Matrix	Duration	Effect (mmol / kg OC)	ENDPOINT	LogKow	FLAG	Reference
1,2,3,4-tetrachlorobenzene	F. candida	reproduction	OECD	28	2.0	EC10	4.43		Geisen et al 2012
1,2,3,5-tetrachlorobenzene	F. candida	reproduction	OECD	28	1.8	EC10	4.47		Geisen et al 2012
1,2,4,5-tetrachlorobenzene	F. candida	reproduction	OECD	28	2.3	EC10	4.43		Geisen et al 2012
Pentachlorobenzene	F. candida	reproduction	OECD	28	2.7	EC10	5.14		Geisen et al 2012
Hexachlorobenzene	F. candida	reproduction	OECD	28	70.2	EC10	6.02	>	Geisen et al 2012
Phenanthrene	C.riparius	Emergence	artificial	28	79.9	LOEC	4.58		Markinovitch et al 2011
Anthracene	A. sativa	Emergence	Soil	14	147.3	LC50	4.55		Mitchell et al. (1988)
Dibenzofuran	L. perenne	Seed emergence	Soil	14	341.9	LC50	3.95		Sverdrup et al. (2003)
Dibenzofuran	L. perenne	Seed growth	Soil	14	178.4	EC50	3.95		Sverdrup et al. (2003)
Dibenzothiophene	L. perenne	Seed growth	Soil	14	301.9	EC50	4.37		Sverdrup et al. (2003)
Fluoranthene	L. perenne	Seed growth	Soil	14	309.0	EC50	5.19	>	Sverdrup et al. (2003)
Fluorene	L. perenne	Seed growth	Soil	14	357.2	EC50	3.93		Sverdrup et al. (2003)
Pyrene	L. perenne	Seed growth	Soil	14	309.0	EC50	5.13	>	Sverdrup et al. (2003)

Table 3. Compiled Effects Data

Compound	Species	Endpoint	Matrix	Duration	Effect (mmol / kg OC)	ENDPOINT	LogKow	FLAG	Reference
Phenanthrene	L. perenne	Seed growth	Soil	14	266.5	EC50	4.58		Sverdrup et al. (2003)
Dibenzofuran	S. alba	Seed growth	Soil	14	185.8	EC50	3.95		Sverdrup et al. (2003)
Dibenzothiophene	S. alba	Seed growth	Soil	14	31.5	EC50	4.37		Sverdrup et al. (2003)
Fluoranthene	S. alba	Seed growth	Soil	14	309.0	EC50	5.19	>	Sverdrup et al. (2003)
Fluorene	S. alba	Seed growth	Soil	14	376.0	EC50	3.93	>	Sverdrup et al. (2003)
Phenanthrene	S. alba	Seed growth	Soil	14	168.3	EC50	4.58		Sverdrup et al. (2003)
Pyrene	S. alba	Seed growth	Soil	14	309.0	EC50	5.13	>	Sverdrup et al. (2003)
Dibenzofuran	T. pratense	Seed growth	Soil	14	59.5	EC50	3.95		Sverdrup et al. (2003)
Dibenzothiophene	T. pratense	Seed growth	Soil	14	31.9	EC50	4.37		Sverdrup et al. (2003)
Fluoranthene	T. pratense	Seed growth	Soil	14	219.4	EC50	5.19		Sverdrup et al. (2003)
Fluorene	T. pratense	Seed growth	Soil	14	135.4	EC50	3.93		Sverdrup et al. (2003)
Phenanthrene	T. pratense	Seed growth	Soil	14	27.7	EC50	4.58		Sverdrup et al. (2003)

