Environment Agency

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Verification of bioaccumulation models for use in environmental standards. Part A: aquatic models

Science Report – SC030197/SR2

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Steve Killeen

Head of Science

Executive summary

This report sets out to verify three methods for predicting the accumulation and concentration of chemicals in aquatic food chains. The three methods are:

- ECOFATE/BIO v1.1/AQUAWEB v1.1 food chain bioaccumulation models;
- the EU Technical Guidance Document (TGD) on risk assessment methods for new and existing chemicals;
- a method published by Voutsas et al. (2002) to predict bioaccumulation in aquatic food webs.

For chemicals with log10 octanol-water partition coefficients (log K_{ow}) up to around five, the contribution from food to the total body burden of top predators such as fish is likely to be small compared with uptake directly from water; in other words, bioconcentration processes dominate the uptake in predatory fish. In these cases, a bioconcentration factor (BCF) value alone would give a reasonably reliable indication of the concentration in predatory fish near the top of the food chain. The BCF value used should preferably be an experimentally determined value, but predicted BCFs could also be considered

For chemicals with a higher log K_{ow} value, a combination of the Voutsas et al. (2002) method for non-metabolised chemicals, along with a generic food chain in the AQUAWEB v1.1 model for substances that are metabolised, is likely to provide the most reliable predictions for chemicals with log K_{ow} values up to around seven. Above a log K_{ow} of seven there are considerable uncertainties in the model and available experimental data, and so it is not possible to recommend any one method for chemicals with very high log K_{ow} values. Problems with predictions for chemicals with such high K_{ow} values may arise not only from uncertainties in the bioaccumulation model, but also from uncertainties over how to estimate the bioavailable fraction in water for such substances.

All methods appear to significantly overestimate bioaccumulation factors (BAFs) derived from the Mersey data set. The reason for this is not clear, although there are significant limitations in this data set. All methods assume that uptake into the organism is governed by partitioning into lipids. Although this is the case for many substances, the methods are not applicable to substances whose uptake is governed by other processes, such as binding to proteins. It should be possible to use the TGD approach provided suitable biomagnification factor (BMF) values can be estimated, but at present no methods for such estimations are available.

Contents

1 Introduction

This project forms part of a broader programme to support the Environment Agency's work in developing standards for the protection of the environment and human health from chemicals (P6-020/U, *A programme of work on environmental and human health standards for chemicals*).

The Environment Agency must derive standards to protect the environment and human health in order to fulfil its statutory pollution control role. This project is intended to help provide a sound scientific basis for setting such standards and to ensure a transparent and consistent approach to setting standards across different functions within the Environment Agency.

Bioaccumulative substances are of concern to the Environment Agency because they have the potential to biomagnify via the food chain and cause effects on organisms at higher trophic levels. Bioaccumulation is of particular concern when the chemical is toxic as well as persistent or continuously released to the environment.

The Environment Agency currently derives standards to protect the aquatic environment based on acute or chronic aquatic toxicity data divided by an extrapolation factor. This approach does not take into account possible effects on organisms higher in the food chain, nor does it consider routes of exposure other than direct contact with water. For highly lipophilic substances that bioaccumulate, water is unlikely to be the only route of exposure for aquatic organisms and top predators, and exposure via contaminated food or sediment may become important. The Environment Agency needs to consider these additional exposure routes when setting aquatic standards for bioaccumulative and persistent substances.

This project will help the Environment Agency's negotiating position at EU meetings to agree environmental quality standards for pollutants and priority substances listed in Annexes VIII to X to the Water Framework Directive (Directive 2000/60/EC).

When setting soil standards, the Environment Agency must consider indirect exposure routes for organisms at the top of the terrestrial food chain. The method used to derive soil standards will feed into the tiered terrestrial ecological risk assessment (ERA) framework that is being developed by the Environment Agency and the Department for Environment, Food and Rural Affairs (Defra). Once finalised, this framework will be used in Part 2A of the Environmental Protection Act 1990 to assess the impacts of soil contamination on wildlife top predators, and it is also likely to have other uses such as under the Habitats Directive.

In addition to aquatic and terrestrial organisms, bioaccumulation in or uptake through the food chain is also important when considering human exposure to contaminants. Methods for determining human exposure to chemicals from some types of soil contamination are already available in the Contaminated Land Exposure Assessment (CLEA) approach (Environment Agency and Defra, 2002). However, equivalent methods for determining exposure to chemicals from other types of soils, and from other routes such as the aquatic food chain, are not generally available.

This work was commissioned by the Environment Agency to validate models suitable for assessing the potential bioaccumulation of organic chemicals when setting environmental standards. The models selected for verification in this report are based on the results of an initial evaluation of a large number of possible models. The initial evaluation is covered in a separate report (Environment Agency, 2007).

This report (Part A) outlines the verification of models and methods for the aquatic environment. Verification of models for the terrestrial environment and for the human

food chain is considered in Parts B and C in this series of reports. Part D of the report summarises the physico-chemical properties of the chemicals modelled in these reports.

For the aquatic environment, the following three methods are considered for verification:

- risk assessments based on the EU Technical Guidance Document;
- a method by Voutsas *et al.* (2002) to predict accumulation in aquatic food webs;
- ECOFATE/BIO v1.1/AQUAWEB v1.1 computer models.

The EU Technical Guidance Document (TGD) outlines the methods used for risk assessments of new and existing chemicals and biocidal products in the EU (European Commission, 2003). Methods in the TGD are implemented in a computer program called the European Union System for Evaluation of Substances, better known as EUSES (EUSES version 2.0.3 was used in this work). The TGD and the EUSES program are freely available from the European Chemicals Bureau website (http://ecb.jrc.it/).

Voutsas *et al.* (2002) have developed a method of predicting bioaccumulation in aquatic food webs. This method is a series of regression equations derived from field data relating the bioaccumulation factor (BAF) to the $\log_{10}$ octanol-water partition coefficient (log K_{ow}). The method considers four generalised trophic levels consisting of plankton (including phytoplankton and zooplankton), benthic invertebrates, planktivorous fish and piscivorous fish. The method is available in a published paper[1].

ECOFATE and Food Chain Bioaccumulation models have been developed by workers at Simon Fraser University in Canada. The Food Chain Bioaccumulation model version 1.1 and ECOFATE model version 1.0β1 both work on very similar principles; however, the first is essentially a steady-state food web model, whereas ECOFATE can also carry out more complex modelling of the fate and behaviour of the chemical in the water/sediment system (that is, steady-state or time-dependent modelling with multiple water/sediment compartments). In this report, only the food web model part of ECOFATE was tested. The ECOFATE and Food Chain Bioaccumulation models are freely available from the Simon Fraser University website (http://www.rem.sfu.ca/toxicology/models/models.htm).

The Food Chain Bioaccumulation model v1.1 that was reviewed previously by the Environment Agency (2007) was available as a stand-alone program. During the course of this work, the Food Chain Bioaccumulation model v1.1 was replaced on the Simon Fraser University website by an updated version called AQUAWEB v1.1. This spreadsheet model incorporates both the original Food Chain Bioaccumulation model v1.1 (called BIO v1.1 in the spreadsheet) and the new AQUAWEB v1.1 model. In order to clarify the precise version of the model used in our calculations[2], the following convention was adopted:

- ECOFATE model – this signifies the ECOFATE model version 1.0β1.
- Food Chain Bioaccumulation model v1.1 – this signifies the original version of the Food Chain Bioaccumulation model that was reviewed by the Environment

[1] In the course of this project, some of the data used in the Voutsas *et al*. (2002) method were checked. This resulted in a number of changes to the data set. However, as these made little difference to the results, the analysis in this report is based on the paper as published. The changes to the data and the revised results are included in Appendix D.

[2] Although all these models are similar in principle, some differences between models were apparent in some of the calculations carried out in this report, particularly at high log K_{ow} values, and so it is necessary to distinguish between the various models.

Agency (2007). This was a stand-alone model but is no longer available from the Simon Fraser University website.

- BIO v1.1 - this signifies the spreadsheet version of the Food Chain Bioaccumulation model (v1.1) that is incorporated into the AQUAWEB v1.1 model.
- AQUAWEB v1.1 – this signifies the updated AQUAWEB v1.1 spreadsheet model.

2 Initial comparison of the models

2.1 TGD/EUSES

The TGD method for the aquatic compartment essentially consists of two parts, an estimated (or measured) bioconcentration factor (BCF) for fish to take account of the uptake in fish via water, and an estimated (or measured) biomagnification factor (BMF) to take account of the uptake via their diet.

BCF values for fish can be estimated by one of the following equations:

$\log BCF = 0.85 \times \log K_{ow} - 0.70$ for $\log K_{ow}$ in the range 2 to 6

$\log BCF = -0.20 \times (\log K_{ow})^2 + 2.74 \times \log K_{ow} - 4.72$ for $\log K_{ow} > 6$

BMF is estimated either from the log K_{ow} or the fish BCF value as follows:

log K_{ow}	**BCF (l kg^{-1})**	**BMF_1**	**BMF_2**
<4.5	<2,000	1	1
4.5-5	2,000-5,000	2	2
5-8	>5,000	10	10
8-9	2,000-5,000	3	3
>9	<2,000	1	1

The fish concentration in the diet of predators such as fish-eating birds and mammals is then estimated using the following equation:

$PEC_{oral,\ predator} = PEC_{water} \times BCF \times BMF_1$

where $PEC_{oral,\ predator}$ = concentration in fish (diet) of fish-eating bird or mammal (mg kg^{-1} wet weight).

BCF = bioconcentration factor (l kg^{-1}).

BMF_1 = biomagnification factor (see above).

PEC_{water} = dissolved concentration of the substance in water (mg l^{-1}).

[For the marine compartment a second BMF is applied to estimate the concentration in top predators, in order to reflect the longer food chains that may be present in the marine environment (the method assumes that the predator itself may also be consumed): $PEC_{oral,\ top\ predator} = PEC_{water} \times BCF \times BMF_1 \times BMF_2$.]

On this basis, the overall bioaccumulation factor in fish (BAF, based on the freely dissolved concentration in water and a wet weight basis in the organism), taking into account exposure via both water and food, can be estimated as follows:

$BAF = BCF \times BMF_1$

[For the marine compartment, the equivalent overall BAF is $BCF \times BMF_1 \times BMF_2$.]

These equations apply equally if experimental BCF values are used instead of estimated ones. It should, however, be noted that the above equations apply only to BMF values estimated using the method outlined in the TGD. These BMF values are essentially 'scaling' factors rather than true biomagnification factors obtained by experiment, from fish feeding studies for example. If actual experimental biomagnification factors are used, then a slightly revised version of the equation needs to be used, as outlined in Environment Agency (2003).

$$PEC_{oral,\ predator} = PEC_{water} \times BCF \times (1 + FAF)$$

where FAF = food accumulation factor in fish derived from a feeding study (that is, the steady-state ratio of the concentration in the organism to the concentration in diet). This is actually the experimentally determined biomagnification factor, but the term FAF has been used here to distinguish this from the default BMFs used in the TGD.

In this case, the BAF would be $BCF \times (1 + FAF)$.

According to the TGD, the BMF (or FAF) from laboratory or field studies should preferably be derived on a lipid normalized basis. Such an approach is useful when investigating whether differences in concentrations in various species occur mainly as a result of differences in lipid content, or result from processes such as biomagnification. However, this then creates a problem when determining the overall BAF using the TGD approach, as BCF values are estimated (and usually measured) on a whole organism (wet weight) basis rather than a lipid weight basis. In addition, when considering the needs of this project, it is more important that the BAFs (and concentrations) are estimated on a whole organism wet weight basis (as this represents the dose that would be consumed by the top predator) than determining whether the concentrations result purely from differences in lipid contents or as a result of biomagnification. Therefore, it is better to use FAF (or BMF) on an organism wet weight basis, leading to an overall BAF with units of l kg^{-1} wet weight, when using this method for setting standards. In cases where the lipid contents of the prey (or food) and predatory organisms are the same, the lipid normalized BMF (or FAF) would be identical to that derived on an organism wet weight basis.

2.2 Voutsas *et al.* (2002)

The Voutsas *et al.* (2002) method gives the following equations for predicting the BAF in an aquatic food web:

Trophic level 1 (phytoplankton and zooplankton)

$$\log BAF_{fd} = -0.1301 \times (\log K_{ow})^2 + 2.5301 \times \log K_{ow} - 3.52$$

$$N_D = 94,\ N_C = 59,\ R^2 = 0.620$$

Trophic level 2 (benthic invertebrates)

$$\log BAF_{fd} = -0.0995 \times (\log K_{ow})^2 + 2.2855 \times \log K_{ow} - 3.1516$$

$$N_D = 352,\ N_C = 82,\ R^2 = 0.713$$

Trophic level 3 (planktivorous fish)

$$\log BAF_{fd} = -0.0977 \times (\log K_{ow})^2 + 2.2855 \times \log K_{ow} - 3.693$$

$$N_D = 325,\ N_C = 61,\ R^2 = 0.912$$

Trophic level 4 $\log BAF_{fd} = -0.0278 \times (\log K_{ow})^2 + 1.6604 \times \log K_{ow} - 1.6135$

(piscivorous fish) $N_D = 103$, $N_C = 64$, $R^2 = 0.929$

where $\log BAF_{fd} = \log_{10}$ of the bioaccumulation factor related to the freely dissolved concentration of the chemical in water and on a organism lipid weight basis (l kg^{-1} lipid).

$\log K_{ow} = \log_{10}$ of the octanol-water partition coefficient.

N_D = number of data points used to construct the regression equation.

N_C = number of chemicals in the data set used to construct the regression equation.

R^2 = correlation coefficient.

These regression equations were tested against an independent test set of field BAF data in the original paper. The results of this validation are summarised below.

Trophic level 1: Number of data points used in validation = 20.

Log K_{ow} range = 3.72 to 7.14.

Average absolute deviation in log BAF = 0.48.

Trophic level 2: Number of data points used in validation = 70.

Log K_{ow} range = 3.42 to 7.14.

Average absolute deviation in log BAF = 0.64,

Trophic level 3: Number of data points used in validation = 57.

Log K_{ow} range = 3.43 to 7.14.

Average absolute deviation in log BAF = 0.52.

Trophic level 4: Number of data points used in validation = 12.

Log K_{ow} range = 3.72 to 7.14.

Average absolute deviation in log BAF = 0.60.

In this case, BAF_{fd} values are given on a lipid normalized basis[3].

[3] In the draft version of Environment Agency (2007), these BAF_{fd} values were incorrectly identified as being on an organism wet weight basis. The further validation work carried out here found that these BAF values are actually derived on lipid normalised basis. This has now been corrected in Environment Agency (2007).

A similar set of equations were also derived by Voutsas *et al.* (2002) for the BAF_t (the lipid normalized bioaccumulation factor on a total concentration in water basis). These are summarised below.

Trophic level 1 (phytoplankton and zooplankton)

$$\log BAF_t = -0.2298 \times (\log K_{ow})^2 + 3.167 \times \log K_{ow} - 3.9242$$

$N_D = 94$, $N_C = 59$, $R^2 = 0.120$

Trophic level 2 (benthic invertebrates)

$$\log BAF_t = -0.2954 \times (\log K_{ow})^2 + 4.2438 \times \log K_{ow} - 8.0573$$

$N_D = 352$, $N_C = 82$, $R^2 = 0.538$

Trophic level 3 (planktivorous fish)

$$\log BAF_t = -0.2707 \times (\log K_{ow})^2 + 4.1253 \times \log K_{ow} - 8.0866$$

$N_D = 325$, $N_C = 61$, $R^2 = 0.857$

Trophic level 4 (piscivorous fish)

$$\log BAF_t = -0.2029 \times (\log K_{ow})^2 + 3.4112 \times \log K_{ow} - 6.0182$$

$N_D = 103$, $N_C = 64$, $R^2 = 0.897$

where $\log BAF_t = \log_{10}$ of the bioaccumulation factor related to the total concentration of the chemical in water and an organism lipid weight basis (l kg^{-1} lipid).

2.3 Food Web Bioaccumulation / ECOFATE /

The Food Web Bioaccumulation model (version 1.1) is a mass balance model for hydrophobic organic chemicals that was developed based on work published by Gobas (1993) and Morrison *et al.* (1996). The ECOFATE version 1.0β1 consists of four integrated modules that include a similar food web bioaccumulation model along with an environmental fate model, a toxicological hazard assessment model and a human health risk assessment model. The main difference between the two models is that the Food Web Bioaccumulation model is a steady-state model, whereas the ECOFATE model can be run both as a steady-state model or a time-dependent model. For the purposes of this report, steady-state predictions are considered most relevant.

The food web in both models consists of the following basic components. The number of species present at each level (with the exception of phytoplankton) can be user-specified.

- phytoplankton
- zooplankton
- filter feeders
- benthic detrivores
- fish.

During the course of this work, an updated version of the Food Web Bioaccumulation model became available. This model is called AQUAWEB v1.1 and is available as a spreadsheet. The spreadsheet also includes a version of the Food Web Bioaccumulation model v1.1 (named BIO v1.1 in the spreadsheet). The main revisions in the development of AQUAWEB v1.1 include a new model for the partitioning of chemicals into organisms, kinetic models for predicting the concentrations in algae, phytoplankton and zooplankton, new allometric relationships for predicting gill ventilation rates in a range of aquatic species, and a new mechanistic model for predicting gastrointestinal magnification of organic chemicals in a range of species. The AQUAWEB model is based on Arnot and Gobas (2004).

A summary of the main features of the AQUAWEB model is given in Appendix A. The main features of the Food Web Bioaccumulation model v1.1 and ECOFATE are summarised in Environment Agency (2007).

The calculations in this section were performed using the original Food Web Bioaccumulation model v1.1. Some of the calculations were repeated with the new spreadsheet version of BIO v1.1 and these gave broadly similar results to those from the original model (data not shown). AQUAWEB v1.1 was not used for this analysis.

2.4 Comparison of predictions using an hypothetical

Predictions for the three main methods under consideration were firstly compared directly by carrying out a series of calculations for a set of hypothetical chemicals with increasing log K_{ow} values (all three methods use log K_{ow} as the starting point to predict accumulation in the food chain).

Figure 2.1 shows a plot of log BAF against log K_{ow} for the TGD method. This shows that the BAF is predicted to increase to a maximum at log K_{ow} of around seven (where the BAF would be approaching 1×10^6 l kg^{-1} wet weight) and then decreases with increasing log K_{ow}.

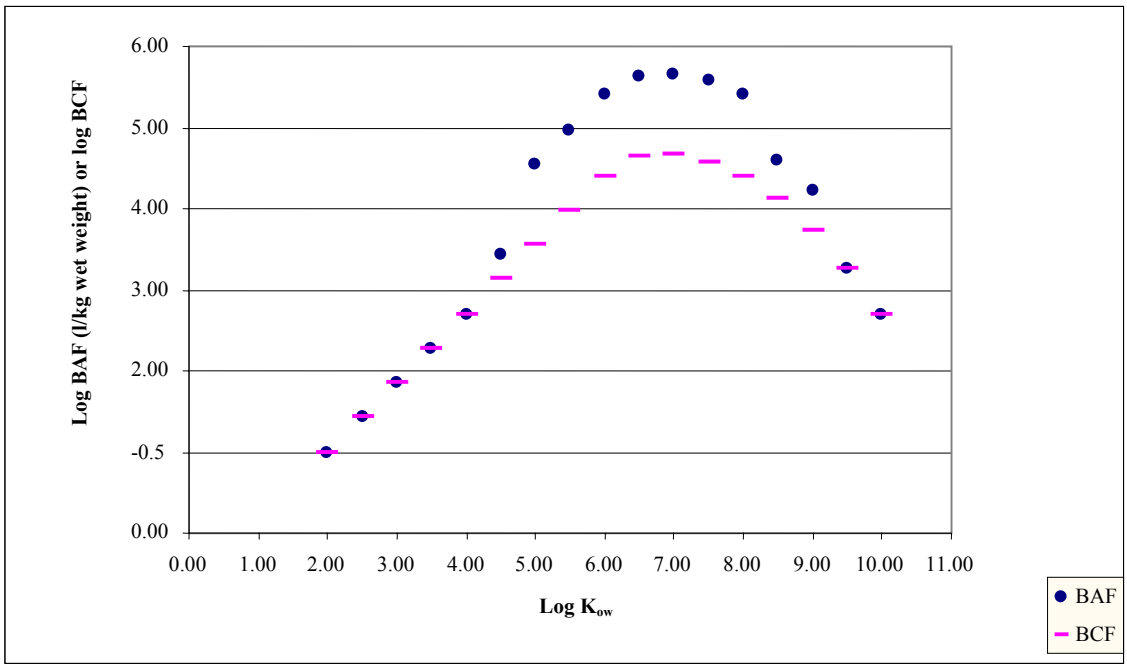

Figure 2.1 Plot of log BAF and log BCF against log K_{ow} for TGD method

From this plot, it is clear that the total accumulation (as measured by the BAF) is substantially higher than would be expected from water-phase-only accumulation (as measured by the BCF) in the log K_{ow} range of 4.5 to 9.

This analysis was carried out for a freshwater food chain, and hence only uses a single BMF_1 value. For the marine food chain, the TGD method introduces a second BMF_2 value. In this case, a similar pattern would be seen in the variation of the log BAF with log K_{ow}, except that the maximum value for log BAF would approach seven (that is, the maximum BAF would approach 1×10^7 l kg^{-1}).

Error! Reference source not found..2 shows a plot of log BAF_{fd} against log K_{ow} for the Voutsas *et al.* (2002) method. This shows that the level of accumulation in each of the four trophic levels considered in the method (phyto- and zooplankton, benthic invertebrates, planktivorous fish and piscivorous fish) is approximately the same until a log K_{ow} of around six, and then increasing accumulation with increasing trophic level is predicted.

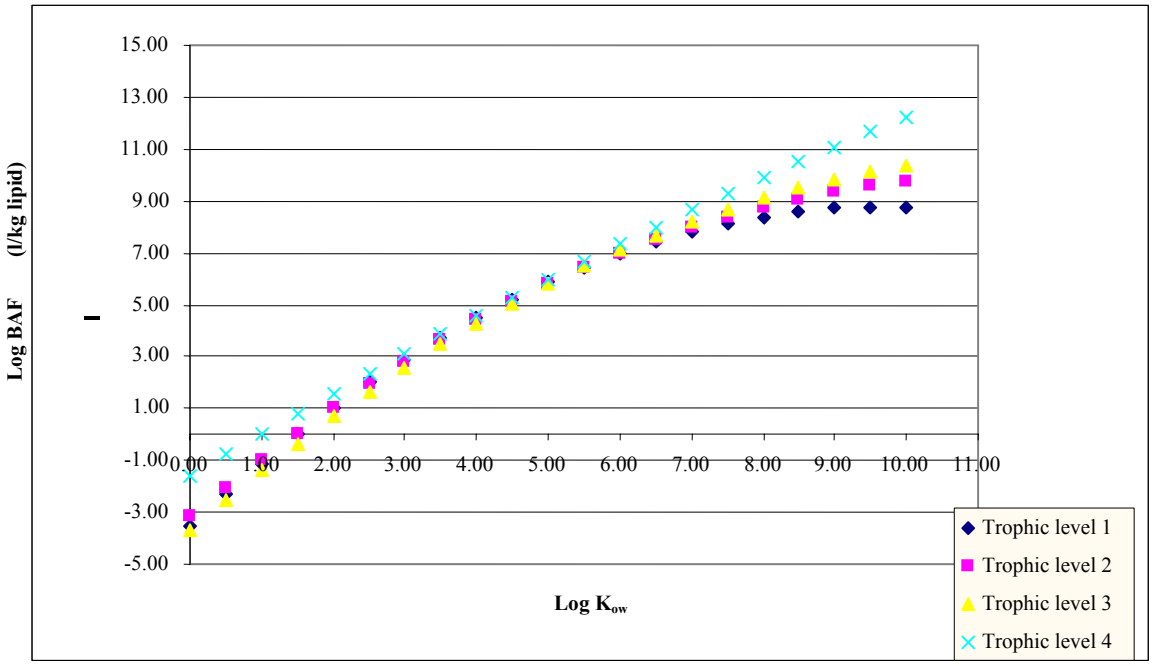

Figure 2.2 Plot of log BAF_{fd} against log K_{ow} for Voutsas *et al.* (2002)

The Voutsas *et al.* (2002) method was developed for a test set of chemicals with log K_{ow} values in the following ranges.

Trophic level 1	log K_{ow} range 5.24 to 8.18
Trophic level 2	log K_{ow} range 4.02 to 8.18
Trophic level 3	log K_{ow} range 4.02 to 8.18
Trophic level 4	log K_{ow} range 4.02 to 8.45

As can be seen, Figure 2.2 has been extrapolated outside of this range, and so the predictions at low and very high log K_{ow} values should be treated with caution. However it is worth noting that the pattern of accumulation predicted with the Voutsas method is different from that predicted with the TGD method at higher log K_{ow} values. For example, the TGD method reaches a maximum BAF of around 1×10^{6} l kg^{-1} wet weight at a log K_{ow} of around seven. For the same log K_{ow} of around seven, the Voutsas *et al.* (2002) method predicts a higher maximum level of accumulation at all trophic levels considered (log BAF_l of around 8 or 9, or a BAF_l of around 1×10^{8} or 1×10^{9} l kg^{-1} lipid; assuming a typical lipid content of around five per cent in the organism, this would be equivalent to a BAF of 5×10^{6} to 5.0×10^{7} l kg^{-1} wet weight). Further, the Voutsas *et al.* (2002) method predicts that the log BAF_l would increase further with increasing log K_{ow} beyond seven (at least up to a log K_{ow} of around 8), with this increase being more marked for the higher trophic levels. This difference between the methods is considered further in Section 2.5

Figure 2.3 shows a plot of log BAF against log K_{ow} for the Food Web Bioaccumulation model v1.1. The food chain used in the calculations was the default food chain in the model based on a Lake Ontario food chain and consisted of phytoplankton, zooplankton (mysids), benthic detrivores (Pontoporeia and oligochaetes), and fish (sculpin, alewife, smelt, lake trout and rainbow trout).

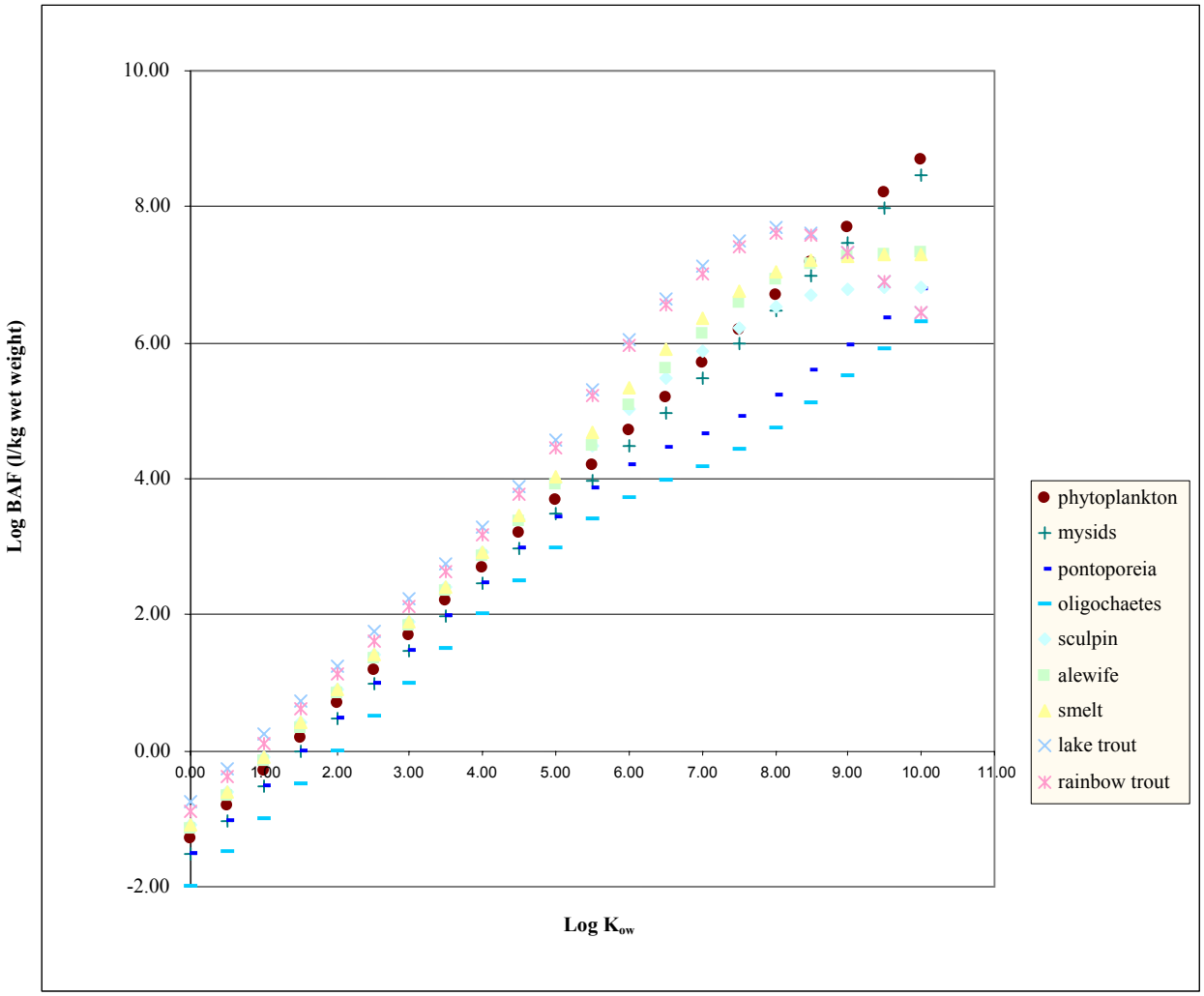

Figure 2.3 Plot of log BAF against log K_{ow} for the default food chain in the FoodWeb Bioaccumulation model (v1.1)

The model requires a concentration in water and a concentration in sediment. In order to ensure that these concentrations were consistent, a standard dissolved concentration in water of 1×10^{-6} g l^{-1} was assumed in all calculations, with the concentration in sediment estimated using the equilibrium partitioning method outlined in the TGD; the QSAR (quantitative structure activity relationship) for predominantly hydrophobic chemicals was used to estimated the organic carbon–water partition coefficient (K_{oc}) needed for the calculations. To ensure that the model treated the input water concentration as dissolved, the concentration of suspended solids in the water was set to zero. Thus for the simulation, the concentration in sediment increased with increasing log K_{ow}, and the pattern of bioaccumulation seen in the model is a function of both the assumptions contained within the model and those made over the choice of sediment concentration. Slightly different patterns of accumulation may be predicted if other assumptions are made.

The model also allows a metabolism rate in fish to be used, but for these hypothetical chemicals, no metabolism in fish was assumed. The input data used in the model simulation are summarised in Table2.1.

The following regression equations were derived from the data in Figure 2.3. These equations allow the BAF to be estimated directly from the log K_{ow} value for any chemical without using the model directly.

Phytoplankton	$\log BAF = \log K_{ow} - 1.301$
Mysids	$\log BAF = \log K_{ow} - 1.523$
Pontoporeia	$\log BAF = 0.002 \times (\log K_{ow})^4 - 0.034 \times (\log K_{ow})^3 + 0.172 \times (\log K_{ow})^2 + 0.744 \times \log K_{ow} - 1.465$
Oligochaete	$\log BAF = 0.002 \times (\log K_{ow})^4 - 0.034 \times (\log K_{ow})^3 + 0.172 \times (\log K_{ow})^2 + 0.744 \times \log K_{ow} - 1.942$
Sculpin	$\log BAF = -0.010 \text{ x } (\log K_{ow})^3 - 0.101 \times (\log K_{ow})^2 + 0.744 \times \log K_{ow} - 0.989$
Alewife	$\log BAF = -0.011 \text{ x } (\log K_{ow})^3 - 0.128 \times (\log K_{ow})^2 + 0.643 \times \log K_{ow} - 0.991$
Smelt	$\log BAF = -0.013 \text{ x } (\log K_{ow})^3 - 0.152 \times (\log K_{ow})^2 + 0.588 \times \log K_{ow} - 0.917$
Lake trout	$\log BAF = -0.003 \times (\log K_{ow})^4 + 0.035 \times (\log K_{ow})^3 - 0.089 \times (\log K_{ow})^2 + 1.011 \times \log K_{ow} - 0.725$
Rainbow trout	$\log BAF = -0.003 \times (\log K_{ow})^4 + 0.036 \times (\log K_{ow})^3 - 0.091 \times (\log K_{ow})^2 + 1.013 \times \log K_{ow} - 0.853$

Table 2.1 Input data used for the simulations with the Food Web Bioaccumulation model v1.1

Parameter			Value	Comment
Molecular weight			250 g mol^{-1}	Value used not important for this simulation.
Log K_{ow}			Range from 0 to 10 in steps of 0.5.	
Henry's law constant			12 Pa m^3 mol^{-1}	Value used not important for this simulation.
Chemical concentration in water			1×10^{-6} g l^{-1}	Taken to be the dissolved water concentration.
Concentration of suspended solids in water			0	This was set to zero as the concentrations in water were taken to be the dissolved concentration.
Organic carbon content of sediment solids			0.10 g g^{-1} (10%)	The default value from the TGD.
Concentration in bottom sediment			Calculated from the dissolved water concentration by equilibrium partitioning using the methods in the TGD.	
pH of water			7	Value used not important for this simulation.
Water temperature			12°C	The default value from the TGD.
Food web	Phytoplankton	Lipid content	0.05 kg kg^{-1} (5%)	This is the default value given in the model. This value appears high as 0.5% is used in the ECOFATE and the spreadsheet versions of BIO v1.1 and AQUAWEB v1.1.
	Zooplankton - Mysids	Lipid content	0.03 kg kg^{-1} (3%)	This is the default value given in the model.
	Benthic detrivore 1 - Pontoporeia	Lipid content	0.03 kg kg^{-1} (3%)	This is the default value given in the model.
	Benthic detrivore 2 – Oligochaetes	Lipid content	0.01 kg kg^{-1} (1%)	This is the default value given in the model.

Parameter			Value	Comment
	Fish 1 – Sculpin	Weight	0.0054 kg	These are the default values given in the model.
		Lipid content	0.08 kg kg^{-1} (8%)	
		Feeding preference (fraction of diet)	0.18 Mysids 0.82 Pontoporeia	
	Fish 2 - Alewife	Weight	0.032 kg	These are the default values given in the model.
		Lipid content	0.07 kg kg^{-1} (7%)	
		Feeding preference (fraction of diet)	0.6 Mysids 0.4 Pontoporeia	
	Fish 3 - Smelt	Weight	0.2 kg	These are the default values given in the model.
		Lipid content	0.08 kg kg^{-1} (8%)	
		Feeding preference (fraction of diet)	0.54 Mysids 0.21 Pontoporeia 0.25 Sculpins	
	Fish 4 – Lake trout	Weight	2.41 kg	These are the default values given in the model.
		Lipid content	0.174 kg kg^{-1} (17.4%)	
		Feeding preference (fraction of diet)	0.1 Sculpins 0.5 Alewife 0.4 Smelt	
	Fish 5 – Rainbow trout	Weight	3.38 kg	These are the default values given in the model.
		Lipid content	0.13 kg kg^{-1} (13%)	
		Feeding preference (fraction of diet)	0.1 Sculpins 0.5 Alewife 0.4 Smelt	

The model also estimates the BCF for the various fish species for exposure via water only. A comparison of the predicted BCF with the predicted BAF for the various species is given in Figure 2.8 to 2.4. These show that the predicted BCF and BAF are very similar up to a log K_{ow} of around five to six, and then the predicted BAF increases relative to the BCF, showing the importance of uptake via the food chain to the overall bioaccumulation potential.