Table 3. Compiled Effects Data

Compound	Species	Endpoint	Matrix	Duration	Effect (mmol / kg OC)	ENDPOINT	LogKow	FLAG	Reference
Pyrene	T. pratense	Seed growth	Soil	14	117.4	EC50	5.13		Sverdrup et al. (2003)
Fluorene	E. eugeniae	Mortality	Soil	14	20.4	LC50	3.93		Neuhauser et al. (1986)
Fluorene	E. fetida	Mortality	Soil	14	17.9	LC50	3.93		Neuhauser et al. (1985) , Neuhauser et al. (1986)
Naphthalene	E. fetida	Mortality	Soil	7	35.1	LC50	3.30		Canada-Wide Standard for PHC
Dibenzofuran	E. veneta	Survival	Soil	21	29.0	LC50	3.95		Sverdrup et al. (2002d)
Dibenzothiophene	E. veneta	Survival	Soil	21	45.1	LC50	4.37		Sverdrup et al. (2002d)
Fluoranthene	E. veneta	Survival	Soil	21	128.5	LC50	5.19		Sverdrup et al. (2002d)
Fluorene	E. veneta	Survival	Soil	21	25.9	LC50	3.93		Sverdrup et al. (2002d)
Phenanthrene	E. veneta	Survival	Soil	21	47.0	LC50	4.58		Sverdrup et al. (2002d)
Pyrene	E. veneta	Survival	Soil	21	47.9	LC50	5.13		Sverdrup et al. (2002d)
Pyrene	L. rubellus	Survival	Soil	42	24.1	LC50	5.13		Brown et al. (2004)
Fluorene	P. excavatus	Mortality	Soil	14	17.6	LC50	3.93		Neuhauser et al. (1986)

Table 3. Compiled Effects Data

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Compound	Species	Endpoint	Matrix	Duration	Effect (mmol / kg OC)	ENDPOINT	LogKow	FLAG	Reference
Anthracene	E. andrei	Mortality	Soil	14	96.7	LC50	4.55	>	Rombke et al. (1994)
Anthracene	E. crypticus	Survival	Soil	28	219.0	LC50	4.55	>	Droge et al. (2006)
Benz[a]anthracene	E. crypticus	Survival	Soil	28	177.0	LC50	5.74	>	Droge et al. (2006)
Benzo[a]pyrene	E. crypticus	Survival	Soil	28	160.4	LC50	6.41	>	Droge et al. (2006)
Dibenzofuran	E. crypticus	Survival	Soil	21	148.6	LC50	3.95		Sverdrup et al. 2002a
Dibenzofuran	E. crypticus	Mortality	Soil	21	144.9	LC50	3.95		Sverdrup et al. 2002a
Dibenzothiophene	E. crypticus	Survival	Soil	21	780.1	LC50	4.37	>	Sverdrup et al. 2002a
Dibenzothiophene	E. crypticus	Mortality	Soil	21	915.8	LC50	4.37	>	Sverdrup et al. 2002a
Fluoranthene	E. crypticus	Survival	Soil	21	772.5	LC50	5.19	>	Sverdrup et al. 2002a
Fluoranthene	E. crypticus	Mortality	Soil	21	741.6	LC50	5.19	>	Sverdrup et al. 2002a
Fluorene	E. crypticus	Survival	Soil	21	601.6	LC50	3.93		Sverdrup et al. 2002a
Fluorene	E. crypticus	Mortality	Soil	21	676.8	LC50	3.93		Sverdrup et al. 2002a
Phenanthrene	E. crypticus	Survival	Soil	21	701.3	LC50	4.58	>	Sverdrup et al. 2002a
Phenanthrene	E. crypticus	Survival	Soil	28	91.7	LC50	4.58		Droge et al. (2006)

Table 3. Compiled Effects Data

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Compound	Species	Endpoint	Matrix	Duration	Effect (mmol / kg OC)	ENDPOINT	LogKow	FLAG	Reference
Pyrene	E. crypticus	Survival	Soil	21	710.7	LC50	5.13	>	Sverdrup et al. 2002a
Pyrene	E. crypticus	Survival	Soil	28	183.4	LC50	5.13	>	Droge et al. (2006)
Anthracene	F. candida	Survival	Soil	28	165.8	LC50	4.55	>	Droge et al. (2006)
Benz[a]anthracene	F. candida	Survival	Soil	28	188.9	LC50	5.74	>	Droge et al. (2006)
Benzo[a]pyrene	F. candida	Survival	Soil	28	160.4	LC50	6.41	>	Droge et al. (2006)
Fluorene	F. candida	Survival	Soil	21	46.6	LC50	3.93		Sorensen TS and Holmstrup M (2005)
Phenanthrene	F. candida	Mortality	Soil	21	15.3	LC50	4.58		Bowmer et al. (1993)
Phenanthrene	F. candida	Mortality	Soil	28	14.0	LC50	4.58		Bowmer et al. (1993)
Phenanthrene	F. candida	Survival	Soil	28	15.9	LC50	4.58		Droge et al. (2006)
Phenanthrene	F. candida	Survival	Soil	28	8.4	LC50	4.58		Paumen et al. (2008b)
Pyrene	F. candida	Survival	Soil	28	1.8	LC50	5.13		Herbert et al. (2004)
Pyrene	F. candida	Survival	Soil	28	32.2	LC50	5.13		Droge et al. (2006)
Pyrene	F. candida	Survival	Soil	21	77.3	LC50	5.13	>	Sorensen TS and Holmstrup M (2005)
Acenaphthene	F. fimetaria	Survival	Soil	21	43.4	LC50	3.88		Sverdrup et al. (2002c)

Table 3. Compiled Effects Data

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Compound	Species	Endpoint	Matrix	Duration	Effect (mmol / kg OC)	ENDPOINT	LogKow	FLAG	Reference
Acenaphthylene	F. fimetaria	Survival	Soil	21	59.5	LC50	3.44		Sverdrup et al. (2002c)
Anthracene	F. fimetaria	Survival	Soil	21	23.5	LC50	4.55		Sverdrup et al. (2002c)
Benz[a]anthracene	F. fimetaria	Survival	Soil	21	268.3	LC50	5.74	>	Sverdrup et al. (2002c)
Benzo[a]pyrene	F. fimetaria	Survival	Soil	21	208.1	LC50	6.41	>	Sverdrup et al. (2002c)
Benzo[b]fluoranthene	F. fimetaria	Survival	Soil	21	89.2	LC50	6.43	>	Sverdrup et al. (2002c)
Benzo[k]fluoranthene	F. fimetaria	Survival	Soil	21	138.7	LC50	6.40	>	Sverdrup et al. (2002c)
Chrysene	F. fimetaria	Survival	Soil	21	282.0	LC50	5.78	>	Sverdrup et al. (2002c)
Dibenz[a,h]anthracene	F. fimetaria	Survival	Soil	21	175.1	LC50	7.13	>	Sverdrup et al. (2002c)
Dibenzofuran	F. fimetaria	Survival	Soil	21	18.6	LC50	3.95		Sverdrup et al. (2001)
Dibenzothiophene	F. fimetaria	Survival	Soil	21	7.1	LC50	4.37		Sverdrup et al. (2001)
Fluoranthene	F. fimetaria	Survival	Soil	21	25.0	LC50	5.19		Sverdrup et al. (2002c)
Fluorene	F. fimetaria	Survival	Soil	21	14.7	LC50	3.93		Sverdrup et al. (2002c)

Table 3. Compiled Effects Data

Compound	Species	Endpoint	Matrix	Duration	Effect (mmol / kg QC)	ENDPOINT	LogKow	FLAG	Reference
Indeno[1,2,3-cd]pyrene	F. fimetaria	Survival	Soil	21	205.8	LC50	6.99	>	Sverdrup et al. (2002c)
Naphthalene	F. fimetaria	Survival	Soil	21	81.4	LC50	3.30		Sverdrup et al. (2002c)
Perylene	F. fimetaria	Survival	Soil	21	138.7	LC50	6.45	>	Sverdrup et al. (2002c)
Phenanthrene	F. fimetaria	Survival	Soil	21	14.4	LC50	4.58		Sverdrup et al. (2002c)
Pyrene	F. fimetaria	Survival	Soil	21	16.4	LC50	5.13		Sverdrup et al. (2002c)
Pyrene	F. fimetaria	Survival	Soil	21	22.9	LC50	5.13		Jensen J and Sverdrup LE (2002c)
Anthracene	C. riparius	Survival	Sediment	28	2.0	LC50	4.55	>	Paumen et al. (2008a)
Phenanthrene	C. riparius	Survival	Sediment	28	8.9	LC50	4.58		Paumen et al. (2008a)
Pentadecane (28 d)	F. candida	survival	Artificial soil	28	320.8	LC50	8.68		CONCAWE. 2011a
n-Octylcyclohexane (28 d)	F. candida	survival	Artificial soil	28	136.5	LC50	7.80		CONCAWE. 2011a
1-Phenylnonane (28 d)	F. candida	survival	Artificial soil	28	74.8	LC50	6.81		CONCAWE. 2011a
Fluoranthene	C. spinicorne	Survival	Sediment	10	14.0	LC50	5.19		Swartz et al. (1990)
1-Methylfluorene	R. abronius	Survival	Sediment	10	10.6	LC50	4.50		Boese et al. (1998)