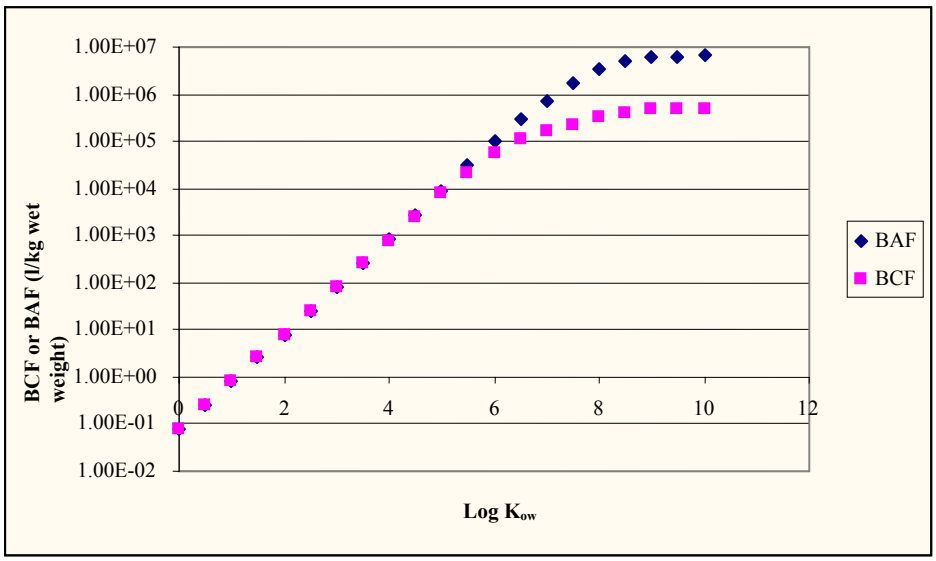

Figure 2.4 Plot of predicted BCF and BAF against log K_{ow} for sculpin using the Food Web Bioaccumulation model (v1.1)

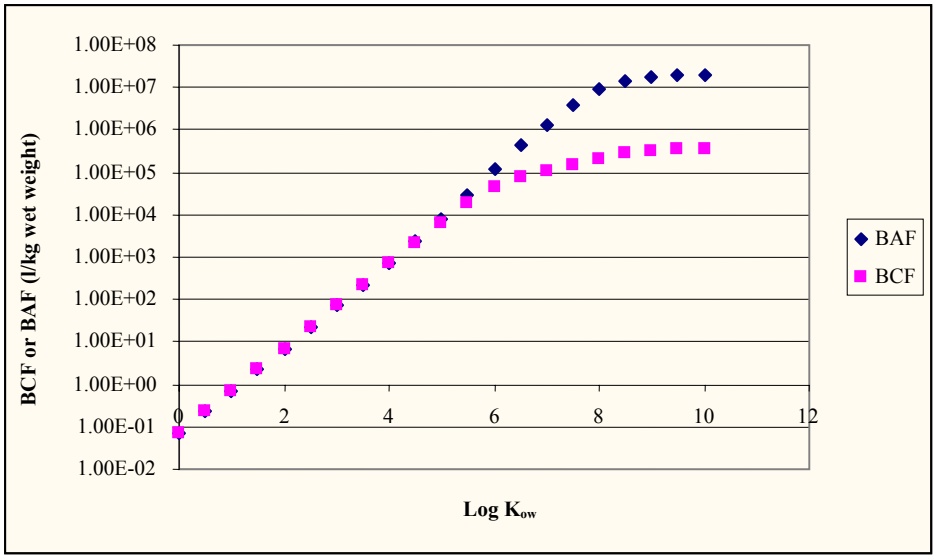

Figure 2.5 Plot of predicted BCF and BAF against log K_{ow} for alewife using the Food Web Bioaccumulation model (v1.1)

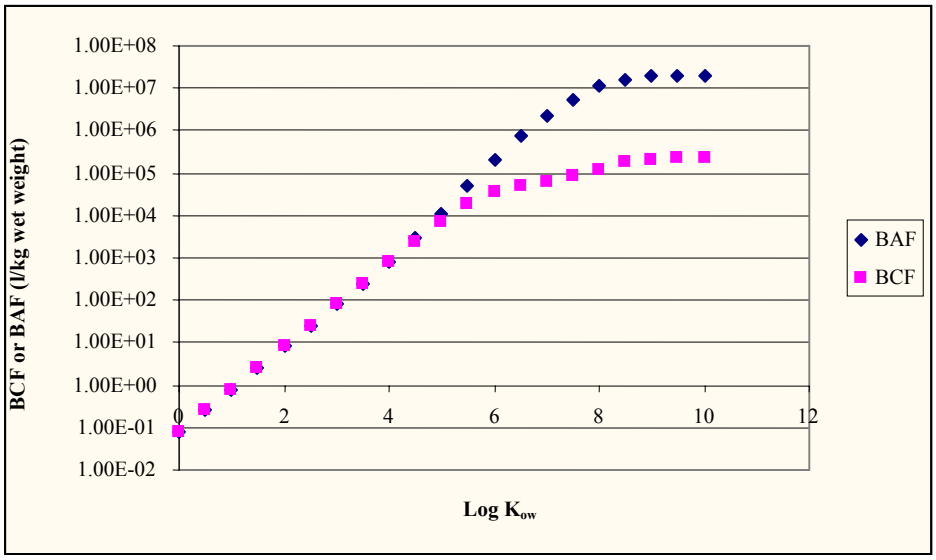

Figure 2.6 Plot of predicted BCF and BAF against log K_{ow} for smelt using the Food Web Bioaccumulation model (v1.1)

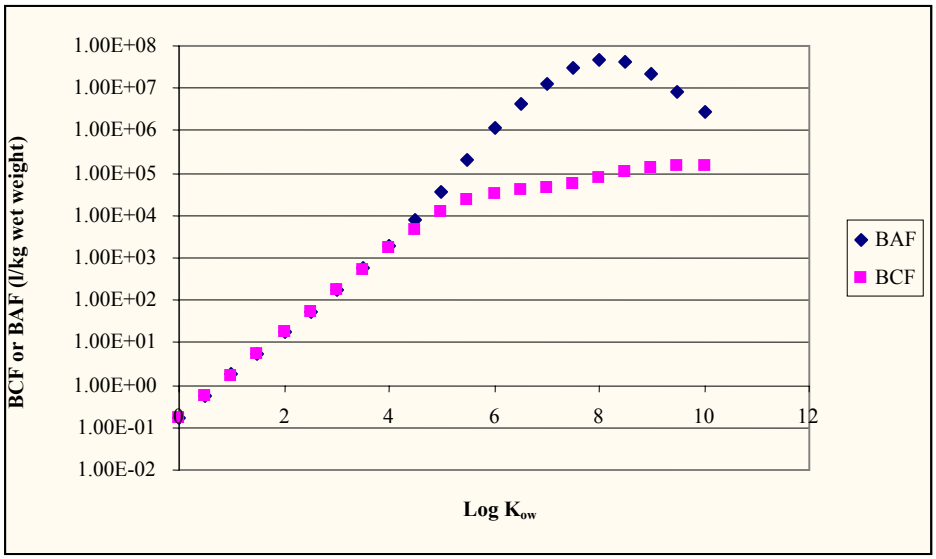

Figure 2.7 Plot of predicted BCF and BAF against log K_{ow} for lake trout using the Food Web Bioaccumulation model (v1.1)

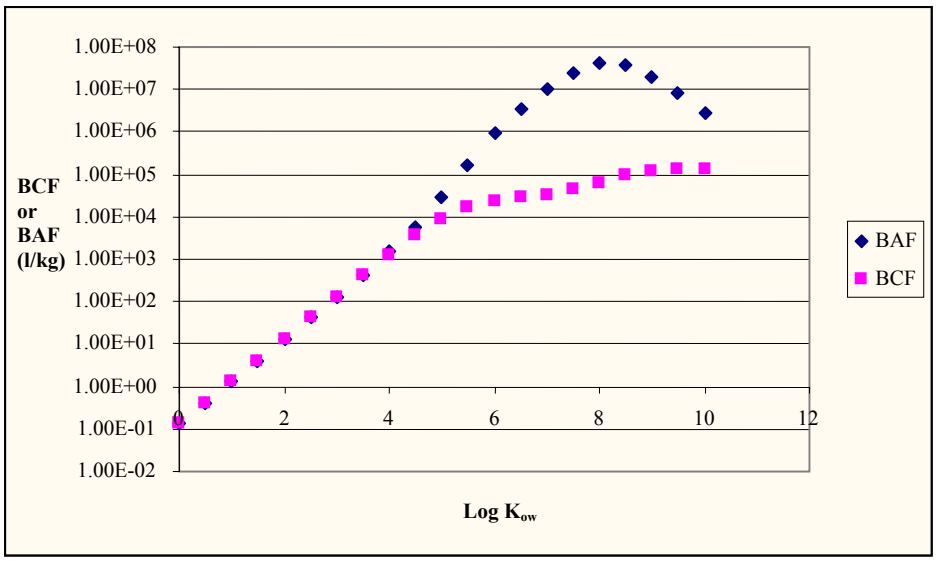

Figure 2.8 Plot of predicted BCF and BAF against log K_{ow} for rainbow trout using the Food Web Bioaccumulation model (v1.1)

The model also predicts that at high log K_{ow} (around eight or above), the BCF tends towards a maximum limit. Similarly, for some species (such as sculpin, alewife and smelt), the BAF shows a similar trend towards a maximum limit, but for other species (such as lake trout and rainbow trout), the predicted BAF reaches a maximum around a log K_{ow} of eight (the maximum BAF is around 1×10^7 to 1×10^8 l kg^{-1} wet weight), and then decreases. The reason for this most probably relates to the diets of the various species. For example, sculpin, alewife and to a lesser extent, smelt are assumed in the model to eat mainly zooplankton or benthic invertebrates. As can be seen in Figure 2.3 accumulation in these prey species is predicted to be almost linear with respect to log K_{ow} over the entire range studied (that is, the concentration in food for sculpin, alewife and smelt increases continuously with increasing log K_{ow} in the model). For lake trout and rainbow trout, however, diet is assumed to be mainly fish (sculpin, alewife and smelt), and for these species the predicted BAF tends towards a limit around a log K_{ow} of eight (that is, the concentration in food for lake trout and rainbow trout reaches a limit at high log K_{ow} in the model). Therefore for sculpin, alewife and smelt, any predicted decreases in uptake kinetics at high log K_{ow} from a decrease in assimilation efficiency is counteracted by increasing concentrations in food, whereas for lake trout and rainbow trout there is no increase in the concentration in food to balance the decrease in uptake kinetics. The shape of the curve is very sensitive to assumptions about the relation between assimilation efficiency and log K_{ow} used in the model.

2.5 Summary of findings

Several conclusions can be drawn from the model hypothetical predictions. Both the TGD approach and the Food Web Bioaccumulation model (and by inference the associated ECOFATE and AQUAWEB models) predict that accumulation in fish over that based on BCF alone is likely to be limited for substances with log K_{ow} of less than 4.5 or 5. For these chemicals, the accumulation in fish near the top of the food chain should be reasonably well predicted from the BCF value.

For chemicals with log K_{ow} greater than 4.5 to 5, increased accumulation via food is important and needs to be taken into account. For these chemicals, a BAF taking into account exposure via both water and food (and in some cases sediment) is needed to predict concentrations that may occur in organisms near the top of the food chain.

Predictions at very high log K_{ow} values (of eight or above) are less certain. Some methods predict a decrease in BAF at high log K_{ow} (for example, the TGD method and the Food Chain Bioaccumulation model), whereas the Voutsas *et al.* (2002) method implies an increasing BAF value with increasing log K_{ow} up to somewhat higher log K_{ow} values. However, there are few reliable data for chemicals at very high log K_{ow} values and as a consequence the methods have generally not been well tested in this range. Therefore it is not currently possible to reliably estimate a BAF for chemicals with log K_{ow} values greater than around eight.

For the magnitude of the BAF values predicted, the TGD method for freshwater aquatic food chains gives a maximum BAF approaching 1×10^6 l kg^{-1} wet weight at a log K_{ow} of around seven. This is significantly lower than predicted by both the Voutsas *et al.* (2002) method (BAF in fish of up to 5×10^7 l kg^{-1} at the same log K_{ow}) and the Food Web Bioaccumulation model (BAF in fish of up to 1×10^7 l kg^{-1} at log K_{ow} of seven, with a maximum BAF of around 1×10^8 l kg^{-1} at log K_{ow} of eight). This implies that the TGD method may be underestimating the true BAF, as the Voutsas *et al.* (2002) method in particular is based on a regression analysis of actual (field) BAF data.

The TGD method is essentially a prediction of bioconcentration from water (BCF) with an additional factor. Although some of the substances used in deriving the TGD BCF equation would be capable of showing biomagnification, they clearly could not do so in bioconcentration tests. Hence the additional factor has to address any biomagnification potential. If the second BMF_2 value is considered in the TGD method (currently only used for marine food chains), then the maximum BAF estimated by TGD would approach 1×10^7 l kg^{-1} at a log K_{ow} of seven, which is more in line with predictions from the other two methods. These results show the importance of the length of the food chain considered, and also that it is difficult to compare methods based on fixed length food chains (such as those based on regression equations) with models including a food web.

3 Testing against laboratory BCF data

3.1 Comparison of predicted and experimental data

A key part of the BIO v1.1/ECOFATE/AQUAWEB v1.1 model and the TGD method estimates the accumulation of chemicals in fish from water – that is, the BCF. This part of the model/method was tested against experimentally determined BCF values for a number of chemicals. BCF values were taken from a selection of published risk assessments[4] carried out under the Existing Substances Regulation (ESR). The values come from a range of tests and involve various species of fish, but all the data are considered reliable as they have been validated as part of the risk assessment process. The chemicals considered, along with experimental and estimated BCF, are shown in 3.1. A similar analysis was carried out using published BCF data for polychlorinated biphenyls (PCBs). These data are summarised in Table 3.2.

For the TGD method, BCF values were estimated using the following equations.

$\log BCF = 0.85 \times \log K_{ow} - 0.70$ for $\log K_{ow}$ in the range 2 to 6

$\log BCF = -0.20 \times (\log K_{ow})^2 + 2.74 \times \log K_{ow} - 4.72$ for $\log K_{ow} > 6$

For the BIO v1.1, ECOFATE and AQUAWEB v1.1 models the calculations were carried out for a fish with a 'typical' lipid content of eight per cent and a wet weight of 0.5 g, taken as representative of the fish species used in BCF tests. The models were run with no sediment or suspended sediment present, and at a temperature of 22°C, in order to mimic the conditions in a standard bioconcentration test. Under these conditions the concentration in water in the model represents the dissolved concentration. The food web used in the models consisted of one fish only and no exposure through the diet was assumed[5]. In addition, no metabolism of the chemicals in the fish was assumed.

Table shows a comparison of the predicted and measured log BCF for the four estimation methods used for the ESR data set. As can be seen from this figure (and the data in Table 3.1), all four methods appear to give good predictions for the BCF for chemicals with a log K_{ow} in the approximate range two to six for the ESR data set.

The data for PCBs are shown in Figure 3.2 (note the ECOFATE model was not used for this comparison). For these substances, predicted BCFs are generally of a similar order of magnitude as experimental ones across the entire range of substances, covering a log K_{ow} range of 3.9 to 8.3. The TGD method appears to give slightly better predictions of BCF than the BIO v1.1 model and AQUAWEB v1.1 model at high log K_{ow} values.

[4] The risk assessment reports are available at http://ecb.jrc.it/.

[5] This was possible with the BIO v1.1 model and the ECOFATE model. For the AQUAWEB model, intake of food was required for the model to be run correctly. In this case the diet was assumed to be 100 per cent phytoplankton. This should not affect the BCF as the model calculates both a BCF and a BAF for fish.

Table 3.1 Experimental and predicted fish BCF values for a test set of ESR chemicals

Chemical	Molecular weight (g mol^{-1})	Log K_{ow}	Experimental fish BCF (l kg^{-1})	Predicted BCF (l kg^{-1})			
				TGD method	ECOFATE	BIO v1.1	AQUAWEB v1.1
Edetic acid	292	-5.01	1.8	1.1×10^{-5}	7.8×10^{-7}	3.3	0.72
Piperizine	86	-1.25	3.9	0.02	4.5×10^{-3}	8.7	1.4
Acrylamide	71	-1.0	1	0.03	0.008	8.7	1.4
1,4-Dioxane	88	-0.27	0.7	0.12	0.04	8.8	1.5
Acrylonitrile	53	0.25	48	0.33	0.14	8.9	1.6
Aniline	74	0.9	2.6	1.2	0.64	9.4	2.1
Tert-butyl methyl ether	88	1.06	1.5	1.6	0.92	9.6	2.4
Phenol	94	1.47	17.5	3.5	2.4	11	4.0
4,4'-Methylenedianiline	198	1.59	14	4.5	3.1	12	4.8
Benzene	78	2.13	11	13	11	20	13
Trichloroethylene	132	2.29	17	18	16	24	18
Tetrachloroethylene	166	2.53	50	28	27	36	31
Toluene	92	2.65	90	36	36	44	40
3,4-Dichloroaniline	162	2.7	45	39	40	49	45
4-Chloro-2-methyphenol	143	3.09	30	84	98	107	108
1,4-Dichlorobenzene	147	3.38	296	149	192	200	210
Bisphenol-A	221	3.4	67	155	201	209	219
Cyclohexane	84	3.44	129	167	220	228	240
Naphthalene	128	3.7	427	279	400	406	436
1,2,4-Trichlorobenzene	181	4.05	2,000	553	897	889	968
Musk ketone	294	4.3	1,380	902	1,593	1,550	1,710
Nonylphenol	220	4.45	1,300	1,209	2,248	2,160	2,390
Dibutylphthalate	278	4.57	1.8	1,529	2,961	2,800	3,130
Musk xylene	297	4.9	4,400	2,917	6,305	5,600	6,460
Di-2-ethylhexyl phthalate (DEHP)	391	7.5	840	38,000	610,00	65,000	109,000
Diisodecylphthalate (DIDP)	447	8.8	14.4	8,017	792,000	139,000	117,000
Benzene, C_{10-13} alkyl derivatives	243	9.12	35	4,304	798,000	149,000	117,000

Table 3.2 Experimental and predicted fish BCF values for a test set of PCBs

Chemical	Molecular weight (g mol^{-1})	Log K_{ow} [a]	Experimental fish BCF (l kg^{-1}) [a]	Predicted BCF (l kg^{-1})		
				TGD method	BIO v1.1	AQUAWEB v1.1
Biphenyl	154	3.90	1,000	412	635	688
PCB 3	189	4.50	590	1,334	2,410	2,680
PCB 4	223	4.90	5,250	2,917	5,600	6,460
PCB 5	223	5.00	12,880	3,548	6,840	8,000
PCB 8	223	5.00	3,550	3,548	6,840	8,000
PCB 9	223	5.10	10,000	4,315	8,300	9,860
PCB 15	223	5.30	3,800	6,383	11,900	14,800
PCB 14	223	5.40	6,610	7,762	14,100	17,900
PCB 18	258	5.60	81,280	11,482	19,000	25,700
PCB 40	292	5.60	48,980	11,482	19,000	25,700
PCB 31	258	5.70	6,760	13,964	21,700	30,400
PCB 50	292	5.75	3,160	15,399	23,000	32,900
PCB 47	292	5.90	12,300	20,654	27,100	41,000
PCB 61	292	5.90	19,500	20,654	27,100	41,000
PCB 70	292	5.90	41,690	20,654	27,100	41,000
PCB 52	292	6.10	18,200	35,645	32,400	52,700
PCB 100	326	6.23	2,340	38,692	35,500	60,400
PCB 101	326	6.40	45,710	42,073	39,200	70,100
PCB 77	292	6.50	7,940	43,652	41,200	75,500
PCB 99	326	6.60	12,300	44,875	43,000	80,600
PCB 153	361	6.90	45,710	46,132	48,500	93,400
PCB 155	361	7.00	4,790	45,709	50,500	96,900
PCB 194	430	7.10	22,390	44,875	52,700	100,000
PCB 209	499	8.26	10,470	18,488	109,000	115,000

a) Data taken from Mackay *et al.* (1992).

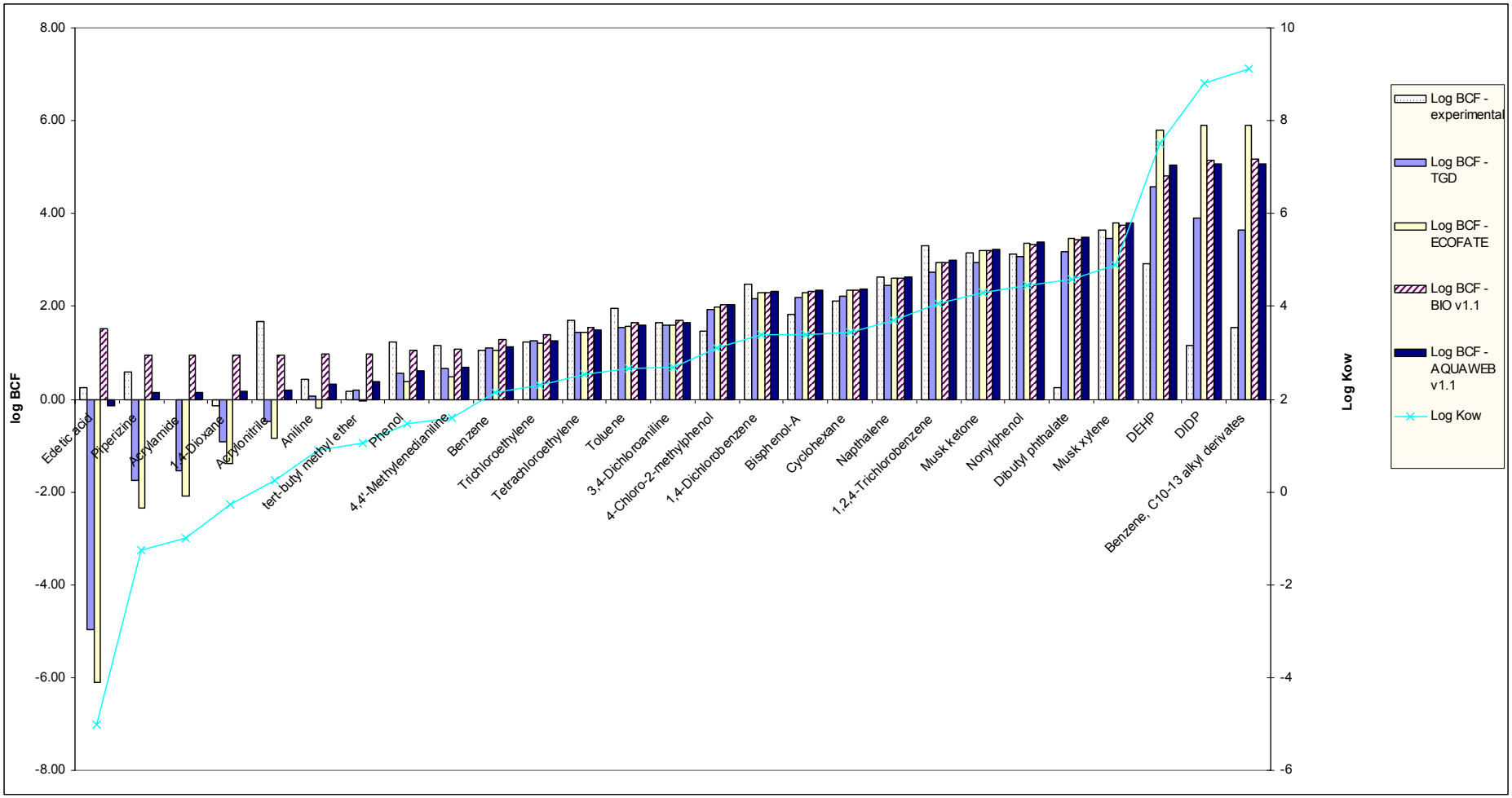

Figure 3.1 Comparison of predicted and experimental fish BCF for the ESR chemicals

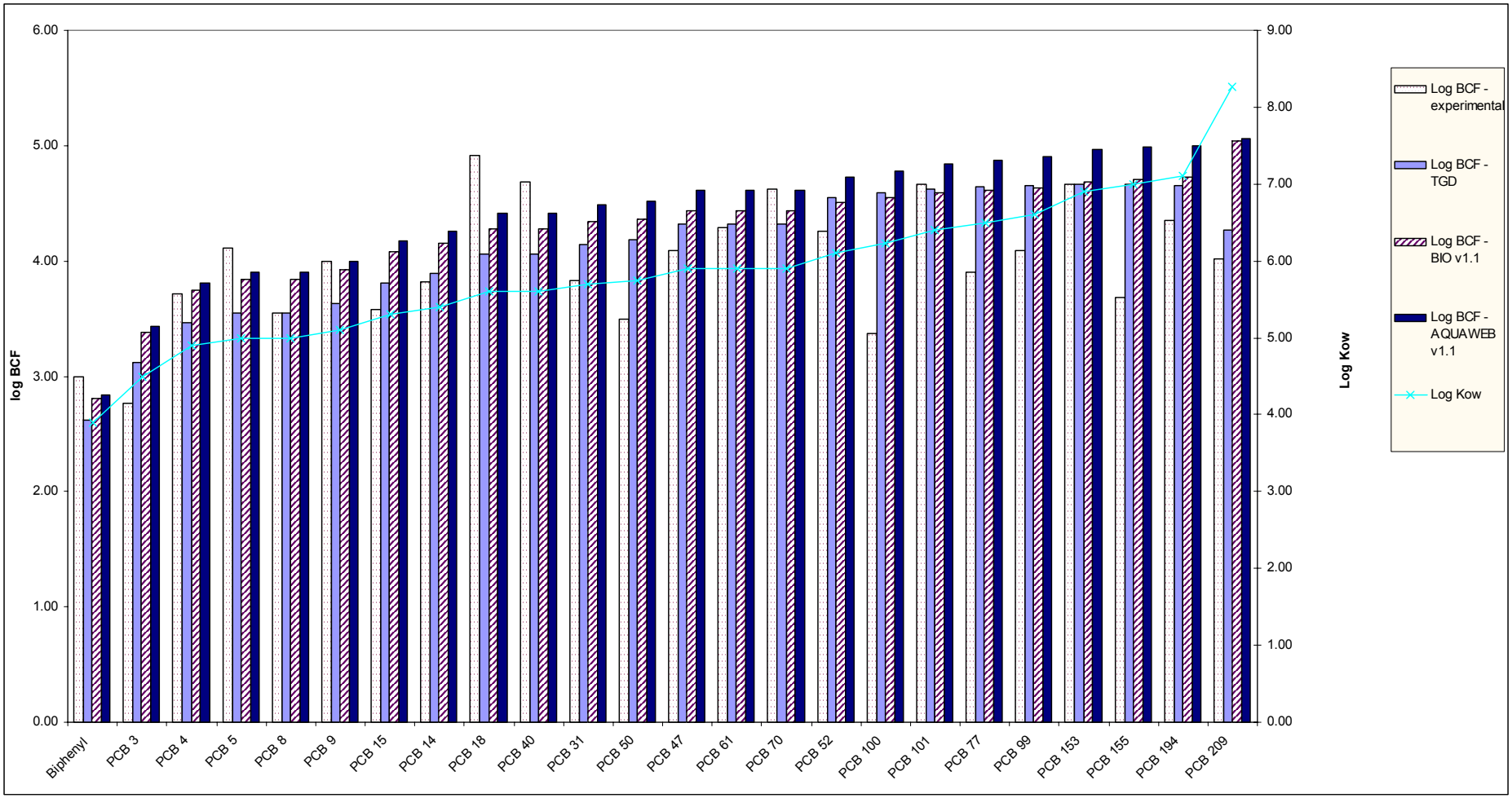

Figure 3.2 Comparison of predicted and experimental fish BCF for PCBs

As the Voutsas *et al.* (2002) method estimates BAF rather than BCF, it is not possible to compare the estimates from this method with the experimental BCF data.

At lower log K_{ow} values (such as a log K_{ow} lower than two), the AQAWEB v1.1 model appears to give slightly better predictions of actual BCF values than the other methods considered, but all methods predict that BCF values will be very low. Therefore, errors in predictions of the actual BCF at the low log K_{ow} end of the spectrum are not likely to be significant in terms of setting standards for these types of chemical. For these chemicals, the accumulation in organisms via both water and the food chain can effectively be ignored. Environmental standards are probably best set for these chemicals based on direct effects on water (and sediment) organisms.

At higher log K_{ow} values, all methods tend to overestimate the actual BCF of some of the chemicals tested in the ESR data set, notably dibutylphthalate, diisodecylphthalate (DIDP), benzene, $C_{10\text{-}13}$ alkyl derivatives, and to a lesser degree di-2-ethylhexyl phthalate (DEHP). One possible explanation for this is that these chemicals may be metabolised in fish, thus reducing their accumulation potential (no metabolism was assumed in the predictions given in 3.1). In order to test this further, information on metabolism in fish for these chemicals was sought from readily available sources.

For dibutylphthalate and DIDP, no information was located. However, for both DEHP and benzene, $C_{10\text{-}13}$ alkyl derivatives the ESR assessments give information on the rate of elimination. For DEHP, the depuration half-lives from a number of fish species were generally found to be in the range 1.8 to 12.2 days. For benzene, $C_{10\text{-}13}$ alkyl derivatives, a first order depuration rate constant of 0.34 per day was reported (equivalent to a depuration half-life of two days).

It should be noted that these half-lives are elimination (depuration) half-lives and not specifically metabolism half-lives. The various versions of the food web model generally consider that elimination from an organism can occur via three main processes: excretion across the gills, metabolism and excretion via faeces[6].

Predicted rate constants for excretion across the gills and excretion via faeces are given in the output from the AQUAWEB v1.1 model. These are as follows.

DEHP

First order rate constant for elimination from gills = 4.9×10^{-4} day^{-1}.

First order rate constant for faecal egestion = 3.7×10^{-4} day^{-1}.

Benzene, $C_{10\text{-}13}$ alkyl derivatives

First order rate constant for elimination from gills = 1.2×10^{-5} day^{-1}.

First order rate constant for faecal egestion = 1.1×10^{-5} day^{-1}.

Thus, the combined first order rate constant for these two elimination processes is 8.6×10^{-4} day^{-1} for DEHP and 2.3×10^{-5} day^{-1} for benzene, $C_{10\text{-}13}$ alkyl derivatives,

[6] A fourth process, growth dilution, is also considered in the models but is not so relevant for the relatively short-term bioconcentration tests, although it can play a role for small fish with very high log K_{ow} substances.

giving a depuration half-life of 806 days and 30,137 days respectively. Clearly the actual rate of elimination for these two substances is much larger than predicted rates considering elimination via the gills and gut (faeces) alone, indicating that metabolism is probably the dominant elimination process for these substances.

Assuming that the actual depuration half-life of DEHP is around 12.2 days, the overall first order rate constant for depuration is 0.057 day^{-1}. For benzene, C_{10-13} alkyl derivatives, the overall first order rate constant for depuration has been determined to be 0.34 day^{-1}. Using these values to represent the metabolism rate constant in the models, the following revised BCFs were estimated. Using BIO v1.1, the revised BCF for DEHP was 21,600 l kg^{-1} and the revised BCF for benzene, C_{10-13} alkyl derivatives was 5,240 l kg^{-1}. Similarly, using the AQUAWEB v1.1 model the revised BCFs were 19,400 l kg^{-1} and 3,820 l kg^{-1} respectively. These are much lower than the estimates obtained assuming no metabolism, but still overestimate the actual BCF by around a factor of 23-25 for DEHP and 110-150 for benzene, C_{10-13} alkyl derivatives.

It is not possible to include metabolism in the TGD method, although if an actual measured BCF was available this could be used in place of the predicted BCF.

3.2 Summary of findings

Overall, the TGD method and the various versions of the Food Web Bioaccumulation model all appear to provide reasonably reliable predictions of fish BCFs, at least in the log K_{ow} range of two to around seven or eight. At relatively high log K_{ow} values (around six), large errors in predictions can occur for chemicals that are readily metabolised[7]. This can be accounted for in the BIO v1.1, ECOFATE and AQUAWEB v1.1 models if a rate constant (or half-life) is included.

In terms of predicting accumulation in the food chain, bioconcentration is only one part, albeit an important one, of the overall accumulation process. Although reliable measured BCF values may be available for some (typically fish) species in the food chain, it is unlikely that they will be available for all species (both fish and non-fish). Since the basic principles used to estimate the accumulation in fish in the AQUAWEB v1.1 model are used for other (non-fish) species, it is reassuring that these methods appear to reliably predict the bioconcentration in fish for many of the chemicals in the test set. Predictions could probably be further improved by including metabolism rate constants in the simulation, and in this respect the BIO v1.1, ECOFATE and AQUAWEB v1.1 models score more highly than the TGD and Voutsas *et al.* (2002) methods, in that such data can be included in the prediction for bioaccumulation throughout the whole food chain if available.

[7] At moderate to low log K_{ow} values, other elimination processes included in the BIO v1.1/ ECOFATE/AQUAWEB v1.1 models (such as excretion across the gills and excretion via faeces) are predicted to be reasonably rapid, and so the addition of another elimination process such as metabolism is probably not quite so important to the overall prediction compared with the situation at high log K_{ow} (where elimination via excretion is predicted to be much less rapid).

4 Testing against field BAF data of Oliver and Niimi (1988)

4.1 Comparison of predicted and field data

Oliver and Niimi (1988) investigated the bioaccumulation of PCBs and other chlorinated organic chemicals in an ecosystem in Lake Ontario. The data set generated by this study was used in the initial development and testing of both the Voutsas *et al.* (2002) method and the Food Web Bioaccumulation model. The data set consists of measured concentrations of individual congeners in several trophic levels in the planktonic food chain (water → plankton → mysid → alewife and smelt → salmonid) and benthic food chain (water → sediment/suspended sediment → amphipod/oligochaete → sculpin → salmonid).

The following samples were included in the study:

- Surface water samples from seven locations sampled in April 1984. Samples were centrifuged to remove suspended sediment prior to extraction and analysis.
- Bottom surficial sediment samples (depth 0-3 cm) from 35 locations sampled in May 1981.
- Suspended sediments from three locations. Samples were collected over winter (between November and April) in sediment traps from six depths. The samples from each depth were combined to give one representative integrated sample for each location for each year between 1982 and 1986.
- Phytoplankton samples from three locations. The samples were collected in July 1982 and would have contained a mixture of phytoplankton and zooplankton, although Oliver and Niimi (1988) expected that phytoplankton would predominate. The lipid content of the phytoplankton was given as 0.5 per cent.
- Mysid samples from two locations. One sample was collected in July 1981 and the second sample was collected in October 1984. The species was identified as *Mysis relicta*. The lipid content of the mysids was given as three per cent.
- Amphipods (*Pontoporeia affinis*) and oligochaete worms (mainly *Tubifex tubifex* and *Limnodrilus hoffmeisteri*) were collected from one location (several samples were collected in sediment box cores at five km intervals in the sampling area) in June 1985. The lipid contents of the amphipods and oligochaetes were given as three per cent and one per cent respectively.
- Slimy sculpin (*Cottus cognatus*) from one location. A single composite sample of five fish was collected in spring 1986. The lipid content of the sculpin was given as eight per cent.

- Alewife (*Alosa pseudoharengus*) from one location. A single composite sample of twelve fish was collected in May 1982. The lipid content of the alewife was given as seven per cent.
- Small rainbow smelt (*Osmerus mordax*). The small smelt weighed around 12 g each and were collected from one location in April 1986. A total of six composite samples were collected, with each composite sample consisting of eight individuals. The lipid content of the smelt was given as four per cent.
- Large rainbow smelt. The large smelt weighed around 16 g. A single composite sample of twenty fish was collected from one location in May 1982.
- Salmonids. A total of 60 salmonids were collected and analysed individually. The samples included ten coho salmon (*Oncorhynchus velinus namaycush*), ten rainbow trout (*Oncorhynchus mykis*) and ten lake trout (*Salvelinus namaycush*) collected in autumn 1981 from one location, and ten coho salmon, ten rainbow trout and ten brown trout (*Salmo trutta*) collected from a second location in April 1982. The lipid content of the salmonids was given as 11 per cent.

Although not all samples were collected from exactly the same locations within the lake (generally samples were taken from the three major basins within the lake), nor at the same time (samples were effectively collected over a five-year period), no significant concentration trends relating to location or sampling time were evident in the data, and Oliver and Niimi (1988) considered the data to be representative of concentrations within the ecosystem over the course of the entire sampling period.

Within the food chain salmonid species are known to feed mainly on alewives, and to a lesser extent on smelt; small lake trout feed mainly on sculpins, and some smelt and alewives during certain times of the year. Smelt feed mainly on mysids. The main food for alewives is mysids, followed by amphipods. Sculpins feed mainly on amphipods but also mysids and chironomids. Mysids feed mainly on zooplankton, while amphipods and oligochaetes feed mainly on detrital matter (Oliver and Niimi, 1988).

As indicated above, these data have been used in the development of the Voutsas *et al.* (2002) method. The performance of the Voutsas *et al.* (2002) method against these data (and the other data used to develop the method) is discussed in Section 2.2. Similarly, the Food Web Bioaccumulation v1.1/BIO v1.1 model and the AQUAWEB v1.1 model have been tested previously against this data set (see Appendix A).

It is, however, possible to use these data to test the TGD method, which predicts the concentration in organisms (fish) near to the top of the food chain. Therefore, the most relevant data from the Oliver and Niimi (1988) study are the concentrations in salmonids, and also possibly large smelt. Relevant data from the Oliver and Niimi (1988) study are given in Table 4.1, along with the estimated overall BAF obtained using the TGD method. The same data are displayed graphically Figure 11.

As can be seen in Table 4.1, predictions from the TGD method are generally within a factor of 10 of the field data for large smelts and around a factor of 30 for the salmonids. However, it is apparent that the TGD-predicted BAF appears to be systematically lower than found in the field data, particularly for PCBs with log K_{ow} values of around six and above (the highest log K_{ow} value in the test set was 7.4) in salmonids. This finding is surprising in that the TGD is designed to be reasonably conservative (it is meant to represent a realistic worst case situation), but it is consistent with the analysis carried out in Section 2. The data of Oliver and Niimi

(1988) suggest that the TGD method currently used for freshwater ecosystems may actually underestimate the concentrations of some substances in predatory fish near the top of the food chain.

Table 4.1 Measured and predicted BAF for the data of Oliver and Niimi (1988)

IUPAC number	Log P	Measured concentrations			Field BAF (l kg^{-1} wet wt.)		Estimated BCF, BMF and BAF using the TGD method		
		Water (mg l^{-1})	Large smelts (mg kg^{-1} wet wt.)	Salmonids (mg kg^{-1} wet wt.)	Large smelts	Salmonids	BCF (l kg^{-1} wet wt.)	BMF	BAF (l kg^{-1} wet wt.)
PCB 8	5.1	1.8×10^{-8}	ND	ND			4.3×10^{3}	10	4.3×10^{4}
PCB 18	5.6	7.2×10^{-8}	ND	4.3×10^{-3}		6.0×10^{4}	1.2×10^{4}	10	1.2×10^{5}
PCB 28	5.8	4.9×10^{-8}	ND	0.036		7.4×10^{5}	1.7×10^{4}	10	1.7×10^{5}
PCB 33	5.8	1.4×10^{-8}	ND	3.0×10^{-4}		2.1×10^{4}	1.7×10^{4}	10	1.7×10^{5}
PCB 40	5.6	3.6×10^{-9}	ND	1.3×10^{-3}		3.6×10^{5}	1.2×10^{4}	10	1.2×10^{5}
PCB 44	6	5.0×10^{-8}	0.015	0.045	$3.0x10^{5}$	9.0×10^{5}	2.5×10^{4}	10	2.5×10^{5}
PCB 47	5.9	4.1×10^{-8}	0.024	0.060	5.9×10^{5}	1.5×10^{6}	2.1×10^{4}	10	2.1×10^{5}
PCB 49	6.1	2.4×10^{-8}	9.0×10^{-3}	0.031	3.8×10^{5}	1.3×10^{6}	3.6×10^{4}	10	3.6×10^{5}
PCB 52	6.1	6.3×10^{-8}	0.018	0.062	2.9×10^{5}	9.8×10^{5}	3.6×10^{4}	10	3.6×10^{5}
PCB 53	5.5	4.6×10^{-9}	ND	1.5×10^{-3}		3.3×10^{5}	9.4×10^{3}	10	9.4×10^{4}
PCB 60	6.31	9.7×10^{-9}	0.039	0.074	4.0×10^{6}	7.6×10^{6}	4.0×10^{4}	10	4.0×10^{5}
PCB 66	5.8	3.1×10^{-8}	0.072	0.16	2.3×10^{6}	5.2×10^{6}	1.7×10^{4}	10	1.7×10^{5}
PCB 87	6.5	2.1×10^{-8}	0.069	0.20	3.3×10^{6}	9.5×10^{6}	4.4×10^{4}	10	4.4×10^{5}
PCB 101	6.4	1.3×10^{-7}	0.079	0.27	6.1×10^{5}	2.1×10^{6}	4.2×10^{4}	10	4.2×10^{5}
PCB 105	6	1.4×10^{-8}	0.038	0.11	2.7×10^{6}	7.9×10^{6}	2.5×10^{4}	10	2.5×10^{5}
PCB 110	6.3	5.5×10^{-8}	0.088	0.23	1.6×10^{6}	4.2×10^{6}	4.0×10^{4}	10	4.0×10^{5}
PCB 136	6.7	1.6×10^{-8}	ND	0.031		1.9×10^{6}	4.6×10^{4}	10	4.6×10^{5}
PCB 153	6.9	5.0×10^{-8}	0.13	0.43	2.6×10^{6}	8.6×10^{6}	4.6×10^{4}	10	4.6×10^{5}
PCB 194	7.4	7.8×10^{-9}	7.3×10^{-3}	0.023	9.4×10^{5}	3.0×10^{6}	4.0×10^{4}	10	4.0×10^{5}

ND = Not detected. The detection limit was not given.