Table 3. Compiled Effects Data

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Compound	Species	Endpoint	Matrix	Duration	Effect (mmol / kg OC)	ENDPOINT	LogKow	FLAG	Reference
2,3,6- Trimethylnaphthalene	R. abronius	Survival	Sediment	10	18.5	LC50	4.65		Boese et al. (1998)
2,6-Dimethylnaphthalene	R. abronius	Survival	Sediment	10	50.2	LC50	4.27		Boese et al. (1998)
2-Methylphenanthrene	R. abronius	Survival	Sediment	10	11.4	LC50	5.04		Boese et al. (1998)
9-Methylanthracene	R. abronius	Survival	Sediment	10	35.7	LC50	5.00		Boese et al. (1998)
Acenaphthene	R. abronius	Survival	Sediment	10	15.7	LC50	3.88		Boese et al. (1998)
Acenaphthene	R. abronius	Survival	Sediment	10	15.0	LC50	3.88		Swartz et al. (1997)
Fluoranthene	R. abronius	Survival	Sediment	10	18.1	LC50	5.19		DeWitt et al. (1992)
Fluoranthene	R. abronius	Survival	Sediment	10	15.4	LC50	5.19		Boese et al. (1998)
Fluoranthene	R. abronius	Survival	Sediment	10	16.4	LC50	5.19		Swartz et al. (1997)
Fluoranthene	R. abronius	Survival	Sediment	10	9.3	LC50	5.19		Swartz et al. (1990)
Fluoranthene	R. abronius	Survival	Sediment	10	10.4	LC50	5.19		Swartz et al. (1990)
Fluoranthene	R. abronius	Survival	Sediment	10	11.0	LC50	5.19		Swartz et al. (1990)
Naphthalene	R. abronius	Survival	Sediment	10	233.0	LC50	3.30		Boese et al. (1998)
Phenanthrene	R. abronius	Survival	Sediment	10	13.2	LC50	4.58		Boese et al. (1998)
Phenanthrene	R. abronius	Survival	Sediment	10	12.5	LC50	4.58		Swartz et al. (1997)
Pyrene	R. abronius	Survival	Sediment	10	15.4	LC50	5.13		Boese et al. (1998)
Pyrene	R. abronius	Survival	Sediment	10	13.9	LC50	5.13		Swartz et al. (1997)
Fluoranthene	Coullana sp.	Survival	Sediment	10	43.5	LC50	5.19		Lotufo GR (1998)
Phenanthrene	N. lacustris	Survival	Sediment	10	25.9	LC50	4.58		Lotufo GR and Fleeger JW (1997)