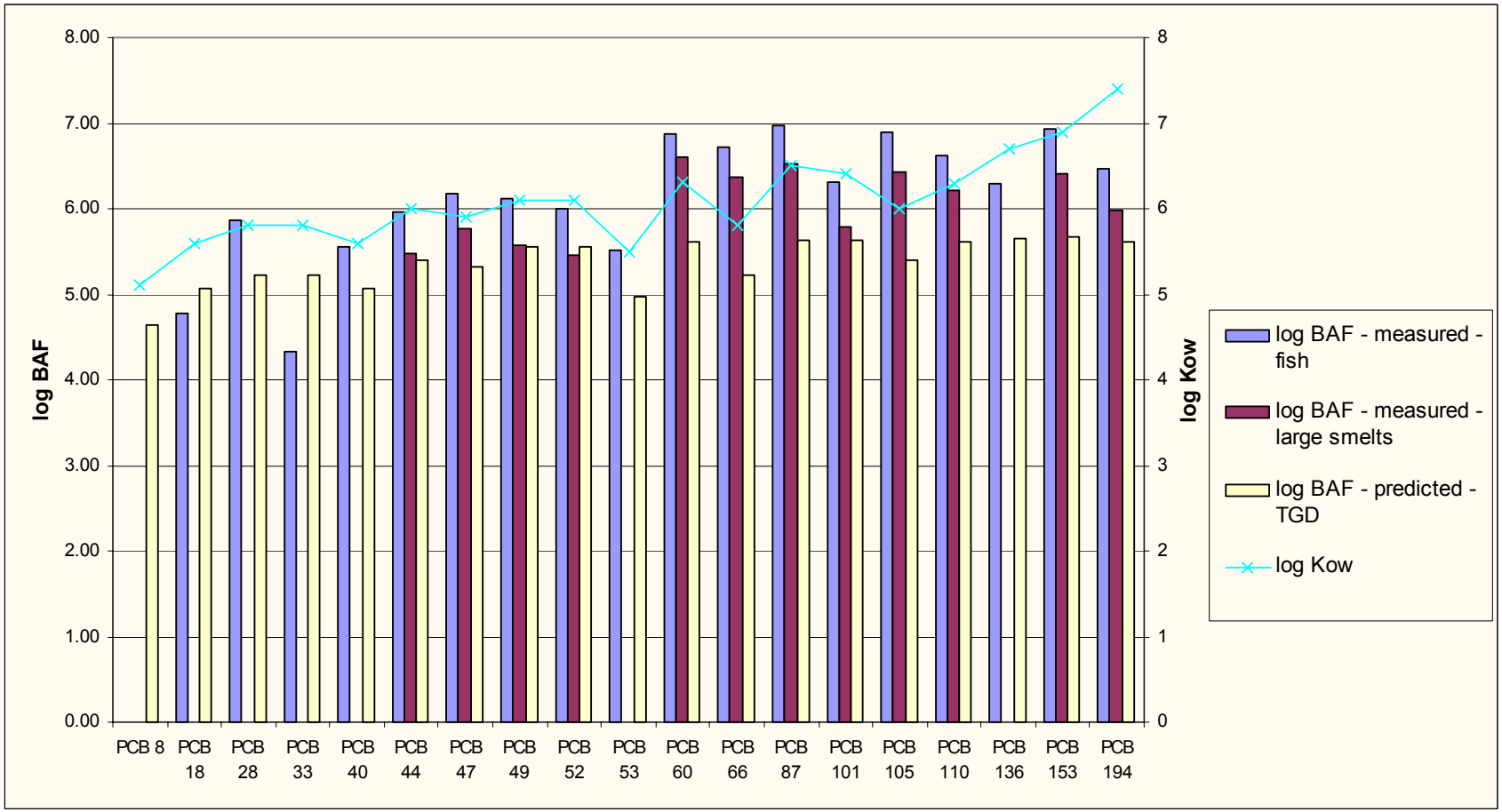

Figure 4.1 Comparison of predicted BAF with field BAF for PCBs[8]

[8]For PCB 8, the substance was measured in water at a concentration of 1.8×10^{-8} mg/l but was not detected in the fish. The detection limit was not given but was probably around 1×10^{-3} mg/kg wet weight or lower. On this basis, the log BAF for PCB 8 would be less than 4.7.

Oliver and Niimi (1988) also investigated the relationship of the BAF obtained for salmonids with log K_{ow} values for six groups of PCB congeners (the groups were tri- to octachloro-congeners) and twelve other chlorinated organic compounds for which suitable data were obtained in the study. The BAF for each congener group was estimated by dividing the sum of the concentrations in salmonids for each group by the sum of the dissolved concentration in water. The following regression equation was obtained:

Salmonids

$$\log BAF = 1.07 \times \log K_{ow} - 0.21$$

$n = 18$, $R^2 = 0.86$, 95% confidence limit of the slope = 0.84 to 1.30.

Similar equations were also derived for other parts of the food chain. These regression equations are summarised below:

(Phyto)plankton

$$\log BAF = 0.68 \times \log K_{ow} + 0.33$$

$n = 26$, $R^2 = 0.83$, 95% confidence limit of the slope = 0.55 to 0.81.

Mysids

$$\log BAF = 0.77 \times \log K_{ow} + 0.53$$

$n = 25$, $R^2 = 0.77$, 95% confidence limit of the slope = 0.59 to 0.94.

Amphipods

$$\log BAF = 0.61 \times \log K_{ow} + 0.61$$

$n = 27$, $R^2 = 0.0.79$, 95% confidence limit of the slope = 0.48 to 0.74.

Oligochaetes

$$\log BAF = 0.73 \times \log K_{ow} + 0.44$$

$n = 26$, $R^2 = 0.67$, 95% confidence limit of the slope = 0.51 to 0.94.

Sculpins

$$\log BAF = 1.08 \times \log K_{ow} - 0.70$$

$n = 21$, $R^2 = 0.83$, 95% confidence limit of the slope = 0.84 to 1.32.

Alewives

$$\log BAF = 0.83 \times \log K_{ow} + 0.81$$

$n = 17$, $R^2 = 0.78$, 95% confidence limit of the slope = 0.59 to 1.06.

Small smelt

$$\log BAF = 0.92 \times \log K_{ow} - 0.02$$

$n = 16$, $R^2 = 0.80$, 95% confidence limit of the slope = 0.66 to 1.17.

Large smelt

$\log BAF = 0.99 \times \log K_{ow} - 0.22$

$n = 17$, $R^2 = 0.82$, 95% confidence limit of the slope = 0.74 to 1.25.

The approach taken here by Oliver and Niimi (1988) is similar to that used in the Voutsas *et al.* (2002) method.

4.2 Summary of findings

This analysis generally shows that the TGD method used for freshwater ecosystems appears to systematically underestimate the actual BAF for PCBs with log K_{ow} values from approximately 6 up to 7.4 (the highest log K_{ow} value tested). This finding is consistent with the analysis carried out in Section 2 of this report, and implies that the use of a single BMF_1 value in the TGD method for (non- or slowly metabolized) chemicals with a log K_{ow} in this range may not be sufficiently conservative.

If a second BMF_2 of around 10 were considered (as would be the case for the marine environment), this would result in predicted BAF around a factor of 10 higher (or a log BAF of one log unit higher) than assumed here for all of the PCBs considered. In this case, reasonably good agreement would then be obtained between the predicted and field BAF for PCBs with log K_{ow} values in the range 6 to 7.4, but the BAF for chemicals with lower log K_{ow} values (close to five) might then be overpredicted.

The results suggest that it may be appropriate to consider the use of a second BMF_2 of around 10 for freshwater food chains (currently this is only applied to marine food chains) in the TGD method for substances with a log K_{ow} of between around six and eight.

5 Testing against the Mersey data set

5.1 Introduction

A set of data covering the measured levels of a range of chemicals in various biota and sediment in the Mersey estuary was made available by the Environment Agency for this project.

The Mersey estuary can be broadly divided into four distinct regions as follows (Environment Agency, 1998):

- Upper estuary. Here, the estuary is a narrow channel of around 17 km in length and runs from Howley Weir in Warrington to the Widnes or Runcorn gap, adjacent to Runcorn Bridge.
- Inner estuary. This is a large shallow basin around 20 km in length and up to five km wide and occurs immediately west of Widnes. At this point the estuary has salt marshes on its southern flank.
- The narrows. This is a straight and narrow channel up to 30 m deep that starts near Pier Head.
- Outer estuary. On the seaward side of the narrows, the channel widens into the outer estuary. The outer estuary is an inter-tidal sand and mud bank through which two channels are maintained by dredging. The outer estuary connects directly with Liverpool Bay and the Irish Sea.

The main sources of water input into the estuary are the River Mersey that enters at Howley Weir and the River Weaver that discharges from the Manchester Ship Canal into the inner estuary at the Weaver sluices.

Dated sediment core samples were collected in 1992 at several sites at Widnes Warth, a salt marsh within the upper estuary, and Ince Marsh, a tidal salt marsh within the inner estuary (Environment Agency, 1998). The results of these analyses are summarised in Appendix B. The levels given generally relate to the concentration found in the upper sediment layers and so reflect the levels present in the early 1990s. No measured concentrations were available for the water phase. Therefore, in order to carry out an analysis of the data set, equivalent concentrations in water were estimated from measured concentrations in the sediment phase using the equilibrium partitioning method outlined in the TGD. These estimated water concentrations are also summarised in Appendix B.

A separate survey of levels of various chemicals in biota was also undertaken (NRA, 1994). The samples were collected over late 1990 to autumn 1991, with some further samples being collected during 1992. The species sampled included shrimps (*Crangon crangon*), mussels (*Mytilus edulis*), starfish (*Asteria rubens*), whelk (*Buccinium undatum*), hermit crab (*Pagurus bernhardus*), plaice (*Pleuronectes platessa*), whiting (*Merlangius merlangus*), dab (*Limanda limanda*), flounder (*Platichthys flesus*), dover sole (*Solea solea*) and cod (*Gadus morhua*). The results of these analyses are summarised in Appendix B. In general, between four and 11 samples of fish were analysed per location per sampling event. Only the edible portions of the fish were analysed. For the invertebrates, pooled whole body samples from several individuals were analysed.

Details of the types of food consumed by these species are summarised in Table 2.1. The data for the fish species were taken from the FISHBASE website[9] and the data for invertebrate species were taken from the British Marine Life Study Society website[10].

For comparison with the model results, it was necessary to assign the species surveyed to one of the trophic levels included in the models. For this purpose, the definitions used by Voutsas *et al.* (2002) were used here, as shown below.

- Trophic level 1: plankton, including both phytoplankton and zooplankton;
- Trophic level 2: benthic invertebrates;
- Trophic level 3: planktivorous fish;
- Trophic level 4: piscivorous fish.

There were difficulties in assigning some of the species to these levels. For example, flat fish tend to feed largely on invertebrates, which does not correspond to either of the fish levels used by Voutsas *et al*. (2002). The allocation used in these cases was based on the FISHBASE trophic level, but this introduced further uncertainty into the results.

Table 2.1 Feeding strategies for the species in the Mersey data set

Species	Food types	Trophic level assumed for Voutsas *et al.* (2002) method	Diet assumed for BIO v1.1/ECOFAE/ AQUAWEB v1.1 model
Mussel (*Mytilus edulis)*	Mussels are filter feeders.	2	Filter feeder
Shrimp (*Crangon vulgaris*)	Shrimps feed on small shellfish, larvae, molluscs, annelids, algae, seaweed and scraps of carrion.	2	Benthic detrivore
Whelk (*Buccinium undatum*)	Whelks can eat a variety of food but most commonly eat molluscs and worms.	2	Benthic detrivore
Hermit crab (*Pagurus bernhardus*)	Hermit crabs are omnivorous scavengers and feed on scraps of carrion, worms and organic detritus. They also filter feed.	2	Filter feeder[a]
Starfish (*Asteria rubens)*	The principle food of starfish is mussels but they will also eat other molluscs, fish eggs and carrion.	2	Benthic detrivore
Dover sole (*Solea solea*)	Dover sole are bottom-dwelling fish and feed mainly on worms, molluscs and small benthic crustaceans (such as amphipods, crabs, isopods, ostracods, shrimps and prawns) at night. Other food items could include small fish, benthic algae/weeds, echinoderms and zooplankton (such as fish	3/4	82.5% worms 12% benthic crustaceans 5.5% molluscs

[9] Available at http://www.fishbase.org/home.htm.
[10] Available at http://www.glaucus.org.uk

Species	Food types	Trophic level assumed for Voutsas *et al.* (2002) method	Diet assumed for BIO v1.1/ECOFAE/ AQUAWEB v1.1 model
	eggs/larvae, mysids and planktonic copepods). FISHBASE gives the trophic level for juveniles and adults as 3.12-3.13[b].		
Flounder (*Platichthys flesus*)	Juveniles of less than one year feed mainly on plankton and larvae of insects. Those older than one year and adults feed mainly on benthic fauna, including small fish, benthic crustaceans (such as amphipods, isopods and prawns), molluscs and worms. Adults burrow in the sand during the day and search for food at night. FISHBASE gives the trophic level for juveniles (>1 year) and adults as 3.16-3.19[b].	3/4	61.5% benthic crustaceans 24.5% worms 13.9% small fish 0.1% phytoplankton
Plaice (*Pleuronectes platessa*)	Plaice live on mixed bottoms and feed mainly on thin-shelled molluscs and worms. Molluscs are the most common items in their diet, but they can also catch bottom-dwelling fish. Other food includes benthic crustaceans (such as amphipods, isopods and prawns), echinoderms (such as starfish/brittle stars) and zooplankton (such as mysids). FISHBASE gives the trophic level for juveniles as 3.26[b].	3/4	83.5% worms 13.1% small fish 3.4% benthic crustaceans
Dab (*Limanda limanda*)	Dab live on sandy bottoms and feed mainly on zoobenthos and small fish. Zoobenthos include benthic crustaceans (such as amphipods, crabs and shrimps/prawns), echinoderms (such as sea cucumbers, starfish/brittle stars and sea urchins), molluscs and worms. FISHBASE gives the trophic level of juveniles as 3.29[b].	3/4	74% benthic crustaceans 22% worms 4% molluscs
Whiting (*Merlangius merlangus*)	Whiting feed mainly on shrimps, crabs, molluscs, small fish, worms and cephalopods. The proportion of fish in the diet increases with age. FISHBASE gives the trophic level of adults as 4.17-4.37[b].	4	87% small fish 8.7% zooplankton 3.8% benthic crustaceans 0.3% worms 0.2% molluscs
Cod (*Gadus morhua*)	Cod are omnivorous, feeding at dawn or dusk mainly on zoobenthos and fish, including young cod. Zoobenthos include benthic crustacean (such as amphipods, copepods, crabs, isopods, lobsters and shrimps/prawns), echinoderms	4	86% small fish 12.9% benthic crustaceans 1% worms 0.1% molluscs

Species	Food types	Trophic level assumed for Voutsas *et al.* (2002) method	Diet assumed for BIO v1.1/ECOFAE/ AQUAWEB v1.1 model
	(such as sea cucumbers, starfish/brittle stars and sea urchins), molluscs and worms. Larvae and juveniles may also feed on zooplankton such as fish eggs/larvae, cladocerans, euphausiids, mysids and planktonic copepods. FISHBASE gives the trophic level of adults as 4.34-4.42[b].		

a) The number of benthic detrivores that can be included in some of the models is currently limited and so for the purposes of this work it was assumed that the species was mainly a filter feeder.

b) FISHBASE gives values for the trophic level of adults as 1 + mean trophic level of the food items, based on the reported diets of the species. For example, phytoplankton are considered to be in trophic level 1, herbivorous zooplankton are considered to be in trophic level 2, and so on.

The Mersey data set was not ideal for the verification of bioaccumulation models for a number of reasons. For example, biota and sediment levels were taken from different locations and at different times, and a relatively large number of chemicals could not be detected in biota samples. In addition, measured levels in sediment were available for only a subset of the chemicals, and these data had to be extrapolated to give an equivalent concentration in water. Overall, this meant that actual sediment and dissolved water concentrations to which the various biota species were exposed were highly uncertain.

A second drawback to this data set was that the fish data related to the concentration found in the edible portions of the fish. This could be partly addressed in the analysis by using the lipid content appropriate to the edible portion of the fish. However, this may have influenced the outcome of some of the more complex models; this is discussed later in relation to the BIO v1.1, ECOFATE and AQUAWEB v1.1 models.

5.2 Comparison of predicted and field data

5.2.1 TGD method

The TGD method could be tested against the Mersey data set only for chemicals where an estimate of the (dissolved) concentration in water could be made. The relevant data are summarised in Table 5.2 (see Appendix B for more details of the data set), along with the concentrations predicted to occur in predatory fish using the TGD method. For the TGD method, a single BMF_1 was used for the analysis. The predicted BAF would be higher than shown for all chemicals with a log K_{ow} in the range 4.5 to to 9 if a second BMF_2 value was used (as is currently recommended in the TGD for the marine environment).

Based on this relatively crude analysis it can be seen that, with the exception of β-hexachlorocyclohexane (β-HCH), the TGD method generally overestimates the BAF by one to two orders of magnitude compared with that obtained based on estimated dissolved water concentrations and measured levels in fish.

Table 5.2 Comparison of TGD predictions with the Mersey data set

Chemical	Log K_{ow}	Field data				Predictions from TGD method	
		Conc. in water (µg l^{-1})	Conc. in fish (µg kg^{-1} wet wt)[a]		BAF – fish[a] (l kg^{-1})	Conc. in fish (µg kg^{-1} wet wt)[b]	BAF – fish (l kg^{-1})[b]
			Species	Value			
Aldrin	6.5	$<4.3\times10^{-5}$	Cod	<0.1		<19 [<0.7-<2.9]	436,520 [16,370-65,480]
			Dab	<0.1			
			Dover sole	<0.1			
			Flounder	<0.1			
			Plaice	<0.1			
			Whiting	<0.1			
α-HCH + γ-HCH	3.7	0.031	Cod	0.5	16	8.7 [0.3-1.3]	279 [10-42]
			Dab	2.0	65		
			Dove sole	1.5	48		
			Flounder	1.6	52		
			Plaice	1.5	48		
			Whiting	1.1	35		
β-HCH	3.7	0.078	Flounder	360	4,615	22 [0.8-3]	279 [10-42]
DDT – Total	6.2	0.022	Cod	0.9	41	8,100 [300-1,220]	377,900 [14,170-56,690]
			Dab	7.7	350		
			Dover sole	8.2	373		
			Flounder	21.8	990		
			Plaice	9.5	432		
			Whiting	3.4	155		
Dieldrin	5.4	$<3.4\times10^{-4}$	Cod	0.4	>1,176	<26 [<1-<4]	77,630 [2,910-11,640]
			Dab	1.9	>5,588		
			Dover sole	1.4	>4,118		
			Flounder	2.3	>6,765		
			Whiting	0.8	>2,353		
Heptachlor	6.1	1.4×10^{-3}	Cod	<0.1	<71	486 [18-73]	356,450 [13,370-53,470]

Chemical	Log K_{ow}	Field data				Predictions from TGD method	
		Conc. in water (µg l^{-1})	Conc. in fish (µg kg^{-1} wet wt)[a]		BAF – fish[a] (l kg^{-1})	Conc. in fish (µg kg^{-1} wet wt)[b]	BAF – fish (l kg^{-1})[b]
			Species	Value			
			Dab	<0.1	<71		
			Dover sole	<0.1	<71		
			Flounder	<0.1	<71		
			Plaice	<0.1	<71		
			Whiting	<0.1	<71		
PCB 28	5.8	3.2×10^{-3}	Dab	0.09	28	540 [20-81]	169,820 [6,370-25,470]
			Dover sole	0.18	56		
			Flounder	1.1	344		
			Plaice	0.55	172		
PCB 52	6.1	4.6×10^{-3}	Dab	0.05	11	1,600 [60-240]	356,450 [13,370-53,470]
			Dover sole	0.51	111		
			Flounder	1.9	413		
			Plaice	0.71	154		
PCB 101	6.4	2.6×10^{-3}	Dab	0.68	148	1,090 [41-164]	420,730 [15,780-63,110]
			Dover sole	1.9	413		
			Flounder	3.7	804		
			Plaice	1.3	283		
PCB 138	6.7	1.8×10^{-3}	Dab	3.1	1,722	815 [31-122]	457,090 [17,140-68,560]
			Dover sole	2.2	1,222		
			Flounder	4.5	2,500		
			Plaice	2.7	1,500		
PCB 153	6.9	1.0×10^{-3}	Dab	2.7	2,700	470 [18-71]	461,320 [17,300-69,200]
			Dover sole	4.1	4,100		
			Flounder	4.8	4,800		
			Plaice	2.9	2,900		
PCB 180	7.2	3.5×10^{-4}	Dab	1.1	3,143	150 [6-23]	436,520 [16,370-65,480]
			Dover sole	1.6	4,571		

Chemical	Log K_{ow}	Field data				Predictions from TGD method	
		Conc. in water (µg l^{-1})	Conc. in fish (µg kg^{-1} wet wt)[a]		BAF – fish[a] (l kg^{-1})	Conc. in fish (µg kg^{-1} wet wt)[b]	BAF – fish (l kg^{-1})[b]
			Species	Value			
			Flounder	2.2	6,286		
			Plaice	1.4	4,000		
ΣPCB - ICES	6.5	8.8×10^{-3}	Cod	1.8	206	3,960 [150-590]	436,520 [16,320-65,480]
			Dab	14.8	1,682		
			Dover sole	13.1	1,489		
			Flounder	18.8	2,136		
			Plaice	11.4	1,295		
			Whiting	4.9	557		

a) Measured levels relate to the edible portions of the fish only. Whole body concentrations would be expected to be higher than reported here.

b) Predicted levels relate to the whole body concentrations in fish. The equivalent predicted BAF for the edible portion of fish alone (assuming that the lipid content of the edible portion is generally around 0.3-1.2 per cent compared with a whole body lipid content of eight per cent) is shown in [ ]

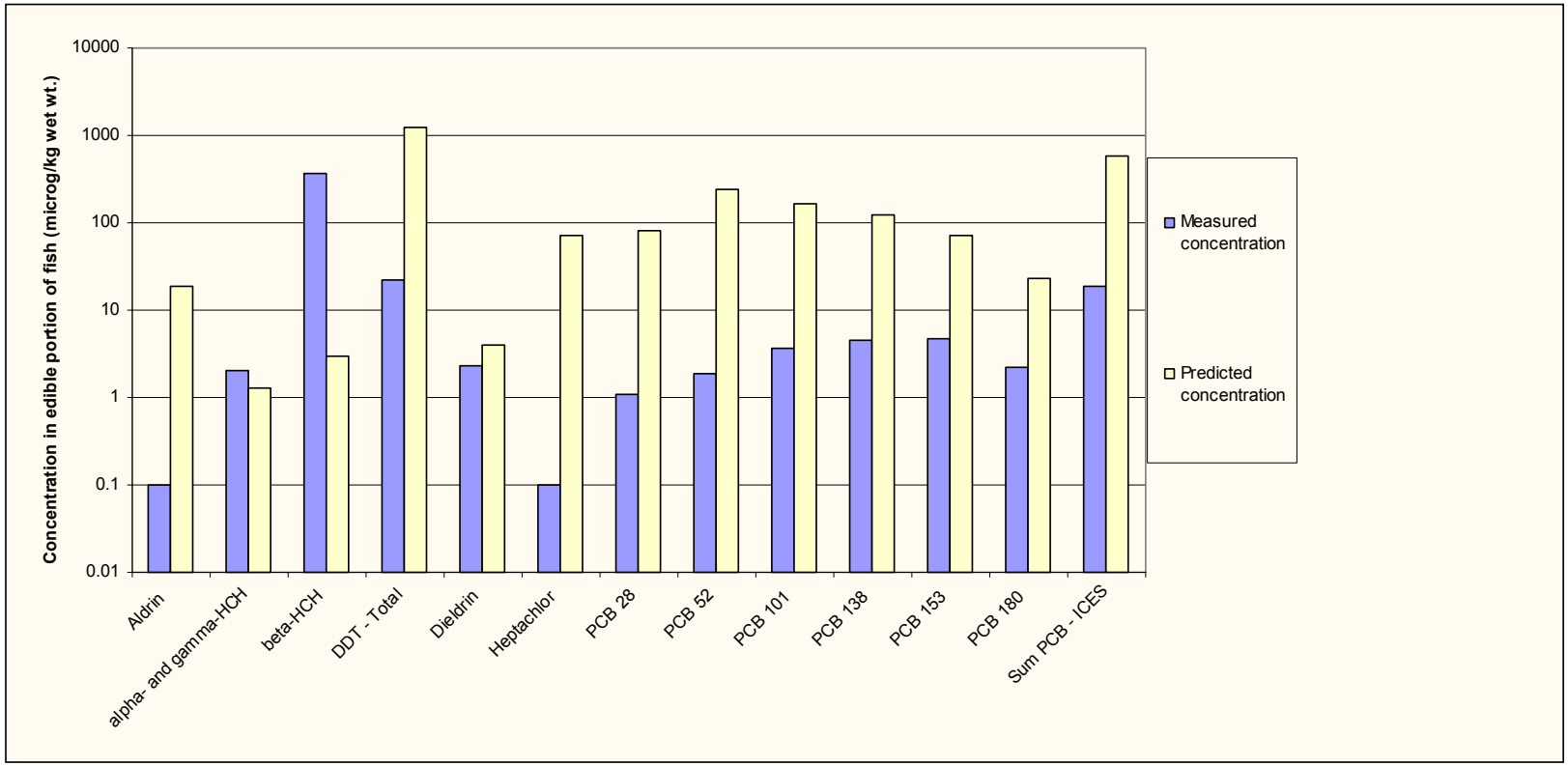

Figure 5.1 Comparison of measured and predicted concentrations in edible portions of fish for the Mersey data set using the TGD method

However, measured concentrations (and BAF) in fish relate to the edible portion of the fish, whereas predicted concentrations and BAF relate to whole body concentrations. The lipid contents of the fish samples analysed were generally in the range 0.3 to 1.2 per cent. Assuming that a typical lipid content of a whole fish is around eight per cent, then the predicted BAF for the edible portion alone would be expected to be lower than that given in Table 5.2 by a factor of around 7 to 27. Equivalent values are shown in [ ] in Table 5.2 and are shown graphically in Figure 5.1. Again, the TGD method appears to overestimate the actual BAF by at least a factor of 10 for many substances. However, predictions for α-HCH and γ-HCH (substances with relatively low log K_{ow} values) and also dieldrin (log K_{ow} of 5.4) on this basis are in close agreement with measured data.

Unfortunately, this analysis was compromised by a lack of reliable data on the actual concentrations in water to which the species were exposed, which introduced a high level of uncertainty into the data.

5.2.2 Voutsas *et al.* (2002) model

As for the TGD method, the Voutsas *et al.* (2002) model could be tested against the Mersey data set only for chemicals where an estimate of the (dissolved) concentration in water could be made. The relevant data are summarised in 5.3 (see Appendix B for more details of the data set), along with the concentrations predicted to occur in predatory fish using the Voutsas *et al.* (2002) method.

The Voutsas *et al.* (2002) method calculates the whole body BAF on a lipid weight basis. Therefore it is most relevant to compare these predictions with measured levels on a lipid weight basis[11]. Predicted and measured concentrations are displayed in Figure 5.2.

As can be seen from Table 5.3, predicted concentrations and BAFs are in good agreement with the measured data only for α-HCH and γ-HCH (and possibly dieldrin, although the measured data represent limit values in this case). For the other chemicals, predicted concentrations and BAFs are well in excess of the field data. This is broadly similar to that found for the TGD predictions in Section 5.2.1; however, in this case predicted concentrations are generally two orders of magnitude higher than would be suggested from the field data.

As with the TGD method, this analysis was compromised by the uncertainties over the actual concentrations in water and sediment to which the organisms were exposed.

[11] Measured concentrations in fish, although reported on a lipid weight basis, relate only to the edible portion of the fish. These concentrations will represent the lipid normalised concentration in the whole fish if it is assumed that the lipid-rich organs (such as liver) that were not analysed in the study contained the same concentration as the edible portions on a lipid weight basis.

Table 5.3 Comparison of Voutsas *et al.* (2002) predictions with the Mersey data set

Chemical	Log K_{ow}	Field data						Predictions– Voutsas et al. (2002) method[b]	
		Conc. in water (µg l^{-1})	Species	Lipid content (%)	Concentration[a]		BAF (l kg^{-1})		Concentration (µg kg^{-1} lipid)	BAF (l kg^{-1} lipid)
					µg kg^{-1} wet wt.	µg kg^{-1} lipid	Wet wt. basis	Lipid basis		
Aldrin	6.5	$<4.3\times10^{-5}$	**Benthic invertebrates**						$<1.4\times10^{3}$	31,642,800
			Blue mussel		<0.1					
			Hermit crab		<0.1					
			Shrimp		<0.1					
			Star fish		<0.1					
			Whelk		<0.1					
			Fish						$<2.1\times10^{3}$ (planktivorous fish) $<4.4x10^{3}$ (piscivorous fish)	48,192,006 (planktivorous fish) 101,053,200 (piscivorous fish)
			Cod		<0.1					
			Dab		<0.1					
			Dover sole		<0.1					
			Flounder		<0.1					
			Plaice		<0.1					
			Whiting		<0.1					
α-HCH + γ-HCH	3.7	0.031	**Benthic invertebrates**						270	8,760
			Blue mussel	0.9	2.7	300	87	9,677		
			Hermit crab	4.7	2.8	60	90	1,935		
			Star fish	1.4	0.7	50	23	1,613		
			Whelk	1.3	1.3	100	42	3,226		
			Fish						190 (planktivorous fish) 439 (piscivorous fish)	6,230 (planktivorous fish) 14,100 (piscivorous fish)
			Cod	0.5	0.5	215	16	6,935		
			Dab	1.0	2.0	191	65	6,161		
			Dove sole	0.3	1.5	555	48	17,903		
			Flounder	0.5	1.6	296	52	9,548		
			Plaice	0.7	1.5	226	48	7,290		
			Whiting	0.3	1.1	387	35	12,483		
β-HCH	3.7	0.078	**Fish**						485 (planktivorous fish) 1,100 (piscivorous fish)	6,230 (planktivorous fish) 14,100 (piscivorous fish)

Chemical	Log K_{ow}	Field data						Predictions– Voutsas et al. (2002) method[b]	
		Conc. in water (µg l^{-1})	Species	Lipid content (%)	Concentration[a]		BAF (l kg^{-1})		Concentration (µg kg^{-1} lipid)	BAF (l kg^{-1} lipid)
					µg kg^{-1} wet wt.	µg kg^{-1} lipid	Wet wt. basis	Lipid basis		
			Flounder	0.5	360	79,721	4,615	1,022,064		
DDT – Total	6.19	0.022	**Benthic invertebrates**						3.3×10^5	15,247,300
			Blue mussel	0.9[d]	30	3,333[d]	1,364	151,500[d]		
			Hermit crab	6.1	33	540	1,500	24,545		
			Star fish	1.3[e]	1.95[e]	150	89[e]	6,818		
			Whelk	1.8	50	2,778[d]	2,273	126,273[d]		
			Fish						4.6×10^5 (planktivorous fish) 8.6×10^5 (piscivorous fish)	21,276,700 (planktivorous fish) 39,736,400 (piscivorous fish)
			Cod	0.3	0.9	356	41	16,182		
			Dab	1.1	7.7	627	350	28,500		
			Dover sole	0.3	8.2	2,526	373	114,818		
			Flounder	0.5	21.8	5,180	990	235,455		
			Plaice	0.6	9.5	1,672	432	76,000		
			Whiting	0.3	3.4	1,241	155	56,409		
Dieldrin	5.4	$<3.4\times10^{-4}$	**Benthic invertebrates**						<652	1,943,900
			Blue mussel	0.9	3.0	320	>8,824	>941,176		
			Hermit crab	5.2	12.9	250	>37,941	>735,294		
			Shrimp	0.7	0.8	120	>2,353	>352,941		
			Star fish	1.4	1.3	90	>3,824	>264,706		
			Whelk	1.5	4.7	310	>13,824	>911,765		
			Fish						<731 (planktivorous fish) <1,170 (piscivorous fish)	2,178,500 (planktivorous fish) 3,483,500 (piscivorous fish)
			Cod	0.3	0.4	132	>1,176	>388,235		
			Dab	1.1	1.9	152	>5,588	>447,059		
			Dover sole	0.3	1.4	443	>4,118	>1,302,941		
			Flounder	0.4	2.3	521	>6,765	>1,532,353		
			Whiting	0.3	0.8	289	>2,353	>850,000		
Heptachlor	6.1	1.4×10^{-3}	**Fish**						2.3×10^4 (planktivorous fish) 4.1×10^4 (piscivorous fish)	16,645,700 (planktivorous fish) 30,234,400 (piscivorous fish)
			Cod		<0.1		<71			
			Dab		<0.1		<71			

Chemical	Log K_{ow}	Field data							Predictions– Voutsas et al. (2002) method[b]	
		Conc. in water (µg l^{-1})	Species	Lipid content (%)	Concentration[a]		BAF (l kg^{-1})		Concentration (µg kg^{-1} lipid)	BAF (l kg^{-1} lipid)
					µg kg^{-1} wet wt.	µg kg^{-1} lipid	Wet wt. basis	Lipid basis		
			Dover sole		<0.1		<71			
			Flounder		<0.1		<71			
			Plaice		<0.1		<71			
			Whiting		<0.1		<71			
PCB 28	5.8	3.2×10^{-3}	**Benthic invertebrates**						1.8×10^{4}	5,716,400
			Star fish	1.3[d]	0.6	46[d]	188	14,375[d]		
			Whelk	1.8[d]	1.2	67[d]	375	20,938[d]		
			Fish						2.3×10^{4} (planktivorous fish) 3.8×10^{4} (piscivorous fish)	7,153,700 (planktivorous fish) 12,067,800 (piscivorous fish)
			Dab	1.2[d]	0.09	7.5[d]	28	2,344[d]		
			Dover sole	0.4[d]	0.18	45[d]	56	14,063[d]		
			Flounder	0.5[d]	1.1	220[d]	344	68,750[d]		
			Plaice	0.7[d]	0.55	79[d]	172	24,688[d]		
PCB 52	6.1	4.6×10^{-3}	**Benthic invertebrates**						5.6×10^{4}	12,233,600
			Star fish	1.3[d]	0.6	46[d]	130	10,000[d]		
			Whelk	1.8[d]	1.0	56[d]	217	12,174[d]		
			Fish						7.6×10^{4} (planktivorous fish) 1.4×10^{5} (piscivorous fish)	16,645,700 (planktivorous fish) 30,234,400 (piscivorous fish)
			Dab	1.2[d]	0.05	4.2[d]	11	913[d]		
			Dover sole	0.4[d]	0.51	128[d]	111	27,826[d]		
			Flounder	0.5[d]	1.9	380[d]	413	82,609[d]		
			Plaice	0.7[d]	0.71	101[d]	154	21,957[d]		
PCB 101	6.4	2.6×10^{-3}	**Benthic invertebrates**						6.5×10^{4}	25,123,492
			Star fish	1.3[d]	1.2	92[d]	462	35,385[d]		
			Whelk	1.8[d]	1.5	83[d]	577	31,923[d]		

Chemical	Log K_{ow}	Field data						Predictions– Voutsas et al. (2002) method[b]	
		Conc. in water (µg l^{-1})	Species	Lipid content (%)	Concentration[a]		BAF (l kg^{-1})		Concentration (µg kg^{-1} lipid)	BAF (l kg^{-1} lipid)
					µg kg^{-1} wet wt.	µg kg^{-1} lipid	Wet wt. basis	Lipid basis		
			Fish						9.7×10^4 (planktivorous fish) 2.0×10^5 (piscivorous fish)	37,195,300 (planktivorous fish) 74,881,000 (piscivorous fish)
			Dab	1.2[d]	0.68	57[d]	148	21,923[d]		
			Dover sole	0.4[d]	1.9	475[d]	413	182,692[d]		
			Flounder	0.5[d]	3.7	740[d]	804	284,615[d]		
			Plaice	0.7[d]	1.3	185[d]	283	71,154[d]		
PCB 138	6.7	1.8×10^{-3}	**Benthic invertebrates**						8.8×10^4	49,510,500
			Star fish	1.3[d]	3.2	246[d]	1,778	136,667[d]		
			Whelk	1.8[d]	32	1,778[d]	17,778	987,778[d]		
			Fish						1.4×10^5 (planktivorous fish) 3.3×10^5 (piscivorous fish)	70.815,500 (planktivorous fish) 183,331,883 (piscivorous fish)
			Dab	1.2[d]	3.1	258[d]	1,722	143,333[d]		
			Dover sole	0.4[d]	2.2	550[d]	1,222	305,556[d]		
			Flounder	0.5[d]	4.5	900[d]	2,500	500,000[d]		
			Plaice	0.7[d]	2.7	386[d]	1,500	214,444[d]		
PCB 153	6.9	1.0×10^{-3}	**Benthic invertebrates**						7.8×10^4	76,059,800
			Star fish	1.3[d]	3.7	285[d]	3,700	285,000[d]		
			Whelk	1.8[d]	37	2,056[d]	37,000	2,056,000[d]		

Chemical	Log K_{ow}	Field data						Predictions– Voutsas et al. (2002) method[b]	
		Conc. in water (µg l^{-1})	Species	Lipid content (%)	Concentration[a]		BAF (l kg^{-1})		Concentration (µg kg^{-1} lipid)	BAF (l kg^{-1} lipid)
					µg kg^{-1} wet wt.	µg kg^{-1} lipid	Wet wt. basis	Lipid basis		
			Fish						1.3×10^5 (planktivorous fish) 3.4×10^5 (piscivorous fish)	129,832,400 (planktivorous fish) 330,904,000 (piscivorous fish)
			Dab	1.2[d]	2.7	225[d]	2,700	225,000[d]		
			Dover sole	0.4[d]	4.1	1,025[d]	4,100	1,025,000[d]		
			Flounder	0.5[d]	4.8	960[d]	4,800	960,000[d]		
			Plaice	0.7[d]	2.9	4,143[d]	2,900	4,143,000[d]		
PCB 180	7.2	3.5×10^{-4}	**Benthic invertebrates**						4.9×10^4	139,933,000
			Star fish	1.3[d]	0.7	54[d]	2,000	154,286[d]		
			Whelk	1.8[d]	17	944[d]	48,571	2,697,143[d]		
			Fish						9.1×10^4 (planktivorous fish) 2.8×10^5 (piscivorous fish)	260,418,600 (planktivorous fish) 794,745,400 (piscivorous fish)
			Dab	1.2[d]	1.1	92[d]	3,143	262,857[d]		
			Dover sole	0.4[d]	1.6	400[d]	4,571	1,142,857[d]		
			Flounder	0.5[d]	2.2	440[d]	6,286	1,257,143[d]		
			Plaice	0.7[d]	1.4	200[d]	4,000	571,429[d]		
ΣPCB - ICES	6.5	8.8×10^{-3}	**Benthic invertebrates**						2.9×10^5	31,642,800
			Blue mussel	0.9	20	2,180	2,273	247,727		
			Hermit crab	6.0	105	1,754	11,832	199,318		

Chemical	Log K_{ow}	Field data						Predictions– Voutsas et al. (2002) method[b]	
		Conc. in water (µg l^{-1})	Species	Lipid content (%)	Concentration[a]		BAF (l kg^{-1})		Concentration (µg kg^{-1} lipid)	BAF (l kg^{-1} lipid)
					µg kg^{-1} wet wt.	µg kg^{-1} lipid	Wet wt. basis	Lipid basis		
			Shrimp	0.7	8.2	1,230	932	139,773		
			Star fish	1.5	9.9	650	1,125	73,864		
			Whelk	1.4	91	6,710	10,341	762,500		
			Fish						4.4×10^5 (planktivorous fish) 9.2×10^5 (piscivorous fish)	48,192,000 (planktivorous fish) 101,053,200 (piscivorous fish)
			Cod	0.3	1.8	765	205	86,932		
			Dab	1.1	14.8	1,237	1,682	140,568		
			Dover sole	0.3	13.1	4,646	1,489	527,955		
			Flounder	0.4	18.8	4,645	2,136	527,841		
			Plaice	0.6	11.4	2,056	1,295	233,636		
			Whiting	0.3	4.9	1,759	557	199,886		

a) Measured levels relate to the edible portions of the fish only. Whole body concentrations would be expected to be higher than reported here.

b) The Voutsas et al. (2002) method gives predictions for the following trophic levels:

- Trophic level 2 – benthic invertebrates
- Trophic level 3 – planktivorous fish
- Trophic level 4 – piscivorous fish

c) The lipid contents given here were estimated from the ratio of the lipid weight and wet weight concentrations reported.

d) No lipid weight concentrations were given for this species and chemical. The lipid content used here is the approximate mean value determined for other chemicals in the same species in the study.

e) No wet weight concentrations were given for this species and chemical. The lipid content used here is the approximate mean value determined for other chemicals in the same species in the study.

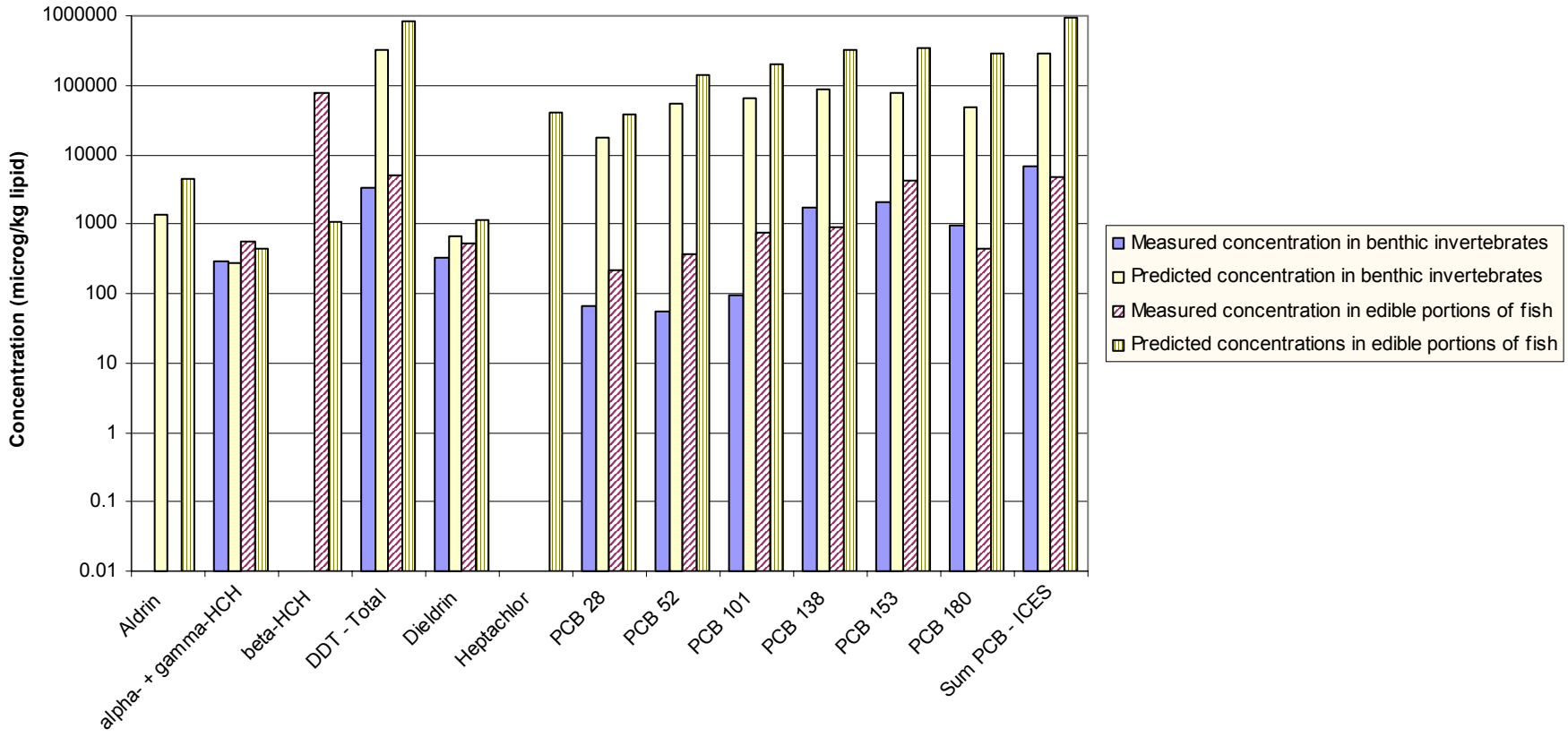

Figure 5.2 Comparison of measured and predicted concentrations in invertebrates and edible portions of fish for the Mersey data set using the Voutsas et al. (2002) method

5.2.3 Food Web Bioaccumulation/ECOFATE/AQUAWEB models

Details of the calculations performed using these models and the Mersey data set are included in Appendix B. A summary of the work and examples are included here.

The same representative ecosystem was set up in each of the models (see Appendix B). As information on the concentrations in water (sediment) was only available for a limited subset of the chemicals for which measured levels in biota were available in the Mersey data set, two approaches were taken. The first was used where sufficient information was available to estimate a concentration in water from the available sediment data. In these cases, concentrations in the food chain were estimated from the concentration in water and BAF values predicted for the relevant organism.

In the second approach, hypothetical concentrations in water were used to calculate the concentrations in each species. These were converted into ratios relative to the predicted concentration in plaice, as the species with the greatest extent of measured levels. The ratios of measured concentrations in species relative to plaice were calculated and the comparison made between ratios of measured and calculated data. This comparison looked more at the ability to predict relative levels in species rather than absolute levels.

Example results are presented for three substances, taken from the results listed in Appendix B.

Hexachlorocyclohexane (HCH)

The relative concentrations measured and predicted for α-HCH and γ-HCH are shown in Figure 5.3. All three of the models appear to predict the observed relative concentrations reasonably well for mussel, cod, dab, dover sole, flounder and whiting. Relative concentrations for hermit crab, starfish and whelk were overpredicted slightly, but even so the relative concentration was generally within a factor of four of the observed ratio. Predictions using AQUAWEB v1.1 were slightly closer to the observed ratios than predictions from the other models. Overall, predictions of the relative concentration across all species were generally within a factor of two to three of the observed ratio.

The concentration of α-HCH and γ-HCH assumed to be present in the dissolved phase in water from the Mersey estuary was estimated to be 0.031 µg l^{-1} (see Appendix B). Predicted BAFs for α-HCH and γ-HCH in the edible portions of plaice were 35 l kg^{-1} wet weight using ECOFATE, 36 l kg^{-1} wet weight using BIO v1.1 and 72 l kg^{-1} wet weight using AQUAWEB v1.1

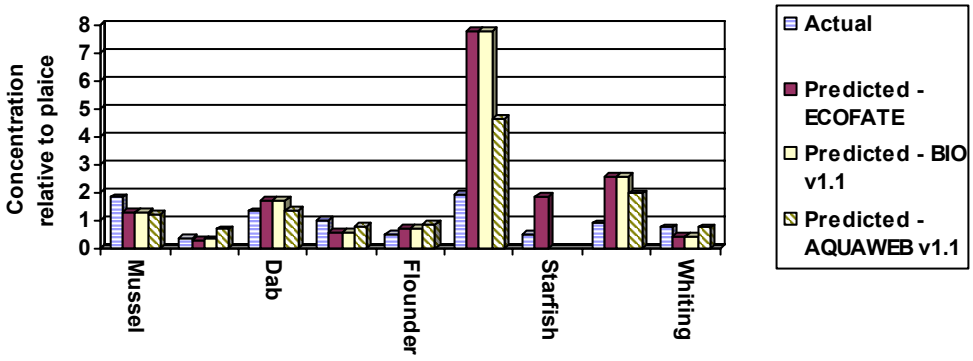

Figure 5.3 Predicted and actual concentrations in biota relative to plaice for α-HCH and γ-HCH

Based on these estimated BAFs and the estimated dissolved concentration in water, the expected concentration of α-HCH and γ-HCH in the edible portion of plaice would be around 1 μg kg^{-1} wet weight using ECOFATE and BIO v1.1 and around 2 μg kg^{-1} wet weight using AQUAWEB v1.1. The actual concentration of α-HCH and γ-HCH measured in the edible portion of plaice was between 0.5 and 3.6 μg kg^{-1} wet weight, with a mean value of around 1.5 μg kg^{-1} wet weight (see Appendix B). There was thus very good agreement between predicted and measured concentrations in plaice. As there was also good agreement between predicted and observed concentrations in the other species surveyed relative to plaice, it can be concluded that concentrations in all species monitored are reasonably well predicted for α- HCH and γ-HCH.

For β-HCH, there was only very limited data available for one species of fish (flounder). Predicted BAFs for the edible portion of this species were 25 l kg^{-1} wet weight using ECOFATE, 26 l kg^{-1} wet weight using BIO v1.1 and 62 l kg^{-1} wet weight using AQUAWEB v1.1. The assumed dissolved concentration of β-HCH in water from the Mersey estuary was 0.078 μg l^{-1} (see Appendix B). Based on these data, the predicted concentration of β-HCH in the edible portion of flounder would be around 2 μg kg^{-1} wet weight based on ECOFATE and BIO v1.1 and 5 μg kg^{-1} wet weight based on AQUAWEB v1.1. The observed concentration in the edible portion of flounder was 360 μg kg^{-1} wet weight. Predicted concentrations were therefore around two orders of magnitude lower than observed. However, for β-HCH the database of measured levels was very small and so it was not clear how representative the measured sample was.

DDT - total

The relative concentrations measured and predicted for total DDT are shown in Figure 5.4. All three models appear to predict the observed relative concentrations reasonably well for dab, dover sole and in some cases cod, hermit crab and whiting. The relative concentration in mussel, flounder, whelk, and in some cases hermit crab were all underpredicted to some extent. Some methods also led to a slight overprediction of the relative concentration in cod and whiting. Overall, with the exception of mussel, cod and whelk, most predictions of the relative concentration across all species were generally within a factor of two to three of the observed ratio.

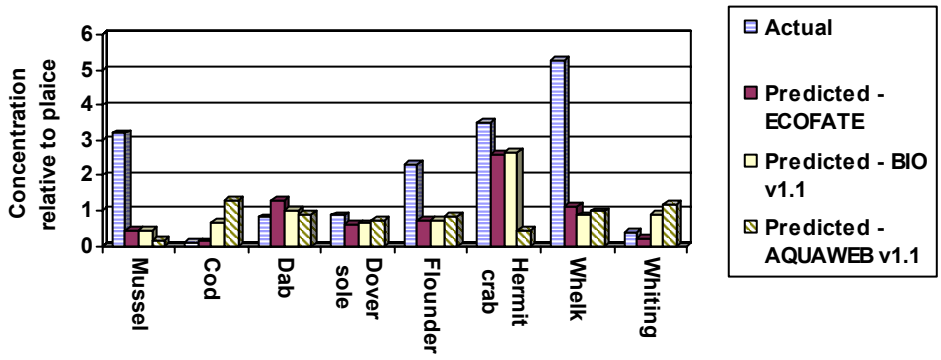

Figure 5.4 Predicted and actual concentrations in biota relative to plaice for DDT

The concentration of total DDT assumed to be present in the dissolved phase in water from the Mersey estuary for modelling purposes was estimated to be 0.022 µg l^{-1} (see Appendix B). Predicted BAFs for total DDT in the edible portions of plaice were 38,000 l kg^{-1} wet weight using ECOFATE, 23,000 l kg^{-1} wet weight using BIO v1.1 and 240,000 l kg^{-1} wet weight using AQUAWEB v1.1

Based on these estimated BAFs and the estimated dissolved concentration in water, the expected concentration of total DDT in the edible portion of plaice would be around 840 µg kg^{-1} wet weight using ECOFATE, 510 µg kg^{-1} wet weight using BIO v1.1 and around 5,300 µg kg^{-1} wet weight using AQUAWEB v1.1. The actual concentration of total DDT measured in the edible portion of plaice was between 5.3 and 14 µg kg^{-1} wet weight, with a mean value of around 9.5 µg kg^{-1} wet weight (see Appendix B). Therefore, predicted concentrations were around 50 to 500 times higher than observed ones. As there was reasonable agreement between predicted and observed concentrations in other species surveyed relative to plaice, it can be concluded that the models would provide a similar level of overprediction of the observed concentration for all other species.

PCB 52

The relative concentrations measured and predicted for PCB 52 are shown in Figure 5.5. All three of the models appear to predict the observed relative concentrations for dover sole, starfish and whelk reasonably well. The relative concentrations in dab appear to be overpredicted to some extent, and the relative concentration in flounder underpredicted. Overall, with the exception of dab, predictions of the relative concentration across all species are generally within a factor of two to three of the observed ratio.

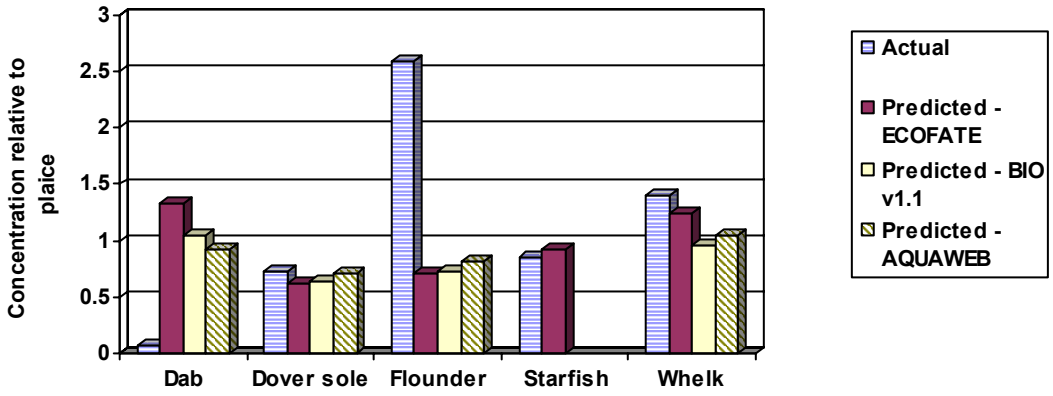

Figure 5.5 Predicted and actual concentrations in biota relative to plaice for PCB 52

The concentration of PCB 52 assumed to be present in the dissolved phase in water from the Mersey estuary for modelling purposes was estimated to be 4.6×10^{-3} µg l^{-1} (see Appendix B). Predicted BAFs for PCB 52 in the edible portions of plaice were 27,000 l kg^{-1} wet weight using ECOFATE, 18,000 l kg^{-1} wet weight using BIO v1.1 and 170,000 l kg^{-1} wet weight using AQUAWEB v1.1

Based on these estimated BAFs and the estimated dissolved concentration in water, the expected concentration of PCB 52 in the edible portion of plaice would be around 120 µg kg^{-1} wet weight using ECOFATE, 80 µg kg^{-1} wet weight using BIO v1.1 and around 800 µg kg^{-1} wet weight using AQUAWEB v1.1. The actual concentration of PCB 52 measured in the edible portion of plaice was 0.71 µg kg^{-1} wet weight (see Appendix B). Therefore, predicted concentrations were around 100 to 1,000 times higher than observed ones. As there was reasonable agreement between predicted and observed concentrations in the other species surveyed relative to the concentration in plaice, it can be concluded that the models would provide a similar level of overprediction of the observed concentration for all other species.

5.3 Summary of findings

Analysis of the Mersey data set was compromised to a large extent by uncertainties over the concentrations in sediment and water to which the various species were exposed. Nevertheless, it was possible to draw some tentative conclusions from the data.

Overall, all three methods resulted in higher predicted concentrations in biota for many of the chemicals considered than were actually found. Given the uncertainties over the exposure concentrations, it is not clear if this resulted from a systematic error in the estimation methods or from assumptions over the dissolved water and sediment concentrations used in the simulations.

ECOFATE, BIO v1.1 and AQUAWEB v1.1 were found to predict reasonably well the level of accumulation that may be expected across a number of species for a range of chemicals. However, it was not possible to establish the absolute predictivity of these models using the Mersey data set owing to uncertainties over the exposure concentrations. In terms of the magnitude of predictions, all three models led to similar BAFs (and hence predicted concentrations) for chemicals with low to

moderate log K_{ow} values, but at higher log K_{ow} values predicted BAFs from AQUAWEB v1.1 were significantly higher than those obtained from both ECOFATE and BIO v1.1 (the latter two models giving broadly similar predictions across all log K_{ow} values as would be expected, given that they are fundamentally the same model). The reason for this apparent discrepancy is not clear, but may be related in part to how the concentrations in suspended matter and the dissolved phase are treated within the various models. In terms of overall ease of use the new spread sheet model, AQUAWEB v1.1, had significant advantages over the ECOFATE model and the original version of the Food Chain Bioaccumulation model v1.1, and indeed allowed simulations to be carried out using BIO v1.1 and AQUAWEB v1.1 simultaneously with only one set of input data.

6 Testing against other data sets

6.1 Comparison of predicted and field data

As well as the Oliver and Niimi (1988) data set discussed in Section 4, other data sets of BAF values were used in the initial development and testing of the Voutsas *et al.* (2002) method. These data sets can also be used to test further both the TGD method and the AQUAWEB v1.1 model. BAF values used for this comparison were taken from the supporting information from Voutsas *et al.* (2002) but were not reviewed or validated in detail for this work. The BAF values in Voutsas *et al.* (2002) were taken from the following sources:

- Metcalfe and Metcalfe (1997). This data set covered PCBs in a Lake Ontario food web, and both pelagic organisms and benthic organisms including plankton, mysids, chironomids, *Diporeia hoyi*, alewife (*Alosa pseudoharengus*), rainbow smelt (*Osmerus mordax*), lake trout (*Salvelinus namaycush*), slimy sculpin (*Cottus cognatus*) and white suckers (*Catostomus commersonii*). The food chain covered was therefore very similar to that in Oliver and Niimi (1988).
- Morrison *et al.* (1996). This data set covered PCBs in benthic invertebrates such as zebra mussels (*Dreissena polymorpha*), caddisfly larvae (*Hydropsyche alterans*), ampiphods (*Gammarus fasciatus*) and crayfish (*Orconectes propinquus*) from Western Lake Erie.
- Burkhard *et al.* (1997). This data set covered chlorinated benzenes, chlorinated butadienes and hexachloroethane in a food chain in the Bayou d'Inde of the Calcasieu River systems in Louisiana, United States. The organisms covered included blue crabs (*Callinectes sapidus*) and fish such as mummichog (*Fundulus heteroclitus*), gulf menhaden (*Brevoortia patronus*) and atlantic croaker (*Micropoganias undulatus*).
- van Hattum *et al.* (1998). This data set covered polycyclic aromatic hydrocarbons in isopods (mainly *Asellus aquaticus*) in eight different sediments/waters in the Netherlands.
- Kidd *et al.* (1998). This data set covered organochlorine compounds (including PCBs) in a freshwater food web in the Canadian Arctic. Biota samples included bulk zooplankton, chironomids, adult Trichotera (*Apatania sp.*) and Plecoptera (*Arcynopteryx sp.*), larval Trichoptera (*Hesperophylax sp.*), Plecopteran nymphs (*Diura bicaudata*), lake trout (*Salvelinus namaycush*), arctic char (*Salvelinus alpinus*), round white fish (*Prosopium cylindraceum*), nine-spine stickleback (*Pungitius pungitius*) and three-spine stickleback (*Gasterosteus aculeatus*).
- Pereira *et al.* (1988). This data set covered halogenated organic compounds (chlorinated benzenes, hexachlorobutadiene, octachlorostyrene and octachloronaphthalene) in a food web from the Calcasieu River estuary, Louisiana, United States. The species included were blue crabs (*Callinectes sapidus*), atlantic croakers (*Micropogonias undulatus*), spotted sea trout (*Cynoscion nebulosis*) and blue catfish (*Ichtalurus furcatus*).

The data from Oliver and Niimi (1998) were not included in this analysis as they are already considered in Section 4.

The use of a mixed data set such as this one can only really give an indication of biomagnification in a food web. The data do not relate to real interactions and feeding patterns and so some of the detail which would be present in data from a real food web is lost. Hence, these results should be interpreted with some caution.

Voutsas *et al.* (2002) derived lipid-normalized BAFs based on both the freely dissolved concentration in water (BAF_{fd}) and the total concentration (BAF_t) in water from these data sources, and then assigned the data to one of four trophic levels:

- Level 1: plankton;
- Level 2: benthic invertebrates;
- Level 3: planktivorous fish;
- Level 4: piscivorous fish.

These same data and assignments were used here to further verify both the TGD method and the AQUAWEB v1.1 model. The TGD method only predicts concentration in fish, and so predictions could only be compared with the available data for planktivorous fish and piscivorous fish. In order to compare TGD predictions with the reported lipid-normalized BAFs, TGD predictions were normalized to an assumed lipid content of five per cent. Some calculations were also carried out using the BIO v1.1 model in order to compare these with the AQUAWEB v1.1 model.

For AQUAWEB v1.1, a 'generic' simple food chain consisting of sediment, water, plankton, benthic invertebrate, planktivorous fish and piscivorous fish was constructed as shown in Table 6.1. The species properties and diet were taken directly from the AQUAWEB v1.1 model. A similar food chain was assumed for calculations using the BIO v1.1 model.

Table 6.1 Generic food chain assumed in AQUAWEB v1.1 model

Organism	Assumed trophic level (as used in Voutsas et al. (2002)	Properties used in model	Diet
Phytoplankton		Lipid content – 0.5% Non-lipid organic carbon content – 6.5% Water content – 93%	Not relevant
Zooplankton	1	Lipid content – 1.2% Organism weight – 5.7×10^{-8} kg Non-lipid organic carbon content – 20% Water content – 78.8%	100% Phytoplankton
Filter feeding invertebrate (such as zebra mussel)	2	Lipid content – 1.3% Organism weight – 1.1×10^{-4} kg Non-lipid organic carbon content – 20% Water content – 78.7%	60% Phytoplankton 30% Sediment/detritus 10% Zooplankton
Benthic invertebrate (such as mayfly)	2	Lipid content – 2.0% Organism weight - 1×10^{-4} kg Non-lipid organic carbon content – 20% Water content – 78.0%	5% Phytoplankton 95% Sediment/detritus
Planktivorous fish (such as alewife)	3	Lipid content – 7.4% Organism weight – 0.116 kg Non-lipid organic carbon content – 20% Water content – 72.6%	100% Zooplankton
Piscivorous fish (such as small mouth bass)	4	Lipid content – 7.5% Organism weight – 0.715 kg Non-lipid organic carbon content – 20% Water content – 72.5%	85% Planktivorous fish 15% Zooplankton

The data set used, along with the predicted BAFs, is summarised in Appendix C.

The AQUAWEB v1.1 model incorporates methods for estimating the partitioning of the chemical between water and dissolved and particulate organic carbon. In addition, the model uses a concentration in sediment as well as a concentration in water. In order to test the importance of these parameters to the overall BAFs estimated, a number of simulations were carried out by varying the concentration in water relative to the concentration in sediment, and by varying the concentrations of dissolved organic matter and particulate organic carbon in water. This was done using the following approaches:

- A dissolved[12] concentration in water of one ng l^{-1} was assumed. The corresponding concentration in sediment was then estimated using the TGD method by: a) calculating the K_{oc} value using the default QSAR (non-hydrophobic chemicals)[13]; and b) calculating the K_{oc} value using the QSAR for predominantly hydrophobic chemicals[14]. The AQUAWEB v1.1 requires a water and sediment concentration to be input and then estimates a sediment pore

[12] The AQUAWEB v1.1 model allows the concentration in water to be entered as either a dissolved concentration (assuming that the water was filtered to remove particulates) or a total concentration (including particulates).
[13] The default QSAR is $\log K_{oc} = (0.52 \times \log K_{ow}) + 1.02$.
[14] This QSAR is $\log K_{oc} = (0.81 \times \log K_{ow}) + 0.10$.

water concentration from the sediment concentration using a different method[15] to TGD, and so the internal sediment pore water concentrations used by the model will not be the same as would be estimated from the above K_{oc} values.

- The water properties required by the AQUAWEB v1.1 model include the mean water temperature, dissolved organic carbon content, particulate organic carbon content, concentration of suspended solids and the sediment organic carbon content. The model was run using two sets of parameters. One set was based on the properties of the Great Lakes (already included in the model by default), and the second set was based on the default properties from the TGD. These are summarised below. A temperature of 12°C was assumed in both cases.

	Great Lakes	TGD
Dissolved organic carbon content	2.2×10^{-6} kg l^{-1}	0 kg l^{-1}
Particulate organic carbon content	5.4×10^{-7} kg l^{-1}	1.5×10^{-6} kg l^{-1}
Concentration of suspended solids	4.0×10^{-5} kg l^{-1}	1.5×10^{-5} kg l^{-1}
Sediment organic carbon content	7.1%	5.0%

[Note: for the properties based on TGD, the particulate organic carbon content was assumed to be 10 per cent of the suspended solids content of the water, in line with the assumption in the TGD method that the organic carbon content of suspended matter is 10 per cent].

This therefore gives four possible combinations of input properties for the simulations.

The AQUAWEB v1.1 model predicts concentrations in the organism on a wet weight basis. In order to convert this to a BAF on a lipid weight basis, the concentration was firstly normalized to the lipid content of the organism in question (using the lipid contents given in Table 6.1) and then divided by the total concentration in water. In these simulations, the concentrations were entered assuming that they represent the concentrations in filtered water: that is, the dissolved concentration. However, even for these concentrations the AQUAWEB v1.1 calculates a "freely" dissolved or "bioavailable" concentration taking into account association with dissolved organic carbon using the following equation:

$$\text{Bioavailable fraction} = \frac{1}{(1+(0.5\times \text{Kow}\times 0.08\times \text{DOC}))}$$

where bioavailable fraction = ratio of the dissolved concentration to the total concentration.
K_{ow} = octanol-water partition coefficient (non-log value).
DOC = dissolved organic carbon concentration (kg l^{-1}).

Thus, even though a concentration in water is entered as filtered, this does not necessarily equate to a freely dissolved or bioavailable concentration unless the dissolved organic carbon concentration is also very low (or zero). Therefore, the BAFs obtained using the Great Lakes water properties incorporate this correction for bioavailability (this correction is only significant at high log K_{ow} values above seven). As the simulations using the TGD properties were carried out assuming the dissolved

[15] Internal sediment pore water concentrations (in ng g^{-1}) used by the model are estimated from the input sediment concentration (in ng g^{-1} dry weight) using the following equation: concentration in pore water = (concentration in sediment × dissolved organic carbon content/organic carbon content)/(0.35 × P).

organic carbon content was zero, the bioavailable fraction was one in all cases, and the BAFs reflected the true dissolved concentration.

The BAFs obtained in this way were compared with the BAF_{fd} values from the Voutsas *et al.* (2002) data set (lipid-normalized BAFs based on the estimated freely dissolved concentration in water).

In cases where the water concentration is input as a total concentration, AQUAWEB v1.1 estimates the dissolved concentration as follows.

$$\text{Bioavailable fraction} = \frac{1}{(1+(\text{POC}\times 0.35\times \text{Kow})+(\text{Kow}\times 0.08\times \text{DOC}))}$$

where bioavailable fraction = ratio of the dissolved concentration to the total concentration.
K_{ow} = octanol-water partition coefficient (non-log value).
POC = particulate organic carbon concentration (kg l^{-1}).
DOC = dissolved organic carbon concentration (kg l^{-1}).

For these calculations, the BAF obtained from AQUAWEB v1.1 represents the BAF related to the total concentration in water (where the total concentration takes into account partitioning to both suspended matter and dissolved organic carbon). These BAFs were compared with the BAF_t values from the Voutsas *et al.* (2002) data set (lipid-normalized BAFs based on the total concentration in water).

Calculations were also carried out using BIOv1.1 for one combination of input data (where the QSAR for predominantly hydrophobic chemicals was used to estimate the sediment concentration, and water properties were based on TGD defaults), for comparison.

Predictions of the BMF for this data set were also obtained using the TGD method, which was only possible for fish (trophic levels 3 and 4). The TGD method gives predictions on a wet weight fish basis; in order to convert these to a lipid weight basis, the lipid contents for trophic level 3 (7.4%) and trophic level 4 (7.5%) from

Table 6.1 were used. Overall BAFs were estimated based on a freely dissolved concentration in water. Equivalent BAFs on a total concentration in water basis were estimated from these data using the suspended sediment-water partitioning properties outlined in the TGD. TGD predictions were carried out using both a BMF_1 value (as recommended for a freshwater food chain) and a BMF_1 and BMF_2 value (as recommended for a marine food chain).

The results of the various simulations are summarised in Appendix C. Equivalent estimates obtained using the Voutsas *et al.* (2002) method are also given.

For the AQUAWEB v1.1 simulations, the predicted BAF (and hence concentration) in the organism does not appear to be highly dependent on the method used to estimate the sediment concentration for the input; very similar results were obtained using sediment concentrations estimated from the TGD default QSAR and the QSAR for predominantly hydrophobics for K_{oc}. Therefore, small differences in the relative ratio of the sediment and water concentrations resulting from the two methods of estimation had little effect on the final outcome; as noted earlier, the model uses a different method for estimating the sediment pore water concentration[15]. Therefore, only the results from simulations using the QSAR for predominantly hydrophobic chemicals are discussed further here (the findings using the default QSAR would be more or less identical to these).

A more marked difference in predicted BAFs was obtained using the water properties of the Great Lakes compared with those obtained using the water properties from the TGD. The most important difference was that the dissolved organic carbon content was set to zero for the TGD simulations (hence, no reduction in the freely dissolved concentration at high log K_{ow}). The following analysis considers this difference further.

A summary of the statistics obtained from an analysis of residuals (defined here as the actual field log BAF from the Voutsas *et al.* (2002) data set – predicted log BAF) is given in Table 6.2. A negative residual indicates that the predictive method overestimated the actual BAF and a positive residual, that the method underestimated the BAF. The statistical analysis also considered the absolute value of the residual, which gives an indication of the agreement between the actual and predicted BAF regardless of whether the prediction is an underestimate or an overestimate. Residuals from the Voutsas *et al* method are also included in the tables, though these cannot be compared to those from the other models, as the data set was used to develop the Voutsas method in the first place.

Table 6.2 Summary statistics for the analysis of residuals for the Voutsas *et al.* (2002) data set (minus the data of Oliver and Niimi, 1988)

Method		Residual[a]				Absolute residual[b]				
		Mean	Standard deviation	Min	Max	Mean	Standard deviation	Min	Max	95th %ile
Trophic level 1 – log BAF_{fd}										
Original Voutsas method		-0.02	0.45	-0.69	0.89	0.38	0.24	0.01	0.89	0.81
AQUAWEB v1.1 – TGD default QSAR for $K_{oc-water}$ properties as given in model	Phytoplankton	0.58	0.62	-0.28	2.27	0.61	0.59	0.00	2.27	1.79
	Zooplankton	0.78	0.50	0.02	1.88	0.78	0.50	0.02	1.88	1.75
AQUAWEB v1.1 – TGD default QSAR for $K_{oc-water}$ properties as for TGD	Phytoplankton	0.37	0.49	-0.36	1.43	0.44	0.43	0.01	1.43	1.35
	Zooplankton	0.57	0.44	-0.07	1.40	0.58	0.43	0.00	1.40	1.30
AQUAWEB v1.1 – TGD predominantly hydrophobics QSAR for $K_{oc-water}$ properties as given in model	Phytoplankton	0.58	0.62	-0.28	2.27	0.61	0.59	0.00	2.27	1.79
	Zooplankton	0.78	0.50	0.02	1.88	0.78	0.50	0.02	1.88	1.75
AQUAWEB v1.1 – TGD predominantly hydrophobics QSAR for K_{oc} – water properties as for TGD	Phytoplankton	0.37	0.49	-0.36	1.43	0.44	0.43	0.01	1.43	1.35
	Zooplankton	0.57	0.44	-0.07	1.40	0.58	0.43	0.00	1.40	1.30
BIO v1.1 – TGD predominantly hydrophobics QSAR for $K_{oc-water}$ properties as for TGD	Phytoplankton	0.84	0.44	-0.02	1.71	0.84	0.44	0.02	1.71	1.58
	Zooplankton	0.84	0.44	-0.02	1.71	0.84	0.44	0.02	1.71	1.58
Trophic level 1 – log BAF_t										
Original Voutsas method		-0.12	0.44	-0.73	0.80	0.38	0.25	0.00	0.80	0.73
AQUAWEB v1.1 – TGD predominantly hydrophobics QSAR for $K_{oc-water}$ properties as for TGD	Phytoplankton	0.27	0.48	-0.45	1.28	0.40	0.37	0.00	1.28	1.20
	Zooplankton	0.47	0.44	-0.19	1.27	0.52	0.38	0.05	1.27	1.15
Trophic level 2 – log BAF_{fd}										
Original Voutsas method		-0.08	0.63	-1.43	1.28	0.53	0.36	0.00	1.43	1.18
AQUAWEB v1.1 – TGD default QSAR for $K_{oc-water}$ properties as given in model	Zebra mussel	0.66	0.71	-0.65	2.44	0.74	0.63	0.00	2.44	2.09
	Mayfly	0.88	0.76	-0.37	2.75	0.91	0.73	0.00	2.75	2.39

Method		Residual[a]				Absolute residual[b]				
		Mean	Standard deviation	Min	Max	Mean	Standard deviation	Min	Max	95th %ile
AQUAWEB v1.1 – TGD default QSAR for $K_{oc-water}$ properties as for TGD	Zebra mussel	0.61	0.65	-0.68	2.13	0.68	0.57	0.01	2.13	1.86
	Mayfly	0.75	0.67	-0.48	2.34	0.78	0.63	0.00	2.34	2.07
AQUAWEB v1.1 – TGD predominantly hydrophobics QSAR for $K_{oc-water}$ properties as given in model	Zebra mussel	0.60	0.68	-0.69	2.29	0.69	0.59	0.00	2.29	1.97
	Mayfly	0.65	0.65	-0.63	2.20	0.72	0.58	0.00	2.20	1.93
AQUAWEB v1.1 – TGD predominantly hydrophobics QSAR for $K_{oc-water}$ properties as for TGD	Zebra mussel	0.59	0.64	-0.71	2.09	0.67	0.56	0.01	2.09	0.67
	Mayfly	0.58	0.63	-0.74	2.04	0.67	0.54	0.00	2.04	1.78
BIO v1.1 – TGD predominantly hydrophobics QSAR for $K_{oc-water}$ properties as for TGD	Zebra mussel	1.55	0.72	0.42	3.2	1.55	0.72	0.42	3.2	2.95
	Mayfly	1.55	0.72	0.42	3.2	1.55	0.72	0.42	3.2	2.95
Trophic level 2 – log BAF_t										
Original Voutsas method		-0.16	0.66	-1.55	1.48	0.55	0.39	0.00	1.55	1.21
AQUAWEB v1.1 – TGD predominantly hydrophobics QSAR for $K_{oc-water}$ properties as for TGD	Zebra mussel	0.39	0.63	-0.94	1.71	0.59	0.44	0.00	1.71	1.47
	Mayfly	0.19	0.64	-1.37	1.30	0.57	0.34	0.00	1.37	1.12
Trophic level 3 – log BAF_{fd}										
Original Voutsas method		0.00	0.45	-1.09	1.35	0.36	0.27	0.00	1.35	0.86
TGD method – BMF_1		0.78	0.75	-0.54	4.15	0.83	0.70	0.00	4.15	2.09
TGD method – BMF_1 and BMF_2		0.21	0.77	-1.54	3.67	0.60	0.52	0.00	3.67	1.43
AQUAWEB v1.1 – TGD default QSAR for $K_{oc-water}$ properties as given in model		0.71	0.69	-0.41	3.80	0.75	0.64	0.00	3.80	1.78
AQUAWEB v1.1 – TGD default QSAR for $K_{oc-water}$ properties as for TGD		0.61	0.55	-0.43	2.65	0.67	0.48	0.00	2.65	1.47
AQUAWEB v1.1 – TGD predominantly hydrophobics QSAR for $K_{oc-water}$ properties as given in model		0.71	0.69	-0.41	3.80	0.75	0.64	0.00	3.80	1.78
AQUAWEB v1.1 – TGD predominantly hydrophobics QSAR for $K_{oc-water}$ properties as for TGD		0.61	0.55	-0.43	2.65	0.67	0.48	0.00	2.65	1.47
BIO v1.1 – TGD predominantly hydrophobics QSAR for $K_{oc-water}$ properties as for TGD		0.89	0.63	-0.34	2.25	0.91	0.60	0.01	2.25	1.85
Trophic level 3 – log BAF_t										
Original Voutsas method		-0.10	0.50	-1.46	1.51	0.38	0.33	0.00	1.51	1.12

Method	Residual[a]				Absolute residual[b]				
	Mean	Standard deviation	Min	Max	Mean	Standard deviation	Min	Max	95th %ile
TGD method – BMF_1	0.50	0.60	-1.09	3.05	0.63	0.46	0.00	3.04	1.38
TGD method – BMF_1 and BMF_2	-0.07	0.76	-2.09	2.57	0.58	0.49	0.00	2.57	1.61
AQUAWEB v1.1 – TGD predominantly hydrophobics QSAR for $K_{oc\ -\ water}$ properties as for TGD	0.49	0.55	-0.73	2.49	0.60	0.42	0.00	2.49	1.30
Trophic level 4 – log BAF_{fd}									
Original Voutsas method	0.07	0.40	-0.93	0.74	0.33	0.22	0.00	0.93	0.74
TGD method – BMF_1	1.19	0.86	0.05	4.52	1.19	0.86	0.05	4.52	2.74
TGD method – BMF_1 and BMF_2	0.61	0.83	-0.85	4.04	0.80	0.64	0.02	4.04	1.74
AQUAWEB v1.1 – TGD default QSAR for $K_{oc\ -\ water}$ properties as given in model	0.72	0.73	-0.63	3.99	0.77	0.67	0.03	3.99	1.77
AQUAWEB v1.1 – TGD default QSAR for $K_{oc\ -\ water}$ properties as for TGD	0.61	0.57	-0.71	2.83	0.68	0.48	0.03	2.83	1.29
AQUAWEB v1.1 – TGD predominantly hydrophobics QSAR for $K_{oc\ -\ water}$ properties as given in model	0.72	0.73	-0.63	3.99	0.77	0.67	0.03	3.99	1.77
AQUAWEB v1.1 – TGD predominantly hydrophobics QSAR for $K_{oc\ -\ water}$ properties as for TGD	0.61	0.57	-0.71	2.83	0.68	0.48	0.03	2.83	1.29
BIO v1.1 – TGD predominantly hydrophobics QSAR for $K_{oc\ -\ water}$ properties as for TGD	1.01	0.57	-0.01	2.23	1.02	0.57	0.01	2.23	1.93
Trophic level 4 – log BAF_t									
Original Voutsas method	-0.03	0.41	-1.02	0.66	0.31	0.26	0.01	1.02	0.77
TGD method – BMF_1	0.88	0.66	-0.42	3.41	0.91	0.63	0.03	3.41	1.91
TGD method – BMF_1 and BMF_2	0.30	0.75	-1.42	2.93	0.91	0.63	0.03	3.41	1.29
AQUAWEB v1.1 – TGD predominantly hydrophobics QSAR for $K_{oc\ -\ water}$ properties as for TGD	0.48	0.57	-0.80	2.68	0.59	0.45	0.01	2.68	1.14

a) Residual = actual log BAF – predicted log BAF.

b) Absolute residual is the difference between the actual log BAF and the predicted log BAF disregarding the sign.

The following section presents some examples of plots comparing field and predicted BAF values using AQUAWEB and the TGD method (where possible) to illustrate the general conclusions in this section. A more extended comparison is given in Appendix C.

For trophic level 1, plots comparing the predicted BAF_{fd} obtained from AQUAWEB v1.1 with the actual BAF_{fd} are shown in Figure 6.1 (using the Great Lakes water properties) and Figure 6.2 (using the TGD water properties). The corresponding residuals in the prediction are shown in Figure 6.2 Predicted BAFfd for trophic level 1 using AQUAWEB (TGD water properties and QSAR for predominantly hydrophobics)

As can be seen from these plots, the field data show a more or less linear increase in the log BAF_{fd} with log K_{ow} (as was found by Voutsas et al., 2002). The predicted log BAF_{fd} depends on the water properties used (the dissolved organic carbon concentration). For simulations using the Great Lakes water properties (where the dissolved organic carbon content was set to 2.2×10^{-6} kg l^{-1}), the predicted log BAF shows a maximum value at a log K_{ow} of around seven and then decreases with increasing log K_{ow}. For simulations carried out using the TGD water properties (where the dissolved organic carbon content was set to zero), the log BAF shows an increasing trend with increasing log K_{ow} across the entire data set, but tends towards a maximum value of log BAF at very high log K_{ow} values (around nine to ten). As discussed previously, the model adjusts the bioavailable fraction of the chemical in water to take account of the association with dissolved organic carbon and this explains the different patterns seen in the two sets of simulations. Only when the dissolved organic carbon content is set to zero will the predicted BAF reflect the BAF on a true dissolved concentration in water.