Table 3. Compiled Effects Data

Compound	Species	Endpoint	Matrix	Duration	Effect (mmol / kg OC)	ENDPOINT	LogKow	FLAG	Reference
Fluoranthene	S. knabeni	Survival	Sediment	10	70.2	LC50	5.19		Lotufo GR (1998)
Phenanthrene	S. knabeni	Survival	Sediment	10	129.0	LC50	4.58		Lotufo GR and Fleeger JW (1997)
Phenanthrene	L. hoffmeisteri	Survival	Sediment	10	238.4	LC50	4.58		Lotufo GR and Fleeger JW (1996)
1,2-Dichlorobenzene	E. andrei	Mortality	Soil	3	3.4	LC50	3.10		Hurdzan CM and Lanno RP (2009)
1,2,4-Trichlorobenzene	E. andrei	Mortality	Soil	5	7.5	LC50	3.72		Hurdzan CM and Lanno RP (2009)
1,2,3,4- Tetrachlorobenzene	E. andrei	Mortality	Soil	8	0.4	LC50	4.43		Hurdzan CM and Lanno RP (2009)
Pentachlorobenzene	E. andrei	Mortality	Soil	10	3.0	LC50	5.14		Hurdzan CM and Lanno RP (2009)
Hexachlorobenzene	F. candida	Survival	Soil	14	47.0	LC50	6.02	>	Hurdzan CM and Lanno RP (2009)
1,2,4-trichlorobenzene	B. caribaeum	Mortality	Sediment	10	148.8	LC50	3.72		Clark et al. (1987)
1,2,3-Trichlorobenzene	E. andrei	Mortality	Sediment	10	16.5	LC50	3.74		Belfroid et al. (1993)
Pentachlorobenzene	E. andrei	Mortality	Sediment	10	10.0	LC50	5.14	>	Belfroid et al. (1993)
Hexachlorobenzene	H. azteca	Mortality	Sediment	10	21.1	LC50	6.02	>	Fuchsman PC et al. (1998)
Pyrene	F. fimetaria	Survival	Askov Soil	21	16.4	LC50	5.13		Sverdrup et al. (2002b)
Pyrene (aged 120 d)	F. fimetaria	Survival	Askov Soil	21	13.6	LC50	5.13		Sverdrup et al. (2002b)

Table 3. Compiled Effects Data

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Compound	Species	Endpoint	Matrix	Duration	Effect (mmol / kg OC)	ENDPOINT	LogKow	FLAG	Reference
Phenanthrene	F. fimetaria	Survival	Askov Soil	21	14.4	LC50	4.58		Sverdrup et al. (2002b)
Phenanthrene (aged 120d)	F. fimetaria	Survival	Askov Soil	21	14.4	LC50	4.58	>	Sverdrup et al. (2002b)
1,2,3-trichlorobenzene	E. andrei	Mortality	Soil KOBG	14	34.4	LC50	3.74		Van Gestel CAM and Ma W (1990)
1,2,3-trichlorobenzene	E. andrei	Mortality	Soil HOLT	14	37.4	LC50	3.74		Van Gestel CAM and Ma W (1990)
1,2,3-trichlorobenzene	E. andrei	Mortality	Soil OECD	14	15.6	LC50	3.74		Van Gestel CAM and Ma W (1990)
1,2,3-trichlorobenzene	E. andrei	Mortality	Soil WAPV	14	33.3	LC50	3.74		Van Gestel CAM and Ma W (1990)
1,2,3-trichlorobenzene	L. rubellus	Mortality	Soil KOBG	14	29.5	LC50	3.74		Van Gestel CAM and Ma W (1990)
1,2,3-trichlorobenzene	L. rubellus	Mortality	Soil HOLT	14	31.2	LC50	3.74		Van Gestel CAM and Ma W (1990)
1,2,3-trichlorobenzene	L. rubellus	Mortality	Soil OECD	14	22.9	LC50	3.74		Van Gestel CAM and Ma W (1990)
1,2,3-trichlorobenzene	L. rubellus	Mortality	Soil WAPV	14	34.3	LC50	3.74		Van Gestel CAM and Ma W (1990)
Hexachlorocyclohexane (Lindane)	L. hoffmeisteri	Mortality	Sediment	3	296.4	LC50	3.39	>	Meller et al. (1998)
1,2,4-trichlorobenzene	A. tuberculata	Mortality	Soil OECD	14	31.0	LC50	3.72		Zolezzi, 2005
1,2,4-trichlorobenzene	E. fetida	Mortality	Soil OECD	14	24.3	LC50	3.72		Zolezzi, 2005

Table 3. Compiled Effects Data

Compound	Species	Endpoint	Matrix	Duration	Effect	ΕΝΙΟΡΟΙΝΤ	LogKow	FLAC	Peference
Compound	Species	Endpoint	Wattix	Duration	kg OC)	ENDFOINT	LOGKOW	TLAG	Kelefence
1,2,4-trichlorobenzene	E. eugeniae	Mortality	Soil OECD	28	15.7	LC50	3.72		Zolezzi, 2005
1,2,4-trichlorobenzene	P. excavatus	Mortality	Soil OECD	28	22.2	LC50	3.72		Zolezzi, 2005
1,2,4-trichlorobenzene	A. sativa	Mortality	Soil OECD	14	29.7	LC50	3.72		Zolezzi, 2005
1,2,4-trichlorobenzene	B. rapa	Mortality	Soil OECD	14	13.6	LC50	3.72		Zolezzi, 2005
chlorobenzene	E. andrei	Mortality	Soil KOBG	14	338.5	LC50	2.52		van Gestel CAM and Ma W (1993)
chlorobenzene	E. andrei	Mortality	Soil OECD	14	152.7	LC50	2.52		van Gestel CAM and Ma W (1993)
1,4-dichlorobenzene	E. andrei	Mortality	Soil KOBG	14	45.1	LC50	3.09		van Gestel CAM and Ma W (1993)
1,4-dichlorobenzene	E. andrei	Mortality	Soil OECD	14	133.0	LC50	3.09		van Gestel CAM and Ma W (1993)
1,2,3-trichlorobenzene	E. andrei	Mortality	Soil KOBG	14	35.8	LC50	3.74		van Gestel CAM and Ma W (1993)
1,2,3-trichlorobenzene	E. andrei	Mortality	Soil HOLT	14	40.4	LC50	3.74		van Gestel CAM and Ma W (1993)
1,2,3-trichlorobenzene	E. andrei	Mortality	Soil OECD	14	16.1	LC50	3.74		van Gestel CAM and Ma W (1993)
1,2,3-trichlorobenzene	E. andrei	Mortality	Soil WAPV	14	34.2	LC50	3.74		van Gestel CAM and Ma W (1993)
1,2,3,4-tetrachlorobenzene	E. andrei	Mortality	Soil KOBG	14	18.8	LC50	4.43		van Gestel CAM and Ma W (1993)
1,2,3,4-tetrachlorobenzene	E. andrei	Mortality	Soil OECD	14	19.8	LC50	4.43		van Gestel CAM and Ma W (1993)

Table 3. Compiled Effects Data

Compound	Species	Endpoint	Matrix	Duration	Effect (mmol / kg OC)	ENDPOINT	LogKow	FLAG	Reference
Pentachlorobenzene	E. andrei	Mortality	Soil KOBG	14	112.4	LC50	5.14		van Gestel CAM and Ma W (1993)
Pentachlorobenzene	E. andrei	Mortality	Soil OECD	14	56.3	LC50	5.14		van Gestel CAM and Ma W (1993)
chlorobenzene	L. rubellus	Mortality	Soil KOBG	14	997.4	LC50	2.52		van Gestel CAM and Ma W (1993)
chlorobenzene	L. rubellus	Mortality	Soil OECD	14	429.7	LC50	2.52		van Gestel CAM and Ma W (1993)
1,4-dichlorobenzene	L. rubellus	Mortality	Soil KOBG	14	66.4	LC50	3.09		van Gestel CAM and Ma W (1993)
1,4-dichlorobenzene	L. rubellus	Mortality	Soil OECD	14	596.2	LC50	3.09		van Gestel CAM and Ma W (1993)
1,2,3-trichlorobenzene	L. rubellus	Mortality	Soil KOBG	14	31.3	LC50	3.74		van Gestel CAM and Ma W (1993)
1,2,3-trichlorobenzene	L. rubellus	Mortality	Soil HOLT	14	33.2	LC50	3.74		van Gestel CAM and Ma W (1993)
1,2,3-trichlorobenzene	L. rubellus	Mortality	Soil OECD	14	22.8	LC50	3.74		van Gestel CAM and Ma W (1993)
1,2,3-trichlorobenzene	L. rubellus	Mortality	Soil WAPV	14	34.2	LC50	3.74		van Gestel CAM and Ma W (1993)
1,2,3,4-tetrachlorobenzene	L. rubellus	Mortality	Soil KOBG	14	27.0	LC50	4.43		van Gestel CAM and Ma W (1993)
1,2,3,4-tetrachlorobenzene	L. rubellus	Mortality	Soil OECD	14	18.1	LC50	4.43		van Gestel CAM and Ma W (1993)