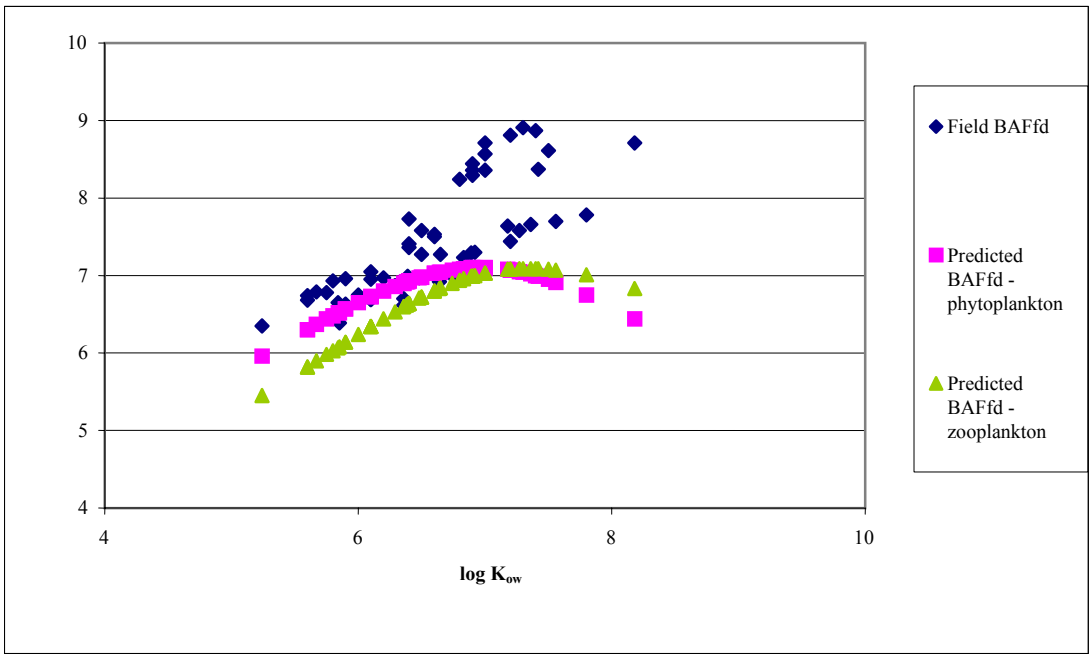

Figure 6.1 Predicted BAF_{fd} for trophic level 1 using AQUAWEB (Great Lakes water properties and QSAR for predominantly hydrophobics)

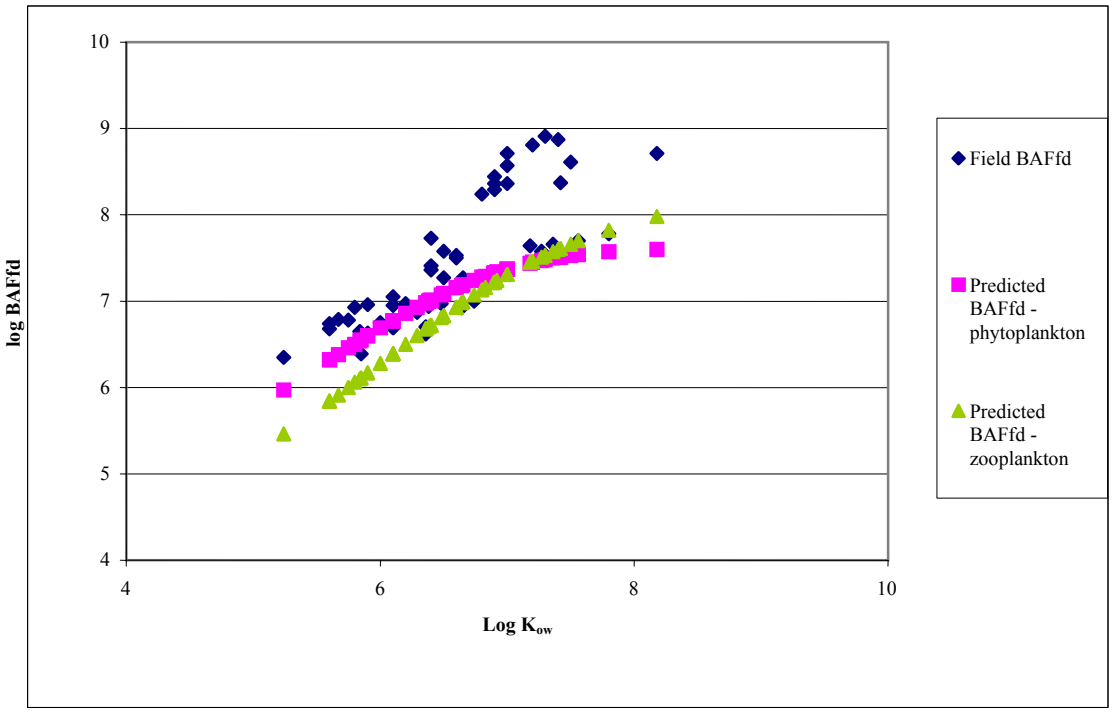

Figure 6.2 **Predicted BAF_{fd} for trophic level 1 using AQUAWEB (TGD water properties and QSAR for predominantly hydrophobics)**

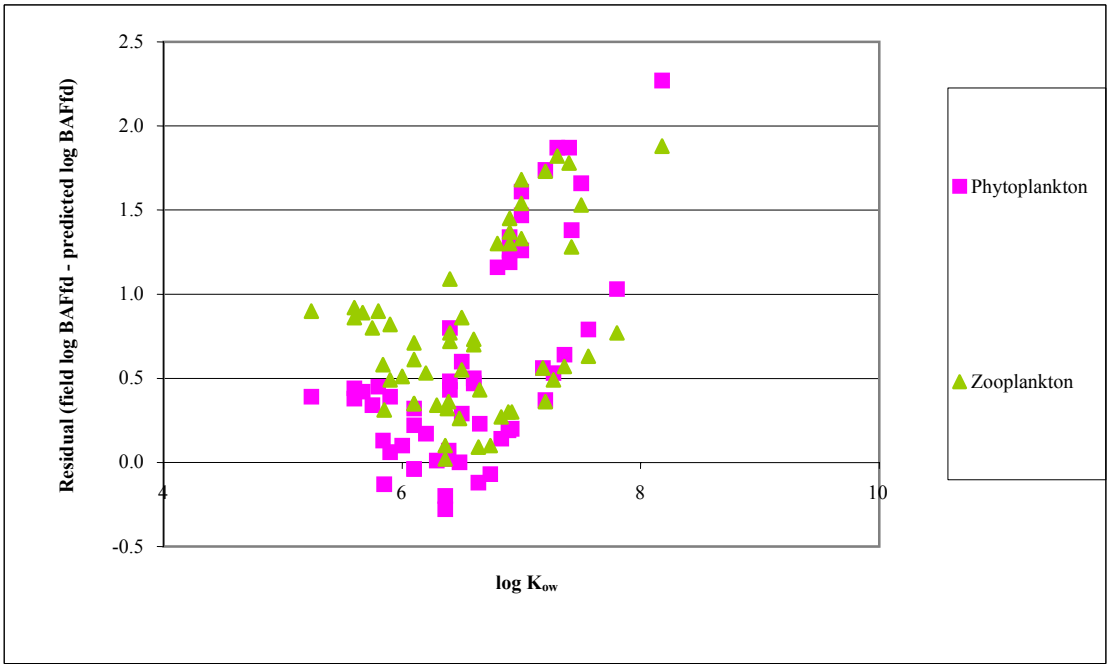

Figure 6.3 Residual in the prediction in log BAF_{fd} for trophic level 1 using AQUAWEB v1.1 (Great Lakes water properties and QSAR for predominantly hydrophobics)

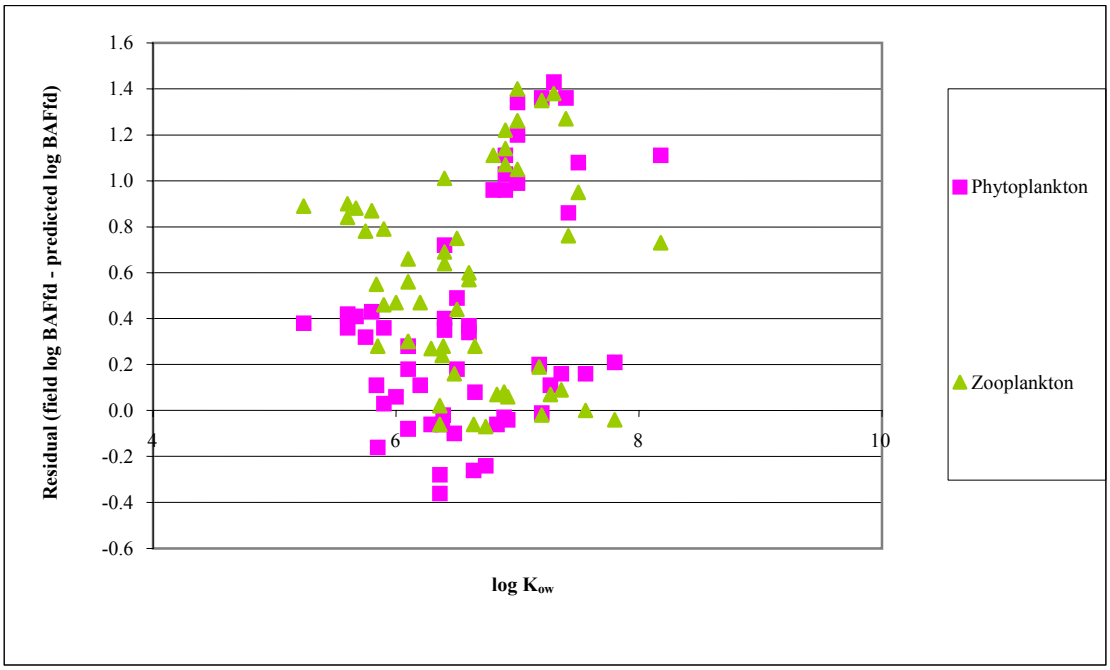

Figure 6.4 Residual in the prediction in log BAF_{fd} for trophic level 1 using AQUAWEB v1.1 (TGD water properties and QSAR for predominantly hydrophobics)

The plots of the residuals against log K_{ow} (Figure 6.2 Predicted BAFfd for trophic level 1 using AQUAWEB (TGD water properties and QSAR for predominantly hydrophobics)

6.3 and 6.4) show no systematic over or underprediction that is log K_{ow} dependent. Analysis of the residuals generally shows that the AQUAWEB v1.1 model performs better than the BIO v1.1 model for this test set.

BAF_{fd} data values presented by Voutsas *et al.* (2002) were generally converted from BAF_t values (lipid-normalized bioaccumulation factors on a total concentration in water) to a freely dissolved basis by assuming an equilibrium partitioning approach. Details of how this was carried out are given in Voutsas *et al.* (2002). In order to test if this data conversion could account for the difference between the predicted and actual BAF_{fd} seen here, a comparison was made between the predicted BAF_t using the Great Lakes water properties and the BAF_t data set. This is shown in 6.5 and 6.6. Here, the predicted log BAF_t shows a maximum at a log K_{ow} of around seven. The scatter in the actual log BAF_t data set is quite large, but it appears to show a similar maximum at a log K_{ow} of around seven. Statistics for the analysis of the residuals (Table 6.2) show that, although the Voutsas *et al.* (2002) method appears to perform better than the AQUAWEB v1.1 method against this data set, the difference in

performance is less marked than that found for the analysis of the log BAF_{fd}. For example, the mean and 95th percentile of the absolute residual from the Voutsas *et al.* (2002) method for the log BAF_{ft} is 0.38 and 0.73 respectively, compared with a mean and 95th percentile for the AQUAWEB predictions for phytoplankton of 0.40 and 1.20 respectively.

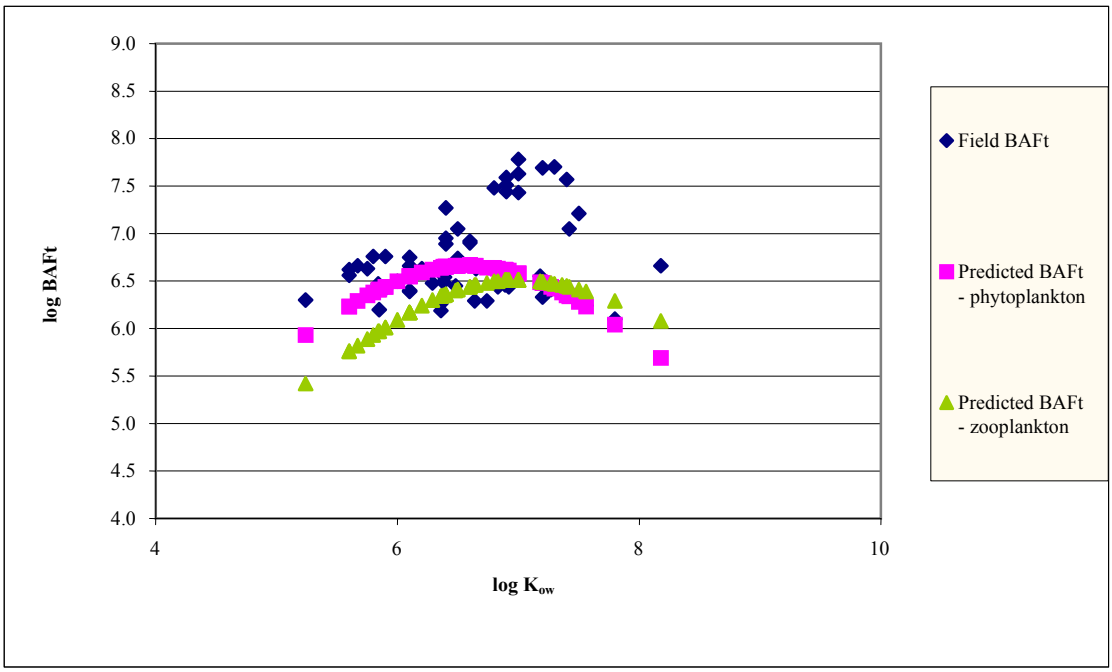

Figure 6.5 Predicted BAF_t for trophic level 1 using AQUAWEB (Great Lakes water properties and QSAR for predominantly hydrophobics)

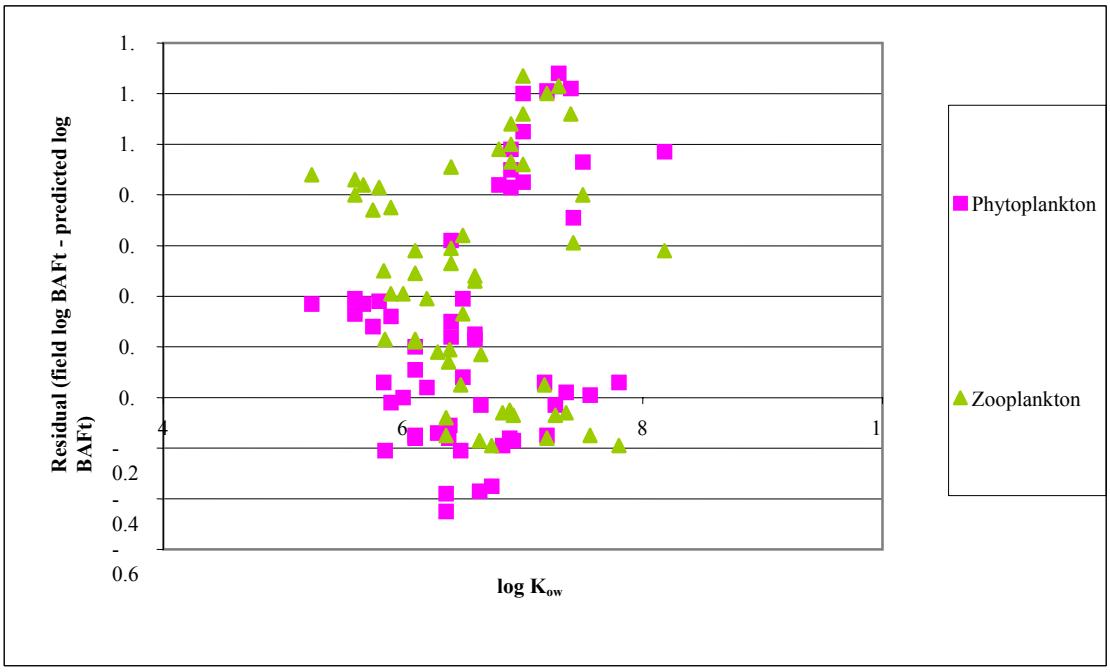

Figure 6.6 Residual in the prediction in log BAF_t for trophic level 1 using AQUAWEB v1.1 (Great Lakes water properties and QSAR for predominantly hydrophobics)

Thus, it is possible that the assumptions made by Voutsas et al. (2002) in converting the data set to BAF_{fd} values may have introduced some further uncertainties into the data set, particularly at log K_{ow} values greater than seven. This may relate to general problems in estimating the freely dissolved or bioavailable fraction in water for highly lipophilic substances.

For an analysis of trophic level 2, see Appendix C.

For trophic level 3, plots comparing the BAF_{fd} estimated using AQUAWEB v1.1 with the actual BAF_{fd} are shown in Figure 6.7 (using the Great Lakes water properties) and Figure 6.8 (using the TGD water properties). The equivalent plot for the BAF_{fd} estimated using the TGD method is shown in **Error! Reference source not found.**6.9. Plots of the residual in the prediction are shown in Figure 6.10 (AQUAWEB v1.1 using the Great Lakes water properties), Figure 6.11 (AQUAWEB v1.1 using the TGD water properties) and Figure 6.12 (TGD method).

As can be seen from these plots, the field data again show a linear increase of log BAF_{fd} with increasing log K_{ow} values. The predictions obtained using AQUAWEB v1.1 appear to follow this increase reasonably well at lower log K_{ow} values, but reach a maximum in the log BAF_{fd} at a log K_{ow} value of around seven or eight depending on the assumptions made on the dissolved organic carbon content of the water – the maximum value is higher and at a higher log K_{ow} value for the TGD water properties. A similar pattern is also evident in the TGD predictions, with a maximum on the predicted BAF_{fd} occurring at a log K_{ow} of around seven.

Analysis of the residuals shows a generally even scatter Figure 6.10 to Figure 6.12), with a tendency to underpredict the BAF value at higher log K_{ow} values – noting that there are only few data at such high log K_{ow} values. The analysis again shows that the AQUAWEB v1.1 model performs better than the BIO v1.1 model for this test set.

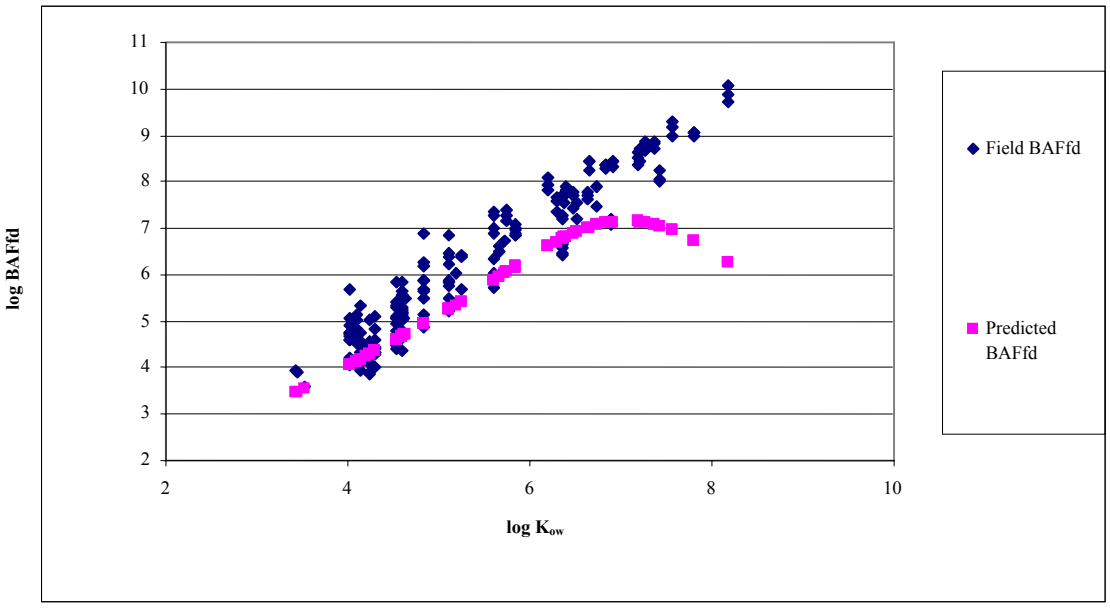

Figure 6.7 Predicted BAF_{fd} for trophic level 3 using AQUAWEB v1.1 (Great Lakes water properties and QSAR for predominantly hydrophobics)

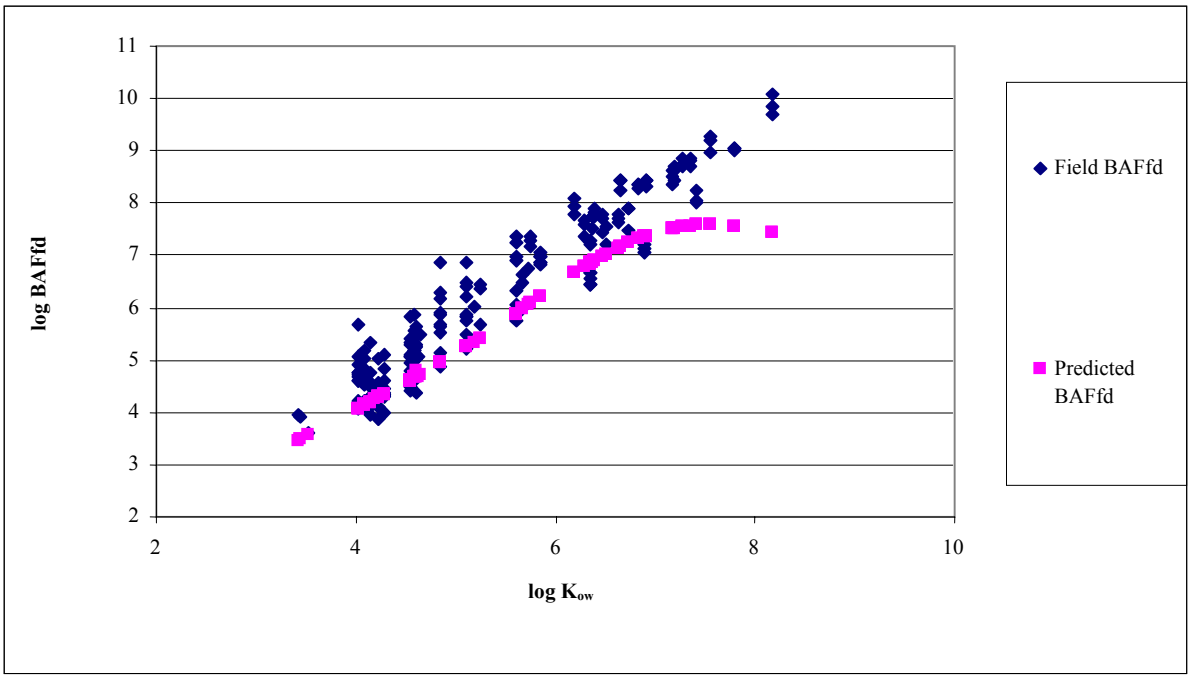

Figure 6.8 Predicted BAF_{fd} for trophic level 3 using AQUAWEB v1.1 (TGD water properties and QSAR for predominantly hydrophobics)

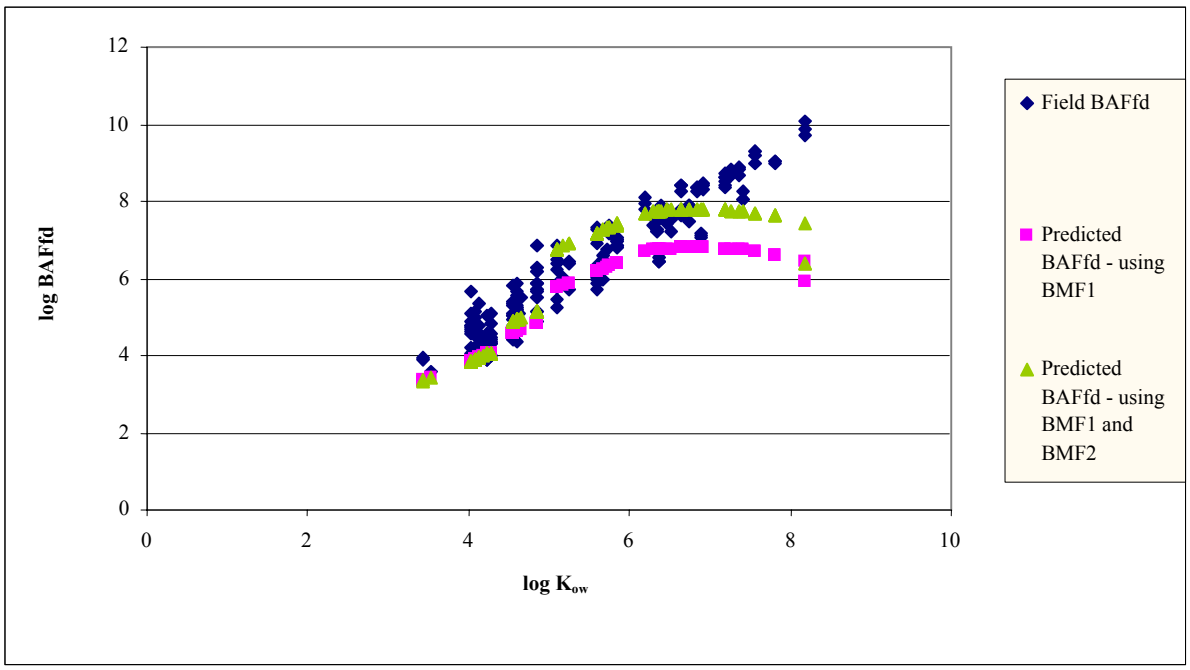

Figure 6.9 Predicted BAF_{fd} for trophic level 3 using the TGD method

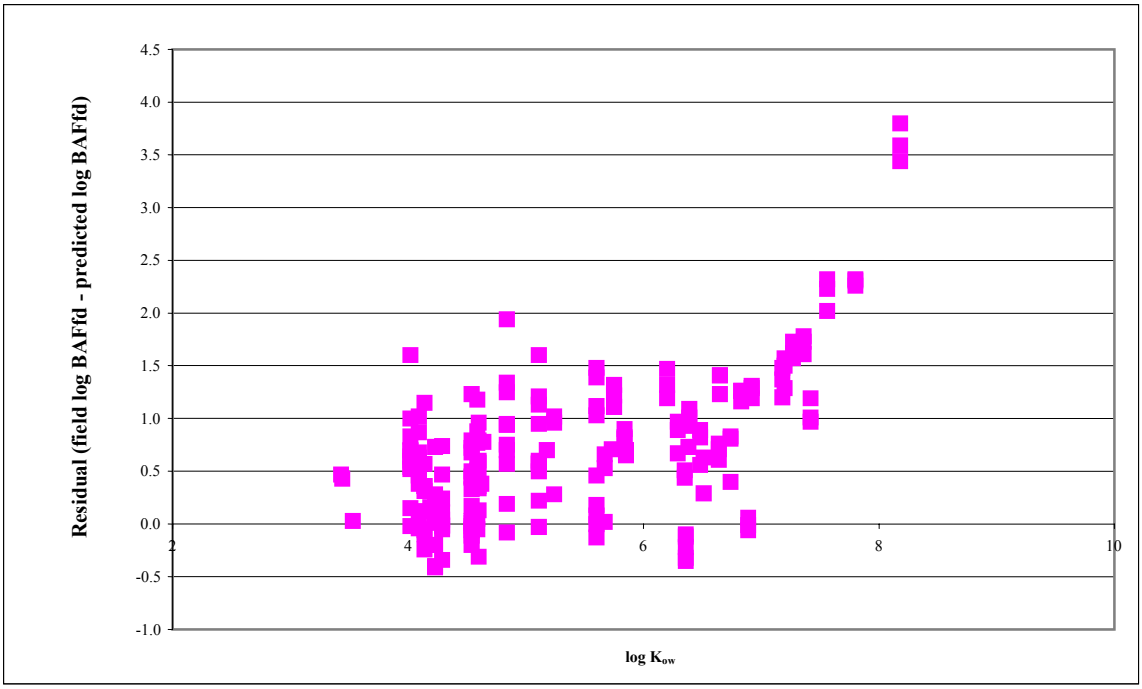

Figure 6.10 Residual in the prediction in log BAF_{fd} for trophic level 3 using AQUAWEB v1.1 (Great Lakes water properties and QSAR for predominantly hydrophobics)

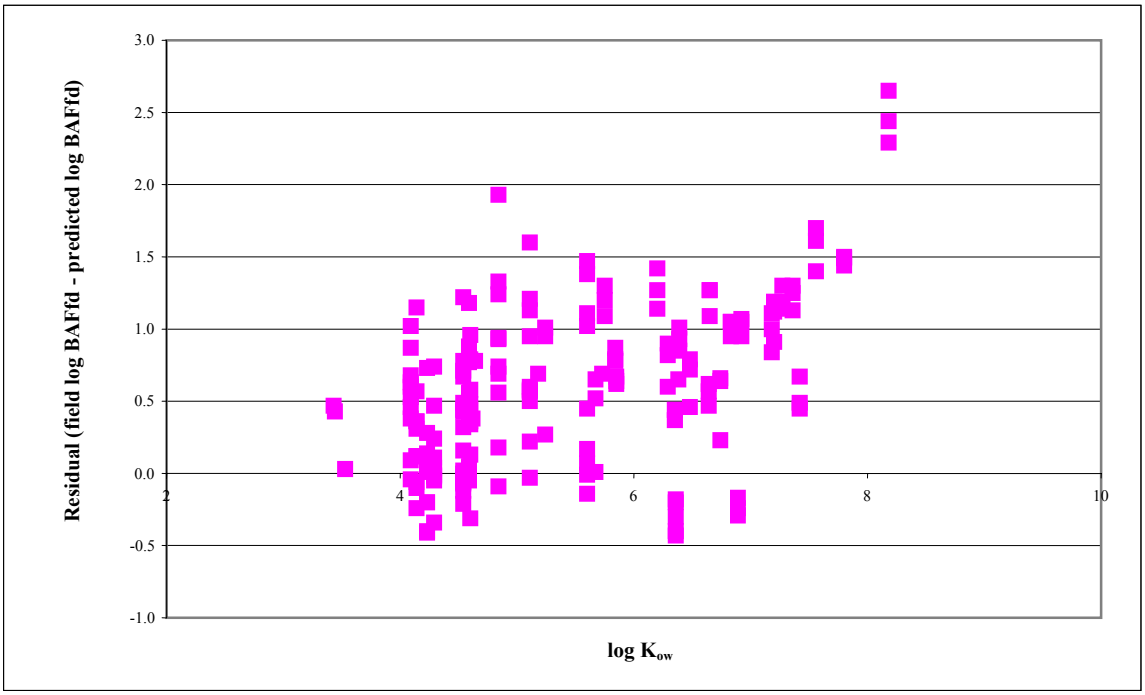

Figure 6.11 Residual in the prediction in log BAFfd for trophic level 3 using AQUAWEB v1.1 (TGD water properties and QSAR for predominantly hydrophobics)

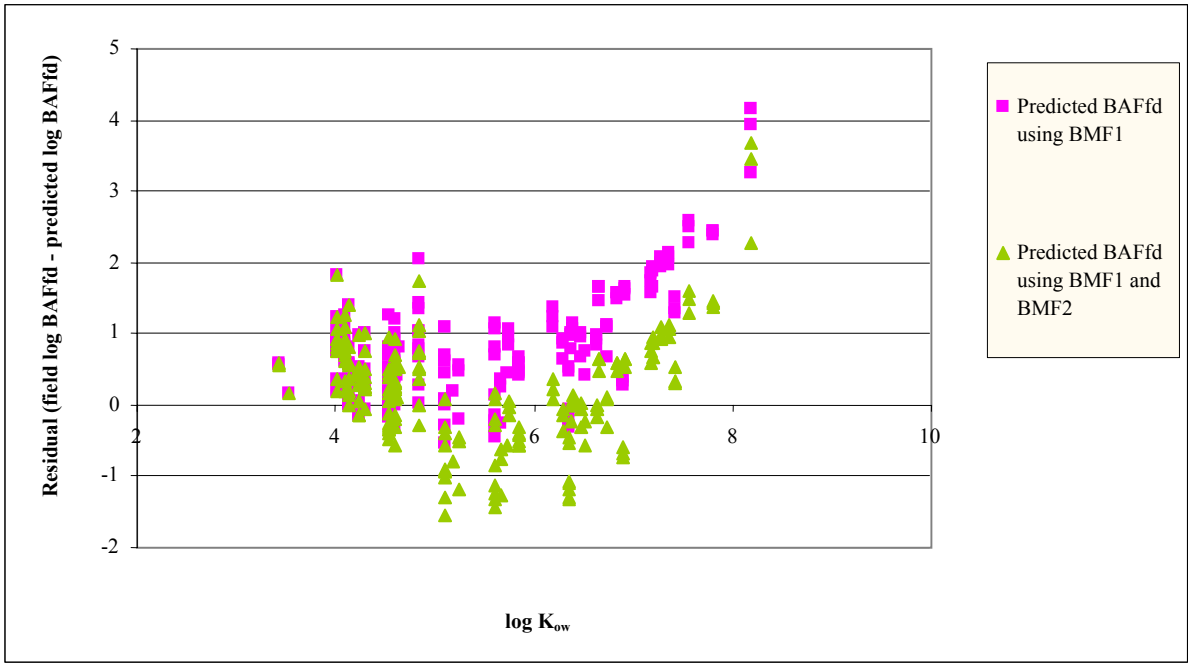

Figure 6.12 Residual in the prediction in log BAF_{fd} for trophic level 3 using the TGD method

Similarly to the preceding trophic levels, an analysis of the predicted BAF_t values was carried out in order to test if the conversion applied by Voutsas *et al.* (2002) could account for the differences between the actual and predicted values. Plots showing the predicted BAF_t and actual BAF_t are given in Figure 6.13 (AQUAWEB v1.1 using the Great Lakes water properties) and Figure 6.14 (TGD method). The corresponding plots for the residuals are given in Figure 6.15 and Figure 6.16 respectively.

As can be seen from the plots, both methods predict a maximum log BAF_t at a log K_{ow} of six to seven. The available data set of actual BAF_t values shows a large degree of scatter, but appears to show an increasing trend in log BAF_t with increasing log K_{ow} (although there is some suggestion of a levelling off of the log BAF_t value at log K_{ow} values above seven). Based on the analysis of residuals given in Table 6.2, the Voutsas et al. (2002) method still appears to perform best against this data set, although the performance of the AQUAWEB v1.1 and TGD method (using both a BMF_1 and BMF_2 value) are much closer in performance to the Voutsas et al. (2002) method than was found for the BAF_{fd} data set. For example, the 95th percentile values for the absolute residuals are 1.12 for the Voutsas et al. (2002) method compared with 1.30 obtained using the AQUAWEB v1.1 model and 1.61 obtained using the TGD method with a BMF_1 and BMF_2 value.

Again, it is possible that the assumptions made by Voutsas et al. (2002) in converting the data set to BAF_{fd} values may have introduced some further uncertainties into the data set, particularly at log K_{ow} values greater than seven.

The TGD method using both a BMF_1 and BMF_2 value (as is currently recommended for extended marine food chains) again appears to perform better against this freshwater data set than the TGD method employing a single BMF_1 value (as is currently recommended for freshwater food chains).