Table 3. Compiled Effects Data

Compound	Species	Endpoint	Matrix	Duration	Effect (mmol / kg OC)	ENDPOINT	LogKow	FLAG	Reference
Pentachlorobenzene	L. rubellus	Mortality	Soil KOBG	14	102.9	LC50	5.14		van Gestel CAM and Ma W (1993)
Pentachlorobenzene	L. rubellus	Mortality	Soil WAPV	14	24.8	LC50	5.14		van Gestel CAM and Ma W (1993)
1,2,4-Trichlorobenzene	B. caribaeum	Survival	Sediment	10	190.1	LC50	3.72		Clark et al. (1987)
Styrene	E. fetida	Survival	Soil OECD	7	59.4	LC50	2.93		Cushman et al. (1997)
Pyrene	Diporeia	Survival	Sediment	8	158.7	LC50	5.13		Landrum et al. (1994)
Fluoranthene	H. azteca	Mortality	Sediment	16	311.4	LC50	5.19		Driscoll SK and Landrum PF (1997)
Diethyl phthalate (DEP)	C. tentans	Mortality	Sediment	10	290.7	LC50	2.41	>	Call et al. (2001)
Di-n-butyl phthalate (DBP)	C. tentans	Mortality	Sediment	10	121.1	LC50	4.46		Call et al. (2001)
Di-n-butyl phthalate (DBP)	C. tentans	Mortality	Sediment	10	124.6	LC50	4.46		Call et al. (2001)
Di-n-butyl phthalate (DBP)	C. tentans	Mortality	Sediment	10	120.5	LC50	4.46		Call et al. (2001)
Di-n-butyl phthalate (DBP)	H. azteca	Mortality	Sediment	10	2551.9	LC50	4.46	>	Call et al. (2001)
Di-n-butyl phthalate (DBP)	H. azteca	Mortality	Sediment	10	2208.3	LC50	4.46	>	Call et al. (2001)
Di-n-butyl phthalate (DBP)	H. azteca	Mortality	Sediment	10	1832.3	LC50	4.46	>	Call et al. (2001)

Table 3. Compiled Effects Data

Compound	Species	Endpoint	Matrix	Duration	Effect (mmol / kg OC)	ENDPOINT	LogKow	FLAG	Reference
Fluoranthene	H. azteca	Mortality	Field Sediment	10	2.5	LC50	5.19		Suedel et al. (1993)
Fluoranthene	C. tentans	Mortality	Field Sediment	10	7.8	LC50	5.19		Suedel et al. (1993)
Fluoranthene	H. azteca	Mortality	Field Sediment	10	7.3	LC50	5.19		Suedel et al. (1993)
Fluoranthene	C. tentans	Mortality	Field Sediment	10	8.6	LC50	5.19		Suedel et al. (1993)
Fluoranthene	H. azteca	Mortality	Field Sediment	10	6.2	LC50	5.19		Suedel et al. (1993)
Fluoranthene	C. tentans	Mortality	Sediment	10	3.4	LC50	5.19		Suedel et al. (1993)
1,4-dichlorobenzene	F. candida	Survival	LUFA soil	28	15.9	LC50	3.09		Geisen et al 2012
1,2,3-trichlorobenzene	F. candida	Survival	LUFA soil	28	15.5	LC50	3.74		Geisen et al 2012
1,2,4-trichlorobenzene	F. candida	Survival	LUFA soil	28	19.8	LC50	3.72		Geisen et al 2012
1,3,5-trichlorobenzene	F. candida	Survival	LUFA soil	28	15.7	LC50	3.76		Geisen et al 2012
1,2,3,4-tetrachlorobenzene	F. candida	Survival	LUFA soil	28	14.7	LC50	4.43		Geisen et al 2012
1,2,3,5-tetrachlorobenzene	F. candida	Survival	LUFA soil	28	17.9	LC50	4.47		Geisen et al 2012
1,2,4,5-tetrachlorobenzene	F. candida	Survival	LUFA soil	28	33.7	LC50	4.43	>	Geisen et al 2012
Pentachlorobenzene	F. candida	Survival	LUFA soil	28	16.1	LC50	5.14		Geisen et al 2012
Hexachlorobenzene	F. candida	Survival	LUFA soil	28	159.6	LC50	6.02	>	Geisen et al 2012
1,4-dichlorobenzene	F. candida	Survival	OECD	28	18.6	LC50	3.09		Geisen et al 2012
1,2,3-trichlorobenzene	F. candida	Survival	OECD	28	14.0	LC50	3.74		Geisen et al 2012