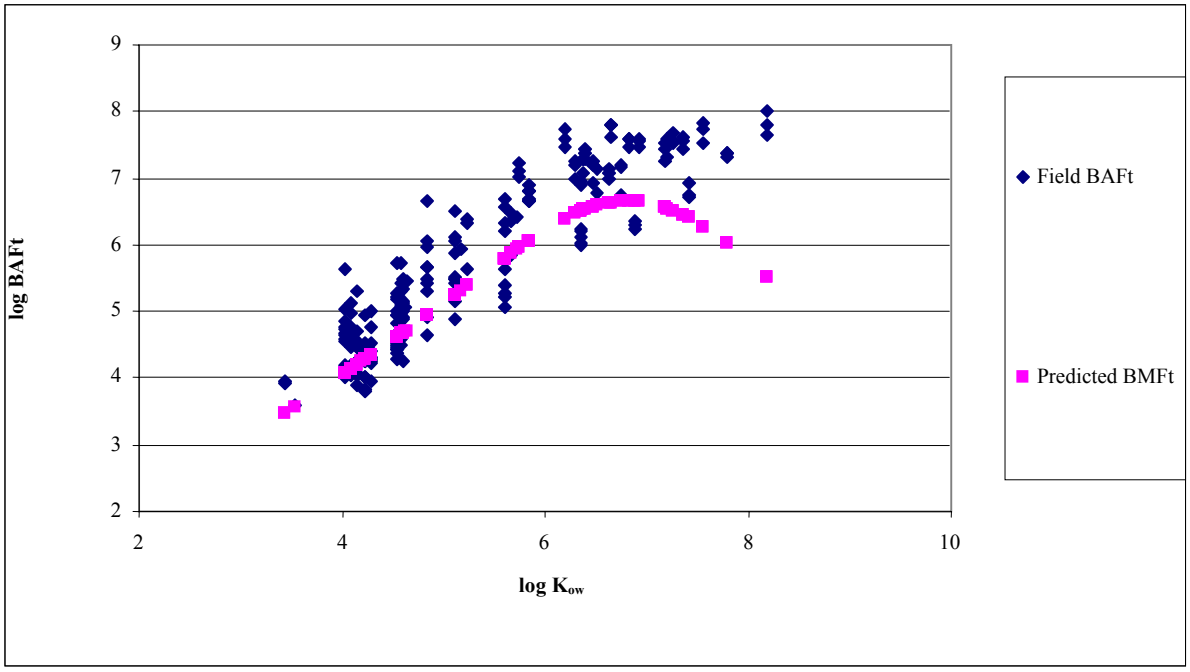

Figure 6.13 Predicted BAF_t for trophic level 3 using AQUAWEB (Great Lakes water properties and QSAR for predominantly hydrophobics)

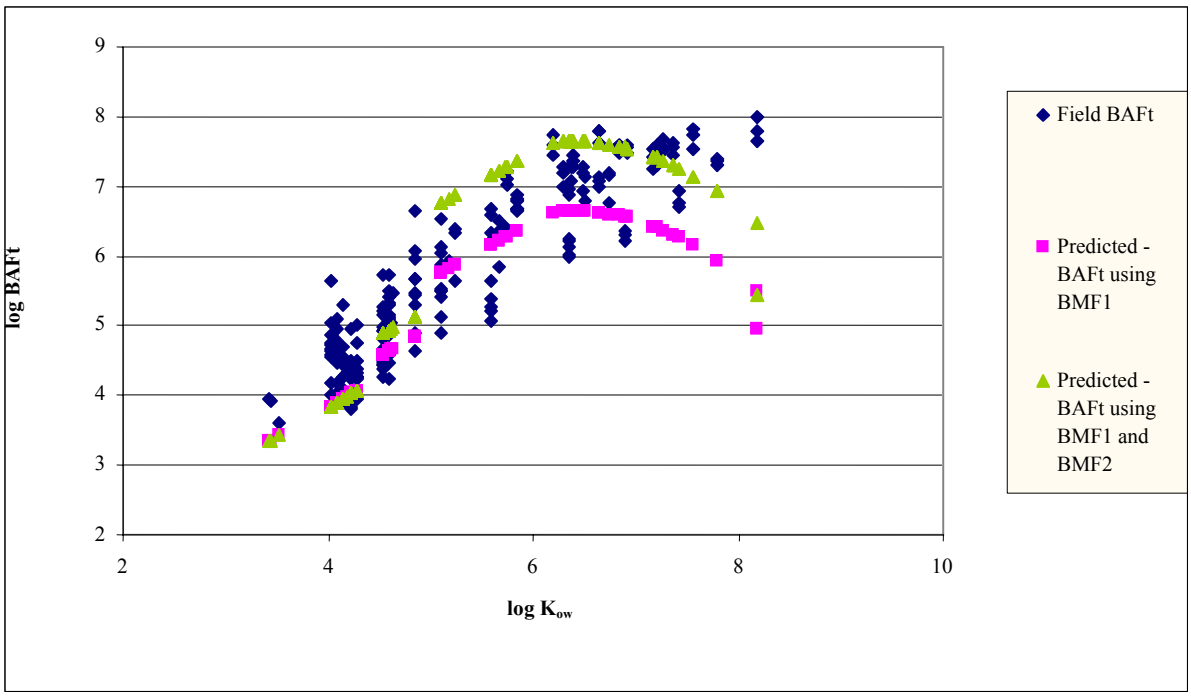

Figure 6.14 Predicted BAF_t for trophic level 3 using the TGD method

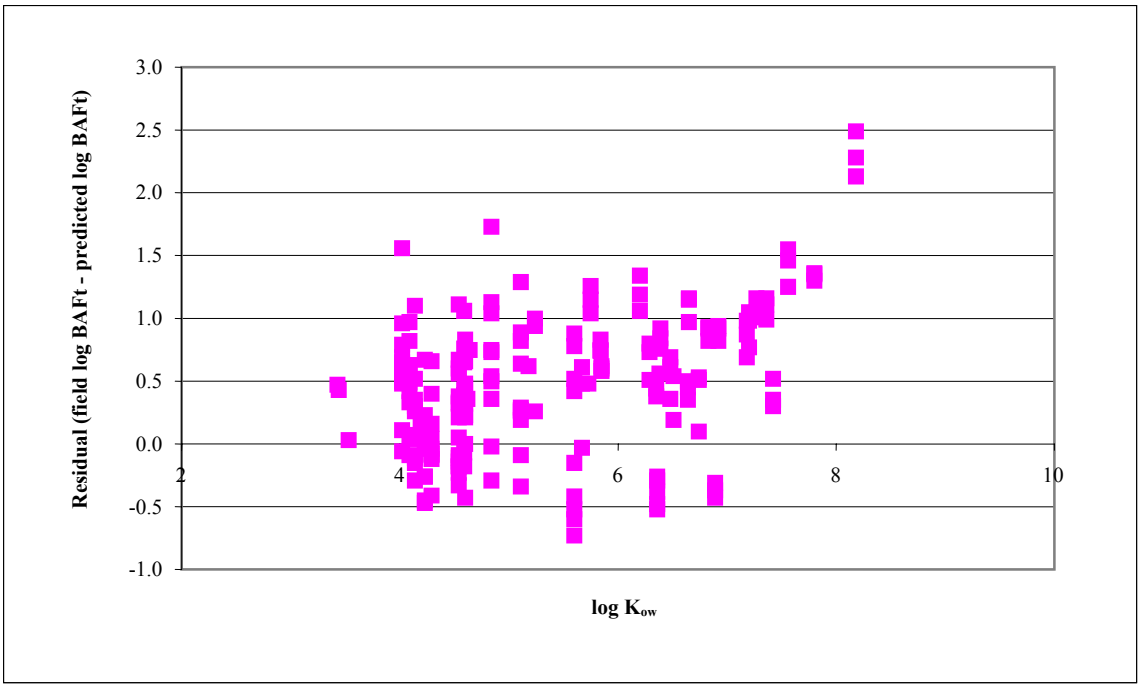

Figure 6.15 Residual in the prediction in log BAF_t for trophic level 3 using AQUAWEB v1.1 (Great Lakes water properties and QSAR for predominantly hydrophobics)

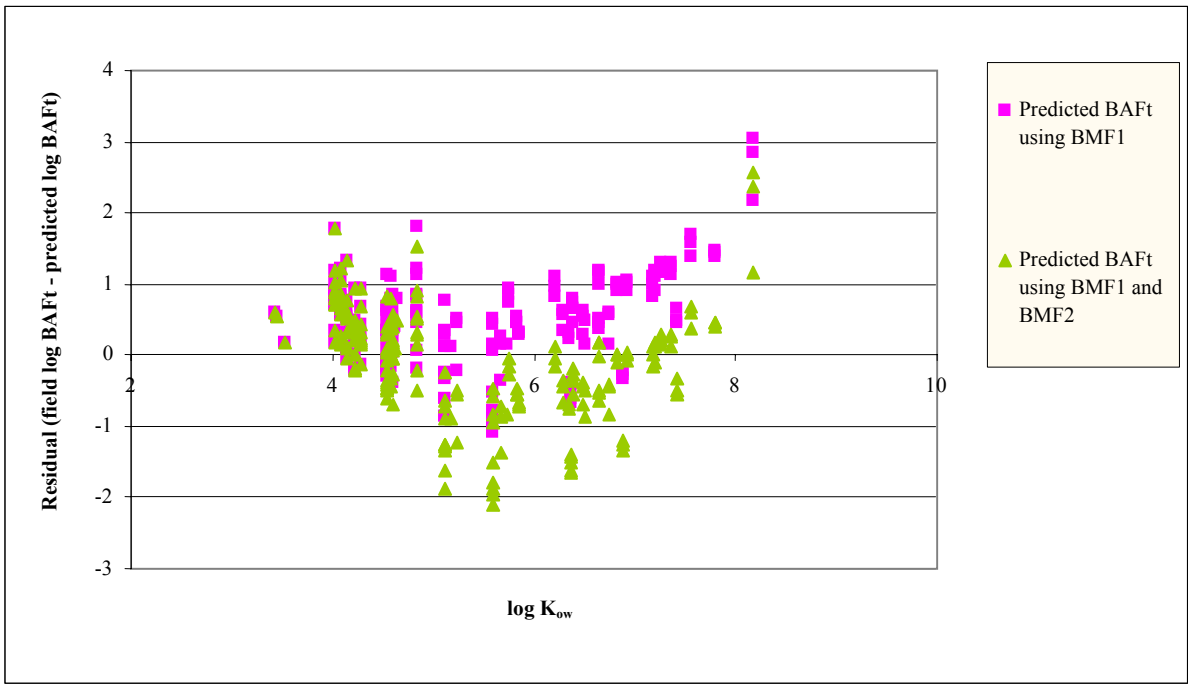

Figure 6.16 Residual in the prediction in log BAF_t for trophic level 3 using the TGD method

The findings for trophic level 4 are very similar to those for trophic level 3.

6.2 Summary of findings

Overall, the Voutsas et al. (2002) method generally gave the best predictions against this data set. This is not altogether surprising as subsets of the data set used here were used by Voutsas et al. (2002) to both develop and test the method. The AQUAWEB v1.1 and TGD method were found to give reasonable predictions for the BAF_{fd} and BAF_t up to a log K_{ow} of around six or seven. At log K_{ow} values higher than seven, a considerable divergence between the predicted and actual BAF_{fd} and BAF_t was apparent.

A comparison of the results from AQUAWEB v1.1 with those from BIOv1.1 shows a generally better performance of AQUAWEB v1.1.

Metabolism data could not be included in the Voutsas et al. (2002) or TGD methods, and the AQUAWEB v1.1 simulations were carried out assuming no metabolism was occurring. For substances that are metabolised significantly, AQUAWEB v1.1 would be expected to provide more reliable predictions of the BAF.

The TGD method using both a BMF_1 and BMF_2 generally performed better against the test set for trophic level 3 and trophic level 4 than the TGD method using only a BMF_1.

The analysis also revealed that the assumptions made over the bioavailable or dissolved fraction of the chemical in water may have an important bearing on the reliability of the predicted BAFs. This is relevant to both the AQUAWEB v1.1 and TGD methods, where the concentration in sediment pore water and the freely dissolved concentration in water are estimated by equilibrium partitioning approaches. Whilst such approaches are known to work satisfactorily in general, their reliability in estimating the bioavailable fraction for substances of extreme lipophilicity (for example, with log K_{ow} of seven or more) or where the absorption potential is not directly related to the log K_{ow}, is unclear, and such errors and uncertainties are probably equally as important as errors in the modelling of subsequent uptake through the food chain for these types of chemicals.

7 Conclusions and recommendations

There are several sources of variability and uncertainty in the data analysed in this study. These include uncertainties in the physico-chemical properties of chemicals used in the models, uncertainties in the actual measured accumulation factors, and uncertainties resulting from assumptions and simplifications in the models. For example, log K_{ow} values for any given chemical can cover a range of one log unit or even more, depending on the measurement or estimation method used. Further, the measurement or estimation of log K_{ow} becomes increasingly difficult with increasing log K_{ow} values. Similarly, variability exists in experimental or field accumulation factors, where concentrations in the exposure medium and biota may vary both spatially and temporally and so lead to uncertainties over the actual value for the BAF. Therefore, model results should not be expected to agree exactly with experimental and field data, but rather should provide a general agreement (to within an order of magnitude) with the data.

The analysis carried out in this report has revealed the following points:

- For chemicals with log K_{ow} values up to around 4.5 to 5, the contribution from food to the total body burden of top predators such as fish is likely to be small compared with uptake directly from water; that is, bioconcentration processes dominate uptake in predatory fish. In these cases, a BCF value alone would give a reasonably reliable indication of the concentration in predatory fish near the top of the food chain. The BCF value used should preferably be an experimentally determined value, but predicted BCFs could also be considered, and could be generated from equations outlined in the TGD or a model such as AQUAWEB v1.1. The AQUAWEB v1.1 model has some advantages over the TGD equations, as it allows metabolism to be taken into account when deriving BCFs. However, in practice the necessary kinetic data on metabolism are only likely to be available for chemicals for which an experimental BCF already exists, as kinetic data are usually generated as part of a BCF study.

- Further verification is needed for the TGD method, the Voutsas et al. (2002) method and the AQUAWEB v1.1 model. Although these appear to work reasonably well when compared with literature BCF or BAF data, at least up to a log K_{ow} value of around six to seven, when used to predict concentrations in the food chain for the Mersey data set all methods significantly overestimated the concentration in biota, particularly for substances with relatively high log K_{ow} values. It is not clear whether this discrepancy between predictions and observations for the Mersey data set results from systematic errors in the prediction methods or from uncertainties in the data set.

- Analysis of the available data shows the importance of assumptions about the partitioning behaviour of the chemical in water (that is, assumptions used to estimate the bioavailable fraction in water) to the predicted BAF, particularly for substances with log K_{ow} values around seven. Although it is possible to predict BAF from the dissolved fraction in water using all three methods, this is potentially important when back-calculating from a concentration of concern in an organism to a concentration in water or sediment using such a predicted BAF (as may be the case when setting a standard).

- In terms of standard setting, for chemicals that are not metabolised the Voutsas et al. (2002) method appears to work reasonably well and provides an estimate of the BAF (either related to the freely dissolved concentration in water or the total concentration

in water) for four generic trophic levels. For substances that are metabolised, the AQUAWEB v1.1 model is preferable (using a relatively generic food chain as considered in Section 6). However, the model appears to underestimate the actual BAF, especially for trophic level 3 and trophic level 4, at log K_{ow} values above seven.

- All methods predict very high BAFs (of the order of 10^6 to 10^7) for certain types of chemicals, which may have implications for the appropriate medium in which to set the standard. For example, high BAFs could result in very low concentrations in water being estimated as a standard. If these concentrations were so low as to not be measurable in practice, then the usefulness of the standard would be limited. It might then be necessary to consider setting the standard based on concentrations in other media (such as sediment) or indeed on the concentration in biota itself. In the latter case, there would be no need for any modelling of uptake through the food chain.
- All methods assume that uptake into the organism is governed by partitioning into lipids, which is the case for many substances. However, such methods will not be reliable for chemicals whose uptake is governed by other factors, such as binding to proteins. This is particularly true for the Voutsas et al. (2002) method, which uses empirically derived equations. It should be possible to use the TGD method with substances where other factors are important, provided that BMF values can be derived either from measurements or through the development of suitable estimation methods; however, at present these are not available.
- The TGD method appears to give more reliable predictions when both a BMF_1 and BMF_2 are used. This approach is currently recommended for marine food chains only. However, our analysis indicates that the use of both a BMF_1 and BMF_2 may also be appropriate for freshwater food chains. This may have implications for the use of the TGD method in risk assessments for secondary poisoning, as well as in setting standards.

In conclusion, a combination of the Voutsas et al. (2002) method for non-metabolised chemicals, along with a generic food chain in the AQUAWEB v1.1 model for metabolised substances, is likely to provide the most reliable predictions for chemicals with log K_{ow} values up to around seven. Above a log K_{ow} of seven, there are considerable uncertainties in the model and experimental data and so it is not possible to recommend any one method for chemicals with very high log K_{ow} values. In particular, the continuing increase in BAF values for log K_{ow} values above seven in the Voutsas et al. equations is at odds with the other models, and as these equations are derived empirically there is no mechanistic framework to support this. Also, uncertainties in the predictions for chemicals with log K_{ow} values above seven do not arise solely from uncertainties in the bioaccumulation models, but also from uncertainties over how to estimate the bioavailable fraction in water for such substances. All methods appeared to significantly overestimate the actual BAFs derived from the Mersey data set; given the reasonable performance of the methods against data sets of BCFs and other BAFs, the reason for this is not clear, although it may be due to limitations in the data set itself.

There is a potential problem with the use of metabolism data in the AQUAWEB v1.1 model, in that most studies looking at metabolism measure the total depuration rate (the total loss of chemical from the organism) rather than metabolism specifically (experimentally, it is very difficult to separate out the different rates of loss processes). As other loss processes (such as respiration and faecal egestion) are already built into the model, rate constants derived from total depuration half-lives in fish may overestimate the rate of metabolism. This would need to be considered when reviewing metabolism data for inclusion in such a model. Alternatively, estimates of the potential rate of metabolism could be used if suitable methods

were developed. A review of such methods was not part of this project; there are programs available which predict possible metabolic pathways for substances, but we are not aware of any tools for predicting the likely breakdown rate for a wide range of substances.

If using the AQUAWEB v1.1 model to obtain BAFs on a freely dissolved basis, it is recommended that the dissolved organic carbon content of water is set to zero, and the concentrations in water are entered as filtered concentrations. The equivalent concentration in sediment used as input can easily be calculated using an equilibrium partitioning approach, as outlined in the TGD. Thus, the predicted concentration in the organism can be used to estimate the BAF directly on a freely dissolved concentration basis (or if needed, can be defined on the basis of the equivalent concentration in sediment).

Suggested modifications to the AQUAWEB v1.1 model to allow it to be used more easily in setting standards include the following[16]:

- Incorporate different methods to estimate the sediment-water partitioning for different types of chemicals or allow a K_{oc} value to be entered directly if one is available. This modification would ensure that the model's sediment-water partitioning properties were consistent with any method used to set standards for the protection of aquatic or sediment organisms. The TGD gives several different QSARs for estimating the K_{oc} value for different types of chemicals that could be considered in this respect (and the TGD method can be readily adapted to use measured K_{oc} values if available).
- Allow the concentration in sediment to be calculated from the concentration in water using the equilibrium partitioning method. At present, the model requires a concentration in water and sediment to be entered separately. When considering use of the model to set standards, it is important that the sediment and water concentrations are in the appropriate ratio. The easiest way to achieve this is by calculating the equivalent sediment concentration from the input water concentration. This would then allow the accumulation factors calculated to be related back to either a concentration in water or a concentration in sediment.
- Incorporate experimental BCF data if available. At present, it is not possible to incorporate actual BCF data for any of the species in the food chain (the model uses an internally calculated BCF value). However, BCF data are likely to be available for a number of chemicals for which standards are being set and it would be preferable to be able to include these. Experimental BCF values can be easily included in the TGD method.
- It would be useful if the output from the AQUAWEB v1.1 model gave the resulting BAFs on a dissolved concentration in water basis as well as the total concentration in water basis. This would illustrate the importance of suspended matter-water partitioning to the final BAF and provide useful information when considering how the standard should be set (it may not be analytically possible to set a standard on a dissolved concentration for some substances, owing to the very low concentrations involved). Such calculations can be easily done within the TGD method.

The BAFs estimated by any of the methods considered here (whether they be on a dissolved concentration or a total concentration basis) are in a form suitable for setting standards. As such, a BAF can be used to readily back-calculate from a 'no observed effect concentration' (NOEC) in food for a fish-eating predator (or some other endpoint derived from mammalian toxicity data) to the associated concentration in water (be it a dissolved concentration or a total concentration). The equivalent concentration in sediment (or conversion of a dissolved concentration to a total concentration and vice versa) can readily

[16] A food web model implemented at RIVM (SimpleWeb) incorporates most of the partitioning improvements listed here, but is not available in a user-friendly form (and was not reviewed as part of this work).

be obtained by applying an equilibrium partitioning approach (such as that outlined in the TGD or any other method already used in connection with setting standards for sediment, for example). This type of approach is recommended by the Environment Agency (2007).

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List of abbreviations

BAF	Bioaccumulation factor
BCF	Bioconcentration factor
BFAF	Biota-food accumulation factor
BMF	Biomagnification factor
BSAF	Biota-sediment accumulation factor
BTF	Biotransfer factor
bw	Bodyweight
CLEA	Contaminated Land Exposure Assessment
DDD	Dichlorodiphenyldichloroethane
DDE	Dichlorodiphenyldichloroethylene
DDT	Dichlorodiphenyltrichloroethane
DDT - Total	Total DDT compounds. Includes all isomers of DDT, DDD (Dichlorodiphenyldichloroethane) and DDE (Dichlorodiphenyldichloroethylene)
Defra	Department for Environment, Food and Rural Affairs
DOC	Dissolved organic carbon
ERA	Ecological risk assessment framework
EU	European Union
EUSES	European Uniform System for Evaluation of Substances
HCH	Hexachlorocyclohexane. Also known as lindane.
K_{aw}	Air-water partition coefficient (also known as dimensionless Henry's Law constant; log K_{aw} = logarithmic value).
K_{oc}	Organic carbon-water partition coefficient (log K_{oc} = logarithmic value)
K_{oa}	Octanol-air partition coefficient (log K_{oa} = logarithmic value)
K_{ow}	Octanol-water partition coefficient (log K_{ow} = logarithmic value) – also known as log K_{ow}
Kp_{soil}	Solids-water partition coefficient for soil (units of l kg^{-1})
$K_{soil\text{-}water}$	Bulk soil-water partition coefficient for wet soil (units of m^3 m^{-3})
MW	Molecular weight
NOAEL	No observed adverse effect level
NOEC	No observed effect concentration
PCB	Polychlorinated biphenyl
ΣPCB	Total PCBs as defined by the International Council for the Exploration of the Sea. These are the congeners PCB 28, PCB 52, PCB 101, PCB 118, PCB

	138, PCB 153 and PCB 180.
PEC	Predicted environmental concentration
POC	Particulate organic carbon
QSAR	Quantitative structure-activity relationship
R^2	Correlation coefficient
wet wt.	Wet weight basis.

Glossary

Adapted from the US Environmental Protection Agency (USEPA, 2000).

Allometric	Relative growth of a part of an organism in relation to the growth of the whole.
Benthic	Referring to organisms living close to the bottom of an ocean, sea, lake or other water body.
Bioaccumulation	The net accumulation of a substance by an organism as a result of uptake from all environmental sources.
Bioaccumulation factor	The ratio of the concentration of a substance in tissue to its concentration in ambient water (or other media). The concentration in the organism can be expressed on a wet or fresh weight basis (BAF = concentration in organism (mg/kg wet weight)/concentration in water (mg/l)) or on a lipid weight basis (BAF = concentration in organism mg/kg lipid/concentration in water (mg/l)). The concentration in water would normally refer to the dissolved concentration, but it is also possible to define BAF on the basis of the total concentration, depending on the system being considered.
Bioconcentration	The net accumulation of a substance by an aquatic organism as a result of uptake directly from the ambient water, through gill membranes or other external body surfaces.
Bioconcentration factor	The ratio of the concentration of a substance in tissue of an aquatic organism to its concentration in the ambient water. It can be expressed in terms of a wet or fresh weight concentration in fish (BCF = concentration in fish (mg/kg wet weight)/concentration in water (mg/l)), or a lipid weight concentration in fish (BCF_{lipid} = concentration in fish (mg/kg lipid)/concentration in water (mg/l)). The concentration in water usually refers to the dissolved concentration.
Biomagnification	The increase in tissue concentration of a chemical in organisms at successive trophic levels through a series of predator-prey associations.
Biomagnification factor	The ratio of the tissue concentration of a chemical in a predator at a particular trophic level to the tissue concentration in its prey at the next lower trophic level for a given water body and chemical exposure. BMF can be expressed in terms of concentrations on a wet or fresh weight basis (BMF = concentration in organism at trophic level x (mg/kg wet weight)/concentration in organism at trophic level y

	(mg/kg wet weight); where x>y) or on a lipid weight basis (BMF_{lipid} = concentration in organism at trophic level x (mg/kg lipid)/concentration in organism at trophic level y (mg/kg lipid)).
Biota-sediment accumulation factor	The ratio of the concentration of a substance in tissue of an aquatic organism to its concentration in surface sediment. The concentrations in the organisms can be expressed on either a fresh weight or lipid weight basis, whereas the concentrations in sediment are normally expressed on a dry weight or organic carbon normalized basis (although wet weight can also be used). The most common types of BSAF are BSAF = concentration in organism (mg/kg wet weight)/concentration in sediment (mg/kg dry weight) and $BSAF_{lipid}$ = concentration in organism (mg/kg lipid)/concentration in sediment (mg/kg organic carbon).
Depuration	The loss of a substance from an organism as a result of any active or passive process.
Hydrophilic	A term that refers to the extent to which a chemical is attracted to partitioning into the water phase. Hydrophilic chemicals have a greater tendency to partition into polar phases (such as water) compared to hydrophobic chemicals
Hydrophobic	A term that refers to the extent to which a chemical avoids partitioning into the water phase. Highly hydrophobic chemicals have a greater tendency to partition into nonpolar phases (lipid, organic carbon) compared with chemicals of lower hydrophobicity.
Lipid-normalized concentration	The total concentration of a contaminant in tissue or whole organism, divided by the lipid fraction in that tissue, organism or media.
Octanol-water partition coefficient	The ratio of the concentration of a substance in the n-octanol phase to its concentration in the aqueous phase in an equilibrated two-phase octanol-water system. The value is often expressed as a base 10 logarithm value (log K_{ow}).
Organic-carbon normalized concentration	For sediments, the total concentration of a contaminant in sediment divided by the fraction of organic carbon in the sediment.
Pelagic	Referring to organisms living near to the surface in oceans, lakes and so on.
Phytoplankton	Vegetable plankton.
Piscivorous	Fish-eating.
Planktivorous	Feeding on plankton.
Uptake	The acquisition by an organism of a substance from the environment as a result of any active or passive process

Zooplankton	Animal plankton

Appendix A – Main features of the AQUAWEB v1.1 model

The AQUAWEB v1.1 model became available during the course of this work. The model is a development of the Food Chain Bioaccumulation model v1.1 (this food web model is also included in the ECOFATE model) and details of the modifications made are reported in Arnot and Gobas (2004). AQUAWEB v1.1 is available as a spreadsheet model. The same spreadsheet also contains a version of the Food Chain Bioaccumulation model called BIO v1.1.

The four main changes made to the model are as follows, based on insights gained from more recent laboratory experiments, analysis of field data and improvements in the data available for model parameterization:

- A new model for the partitioning of chemicals into organisms. This now takes into account partitioning into both lipid and non-lipid organic matter (such as proteins and carbohydrates) within the organism. The Food Chain Bioaccumulation model v1.1 only considered partitioning into lipid. In addition, the AQUAWEB v1.1 model takes into account partitioning to both particulate organic carbon and dissolved organic carbon in the water phase, whereas only the former appears to have been included in the Food Chain Bioaccumulation model v1.1. AQUAWEB v1.1 also takes into account the fact that organisms in close contact with bottom sediments can be exposed to higher concentrations of the chemical in pore water than from the overlying water.
- A new kinetic model for predicting concentrations in phytoplankton. The model is based on a water-organic carbon two phase-resistance model. In addition, kinetic models are also included for zooplankton and invertebrates. The Food Chain Bioaccumulation model v1.1 essentially used an equilibrium partitioning approach between the water phase and the lipid phase of the phytoplankton, zooplankton and invertebrates.
- New allometric relationships for predicting gill and skin ventilation rates in a wide range of aquatic species.
- A new mechanistic model for predicting the gastrointestinal magnification of organic chemicals. The Food Web Bioaccumulation model v1.1 used a constant gastrointestinal magnification factor for all species.

The basic assumption in the AQUAWEB model is similar to that used in the Food Chain Bioaccumulation model, in that the exchange of non-ionic chemicals between an organism and its ambient environment can be described by a single equation as follows.

$$\frac{dM_B}{dt} = \left\{W_B \times \left(k_1 \times \left[m_O \times \Phi \times C_{WTO} + m_P \times C_{WD,S}\right] + k_D \times \sum\left(P_i \times C_{D,i}\right)\right\} - \left(k_2 + k_E + k_G + k_M\right) \times M_B$$

where M_B = the mass of the chemical in the organism (g).

dM_B/dt = the net flux of chemical adsorbed or depurated by the organism at any point in time (t; days).

W_B = weight of organism at time t (kg).

k_1 = rate constant for uptake via the respiratory area (such as gills and/or skin) (l kg^{-1} day^{-1}).

m_O = fraction of the respiratory ventilation that involves overlying water.

m_P = fraction of the respiratory ventilation that involves sediment-associated pore water.

Φ = fraction of the total chemical concentration in the overlying water that is freely dissolved and can be absorbed via membrane diffusion.

$C_{WT,O}$ = total concentration of the chemical in the water column above the sediment (g l^{-1}).

$C_{WD,S}$ = freely dissolved chemical concentration in the sediment-associated pore water (g l^{-1}).

k_D = rate constant for chemical uptake via ingestion of food and water (kg kg^{-1} day^{-1}).

P_i = fraction of diet consisting of prey item i.

$C_{D,\ i}$ = concentration of chemical in prey item i (g kg^{-1}).

k_2 = rate constant for chemical elimination via the respiratory area (day^{-1}).

k_E = rate constant for chemical elimination via excretion into egested faeces (day^{-1}).

k_G = rate constant for growth dilution (day^{-1}).

k_M = rate constant for metabolic transformation of the chemical (day^{-1}).

The steady-state solution to this equation allows the chemical concentration in the organism C_B (g kg^{-1} wet weight) to be calculated as follows.

$$C_B = \frac{\left\{k_1 \times (m_O \times \Phi \times C_{WT,O} + m_P \times C_{WD,S}) + k_D \times \sum \left\{P_i \times C_{D,i}\right\}\right\}}{(k_2 + k_E + k_G + k_M)}$$

In terms of the input data needed to run the AQUAWEB model compared with the Food Chain Bioaccumulation model, only a relatively limited amount of data are required. These are mainly as follows.

- Phytoplankton – one species can be included in the model. Default values are given.
    - non-lipid carbon content.
    - water content.
    - growth rate constant.
- Zooplankton – one species can be included in the model. Default values are given.

- wet weight of organism.
- lipid content.
- fraction pore water ventilated.
- composition of diet.

- Invertebrates – a total of five species can be included (two filter feeders and three detrivores/scavengers). Default values are given for two filter feeders (zebra mussel and caddis fly larvae) and three detrivores/scavengers (may fly, gammarus and crayfish).
  - wet weight of organism.
  - lipid content.
  - fraction pore water ventilated.
  - composition of diet.
- Fish – a total of fourteen species can be included in the model. Default values are given for yoy, emerald shiner, alewife, trout-perch, small white sucker, black crappie, white perch, yellow perch, adult white sucker, freshwater drum, gizzard shad, small mouth bass, large mouth bass and walleye.
  - wet weight of organism.
  - lipid content.
  - fraction pore water ventilated.
  - composition of diet.
- Environmental properties – typical values are given for Western Lake Erie.
  - mean water temperature.
  - dissolved organic carbon content of water body.
  - particulate organic carbon content of water body.
  - concentration of suspended solids in water body.
  - sediment organic carbon content.
- Chemical-specific properties.
  - molecular weight.
  - Henry's law constant.
  - log K_{ow}.
  - total concentration in water (ng l^{-1}).
  - sediment concentration (ng g^{-1} dry weight).
  - metabolic transformation rate constant in phytoplankton, zooplankton, invertebrates and fish (day^{-1}). A value of zero is used if the substance is not metabolized.

Arnot and Gobas (2004) carried out an extensive comparison of the performance of the AQUAWEB v1.1 model against the BIO v1.1 model using measured data sets from Lake Ontario, Lake Erie and Lake St. Claire in North America. In total, actual bioaccumulation factors were available for 59 chemicals in eight species from Lake Ontario (total number of data points 408), 25 chemicals in 20 species from Lake Erie (total number of data points 483) and six chemicals in 22 species from Lake St. Clare (total number of data points 128).

Both models were used to predict BAFs for the species present in each lake, and the predictions were compared with the actual bioaccumulation factors. The performance of the models was determined in terms of the overall modal bias (MB), which was effectively the geometric mean of the ratio of predicted and observed chemicals in all species for which actual data were available. A MB of greater than one indicates a systematic overprediction (for example, a MB of two indicates that the model generally overpredicts the actual BAF by a factor of two). Whereas an MB less than one indicates a systematic underprediction (for example, a MB of 0.5 indicates that the model generally underpredicts the actual BAF by a factor of two). For the analysis, a total of six sequential scenarios were run, where each scenario investigated the effect of one particular model modification compared to base line predictions from the BIO v1.1 model. A summary of the results of this analysis is given in Table A1. This type of analysis represents all sources of error, including the natural, spatial and temporal variability in the actual BAFs derived from field data, as well as errors in the model structure, parameterization and so on.

Table A1 Results of model evaluation carried out by Arnot and Gobas (2004)

Step-wise modification	**Model bias (MB)**					
	Lake Ontario		**Lake Erie**		**Lake St. Clair**	
	Original	**Revised**	**Original**	**Revised**	**Original**	**Revised**
Kinetic model applied to phytoplankton	**0.15**	**1.20**	**0.12**	**0.72**	**No data**	**No data**
Bioaccumulation model applied to zooplankton	No data	No data	No data	No data	0.42	1.17
Bioaccumulation model applied to invertebrates	1.95	1.04	0.3	1.13	0.37	0.92
Organism composition model (lipids and non-lipids) applied to fish	0.45	0.47	0.34	0.45	0.25	0.37
Allometric gill ventilation rate applied to fish		0.52		0.48		0.40
Diet digestion model applied to fish		1.00		1.05		0.71
Overall model comparison (all species)	0.86	1.04[a]	0.16	1.05[b]	0.17	0.78[c]

a) 95% confidence interval for the overall model bias was 0.13-8.08.

b) 95% confidence interval for the overall model bias was 0.24-4.64.

c) 95% confidence interval for the overall model bias was 0.08-7.89.

For phytoplankton, the AQUAWEB v1.1 model was found to improve the predicted BAF compared with the BIO v1.1 model. Around 65% (out of a total number of 65) of the model predictions were found to be within a factor of two of the observed BAFs, and 88% were found to be within a factor of 10 of the observed BAF (the equivalent figures for the original model were 6% and 43% within a factor of two and 10 of the observed). The improvements to the predictivity made in AQUAWEB v1.1 were thought to result mainly from the new model predicting higher BAFs at low log K_{ow} values than the original model (as a result of inclusion of non-lipid organic carbon in the model), and calculating lower BAFs at high log

K_{ow} values than the original model (as a result of including phytoplankton growth in the model).

For zooplankton, only a relatively small data set was available but this again showed an improvement in predictivity for the AQUAWEB v1.1 model compared with the BIO v1.1 model. This improvement was thought to result from the inclusion of dietary magnification in the new model (the original model only considered equilibrium partitioning into the organism from water).

For aquatic invertebrates, improvements were again seen in the predictivity of AQUAWEB 1.1 compared with the original model. These improvements were thought to result from the inclusion of a kinetic bioaccumulation model rather than the equilibrium partitioning model used previously. The majority of model predictions with AQUAWEB v1.1 for both filter feeders and detritus feeders were within a factor of two of the observed BAFs, with 60% and 90% of the predicted BAFs for nine species and 64 chemicals (total number of data points was 324) being found to be within a factor of two and 10 respectively of the actual BAFs (the equivalent statistics for the original model were 37% of predictions within a factor of two and 89% of predictions within a factor of 10 of the observed BAF).

For fish, the AQUAWEB v1.1 model was found to give a higher predictivity than the BIO v1.1 model. Of the modifications made to the fish accumulation part of the model, the inclusion of a mechanistic gastrointestinal magnification model into the overall model resulted in the largest improvements to the predictivity of the model.

Overall, Arnot and Gobas (2004) concluded that revisions in the AQUAWEB v1.1 model produced improvements in the model accuracy over the BIO v1.1 model. The model was recommended for use with chemicals with a log K_{ow} from one to around nine.

Appendix B – Mersey data set

This appendix presents the data which form the Mersey data set and the results of the testing of the ECOFATE/AQUAWEB models against the data.

B1. Data

The Mersey data set was taken from Environment Agency (1998) (sediment levels) and NRA (1994) (biota levels). The chemicals in the data set are summarised in

Table B1. The levels measured in the sediment are summarised in Table B2 and the levels in the various biota samples are summarised in Table B3.

Table B1 Chemicals in the Mersey data set

Name	Physico-chemical properties		Comment/Reference
1,2,4,5-Tetrachloro benzene	Molecular weight (g mol^{-1})	216	Mackay et al. (1992)
	Solubility at 25°C (mg l^{-1})	1.3	
	Vapour pressure at 25°C (Pa)[a]	9.6	
	Log K_{ow}	4.5	
1,2,4-Trichlorobenzene	Molecular weight (g mol^{-1})	182	Mackay et al. (1992)
	Solubility at 25°C (mg l^{-1})	41	
	Vapour pressure at 25°C (Pa)[a]	61	
	Log K_{ow}	4.1	
1,4-Dichlorobenzene	Molecular weight (g mol^{-1})	157	Mackay et al. (1992)
	Solubility at 25°C (mg l^{-1})	83	
	Vapour pressure at 25°C (Pa)[a]	170	
	Log K_{ow}	3.4	
Aldrin	Molecular weight (g mol^{-1})	365	
	Solubility at 25°C (mg l^{-1})	0.010	Verschueren (1983)
	Vapour pressure at 25°C (Pa)	8.6×10^{-3}	Value at 20°C - Richardson and Gangolli (1992)
	Log K_{ow}	6.5	HSDB (2006)
α- and γ-Hexachlorocyclohexane (HCH)	Molecular weight (g mol^{-1})	291	
	Solubility at 25°C (mg l^{-1})	17	Verschueren (1983)
	Vapour pressure at 25°C (Pa)	1.3×10^{-3}	Worthing (1979)
	Log K_{ow}	3.7	Values related mainly to γ-HCH - WHO (1991)
β-HCH	Molecular weight (g mol^{-1})	291	Assumed to be the same as for γ-HCH
	Solubility at 25°C (mg l^{-1})	17	
	Vapour pressure at 25°C (Pa)	1.3×10^{-3}	
	Log K_{ow}	3.7	
cis-Chlordane	Molecular weight (g mol^{-1})	410	
	Solubility at 25°C (mg l^{-1})	0.056	Value for "chlordane" - HSDB (2006)
	Vapour pressure at 25°C (Pa)	1.3×10^{-3}	Worthing (1979)
	Log K_{ow}	6.16	Value for "chlordane" - HSDB (2006)
trans-Chlordane	Molecular weight (g mol^{-1})	410	Assumed to be the same as for cis-chlordane
	Solubility at 25°C (mg l^{-1})	0.056	
	Vapour pressure at 25°C (Pa)	1.3×10^{-3}	
	Log K_{ow}	6.16	
DDT – Total (refers to the sum of all isomers of DDT, DDD and DDE)	Molecular weight (g mol^{-1})	355	Values for DDT were used
	Solubility at 25°C (mg l^{-1})	3.4×10^{-3}	Verschueren (1983)
	Vapour pressure at 25°C (Pa)	2.5×10^{-5}	Value at 20°C - Verschueren (1983)

Name	Physico-chemical properties		Comment/Reference
	Log K_{ow}	6.19	Verschueren (1983)
Dieldrin	Molecular weight (g mol^{-1})	381	
	Solubility at 25°C (mg l^{-1})	0.10	Verschueren (1983)
	Vapour pressure at 25°C (Pa)	2.4×10^{-5}	Verschueren (1983)
	Log K_{ow}	5.4	HSDB (2006)
Endrin	Molecular weight (g mol^{-1})	381	
	Solubility at 25°C (mg l^{-1})	0.23	WHO (1992)
	Vapour pressure at 25°C (Pa)	2.7×10^{-5}	Verschueren (1983)
	Log K_{ow}	5.6	Verschueren (1983)
Heptachlor	Molecular weight (g mol^{-1})	373	
	Solubility at 25°C (mg l^{-1})	0.056	Worthing (1979)
	Vapour pressure at 25°C (Pa)	0.040	Verschueren (1983)
	Log K_{ow}	6.1	HSDB (2006)
Hexachlorobenzene	Molecular weight (g mol^{-1})	285	Mackay et al. (1992)
	Solubility at 25°C (mg l^{-1})	5.0×10^{-3}	
	Vapour pressure at 25°C (Pa)[a]	0.25	
	Log K_{ow}	5.5	
Hexachlorobutadiene	Molecular weight (g mol^{-1})	261	Mackay et al. (1993)
	Solubility at 25°C (mg l^{-1})	3.2	
	Vapour pressure at 25°C (Pa)[a]	20	
	Log K_{ow}	4.7	
Isodrin	Molecular weight (g mol^{-1})	365	
	Solubility at 25°C (mg l^{-1})		
	Vapour pressure at 25°C (Pa)	8.0×10^{-4}	Temperature unclear - HSDB (2006)
	Log K_{ow}	6.5	Value for aldrin - HSDB (2006)
Methoxychlor	Molecular weight (g mol^{-1})	346	
	Solubility at 25°C (mg l^{-1})	0.040	Verschueren (1983)
	Vapour pressure at 25°C (Pa)		
	Log K_{ow}	5.08	HSDB (2006)
Mirex	Molecular weight (g mol^{-1})	546	
	Solubility at 25°C (mg l^{-1})	0.20	Verschueren (1983)
	Vapour pressure at 25°C (Pa)	4.0×10^{-5}	WHO (1984)
	Log K_{ow}	5.28	HSDB (2006)
Oxychlordane	Molecular weight (g mol^{-1})	424	Values estimated using the EPIWIN version 3.12 (USEPA, 2000)
	Solubility at 25°C (mg l^{-1})	0.014	
	Vapour pressure at 25°C (Pa)	9.3×10^{-4}	
	Log K_{ow}	5.48	
PCB 28	Molecular weight (g mol^{-1})	258	Mackay et al. (1992)
	Solubility at 25°C (mg l^{-1})	0.16	
	Vapour pressure at 25°C (Pa)[a]	0.026	
	Log K_{ow}	5.8	
PCB 52	Molecular weight (g mol^{-1})	292	Mackay et al. (1992)
	Solubility at 25°C (mg l^{-1})	0.030	
	Vapour pressure at 25°C (Pa)[a]	2.0×10^{-3}	
	Log K_{ow}	6.1	
PCB 101	Molecular weight (g mol^{-1})	326	Mackay et al. (1992)
	Solubility at 25°C (mg l^{-1})	0.010	
	Vapour pressure at 25°C (Pa)[a]	3.5×10^{-3}	
	Log K_{ow}	6.4	
PCB 138	Molecular weight (g mol^{-1})	361	Mackay et al. (1992)
	Solubility at 25°C (mg l^{-1})	1.5×10^{-3}	
	Vapour pressure at 25°C (Pa)[a]	5.0×10^{-4}	
	Log K_{ow}	6.7	
PCB 153	Molecular weight (g mol^{-1})	361	Mackay et al. (1992)
	Solubility at 25°C (mg l^{-1})	1.0×10^{-3}	
	Vapour pressure at 25°C (Pa)[a]	7.0×10^{-4}	
	Log K_{ow}	6.9	
PCB 180	Molecular weight (g mol^{-1})	395	Mackay et al. (1992)
	Solubility at 25°C (mg l^{-1})	3.1×10^{-4}	
	Vapour pressure at 25°C (Pa)[a]	1.3×10^{-4}	

Name	Physico-chemical properties		Comment/Reference
	Log K_{ow}	7.2	
ΣPCB - ICES	Molecular weight (g mol^{-1})	292	Average of the values for the six PCB congeners included (PCB 28, PCB 52, PCB 101, PCB 138, PCB 153 and PCB 180)
	Solubility at 25°C (mg l^{-1})	0.030	
	Vapour pressure at 25°C (Pa)[a]	2×10^{-3}	
	Log K_{ow}	6.5	

a) Values for the vapour pressure from Mackay et al. (1992 and 1993) all refer to the vapour pressure for the sub-cooled liquid. The basis for the vapour pressures from the other sources (solid or sub-cooled liquid) is not clear.

Table B2 Levels of selected chemicals in sediment from the Mersey estuary

Chemical	Measured sediment levels (µg kg^{-1} dry weight)			Estimated K_{OC}[a] ($l\ kg^{-1}$)	Estimated dissolved concentration[b] (µg l^{-1})
	Upper estuary	Inner estuary	Value assumed for modelling		
1,2,4,5-Tetrachlorobenzene	no data	no data	no data	5,559	no data
1,2,4-Trichlorobenzene	no data	no data	no data	2,636	no data
1,4-Dichlorobenzene	no data	no data	no data	715	no data
Aldrin	<0.1	no data	<0.1	231,739	$<4.3\times10^{-5}$
α- and γ-HCH	no data	0.4	0.4	1,250	0.031
β-HCH	1.5	1.0	1.0	1,250	0.078
cis-Chlordane	no data	no data	no data	122,914	no data
trans-Chlordane	no data	no data	no data	122,914	no data
DDT - Total	30	28	28	129,987	0.022
Dieldrin	<0.1	no data	<0.1	29,785	$<3.4\times10^{-4}$
Endrin	no data	no data	no data	43,251	no data
Heptachlor	1.5	no data	1.5	109,901	1.4×10^{-3}
Hexachlorobenzene	no data	no data	no data	35,892	no data
Hexachlorobutadiene	no data	no data	no data	8,072	no data
Isodrin	no data	no data	no data	231,739	no data
Methoxychlor	no data	no data	no data	16,398	no data
Mirex	no data	no data	no data	23,812	no data
Oxychlordane	no data	no data	no data	34,578	no data
PCB 28	2	no data	2	62,806	3.2×10^{-3}
PCB 52	5	no data	5	109,901	4.6×10^{-3}
PCB 101	5	no data	5	192,309	2.6×10^{-3}
PCB 138	6	no data	6	336,512	1.8×10^{-3}
PCB 153	5	no data	5	488,652	1.0×10^{-3}
PCB 180	3	no data	3	855,067	3.5×10^{-4}
ΣPCB - ICES	30	21	21	239,056	8.8×10^{-3}

a) K_{oc} was estimated using the methods in the TGD. The equation for predominantly hydrophobic chemicals was used.

b) The dissolved water concentration was estimated using the equilibrium partitioning method outlined in the TGD.

Table B3 Measured levels in biota from the Mersey estuary

Chemical	Species	Location		Concentration (µg kg^{-1})				Lipid content
		Name	Designation	Wet weight		Lipid		%
				Mean	Standard deviation	Mean	Standard deviation	
1,2,4,5-Tetrachlorobenzene	Blue mussel	New Ferry	Inner estuary	0.4		40		1.0
	Dover sole	Garston	Inner estuary	0.17		25		0.7
	Flounder	Gt. Burbo Bank	Outer estuary	0.19		35		0.5
	Hermit crab	Gt. Burbo Bank	Outer estuary	1.7		30		5.7
	Plaice	Rock Channel	Narrows/outer estuary	0.7		95		0.7
	Plaice	Gt. Burbo Bank	Outer estuary	0.19		60		0.3
	Plaice - species mean			0.45	0.26	78	18	0.5
	Shrimp	New Ferry	Inner estuary	0.5		80		0.6
	Whelk	Gt. Burbo Bank	Outer estuary	0.3		10		3.0
1,2,4-Trichlorobenzene	Blue mussel	New Ferry	Inner estuary	1.1	0.4	120	49	0.9
	Dover sole	Eastham	Inner estuary	0.4	0.1	165	450	0.2
	Plaice	Eastham	Inner estuary	0.4	0.8	31	54	1.3
	Shrimp	New Ferry	Inner estuary	4.8	4	760	705	0.6
1,4-Dichlorobenzene	Blue mussel	New Ferry	Inner estuary	23.3	8.4	2,520	913	0.9
	Cod	Rock Channel	Narrows/outer estuary	<0.1				
	Dab	Rock Channel	Narrows/outer estuary	13		2,642		0.5

Chemical	Species	Location		Concentration (µg kg^{-1})				Lipid content
		Name	Designation	Wet weight		Lipid		%
				Mean	Standard deviation	Mean	Standard deviation	
1,4-Dichlorobenzene (cont.)	Dab	Gt. Burbo Bank	Outer estuary	75		7,870		1.0
	Dab – species mean			44	31	5,256	2,614	0.8
	Dover Sole	Eastham	Inner estuary	3		990		0.3
	Dover Sole	Garston	Inner estuary	14		3,965		0.4
	Dover Sole	Gt. Burbo Bank	Outer estuary	30		8,170		0.4
	Dover sole – species mean			16	11	4,375	2,946	0.4
	Flounder	Gt. Burbo Bank	Outer estuary	7		1,940		0.4
	Hermit crab	Gt. Burbo Bank	Outer estuary	71.8	69	1,100	940	6.5
	Plaice	Eastham	Inner estuary	1		1,480		0.1
	Plaice	Garston	Inner estuary	3		760		0.4
	Plaice	Rock Channel	Narrows/outer estuary	15		2,248		0.7
	Plaice	Gt. Burbo Bank	Outer estuary	3		681		0.4
	Plaice – species mean			7	5.7	1,230	721	0.5
	Shrimp	New Ferry	Inner estuary	42	44	6,530	7,218	0.6
	Whelk	Gt. Burbo Bank	Outer estuary	<0.1				
	Whiting	Rock Channel	Narrows/outer estuary	41.9	28	20,463	14,630	0.2
	Whiting	Gt. Burbo Bank	Outer estuary	39.2	24.4			

Chemical	Species	Location		Concentration (µg kg^{-1})				Lipid content
		Name	Designation	Wet weight		Lipid		%
				Mean	Standard deviation	Mean	Standard deviation	
1,4-Dichlorobenzene (cont.)	Whiting – species mean			40.6	1.4			
Aldrin	Blue mussel	New Ferry	Inner estuary	<0.1				
	Cod	Rock Channel	Narrows/outer estuary	<0.1				
	Cod	Rock Channel	Narrows/outer estuary	<0.1				
	Cod – species mean			<0.1				
	Dab	Gt. Burbo Bank	Inner estuary	<0.1				
	Dab	Gt. Burbo Bank	Inner estuary	<0.1				
	Dab	Gt. Burbo Bank	Inner estuary	<0.1				
	Dab	Rock Channel	Narrows/outer estuary	<0.1				
	Dab	Gt. Burbo Bank	Outer estuary	<0.1				
	Dab – species mean			<0.1				
	Dover sole	Eastham	Inner estuary	<0.1				
	Dover sole	Garston	Inner estuary	<0.1				
	Dover sole	Garston	Inner estuary	<0.1				
	Dover sole	Gt. Burbo Bank	Outer estuary	<0.1				
	Dover sole	Gt. Burbo Bank	Outer estuary	<0.1				
	Dover sole – species mean			<0.1				

Chemical	Species	Location		Concentration (µg kg^{-1})				Lipid content
		Name	Designation	Wet weight		Lipid		%
				Mean	Standard deviation	Mean	Standard deviation	
Aldrin (cont.)	Flounder	Garston	Inner estuary	<0.1				
	Flounder	Rock Channel	Narrows/outer estuary	<0.1				
	Flounder	Gt. Burbo Bank	Outer estuary	<0.1				
	Flounder	Gt. Burbo Bank	Outer estuary	<0.1				
	Flounder	Gt. Burbo Bank	Outer estuary	<0.1				
	Flounder – species mean			<0.1				
	Hermit crab	Gt. Burbo Bank	Outer estuary	<0.1				
	Plaice	Eastham	Inner estuary	<0.1				
	Plaice	Garston	Inner estuary	<0.1				
	Plaice	Garston	Inner estuary	<0.1				
	Plaice	Rock Channel	Narrows/outer estuary	<0.1				
	Plaice	Rock Channel	Narrows/outer estuary	<0.1				
	Plaice	Rock Channel	Narrows/outer estuary	<0.1				
	Plaice	Gt. Burbo Bank	Outer estuary	<0.1				
	Plaice	Gt. Burbo Bank	Outer estuary	<0.1				
	Plaice	Gt. Burbo Bank	Outer estuary	<0.1				
	Plaice	Gt. Burbo Bank	Outer estuary	<0.1				

Chemical	Species	Location		Concentration (µg kg^{-1})				Lipid content
		Name	Designation	Wet weight		Lipid		%
				Mean	Standard deviation	Mean	Standard deviation	
Aldrin (cont.)	Plaice – species mean			<0.1				
	Shrimp	New Ferry	Inner estuary	<0.1				
	Starfish	Gt. Burbo Bank	Outer estuary	<0.1				
	Whelk	Gt. Burbo Bank	Outer estuary	<0.1				
	Whiting	Eastham	Inner estuary	<0.1				
	Whiting	Eastham	Inner estuary	<0.1				
	Whiting	Garston	Inner estuary	<0.1				
	Whiting	Garston	Inner estuary	<0.1				
	Whiting	Rock Channel	Narrows/outer estuary	<0.1				
	Whiting	Rock Channel	Narrows/outer estuary	<0.1				
	Whiting	Gt. Burbo Bank	Outer estuary	<0.1				
	Whiting – species mean			<0.1				
α- and γ-HCH	Blue mussel	New Ferry	Inner estuary	2.7		300		0.9
	Cod	Rock Channel	Narrows/outer estuary	0.2	0.2	102	88	0.2
	Cod	Rock Channel	Narrows/outer estuary	0.7	0.4	327	233	0.2
	Cod – species mean			0.5	0.3	215	113	0.2
	Dab	Rock Channel	Narrows/outer estuary	4.0	1.0	418	248	1.0

Chemical	Species	Location		Concentration (µg kg^{-1})				Lipid content
		Name	Designation	Wet weight		Lipid		%
				Mean	Standard deviation	Mean	Standard deviation	
α- and γ-HCH (cont.)	Dab	Gt. Burbo Bank	Outer estuary	0.5	0.1	62	9	0.8
	Dab	Gt. Burbo Bank	Outer estuary	2.4	0.6	207	41	1.2
	Dab	Gt. Burbo Bank	Outer estuary	0.7	0.2	89	19	0.8
	Dab	Gt. Burbo Bank	Outer estuary	2.2	0.3	180	30	1.2
	Dab – species mean			2.0	1.3	191	126	1.0
	Dover sole	Eastham	Inner estuary	2.0	0.6	1,055	528	0.2
	Dover sole	Garston	Inner estuary	1.9	0.2	510	83	0.4
	Dover sole	Garston	Inner estuary	2.1	0.5	810	588	0.3
	Dover sole	Gt. Burbo Bank	Outer estuary	0.7	0.2	180	50	0.4
	Dover sole	Gt. Burbo Bank	Outer estuary	0.9	0.3	220	31	0.4
	Dover sole – species mean			1.5	0.6	555	338	0.3
	Flounder	Garston	Inner estuary	4.6	0.8	522	224	0.9
	Flounder	Rock Channel	Narrows/outer estuary	0.8	0.2	320	165	0.3
	Flounder	Gt. Burbo Bank	Outer estuary	1.0	0.4	180	51	0.6
	Flounder	Gt. Burbo Bank	Outer estuary	1.3	0.5	280	167	0.5
	Flounder	Gt. Burbo Bank	Outer estuary	0.5	0.2	180	46	0.3
	Flounder – species mean			1.6	1.5	296	126	0.5

Chemical	Species	Location		Concentration (µg kg^{-1})				Lipid content
		Name	Designation	Wet weight		Lipid		%
				Mean	Standard deviation	Mean	Standard deviation	
α- and γ-HCH (cont.)	Hermit crab	Gt. Burbo Bank	Outer estuary	2.8		60		4.7
	Plaice	Eastham	Inner estuary	3.6	0.8	336	88	1.1
	Plaice	Garston	Inner estuary	1.5	0.5	261	43	0.6
	Plaice	Garston	Inner estuary	1.2	0.3	292	113	0.4
	Plaice	Rock Channel	Narrows/outer estuary	1.8	0.2	102	88	1.8
	Plaice	Rock Channel	Narrows/outer estuary	1.8	0.2	310	48	0.6
	Plaice	Rock Channel	Narrows/outer estuary	2.4	0.8	320	113	0.8
	Plaice	Rock Channel	Narrows/outer estuary	1.2	0.2	210	37	0.6
	Plaice	Gt. Burbo Bank	Outer estuary	0.5	0.3	126	27	0.4
	Plaice	Gt. Burbo Bank	Outer estuary	0.8	0.3	160	25	0.5
	Plaice	Gt. Burbo Bank	Outer estuary	0.5	0.2	140	22	0.4
	Plaice	Gt. Burbo Bank	Outer estuary	0.8	0.1	230	28	0.3
	Plaice – species mean			1.5	0.9	226	80	0.7
	Starfish	Gt. Burbo Bank	Outer estuary	0.7		50		1.4
	Whelk	Gt. Burbo Bank	Outer estuary	1.3		100		1.3
	Whiting	Eastham	Inner estuary	2.1	0.4	637	156	0.3
	Whiting	Eastham	Inner estuary	1.3	0.3	546	108	0.2

Chemical	Species	Location		Concentration (µg kg^{-1})				Lipid content
		Name	Designation	Wet weight		Lipid		%
				Mean	Standard deviation	Mean	Standard deviation	
α- and γ-HCH (cont.)	Whiting	Garston	Inner estuary	1.6	0.3	822	307	0.2
	Whiting	Garston	Inner estuary	1.9	0.2	258	148	0.7
	Whiting	Rock Channel	Narrows/outer estuary	0.5	0.1	146	46	0.3
	Whiting	Rock Channel	Narrows/outer estuary	0.3	0.2	201	85	0.1
	Whiting	Gt. Burbo Bank	Outer estuary	0.3	0.1	97	54	0.3
	Whiting – species mean			1.1	0.7	387	259	0.3
β-HCH	Flounder	Garston	Inner estuary	360.0		79,721		0.5
cis-Chlordane	Blue mussel	New Ferry	Inner estuary	1.0	0.4	110	45	0.9
	Cod	Rock Channel	Narrows/outer estuary	<0.1				
	Cod	Rock Channel	Narrows/outer estuary	<0.1				
	Cod – species mean			<0.1				
	Dab	Rock Channel	Narrows/ outer estuary	0.3	0.4	15	20	2.0
	Dab	Gt. Burbo Bank	Outer estuary	<0.1				
	Dab	Gt. Burbo Bank	Outer estuary	0.1	0.3	9	15	1.1
	Dab	Gt. Burbo Bank	Outer estuary	<0.1				
	Dab	Gt. Burbo Bank	Outer estuary	<0.1				
	Dab – species mean			0.1[a]	0.1	12	3	1.6

Chemical	Species	Location		Concentration (µg kg^{-1})				Lipid content
		Name	Designation	Wet weight		Lipid		%
				Mean	Standard deviation	Mean	Standard deviation	
cis-Chlordane (cont.)	Dover sole	Eastham	Inner estuary	<0.1				
	Dover sole	Garston	Inner estuary	0.4	0.3	130	219	0.3
	Dover sole	Garston	Inner estuary	0.2	0.2	70	63	0.3
	Dover sole	Gt. Burbo Bank	Outer estuary	0.1	0.2	30	52	0.3
	Dover sole	Gt. Burbo Bank	Outer estuary	<0.1				
	Dover sole – species mean			0.2[a]	0.1	77	41	0.3
	Flounder	Garston	Inner estuary	0.8	0.4	195	113	0.4
	Flounder	Rock Channel	Narrows/outer estuary	0.4	0.2	90	61	0.4
	Flounder	Gt. Burbo Bank	Outer estuary	0.5	0.3	160	151	0.3
	Flounder	Gt. Burbo Bank	Outer estuary	0.4	0.9	50	64	0.8
	Flounder	Gt. Burbo Bank	Outer estuary	0.4	0.4	90	90	0.4
	Flounder – species mean			0.5	0.2	117	53	0.5
	Hermit crab	Gt. Burbo Bank	Outer estuary	3.5	5.2	70	74	5.0
	Plaice	Eastham	Inner estuary	0.1	0.2	9	15	1.1
	Plaice	Garston	Inner estuary	<0.1				
	Plaice	Garston	Inner estuary	<0.1				
	Plaice	Rock Channel	Narrows/outer estuary	0.7	0.7	95	93	0.7

Chemical	Species	Location		Concentration (µg kg^{-1})				Lipid content
		Name	Designation	Wet weight		Lipid		%
				Mean	Standard deviation	Mean	Standard deviation	
cis-Chlordane (cont.)	Plaice	Rock Channel	Narrows/outer estuary	0.7	0.4	110	65	0.6
	Plaice	Rock Channel	Narrows/outer estuary	0.2	0.2	30	25	0.7
	Plaice	Gt. Burbo Bank	Outer estuary	<0.1				
	Plaice	Gt. Burbo Bank	Outer estuary	<0.1				
	Plaice	Gt. Burbo Bank	Outer estuary	0.2	0.2	30	40	0.7
	Plaice	Gt. Burbo Bank	Outer estuary	<0.1				
	Plaice – species mean			0.2[a]	0.2	55	40	0.8
	Shrimp	New Ferry	Inner estuary	<0.1				
	Starfish	Gt. Burbo Bank	Outer estuary	<0.1				
	Whelk	Gt. Burbo Bank	Outer estuary	0.2	0.2	10	10	2.0
	Whiting	Eastham	Inner estuary	<0.1				
	Whiting	Eastham	Inner estuary	0.2	0.1	77	34	0.3
	Whiting	Garston	Inner estuary	0.1	0.1	29	16	0.3
	Whiting	Garston	Inner estuary	<0.1				
	Whiting	Rock Channel	Narrows/outer estuary	<0.1				
	Whiting	Rock Channel	Narrows/outer estuary	<0.1				
	Whiting	Gt. Burbo Bank	Outer estuary	<0.1				

Chemical	Species	Location		Concentration (µg kg^{-1})				Lipid content
		Name	Designation	Wet weight		Lipid		%
				Mean	Standard deviation	Mean	Standard deviation	
cis-Chlordane (cont.)	Whiting – species mean			0.1[a]	0.1	39	28	0.9
trans-Chlordane	Blue mussel	New Ferry	Inner estuary	1.7	0.6	180	63	0.9
	Cod	Rock Channel	Narrows/outer estuary	<0.1				
	Cod	Rock Channel	Narrows/ outer estuary	<0.1				
	Cod – species mean			<0.1				
	Dab	Rock Channel	Narrows/outer estuary	1.0	0.9	46	45	2.2
	Dab	Gt. Burbo Bank	Outer estuary	<0.1				
	Dab	Gt. Burbo Bank	Outer estuary	0.3	0.8	20	51	1.5
	Dab	Gt. Burbo Bank	Outer estuary	<0.1				
	Dab	Gt. Burbo Bank	Outer estuary	<0.1				
	Dab – species mean			0.3[a]	0.4	33	13	1.9
	Dover sole	Eastham	Inner estuary	<0.1				
	Dover sole	Garston	Inner estuary	0.3	0.3	70	81	0.4
	Dover sole	Garston	Inner estuary	0.3	0.1	70	35	0.4
	Dover sole	Gt. Burbo Bank	Outer estuary	0.1	0.1	10	28	1.0
	Dover sole	Gt. Burbo Bank	Outer estuary	0.2	0.2	50	47	0.4
	Dover sole – species mean			0.2[a]	0.1	50	24	0.6

Chemical	Species	Location		Concentration (µg kg^{-1})				Lipid content
		Name	Designation	Wet weight		Lipid		%
				Mean	Standard deviation	Mean	Standard deviation	
trans-Chlordane (cont.)	Flounder	Garston	Inner estuary	2.2	1.0	488	259	0.5
	Flounder	Rock Channel	Narrows/outer estuary	0.5	0.3	180	95	0.3
	Flounder	Gt. Burbo Bank	Outer estuary	0.2	0.2	50	38	0.4
	Flounder	Gt. Burbo Bank	Outer estuary	<0.1				
	Flounder	Gt. Burbo Bank	Outer estuary	0.6	0.4	50	38	1.2
	Flounder – species mean			0.7[a]	0.8	192	179	0.6
	Hermit crab	Gt. Burbo Bank	Outer estuary	0.5	0.5	10	13	5.0
	Plaice	Eastham	Inner estuary	1.2	0.9	109	107	1.1
	Plaice	Garston	Inner estuary	<0.1				
	Plaice	Garston	Inner estuary	<0.1				
	Plaice	Rock Channel	Narrows/outer estuary	0.2	0.3	8	15	2.4
	Plaice	Rock Channel	Narrows/outer estuary	0.4	0.2	60	16	0.7
	Plaice	Rock Channel	Narrows/outer estuary	0.5	0.3	60	16	0.8
	Plaice	Gt. Burbo Bank	Outer estuary	0.1	0.1	30	27	0.3
	Plaice	Gt. Burbo Bank	Outer estuary	0.1	0.2	15	23	0.7
	Plaice	Gt. Burbo Bank	Outer estuary	0.3	0.3	40	48	0.8
	Plaice	Gt. Burbo Bank	Outer estuary	<0.1				

Chemical	Species	Location		Concentration (µg kg^{-1})				Lipid content
		Name	Designation	Wet weight		Lipid		%
				Mean	Standard deviation	Mean	Standard deviation	
trans-Chlordane (cont.)	Plaice – species mean			0.3[a]	0.3	46	32	1.0
	Shrimp	New Ferry	Inner estuary	0.1	0.1	110	19	0.1
	Starfish	Gt. Burbo Bank	Outer estuary	0.1	0.1	10	5	1.0
	Whelk	Gt. Burbo Bank	Outer estuary	0.8	0.5	60	36	1.3
	Whiting	Eastham	Inner estuary	<0.1				
	Whiting	Eastham	Inner estuary	0.5	0.2	185	56	0.3
	Whiting	Garston	Inner estuary	0.1	0.1	29	25	0.3
	Whiting	Garston	Inner estuary	<0.1				
	Whiting	Rock Channel	Narrows/outer estuary	<0.1				
	Whiting	Rock Channel	Narrows/outer estuary	<0.1				
	Whiting	Gt. Burbo Bank	Outer estuary	<0.1				
	Whiting – species mean			0.1[a]	0.2	107	78	0.3
DDT - Total	Blue mussel	New Ferry	Inner estuary	30.0				
	Cod	Rock Channel	Narrows/outer estuary	0.5	0.2	245	212	0.2
	Cod	Rock Channel	Narrows/outer estuary	1.2	0.4	466	287	0.3
	Cod – species mean			0.9	0.4	356	110	0.3
	Dab	Rock Channel	Narrows/outer estuary	24.0	0.8	1,794	1,023	1.3

Chemical	Species	Location		Concentration (µg kg^{-1})				Lipid content
		Name	Designation	Wet weight		Lipid		%
				Mean	Standard deviation	Mean	Standard deviation	
DDT – Total (cont.)	Dab	Gt. Burbo Bank	Outer estuary	2.2	0.8	261	197	0.8
	Dab	Gt. Burbo Bank	Outer estuary	3.4	1.6	270	195	1.3
	Dab	Gt. Burbo Bank	Outer estuary	3.8	1.1	431	269	0.9
	Dab	Gt. Burbo Bank	Outer estuary	4.7	1.4	381	211	1.2
	Dab – species mean			7.7	8.2	627	587	1.1
	Dover sole	Eastham	Inner estuary	9.4	8.1	4,082	5,133	0.2
	Dover sole	Garston	Inner estuary	11.9	6.2	3,080	2,413	0.4
	Dover sole	Garston	Inner estuary	7.6	2.0	2,010	1,215	0.4
	Dover sole	Gt. Burbo Bank	Outer estuary	5.4	1.0	1,550	1,055	0.3
	Dover sole	Gt. Burbo Bank	Outer estuary	6.8	1.2	1,910	1,183	0.4
	Dover sole – species mean			8.2	2.2	2,526	930	0.3
	Flounder	Garston	Inner estuary	38.4	17.0	8,530	5,257	0.5
	Flounder	Rock Channel	Narrows/outer estuary	18.4	6.0	6,490	4,751	0.3
	Flounder	Gt. Burbo Bank	Outer estuary	23.0	14.4	3,450	2,026	0.7
	Flounder	Gt. Burbo Bank	Outer estuary	18.8	7.2	4,430	3,259	0.4
	Flounder	Gt. Burbo Bank	Outer estuary	10.6	3.3	3,000	1,977	0.4
	Flounder – species mean			21.8	9.2	5,180	2,061	0.5

Chemical	Species	Location		Concentration (µg kg^{-1})				Lipid content
		Name	Designation	Wet weight		Lipid		%
				Mean	Standard deviation	Mean	Standard deviation	
DDT – Total (cont.)	Hermit crab	Gt. Burbo Bank	Outer estuary	33.0		540		6.1
	Plaice	Eastham	Inner estuary	10.9	2.1	1,092	634	1.0
	Plaice	Garston	Inner estuary	9.3	2.0	1,635	928	0.6
	Plaice	Garston	Inner estuary	7.3	2.1	1,729	1,653	0.4
	Plaice	Rock Channel	Narrows/outer estuary	12.4	3.0	1,940	629	0.6
	Plaice	Rock Channel	Narrows/outer estuary	12.3	5.5	1,294	810	1.0
	Plaice	Rock Channel	Narrows/outer estuary	13.9	3.1	2,430	1,124	0.6
	Plaice	Gt. Burbo Bank	Outer estuary	7.8	2.1	1,725	846	0.5
	Plaice	Gt. Burbo Bank	Outer estuary	7.1	1.4	1,790	677	0.4
	Plaice	Gt. Burbo Bank	Outer estuary	9.0	3.9	1,630	803	0.6
	Plaice	Gt. Burbo Bank	Outer estuary	5.3	0.9	1,450	569	0.4
	Plaice – species mean			9.5	2.6	1,672	346	0.6
	Starfish	Gt. Burbo Bank	Outer estuary			150		
	Whelk	Gt. Burbo Bank	Outer estuary	50.4				
	Whiting	Eastham	Inner estuary	5.9	0.8	1,818	753	0.3
	Whiting	Eastham	Inner estuary	5.4	0.9	2,149	665	0.3
	Whiting	Garston	Inner estuary	3.6	0.6	1,796	535	0.2

Chemical	Species	Location		Concentration (µg kg^{-1})				Lipid content
		Name	Designation	Wet weight		Lipid		%
				Mean	Standard deviation	Mean	Standard deviation	
DDT – Total (cont.)	Whiting	Garston	Inner estuary	1.6	0.5	822	307	0.2
	Whiting	Garston	Inner estuary	5.1	0.6	1,370	487	0.4
	Whiting	Rock Channel	Narrows/outer estuary	3.2	1.1	927	755	0.3
	Whiting	Rock Channel	Narrows/outer estuary	1.0	0.3	687	357	0.1
	Whiting	Gt. Burbo Bank	Outer estuary	1.0	0.4	360	175	0.3
	Whiting – species mean			3.4	1.9	1,241	596	0.3
Dieldrin	Blue mussel	New Ferry	Inner estuary	3.0		320		0.9
	Cod	Rock Channel	Narrows/outer estuary	0.2	0.1	70	52	0.3
	Cod	Rock Channel	Narrows/outer estuary	0.5	0.3	193	102	0.3
	Cod – species mean			0.4	0.2	132	62	0.3
	Dab	Rock Channel	Narrows/outer estuary	4.5	2.9	295	142	1.5
	Dab	Gt. Burbo Bank	Outer estuary	0.8	0.2	87	18	0.9
	Dab	Gt. Burbo Bank	Outer estuary	1.6	0.7	129	36	1.2
	Dab	Gt. Burbo Bank	Outer estuary	1.0	0.3	121	22	0.8
	Dab	Gt. Burbo Bank	Outer estuary	1.6	0.5	127	31	1.3
	Dab – species mean			1.9	1.3	152	73	1.1
	Dover sole	Eastham	Inner estuary	1.6	1.5	774	987	0.2

Chemical	Species	Location		Concentration (µg kg^{-1})				Lipid content
		Name	Designation	Wet weight		Lipid		%
				Mean	Standard deviation	Mean	Standard deviation	
Dieldrin (cont.)	Dover sole	Garston	Inner estuary	2.0	1.6	590	712	0.3
	Dover sole	Garston	Inner estuary	1.4	0.4	370	119	0.4
	Dover sole	Gt. Burbo Bank	Outer estuary	0.8	0.2	220	53	0.4
	Dover sole	Gt. Burbo Bank	Outer estuary	1.0	0.4	260	148	0.4
	Dover sole – species mean			1.4	0.4	443	210	0.3
	Flounder	Garston	Inner estuary	5.3	2.1	1,146	486	0.5
	Flounder	Rock Channel	Narrows/outer estuary	1.6	0.8	500	225	0.3
	Flounder	Gt. Burbo Bank	Outer estuary	2.2	2.8	320	178	0.7
	Flounder	Gt. Burbo Bank	Outer estuary	1.7	1.0	400	250	0.4
	Flounder	Gt. Burbo Bank	Outer estuary	0.8	0.4	240	180	0.3
	Flounder – species mean			2.3	1.6	521	324	0.4
	Hermit crab	Gt. Burbo Bank	Outer estuary	12.9	6.9	250	173	5.2
	Shrimp	New Ferry	Inner estuary	0.8		120		0.7
	Starfish	Gt. Burbo Bank	Outer estuary	1.3		90		1.4
	Whelk	Gt. Burbo Bank	Outer estuary	4.7	2.4	310	104	1.5
	Whiting	Eastham	Inner estuary	1.3	0.4	406	75	0.3
	Whiting	Eastham	Inner estuary	1.0	0.4	409	96	0.2

Chemical	Species	Location		Concentration (µg kg^{-1})				Lipid content
		Name	Designation	Wet weight		Lipid		%
				Mean	Standard deviation	Mean	Standard deviation	
Dieldrin (cont.)	Whiting	Garston	Inner estuary	0.7	0.2	361	61	0.2
	Whiting	Garston	Inner estuary	1.3	0.3	348	74	0.4
	Whiting	Rock Channel	Narrows/outer estuary	0.5	0.3	147	103	0.3
	Whiting	Rock Channel	Narrows/outer estuary	0.3	0.1	234	49	0.1
	Whiting	Gt. Burbo Bank	Outer estuary	0.3	0.1	120	46	0.3
	Whiting – species mean			0.8	0.4	289	112	0.3
Endrin	Blue mussel	New Ferry	Inner estuary	<0.1				
	Cod	Rock Channel	Narrows/outer estuary	<0.1				
	Cod	Rock Channel	Narrows/outer estuary	<0.1				
	Cod – species mean			<0.1				
	Dab	Rock Channel	Narrows/outer estuary	<0.1				
	Dab	Gt. Burbo Bank	Outer estuary	<0.1				
	Dab	Gt. Burbo Bank	Outer estuary	<0.1				
	Dab	Gt. Burbo Bank	Outer estuary	<0.1				
	Dab	Gt. Burbo Bank	Outer estuary	<0.1				
	Dab – species mean			<0.1				
	Dover sole	Eastham	Inner estuary	<0.1				

Chemical	Species	Location		Concentration (µg kg^{-1})				Lipid content
		Name	Designation	Wet weight		Lipid		%
				Mean	Standard deviation	Mean	Standard deviation	
Endrin (cont.)	Dover sole	Garston	Inner estuary	<0.1				
	Dover sole	Garston	Inner estuary	<0.1				
	Dover sole	Gt. Burbo Bank	Outer estuary	<0.1				
	Dover sole	Gt. Burbo Bank	Outer estuary	<0.1				
	Dover sole – species mean			<0.1				
	Flounder	Garston	Inner estuary	<0.1				
	Flounder	Rock Channel	Narrows/outer estuary	<0.1				
	Flounder	Gt. Burbo Bank	Outer estuary	<0.1				
	Flounder	Gt. Burbo Bank	Outer estuary	<0.1				
	Flounder	Gt. Burbo Bank	Outer estuary	<0.1				
	Flounder – species mean			<0.1				
	Hermit crab	Gt. Burbo Bank	Outer estuary	0.3				
	Plaice	Eastham	Inner estuary	<0.1				
	Plaice	Garston	Inner estuary	<0.1				
	Plaice	Garston	Inner estuary	<0.1				
	Plaice	Rock Channel	Narrows/outer estuary	<0.1				
	Plaice	Rock Channel	Narrows/outer estuary	<0.1				

Chemical	Species	Location		Concentration (µg kg^{-1})				Lipid content
		Name	Designation	Wet weight		Lipid		%
				Mean	Standard deviation	Mean	Standard deviation	
Endrin (cont.)	Plaice	Rock Channel	Narrows/outer estuary	<0.1				
	Plaice	Gt. Burbo Bank	Outer estuary	<0.1				
	Plaice	Gt. Burbo Bank	Outer estuary	<0.1				
	Plaice	Gt. Burbo Bank	Outer estuary	<0.1				
	Plaice	Gt. Burbo Bank	Outer estuary	<0.1				
	Plaice – species mean			<0.1				
	Shrimp	New Ferry	Inner estuary	0.8				
	Starfish	Gt. Burbo Bank	Outer estuary	<0.1				
	Whelk	Gt. Burbo Bank	Outer estuary	0.2				
	Whiting	Eastham	Inner estuary	<0.1				
	Whiting	Eastham	Inner estuary	<0.1				
	Whiting	Garston	Inner estuary	<0.1				
	Whiting	Garston	Inner estuary	<0.1				
	Whiting	Rock Channel	Narrows/outer estuary	<0.1				
	Whiting	Rock Channel	Narrows/outer estuary	<0.1				
	Whiting	Gt. Burbo Bank	Outer estuary	<0.1				
	Whiting – species mean			<0.1				

Chemical	Species	Location		Concentration (µg kg^{-1})				Lipid content
		Name	Designation	Wet weight		Lipid		%
				Mean	Standard deviation	Mean	Standard deviation	
Heptachlor	Cod	Rock Channel	Narrows/outer estuary	<0.1				
	Cod	Rock Channel	Narrows/outer estuary	<0.1				
	Cod – species mean			<0.1				
	Dab	Rock Channel	Narrows/outer estuary	<0.1				
	Dab	Gt. Burbo Bank	Outer estuary	<0.1				
	Dab	Gt. Burbo Bank	Outer estuary	<0.1				
	Dab	Gt. Burbo Bank	Outer estuary	<0.1				
	Dab	Gt. Burbo Bank	Outer estuary	<0.1				
	Dab – species mean			<0.1				
	Dover sole	Eastham	Inner estuary	<0.1				
	Dover sole	Garston	Inner estuary	<0.1				
	Dover sole	Garston	Inner estuary	<0.1				
	Dover sole	Gt. Burbo Bank	Outer estuary	<0.1				
	Dover sole	Gt. Burbo Bank	Outer estuary	<0.1				
	Dover sole – species mean			<0.1				
	Flounder	Garston	Inner estuary	<0.1				
	Flounder	Rock Channel	Narrows/outer estuary	<0.1				

Chemical	Species	Location		Concentration (µg kg^{-1})				Lipid content
		Name	Designation	Wet weight		Lipid		%
				Mean	Standard deviation	Mean	Standard deviation	
Heptachlor (cont.)	Flounder	Gt. Burbo Bank	Outer estuary	<0.1				
	Flounder	Gt. Burbo Bank	Outer estuary	<0.1				
	Flounder	Gt. Burbo Bank	Outer estuary	<0.1				
	Flounder – species mean			<0.1				
	Plaice	Eastham	Inner estuary	<0.1				
	Plaice	Garston	Inner estuary	<0.1				
	Plaice	Garston	Inner estuary	<0.1				
	Plaice	Rock Channel	Narrows/outer estuary	<0.1				
	Plaice	Rock Channel	Narrows/outer estuary	<0.1				
	Plaice	Rock Channel	Narrows/outer estuary	<0.1				
	Plaice	Gt. Burbo Bank	Outer estuary	<0.1				
	Plaice	Gt. Burbo Bank	Outer estuary	<0.1				
	Plaice	Gt. Burbo Bank	Outer estuary	<0.1				
	Plaice	Gt. Burbo Bank	Outer estuary	<0.1				
	Plaice – species mean			<0.1				
	Whiting	Eastham	Inner estuary	<0.1				
	Whiting	Eastham	Inner estuary	<0.1				

Chemical	Species	Location		Concentration (µg kg^{-1})				Lipid content
		Name	Designation	Wet weight		Lipid		%
				Mean	Standard deviation	Mean	Standard deviation	
Heptachlor (cont.)	Whiting	Garston	Inner estuary	<0.1				
	Whiting	Garston	Inner estuary	<0.1				
	Whiting	Rock Channel	Narrows/outer estuary	<0.1				
	Whiting	Rock Channel	Narrows/outer estuary	<0.1				
	Whiting	Gt. Burbo Bank	Outer estuary	<0.1				
	Whiting – species mean			<0.1				
Hexachlorobenzene	Blue mussel	New Ferry	Inner estuary	1.1	0.4	120	42	0.9
	Cod	Rock Channel	Narrows/outer estuary	<0.1				
	Cod	Rock Channel	Narrows/outer estuary	<0.1				
	Cod – species mean			<0.1				
	Dab	Rock Channel	Narrows/outer estuary	1.1	0.9	57	44	1.9
	Dab	Gt. Burbo Bank	Outer estuary	0.2	0.1	14	6	1.4
	Dab	Gt. Burbo Bank	Outer estuary	0.1	0.1	11	7	0.9
	Dab	Gt. Burbo Bank	Outer estuary	0.1	0.1	15	9	0.7
	Dab	Gt. Burbo Bank	Outer estuary	<0.1				
	Dab – species mean			0.3[a]	0.4	24	19	1.2
	Dover sole	Eastham	Inner estuary	<0.1				

Chemical	Species	Location		Concentration (µg kg^{-1})				Lipid content
		Name	Designation	Wet weight		Lipid		%
				Mean	Standard deviation	Mean	Standard deviation	
Hexachlorobenzene (cont.)	Dover sole	Garston	Inner estuary	<0.1				
	Dover sole	Garston	Inner estuary	<0.1				
	Dover sole	Gt. Burbo Bank	Outer estuary	<0.1				
	Dover sole	Gt. Burbo Bank	Outer estuary	<0.1				
	Dover sole – species mean			<0.1				
	Flounder	Garston	Inner estuary	2.5	0.6	565	179	0.4
	Flounder	Rock Channel	Narrows/outer estuary	0.6	0.4	200	116	0.3
	Flounder	Gt. Burbo Bank	Outer estuary	0.1	0.1	40	56	0.3
	Flounder	Gt. Burbo Bank	Outer estuary	0.7	1.4	90	97	0.8
	Flounder	Gt. Burbo Bank	Outer estuary	0.6	0.6	120	105	0.5
	Flounder – species mean			0.9	0.8	203	188	0.5
	Plaice	Eastham	Inner estuary	0.3	0.2	23	17	1.3
	Plaice	Garston	Inner estuary	0.2	0.2	42	32	0.5
	Plaice	Garston	Inner estuary	0.8	0.3	182	136	0.4
	Plaice	Rock Channel	Narrows/outer estuary	0.9	0.1	58	44	1.6
	Plaice	Rock Channel	Narrows/outer estuary	0.2	0.1	40	17	0.5
	Plaice	Rock Channel	Narrows/outer estuary	0.3	0.2	500	15	0.1