Table 3. Compiled Effects Data
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Compound	Species	Endpoint	Matrix	Duration	Effect (mmol / kg OC)	ENDPOINT	LogKow	FLAG	Reference
1,2,4-trichlorobenzene	F. candida	Survival	OECD	28	9.0	LC50	3.72		Geisen et al 2012
1,3,5-trichlorobenzene	F. candida	Survival	OECD	28	13.6	LC50	3.76		Geisen et al 2012
1,2,3,4-tetrachlorobenzene	F. candida	Survival	OECD	28	16.6	LC50	4.43		Geisen et al 2012
1,2,3,5-tetrachlorobenzene	F. candida	Survival	OECD	28	12.5	LC50	4.47		Geisen et al 2012
1,2,4,5-tetrachlorobenzene	F. candida	Survival	OECD	28	14.8	LC50	4.43	>	Geisen et al 2012
Pentachlorobenzene	F. candida	Survival	OECD	28	18.0	LC50	5.14		Geisen et al 2012
Hexachlorobenzene	F. candida	Survival	OECD	28	70.2	LC50	6.02	>	Geisen et al 2012
Phenanthrene	C.riparius	Emergence	artificial	28	119.5	LC50	4.58		Markinovitch et al 2011
phenanthrene	E. fetida	Mortality	soil	14	11.4	LC50	4.58		Wu et al 2011

Table 3. Compiled Effects Data

FIGURES



Figure 1a. Acute toxicity (LC50) vs. $\log K_{ow}$. Lines represent TLM-EqP relationship with and without the Kmw adjustment. Filled symbols are definitive LC50s, > symbols are tests where no toxic effects were seen at the tested concentration.



Figure 1b. Acute toxicity (LC50) vs $\log K_{\text{OW}}$. Lines represent TLM-EqP relationship with and without the Kmw adjustment. Filled symbols are definitive LC50s, > symbols are tests where no toxic effects were seen at the tested concentration.



Figure 1c. Acute toxicity (LC50) vs $\log K_{\text{OW}}$. Lines represent TLM-EqP relationship with and without the Kmw adjustment. Filled symbols are definitive LC50s, > symbols are tests where no toxic effects were seen at the tested concentration.



Figure 2. Comparison of CTLBBs from aquatic and the combined soil and sediment database. Note, the soil (dark blue) and sediment (light blue) CTLBBs have been multiplied by the ACR = 4.5 for a consistent comparison due to differences in test durations.



Figure 3. Comparison of TLM-estimated CTLBBs and measured CBBs for sediment invertebrates.



Figure 4. Aqueous LC50 data and TLM fit for C.riparius in 48 hr acute, aqueous exposures.



Figure 5. Acute to chronic ratios for combined soil and sediment data compared to ACRs from aquatic database.



Figure 6. ACR vs $\log K_{\rm OW}$ for aquatic and soil/sediment databases.



Figure 7. NOECs from soil and sediment exposures compared to HC5-EqP. Lines represent TLM-EqP relationship with and without the K_{LW} adjustment. The estimated solubility limit for soil and sediment exposures is also provided. Filled symbols are definitive LC50s, > symbols are tests where no toxic effects were seen at the tested concentration.



Figure 8. Fraction of entries that are $< HC5 vs \log K_{OW}$ in 0.5 log unit bins.



Figure 9. Fraction of entries that are non-toxic at max tested concentration (\blacktriangle)vs $\log K_{\rm OW}$ in 0.5 log unit bins.



Figure 10. Comparison of effects data against the duration of the pre-equilibration step after mixing of the chemical with the soil, prior to addition of test organisms.



Figure 11. The ratio between the effects data derived from shorter pre-equilibration times to longer pre-equilibration times generally increases with increasing $\log K_{ow}$.

Appendix 1

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