Chemical	Species	Location		Concentration (µg kg^{-1})				Lipid content
		Name	Designation	Wet weight		Lipid		%
				Mean	Standard deviation	Mean	Standard deviation	
Hexachlorobenzene (cont.)	Plaice	Gt. Burbo Bank	Outer estuary	0.2	0.2	40	20	0.5
	Plaice	Gt. Burbo Bank	Outer estuary	<0.1				
	Plaice	Gt. Burbo Bank	Outer estuary	0.4	0.3	70	23	0.6
	Plaice	Gt. Burbo Bank	Outer estuary	0.1	0.1	200	19	0.1
	Plaice – species mean			0.3[a]	0.3	128	145	0.6
	Shrimp	New Ferry	Inner estuary	0.5				
	Starfish	Gt. Burbo Bank	Outer estuary	0.5				
	Whelk	Gt. Burbo Bank	Outer estuary	0.5				
	Whiting	Eastham	Inner estuary	<0.1				
	Whiting	Eastham	Inner estuary	0.7	0.3	291	100	0.2
	Whiting	Garston	Inner estuary	1.5	0.4	398	123	0.4
	Whiting	Garston	Inner estuary	0.8	0.3	395	132	0.2
	Whiting	Rock Channel	Narrows/outer estuary	0.2	0.2	63	62	0.3
	Whiting	Rock Channel	Narrows/outer estuary	<0.1				
	Whiting	Gt. Burbo Bank	Outer estuary	<0.1				
	Whiting – species mean			0.5[a]	0.5	287	136	0.3
Hexachlorobutadiene	Blue Mussel	New Ferry	Inner estuary	0.5		60		0.8

Chemical	Species	Location		Concentration (µg kg^{-1})				Lipid content
		Name	Designation	Wet weight		Lipid		%
				Mean	Standard deviation	Mean	Standard deviation	
Hexachlorobutadiene (cont.)	Dab	Rock Channel	Narrows/outer estuary	0.3	0.9			
	Dab	Gt. Burbo Bank	Outer estuary	<0.1				
	Dab – species mean			0.2[a]	0.1			
	Flounder	Garston	Inner estuary	2.5	0.6			
	Flounder	Gt. Burbo Bank	Outer estuary	<0.1				
	Flounder – species mean			1.3[a]	1.2			
	Hermit crab	Gt. Burbo Bank	Outer estuary	<0.1				
	Plaice	Eastham	Inner estuary	0.1	0.1			
	Plaice	Garston	Inner estuary	<0.1				
	Plaice	Gt. Burbo Bank	Outer estuary	0.2	0.4			
	Plaice – species mean			0.1[a]	0.1			
	Shrimp	New Ferry	Inner estuary	0.5		80		0.6
	Starfish	Gt. Burbo Bank	Outer estuary	<0.1				
	Whelk	Gt. Burbo Bank	Outer estuary	<0.1				
	Whiting	Eastham	Inner estuary	1.0	0.2			
	Whiting	Eastham	Inner estuary	0.7	0.3			
	Whiting	Garston	Inner estuary	0.8	0.3			

Chemical	Species	Location		Concentration (µg kg^{-1})				Lipid content
		Name	Designation	Wet weight		Lipid		%
				Mean	Standard deviation	Mean	Standard deviation	
Hexachlorobutadiene (cont.)	Whiting	Garston	Inner estuary	1.4	0.4			
	Whiting – species mean			1.0	0.3			
Isodrin	Blue mussel	New Ferry	Inner estuary	<0.1				
	Cod	Rock Channel	Narrows/outer estuary	<0.1				
	Cod	Rock Channel	Narrows/outer estuary	<0.1				
	Cod – species mean			<0.1				
	Dab	Rock Channel	Narrows/outer estuary	<0.1				
	Dab	Gt. Burbo Bank	Outer estuary	<0.1				
	Dab	Gt. Burbo Bank	Outer estuary	<0.1				
	Dab	Gt. Burbo Bank	Outer estuary	<0.1				
	Dab	Gt. Burbo Bank	Outer estuary	<0.1				
	Dab – species mean			<0.1				
	Dover sole	Eastham	Inner estuary	<0.1				
	Dover sole	Garston	Inner estuary	<0.1				
	Dover sole	Garston	Inner estuary	<0.1				
	Dover sole	Gt. Burbo Bank	Outer estuary	<0.1				
	Dover sole	Gt. Burbo Bank	Outer estuary	<0.1				

Chemical	Species	Location		Concentration (µg kg^{-1})				Lipid content
		Name	Designation	Wet weight		Lipid		%
				Mean	Standard deviation	Mean	Standard deviation	
Isodrin (cont.)	Dover sole – species mean			<0.1				
	Flounder	Garston	Inner estuary	<0.1				
	Flounder	Rock Channel	Narrows/outer estuary	<0.1				
	Flounder	Gt. Burbo Bank	Outer estuary	<0.1				
	Flounder	Gt. Burbo Bank	Outer estuary	<0.1				
	Flounder	Gt. Burbo Bank	Outer estuary	<0.1				
	Flounder – species mean			<0.1				
	Hermit crab	Gt. Burbo Bank	Outer estuary	<0.1				
	Plaice	Eastham	Inner estuary	<0.1				
	Plaice	Garston	Inner estuary	<0.1				
	Plaice	Garston	Inner estuary	<0.1				
	Plaice	Rock Channel	Narrows/outer estuary	<0.1				
	Plaice	Rock Channel	Narrows/outer estuary	<0.1				
	Plaice	Rock Channel	Narrows/outer estuary	<0.1				
	Plaice	Gt. Burbo Bank	Outer estuary	<0.1				
	Plaice	Gt. Burbo Bank	Outer estuary	<0.1				
	Plaice	Gt. Burbo Bank	Outer estuary	<0.1				

Chemical	Species	Location		Concentration (µg kg^{-1})				Lipid content
		Name	Designation	Wet weight		Lipid		%
				Mean	Standard deviation	Mean	Standard deviation	
Isodrin (cont.)	Plaice	Gt. Burbo Bank	Outer estuary	<0.1				
	Plaice – species mean			<0.1				
	Shrimp	New Ferry	Inner estuary	<0.1				
	Starfish	Gt. Burbo Bank	Outer estuary	<0.1				
	Whelk	Gt. Burbo Bank	Outer estuary	<0.1				
	Whiting	Eastham	Inner estuary	<0.1				
	Whiting	Eastham	Inner estuary	<0.1				
	Whiting	Garston	Inner estuary	<0.1				
	Whiting	Garston	Inner estuary	<0.1				
	Whiting	Rock Channel	Narrows/outer estuary	<0.1				
	Whiting	Rock Channel	Narrows/outer estuary	<0.1				
	Whiting	Gt. Burbo Bank	Outer estuary	<0.1				
	Whiting – species mean			<0.1				
Methoxychlor	Dab	Rock Channel	Narrows/outer estuary	<0.1				
	Dab	Gt. Burbo Bank	Outer estuary	<0.1				
	Dab	Gt. Burbo Bank	Outer estuary	<0.1				
	Dab	Gt. Burbo Bank	Outer estuary	<0.1				

Chemical	Species	Location		Concentration (µg kg^{-1})				Lipid content
		Name	Designation	Wet weight		Lipid		%
				Mean	Standard deviation	Mean	Standard deviation	
Methoxychlor (cont.)	Dab	Gt. Burbo Bank	Outer estuary	<0.1				
	Dab – species mean			<0.1				
	Dover sole	Eastham	Inner estuary	<0.1				
	Dover sole	Garston	Inner estuary	<0.1				
	Dover sole	Garston	Inner estuary	<0.1				
	Dover sole	Gt. Burbo Bank	Outer estuary	<0.1				
	Dover sole	Gt. Burbo Bank	Outer estuary	<0.1				
	Dove sole – species mean			<0.1				
	Flounder	Garston	Inner estuary	<0.1				
	Flounder	Rock Channel	Narrows/outer estuary	<0.1				
	Flounder	Gt. Burbo Bank	Outer estuary	<0.1				
	Flounder	Gt. Burbo Bank	Outer estuary	<0.1				
	Flounder	Gt. Burbo Bank	Outer estuary	<0.1				
	Flounder – species mean			<0.1				
	Plaice	Eastham	Inner estuary	<0.1				
	Plaice	Garston	Inner estuary	<0.1				
	Plaice	Garston	Inner estuary	<0.1				

Chemical	Species	Location		Concentration (µg kg^{-1})				Lipid content
		Name	Designation	Wet weight		Lipid		%
				Mean	Standard deviation	Mean	Standard deviation	
Methoxychlor (cont.)	Plaice	Rock Channel	Narrows/outer estuary	<0.1				
	Plaice	Rock Channel	Narrows/outer estuary	<0.1				
	Plaice	Rock Channel	Narrows/outer estuary	<0.1				
	Plaice	Gt. Burbo Bank	Outer estuary	<0.1				
	Plaice	Gt. Burbo Bank	Outer estuary	<0.1				
	Plaice	Gt. Burbo Bank	Outer estuary	<0.1				
	Plaice	Gt. Burbo Bank	Outer estuary	<0.1				
	Plaice – species mean			<0.1				
	Whiting	Eastham	Inner estuary	<0.1				
	Whiting	Eastham	Inner estuary	<0.1				
	Whiting	Garston	Inner estuary	<0.1				
	Whiting	Garston	Inner estuary	<0.1				
	Whiting	Rock Channel	Narrows/outer estuary	<0.1				
	Whiting	Rock Channel	Narrows/outer estuary	<0.1				
	Whiting	Gt. Burbo Bank	Outer estuary	<0.1				
	Whiting – species mean			<0.1				
Mirex	Cod	Rock Channel	Narrows/outer estuary	<0.1				

Chemical	Species	Location		Concentration (µg kg^{-1})				Lipid content
		Name	Designation	Wet weight		Lipid		%
				Mean	Standard deviation	Mean	Standard deviation	
Mirex (cont.)	Cod	Rock Channel	Narrows/outer estuary	<0.1				
	Cod – species mean			<0.1				
	Dab	Rock Channel	Narrows/outer estuary	<0.1				
	Dab	Gt. Burbo Bank	Outer estuary	<0.1				
	Dab	Gt. Burbo Bank	Outer estuary	<0.1				
	Dab	Gt. Burbo Bank	Outer estuary	<0.1				
	Dab	Gt. Burbo Bank	Outer estuary	<0.1				
	Dab – species mean			<0.1				
	Dover sole	Eastham	Inner estuary	<0.1				
	Dover sole	Garston	Inner estuary	<0.1				
	Dover sole	Garston	Inner estuary	<0.1				
	Dover sole	Gt. Burbo Bank	Outer estuary	<0.1				
	Dover sole	Gt. Burbo Bank	Outer estuary	<0.1				
	Dover sole – species mean			<0.1				
	Flounder	Garston	Inner estuary	<0.1				
	Flounder	Rock Channel	Narrows/outer estuary	<0.1				
	Flounder	Gt. Burbo Bank	Outer estuary	<0.1				

Chemical	Species	Location		Concentration (µg kg^{-1})				Lipid content
		Name	Designation	Wet weight		Lipid		%
				Mean	Standard deviation	Mean	Standard deviation	
Mirex (cont.)	Flounder	Gt. Burbo Bank	Outer estuary	<0.1				
	Flounder	Gt. Burbo Bank	Outer estuary	<0.1				
	Flounder – species mean			<0.1				
	Plaice	Eastham	Inner estuary	<0.1				
	Plaice	Garston	Inner estuary	<0.1				
	Plaice	Garston	Inner estuary	<0.1				
	Plaice	Rock Channel	Narrows/outer estuary	<0.1				
	Plaice	Rock Channel	Narrows/outer estuary	<0.1				
	Plaice	Rock Channel	Narrows/outer estuary	<0.1				
	Plaice	Gt. Burbo Bank	Outer estuary	<0.1				
	Plaice	Gt. Burbo Bank	Outer estuary	<0.1				
	Plaice	Gt. Burbo Bank	Outer estuary	<0.1				
	Plaice	Gt. Burbo Bank	Outer estuary	<0.1				
	Plaice – species mean			<0.1				
	Whiting	Eastham	Inner estuary	<0.1				
	Whiting	Eastham	Inner estuary	<0.1				
	Whiting	Garston	Inner estuary	<0.1				

Chemical	Species	Location		Concentration (µg kg^{-1})				Lipid content
		Name	Designation	Wet weight		Lipid		%
				Mean	Standard deviation	Mean	Standard deviation	
Mirex (cont.)	Whiting	Garston	Inner estuary	<0.1				
	Whiting	Rock Channel	Narrows/outer estuary	<0.1				
	Whiting	Rock Channel	Narrows/outer estuary	<0.1				
	Whiting	Gt. Burbo Bank	Outer estuary	<0.1				
	Whiting – species mean			<0.1				
Oxychlordane	Blue mussel	New Ferry	Inner estuary	<0.1				
	Cod	Rock Channel	Narrows/outer estuary	<0.1				
	Cod	Rock Channel	Narrows/outer estuary	<0.1				
	Cod – species mean			<0.1				
	Dab	Rock Channel	Narrows/outer estuary	<0.1				
	Dab	Gt. Burbo Bank	Outer estuary	<0.1				
	Dab	Gt. Burbo Bank	Outer estuary	<0.1				
	Dab	Gt. Burbo Bank	Outer estuary	<0.1				
	Dab	Gt. Burbo Bank	Outer estuary	<0.1				
	Dab – species mean			<0.1				
	Dover sole	Eastham	Inner estuary	<0.1				
	Dover sole	Garston	Inner estuary	<0.1				

Chemical	Species	Location		Concentration (µg kg^{-1})				Lipid content
		Name	Designation	Wet weight		Lipid		%
				Mean	Standard deviation	Mean	Standard deviation	
Oxychlordane (cont.)	Dover sole	Garston	Inner estuary	<0.1				
	Dover sole	Gt. Burbo Bank	Outer estuary	<0.1				
	Dover sole	Gt. Burbo Bank	Outer estuary	<0.1				
	Dover sole – species mean			<0.1				
	Flounder	Garston	Inner estuary	<0.1				
	Flounder	Rock Channel	Narrows/outer estuary	<0.1				
	Flounder	Gt. Burbo Bank	Outer estuary	<0.1				
	Flounder	Gt. Burbo Bank	Outer estuary	<0.1				
	Flounder	Gt. Burbo Bank	Outer estuary	<0.1				
	Flounder – species mean			<0.1				
	Hermit crab	Gt. Burbo Bank	Outer estuary	<0.1				
	Plaice	Eastham	Inner estuary	<0.1				
	Plaice	Garston	Inner estuary	<0.1				
	Plaice	Garston	Inner estuary	<0.1				
	Plaice	Rock Channel	Narrows/outer estuary	<0.1				
	Plaice	Rock Channel	Narrows/outer estuary	<0.1				
	Plaice	Rock Channel	Narrows/outer estuary	<0.1				

Chemical	Species	Location		Concentration (µg kg^{-1})				Lipid content
		Name	Designation	Wet weight		Lipid		%
				Mean	Standard deviation	Mean	Standard deviation	
Oxychlordane (cont.)	Plaice	Gt. Burbo Bank	Outer estuary	<0.1				
	Plaice	Gt. Burbo Bank	Outer estuary	<0.1				
	Plaice	Gt. Burbo Bank	Outer estuary	<0.1				
	Plaice	Gt. Burbo Bank	Outer estuary	<0.1				
	Plaice – species mean			<0.1				
	Shrimp	New Ferry	Inner estuary	<0.1				
	Starfish	Gt. Burbo Bank	Outer estuary	<0.1				
	Whelk	Gt. Burbo Bank	Outer estuary	<0.1				
	Whiting	Eastham	Inner estuary	<0.1				
	Whiting	Eastham	Inner estuary	<0.1				
	Whiting	Garston	Inner estuary	<0.1				
	Whiting	Garston	Inner estuary	<0.1				
	Whiting	Rock Channel	Narrows/outer estuary	<0.1				
	Whiting	Rock Channel	Narrows/outer estuary	<0.1				
	Whiting	Gt. Burbo Bank	Outer estuary	<0.1				
	Whiting – species mean			<0.1				
PCB 28	Dab	Gt. Burbo Bank	Outer estuary	0.09				

Chemical	Species	Location		Concentration (µg kg^{-1})				Lipid content
		Name	Designation	Wet weight		Lipid		%
				Mean	Standard deviation	Mean	Standard deviation	
PCB 28 (contd.)	Dover sole	Gt. Burbo Bank	Outer estuary	0.18				
	Flounder	Gt. Burbo Bank	Outer estuary	1.1				
	Plaice	Gt. Burbo Bank	Outer estuary	0.55				
	Starfish	Gt. Burbo Bank	Outer estuary	0.6				
	Whelk	Gt. Burbo Bank	Outer estuary	1.2				
PCB 52	Dab	Gt. Burbo Bank	Outer estuary	0.05				
	Dover sole	Gt. Burbo Bank	Outer estuary	0.51				
	Flounder	Gt. Burbo Bank	Outer estuary	1.9				
	Plaice	Gt. Burbo Bank	Outer estuary	0.71				
	Starfish	Gt. Burbo Bank	Outer estuary	0.6				
	Whelk	Gt. Burbo Bank	Outer estuary	1				
PCB 101	Dab	Gt. Burbo Bank	Outer estuary	0.68				
	Dover sole	Gt. Burbo Bank	Outer estuary	1.9				
	Flounder	Gt. Burbo Bank	Outer estuary	3.7				
	Plaice	Gt. Burbo Bank	Outer estuary	1.3				
	Starfish	Gt. Burbo Bank	Outer estuary	1.2				
	Whelk	Gt. Burbo Bank	Outer estuary	1.5				

Chemical	Species	Location		Concentration (µg kg^{-1})				Lipid content
		Name	Designation	Wet weight		Lipid		%
				Mean	Standard deviation	Mean	Standard deviation	
PCB 138	Dab	Gt. Burbo Bank	Outer estuary	3.1				
	Dover sole	Gt. Burbo Bank	Outer estuary	2.2				
	Flounder	Gt. Burbo Bank	Outer estuary	4.5				
	Plaice	Gt. Burbo Bank	Outer estuary	2.7				
	Starfish	Gt. Burbo Bank	Outer estuary	3.2				
	Whelk	Gt. Burbo Bank	Outer estuary	32				
PCB 153	Dab	Gt. Burbo Bank	Outer estuary	2.7				
	Dover sole	Gt. Burbo Bank	Outer estuary	4.1				
	Flounder	Gt. Burbo Bank	Outer estuary	4.8				
	Plaice	Gt. Burbo Bank	Outer estuary	2.9				
	Starfish	Gt. Burbo Bank	Outer estuary	3.7				
	Whelk	Gt. Burbo Bank	Outer estuary	37				
PCB 180	Dab	Gt. Burbo Bank	Outer estuary	1.1				
	Dover sole	Gt. Burbo Bank	Outer estuary	1.6				
	Flounder	Gt. Burbo Bank	Outer estuary	2.2				
	Plaice	Gt. Burbo Bank	Outer estuary	1.4				
	Starfish	Gt. Burbo Bank	Outer estuary	0.7				

Chemical	Species	Location		Concentration (µg kg^{-1})				Lipid content
		Name	Designation	Wet weight		Lipid		%
				Mean	Standard deviation	Mean	Standard deviation	
PCB 180 (contd.)	Whelk	Gt. Burbo Bank	Outer estuary	17				
ΣPCBs - ICES	Blue Mussel	New Ferry	Inner estuary	20	1.1	2,180	123	0.9
	Cod	Rock Channel	Narrows/outer estuary	1.6	0.5	746	690	0.2
	Cod	Rock Channel	Narrows/outer estuary	2.0	0.7	783	537	0.3
	Cod – species mean			1.8	0.2	765	19	0.3
	Dab	Rock Channel	Narrows/outer estuary	43.4	13.5	3,283	2,159	1.3
	Dab	Gt. Burbo Bank	Outer estuary	5.6	0.9	633	352	0.9
	Dab	Gt. Burbo Bank	Outer estuary	6.1	1.3	504	273	1.2
	Dab	Gt. Burbo Bank	Outer estuary	8.9	1.6	1,025	475	0.9
	Dab	Gt. Burbo Bank	Outer estuary	10.1	9.7	739	692	1.4
	Dab – species mean			14.8	14.4	1,237	1,037	1.1
	Dover sole	Eastham	Inner estuary	11.3	2.9	6,051	9,059	0.2
	Dover sole	Garston	Inner estuary	17.9	2.5	5,980	11,442	0.3
	Dover sole	Garston	Inner estuary	11.0	2.3	3,110	2,741	0.4
	Dover sole	Gt. Burbo Bank	Outer estuary	10.4	3.0	3,370	3,884	0.3
	Dover sole	Gt. Burbo Bank	Outer estuary	15.0	2.8	4,720	4,160	0.3
	Dover sole – species mean			13.1	2.9	4,646	1,245	0.3

Chemical	Species	Location		Concentration (µg kg^{-1})				Lipid content
		Name	Designation	Wet weight		Lipid		%
				Mean	Standard deviation	Mean	Standard deviation	
ΣPCBs – ICES (cont.)	Flounder	Garston	Inner estuary	25.2	2.1	5,653	1,824	0.4
	Flounder	Rock Channel	Narrows/outer estuary	14.9	2.1	5,880	5,345	0.3
	Flounder	Gt. Burbo Bank	Outer estuary	12.6	2.4	3,480	1,965	0.4
	Flounder	Gt. Burbo Bank	Outer estuary	21.8	4.5	3,600	2,040	0.6
	Flounder	Gt. Burbo Bank	Outer estuary	19.3	2.3	4,610	2,920	0.4
	Flounder – species mean			18.8	4.6	4,645	999	0.4
	Hermit crab	Gt. Burbo Bank	Outer estuary	105	12	1,754	123	6.0
	Plaice	Eastham	Inner estuary	10.1	1.2	1,016	412	1.0
	Plaice	Garston	Inner estuary	9.1	1.9	1,662	1,469	0.5
	Plaice	Garston	Inner estuary	11.1	2.5	2,575	2,794	0.4
	Plaice	Rock Channel	Narrows/outer estuary	18.9	6.2	1,387	890	1.4
	Plaice	Rock Channel	Narrows/outer estuary	12.7	1.4	2,070	601	0.6
	Plaice	Rock Channel	Narrows/outer estuary	13.8	1.3	2,600	1,551	0.5
	Plaice	Gt. Burbo Bank	Outer estuary	10.6	2.3	2,585	1,825	0.4
	Plaice	Gt. Burbo Bank	Outer estuary	8.8	0.9	2,240	822	0.4
	Plaice	Gt. Burbo Bank	Outer estuary	11.2	1.9	2,230	977	0.5
	Plaice	Gt. Burbo Bank	Outer estuary	7.9	1.3	2,190	1,102	0.4

Chemical	Species	Location		Concentration (µg kg^{-1})				Lipid content
		Name	Designation	Wet weight		Lipid		%
				Mean	Standard deviation	Mean	Standard deviation	
ΣPCBs – ICES (cont.)	Plaice – species mean			11.4	3.0	2,056	511	0.6
	Shrimp	New Ferry	Inner estuary	8.2	6.2	1,230	128	0.7
	Starfish	Gt. Burbo Bank	Outer estuary	9.9	6	650	49	1.5
	Whelk	Gt. Burbo Bank	Outer estuary	91	6.6	6,710	622	1.4
	Whiting	Eastham	Inner estuary	7.6	0.5	2,353	693	0.3
	Whiting	Eastham	Inner estuary	8.0	0.7	3,030	309	0.3
	Whiting	Garston	Inner estuary	7.1	0.8	1,903	784	0.4
	Whiting	Garston	Inner estuary	5.3	0.7	2,604	1,059	0.2
	Whiting	Rock Channel	Narrows/outer estuary	3.2	0.6	913	858	0.4
	Whiting	Rock Channel	Narrows/outer estuary	1.2	0.3	871	463	0.1
	Whiting	Gt. Burbo Bank	Outer estuary	1.7	0.2	637	387	0.3
	Whiting – species mean			4.9	2.6	1,759	884	0.3

a) For the calculation of the species mean, a not detected result (<0.1 µg kg^{-1}) was taken as 0.05 µg kg^{-1}.

B2 Results for BIO v1.1, ECOFATE and AQUAWEB v1.1 models

In order to run the BIO v1.1, ECOFATE and AQUAWEB v1.1 models for the Mersey data sets, the same representative ecosystem was constructed within each model. The properties of the species used are summarised in Table B4.

Table B4 Model ecosystem used for the Mersey data set

Species	Lipid content (%)	Organism wet weight[d] (kg)	Diet assumed for modelling purposes	Comment
Phytoplankton	0.5[a]	Not relevant	Not relevant	The model assumes uptake occurs from water.
Zooplankton (such as mysid)	3[a]	5.7×10^{-8} [a]	Not relevant	The model assumes that uptake occurs from water.
Mussel	0.9[b]	1.1×10^{-4} [a]	Filter feeder – 100% phytoplankton	
Hermit crab	5.5[b]	0.010	Filter feeder – 100% phytoplankton	
Oligochaete	1.0[a]	1×10^{-3}	Benthic detrivore – 100% sediment/detritus	
Shrimp	0.6[b]	5×10^{-4}	Benthic detrivore – 100% sediment/detritus	
Whelk	1.8[b]	0.020	Benthic detrivore – 100% sediment/detritus	
Star fish[c]	1.3[b]	Not needed[c]	Benthic detrivore – 100% sediment/detritus	
Dab	1.2[b]	0.3	74% Shrimp 22% Oligochaete 4% Mussel (based on Table 2)	
Plaice	0.7	0.5	83.5% Oligochaete 13.1% Small fish 3.4% Shrimp (based on Table 2)	The fish in diet was assumed to be composed equally of all fish species in the ECOFATE model and entirely of dab in the BIO v1.1 and AQUAWEB v1.1 models.[e]
Dover sole	0.4[b]	1	82.5% Oligochaete 12% Shrimp 5.5% Mussel (based on Table 2)	
Flounder	0.5[b]	1.5	61.5 Shrimp 24.5% Oligochaete 13.9% small fish 0.1% Phytoplankton (based on Table 2)	The fish in diet was assumed to be composed equally of all fish species in the ECOFATE model

Species	Lipid content (%)	Organism wet weight[d] (kg)	Diet assumed for modelling purposes	Comment
				and equally of dab, plaice and dover sole in the BIO v1.1 and AQUAWEB v1.1 models.[e]
Whiting	0.3	1	87% Small fish 8.7% zooplankton (mysids) 3.8% Shrimp 0.3% Oligochaete 0.2% Mussel (based on Table 2)	The fish in diet was assumed to be composed equally of all fish species in the ECOFATE model and equally of dab, plaice, dover sole and flounder in the BIO v1.1 and AQUAWEB v1.1 models.[e]
Cod	0.2[b]	3	86% Small fish 12.9% Shrimp 1% Oligochaete 0.1% Mussel (based on Table 2)	The fish in diet was assumed to be composed equally of all fish species in the ECOFATE model and equally of dab, plaice, dover sole, flounder and whiting in the BIO v1.1 and AQUAWEB v1.1 models.[e]

a) Typical values taken from the ECOFATE model.

b) Typical values taken from Mersey data set. The fish lipid contents refer to the edible portion of the fish. Example calculations were also run assuming that all fish had a whole body lipid content of around eight per cent in order to evaluate the concentration on a whole body basis.

c) Star fish were only included in the simulations using ECOFATE. The current spreadsheet version of the BIO v1.1 and the AQUAWEB model v1.1 only allows for a total of five invertebrates (filter feeders and benthic detrivores) to be included.

d) No actual data were available. The values that were assumed in this simulation are given. The weights of zooplankton and invertebrates are not needed for the BIO v1.1 and the ECOFATE model.

e) The BIO v1.1 and AQUAWEB V1.1 models only allow fish to consume prey at the preceding trophic levels, whereas the ECOFATE model allows fish to consume any other fish. It is possible to include cannibalism in the BIO v1.1 and AQUAWEB v1.1 models by introducing different age groups.

As information on the concentrations in water (sediment) was only available for a limited subset of the chemicals for which measured levels in biota were available in the Mersey data set, two approaches were used for the modelling exercise. Firstly, in order to test if the models could predict the relative[17] accumulation of each given chemical within the available species, the model was run assuming a hypothetical dissolved water concentration along with the equivalent concentration in sediment. These concentrations were estimated using the ECOFATE model with a standard emission of one g day^{-1} into a water body of 100 m $\times$100 m and depth of 10 m, with a nominal flow of 100,000 l day^{-1}. The actual concentrations used are not important to the final outcome but the relative concentrations in water and sediment are important.

[17] The concentrations relative to the concentration in plaice were used for this analysis as data for plaice was the most abundant within the data set.

A sediment organic carbon content of five per cent, depth of sediment of 10 cm, a suspended sediment concentration of 1.5×10^{-5} kg l^{-1} and a temperature of 12°C were used in the model simulations (based on the assumptions in the TGD). These same concentrations were used as inputs to the BIO v1.1 and AQUAWEB v1.1 models to allow the results to be compared directly (for these models, the dissolved organic carbon concentration and the particulate organic carbon concentrations were set to zero in order to allow a direct comparison to be made). The chemical concentrations assumed as input are shown in Table b5.

Table B5 Hypothetical concentrations used as input for modelling of the Mersey dataset

Substance	Dissolved concentration in water (g l^{-1})	Concentration in sediment solids (g kg^{-1} dry)
1,2,4,5-Tetrachlorobenzene	8.5×10^{-6}	0.013
1,2,4-Trichlorobenzene	9.3×10^{-6}	5.9×10^{-3}
1,4-Dichlorobenzene	9.8×10^{-6}	1.3×10^{-3}
Aldrin	8.0×10^{-7}	0.068
α- and γ-HCH	9.7×10^{-6}	2.5×10^{-3}
β - HCH	9.7×10^{-6}	2.5×10^{-3}
cis-Chlordane	1.4×10^{-6}	0.071
trans-Chlordane	1.4×10^{-6}	0.071
DDT - Total	1.3×10^{-6}	0.071
Dieldrin	4.3×10^{-6}	0.051
Endrin	3.3×10^{-6}	0.059
Heptachlor	1.5×10^{-6}	0.071
Hexachlrorobenzene	3.8×10^{-6}	0.055
Hexachlorobutadiene	7.9×10^{-6}	0.019
Isodrin	8.0×10^{-7}	0.068
Methoxychlor	6.1×10^{-6}	0.035
Mirex	5.0×10^{-6}	0.045
Oxychlor	3.9×10^{-6}	0.055
PCB28	2.5×10^{-6}	0.066
PCB52	1.5×10^{-6}	0.071
PCB101	9.4×10^{-7}	0.070
PCB138	5.9×10^{-7}	0.063
PCB153	4.4×10^{-7}	0.055
PCB180	2.7×10^{-7}	0.041
$\sum$PCB - ICES	8.0×10^{-7}	0.068

The second approach taken was, for chemicals where sufficient information was available, to estimate a likely concentration in water from the available sediment data; concentrations in the food chain were estimated from the concentration in water (taken from Table B2) and the BAF predicted for the relevant organism (taken from Table B6 to Table B11.

Predicted BAFs for species included in the food chain constructed within ECOFATE using the hypothetical input concentrations for water and sediment are summarised in Table B6 for plankton, crustacean and molluscs and in Table B7 for fish. Equivalent BAFs obtained using BIO v1.1 are summarised in Table B8 and Table B9 respectively and those obtained using AQUAWEB v1.1 are summarised in Table B10 and Table B11 respectively.

The resulting predictions are considered in relation to the available measured data for each chemical in turn.

Table B6 Bioaccumulation factors predicted by ECOFATE for plankton, crustacean and molluscs in the Mersey data set

Chemical	BAF (l kg^{-1} wet weight)							
	Phyto-plankton (algae)	Zooplankton (mysid)	Hermit crab	Mussel	Worm	Shrimp	Whelk	Starfish
1,2,4,5-Tetrachlorobenzene	160	950	1,700	290	330	200	590	424
1,2,4-Trichlorobenzene	63	380	690	110	130	76	230	166
1,4-Dichlorobenzene	13	75	140	23	25	15	45	33
Aldrin	16,000	95,000	220,000	36,000	46,000	27,000	82,000	60,000
α- and γ-HCH	25	150	280	45	50	30	91	65
β-HCH	25	150	280	45	50	30	91	65
cis-Chlordane	7,200	43,000	90,000	15,000	22,000	13,000	40,000	29,000
trans-Chlordane	7,200	43,000	90,000	15,000	22,000	13,000	40,000	29,000
DDT – Total	7,700	46,000	98,000	16,000	24,000	14,000	43,000	31,000
Dieldrin	1,300	7,500	14,000	2,300	3,000	1,800	5,400	3,900
Endrin	2,000	12,000	23,000	3,700	5,100	3,100	9,200	6,700
Heptachlor	6,300	38,000	78,000	13,000	19,000	11,000	34,000	25,000
Hexachlorobenzene	1,600	9,500	18,000	2,900	3,900	2,400	7,100	5,100
Hexachlorobutadiene	250	1,500	2,800	450	520	310	940	680
Isodrin	16,000	95,000	220,000	36,000	46,000	27,000	82,000	60,000
Methoxychlor	600	3,600	6,700	1,100	1,300	800	2,400	1,700
Mirex	950	5,700	11,000	1,700	2,200	1,300	4,000	2,900
Oxychlordane	1,500	9,100	17,000	2,800	3,700	2,200	6,700	4,800
PCB 28	3,200	19,000	37,000	6,000	8,700	5,200	16,000	11,000
PCB 52	6,300	38,000	78,000	13,000	19,000	11,000	34,000	25,000
PCB 101	13,000	75,000	170,000	28,000	38,000	23,000	68,000	49,000
PCB 138	25,000	150,000	390,000	64,000	64,000	38,000	110,000	83,000
PCB 153	40,000	240,000	700,000	110,000	82,000	49,000	150,000	110,000
PCB 180	79,000	480,000	1,700,000	280,000	110,000	64,000	190,000	140,000
ΣPCB - ICES	16,000	95,000	220,000	36,000	46,000	27,000	82,000	60,000

Table B7 Bioaccumulation factors predicted by ECOFATE for fish in the Mersey data set

Chemical	BAF (l kg^{-1} wet weight)											
	Plaice		Flounder		Dover sole		Dab		Whiting		Cod	
	Lipid content		Lipid content		Lipid content		Lipid content		Lipid content		Lipid content	
	0.7%	8%	0.5%	8%	0.4%	8%	1.2%	8%	0.3%	8%	0.2%	8%
1,2,4,5-Tetrachloro-benzene	230	2,700	170	2,700	130	2,600	390	2,600	97	2,700	64	2,500
1,2,4-Trichloro-benzene	90	1,000	64	1,000	51	1,000	150	1,000	38	1,000	25	1,000
1,4-Dichloro-benzene	18	200	13	200	10	200	30	200	7.5	300	5	200
Aldrin	100,000	1,300,000	73,000	1,100,000	61,000	730,000	130,000	560,000	23,000	540,000	11,000	180,000
α- + γ-HCH	35	410	25	410	20	400	60	400	15	410	10	400
β-HCH	35	410	25	410	20	400	60	400	15	410	10	400
cis-Chlordane	34,000	480,000	24,000	420,000	21,000	300,000	44,000	220,000	7,600	240,000	4,200	95,000
trans-Chlordane	34,000	480,000	24,000	420,000	21,000	300,000	44,000	220,000	7,600	240,000	4,200	95,000
DDT – Total	38,000	530,000	27,000	460,000	23,000	320,000	49,000	240,000	8,300	260,000	4,500	100,000
Dieldrin	2,500	33,000	1,700	32,000	1,500	27,000	3,800	24,000	860	29,000	530	19,000
Endrin	4,700	64,000	3,300	62,000	2,900	50,000	6,900	41,000	1,500	50,000	880	29,000
Heptachlor	27,000	390,000	19,000	350,000	17,000	250,000	36,000	190,000	6,300	200,000	3,500	84,000
Hexachloro-benzene	3,400	46,000	2,400	44,000	2,100	37,000	5,100	31,000	1,100	28,000	680	23,000
Hexachloro-butadiene	380	4,500	270	4,500	220	4,300	630	4,100	150	4,400	100	3,900
Isodrin	100,000	1,300,000	73,000	1,100,000	61,000	730,000	130,000	560,000	23,000	540,000	11,000	180,000
Methoxy-chlor	1,000	12,000	710	12,000	590	11,000	1,600	10,000	390	12,000	250	9,300
Mirex	1,700	23,000	1,200	22,000	1,000	19,000	2,700	17,000	630	20,000	400	14,000

Chemical	BAF (l kg^{-1} wet weight)											
	Plaice		Flounder		Dover sole		Dab		Whiting		Cod	
	Lipid content		Lipid content		Lipid content		Lipid content		Lipid content		Lipid content	
	0.7%	8%	0.5%	8%	0.4%	8%	1.2%	8%	0.3%	8%	0.2%	8%
Oxychlor-dane	3,200	43,000	2,200	42,000	1,900	35,000	4,800	30,000	1,100	36,000	650	22,000
PCB 28	9,300	130,000	6,500	120,000	5,800	94,000	13,000	75,000	2,600	89,000	1,500	45,000
PCB 52	27,000	390,000	19,000	350,000	17,000	250,000	36,000	190,000	6,300	200,000	3,500	84,000
PCB 101	77,000	1,000,000	54,000	860,000	46,000	580,000	97,000	440,000	16,000	430,000	8,500	150,000
PCB 138	180,000	2,100,000	130,000	1,700,000	100,000	1,100,000	220,000	850,000	43,000	800,000	20,000	250,000
PCB 153	270,000	2,800,000	190,000	2,300,000	150,000	1,500,000	330,000	1,200,000	78,000	1,100,000	32,000	310,000
PCB 180	410,000	3,700,000	300,000	3,000,000	230,000	2,000,000	520,000	1,600,000	180,000	1,500,000	57,000	370,000
ΣPCB - ICES	100,000	1,300,000	73,000	1,100,000	61,000	730,000	130,000	560,000	23,000	540,000	11,000	180,000

Table B8 Bioaccumulation factors predicted by BIO v1.1 for plankton, crustacean and molluscs in the Mersey data set

Chemical	BAF (l kg^{-1} wet weight)						
	Phyto-plankton (algae)	Zooplankton (mysid)	Hermit crab	Mussel	Worm	Shrimp	Whelk
1,2,4,5-Tetrachlorobenzene	160	950	1,700	280	320	190	570
1,2,4-Trichlorobenzene	63	380	680	110	130	76	230
1,4-Dichlorobenzene	13	75	150	24	26	16	47
Aldrin	16,000	95,000	93,000	15,000	17,000	10,000	31,000
α- and γ-HCH	25	150	280	46	51	31	92
β-HCH	25	150	280	46	51	31	92
cis-Chlordane	7,200	43,000	57,000	9,300	10,000	6,200	19,000
trans-Chlordane	7,200	43,000	57,000	9,300	10,000	6,200	19,000
DDT – Total	7,700	47,000	60,000	9,800	11,000	6,500	20,000
Dieldrin	1,300	7,500	13,000	2,100	2,400	1,400	4,200
Endrin	2,000	12,000	20,000	3,200	3,600	2,200	6,500
Heptachlor	6,300	38,000	52,000	8,400	9,400	5,600	17,000
Hexachlorobenzene	1,600	9,500	16,000	2,600	2,900	1,800	5,200
Hexachlorobutadiene	250	1,500	2,700	450	500	300	890
Isodrin	16,000	95,000	93,000	15,000	17,000	10,000	31,000
Methoxychlor	600	3,600	6,400	1,100	1,200	700	2,100
Mirex	950	5,700	10,000	1,600	1,800	1,100	3,300
Oxychlordane	1,500	9,100	15,000	2,500	2,800	1,700	5,000
PCB 28	3,200	19,000	29,000	4,800	5,400	3,200	9,700
PCB 52	6,300	38,000	52,000	8,400	9,400	5,600	17,000
PCB 101	13,000	75,000	82,000	13,000	15,000	8,900	27,000
PCB 138	25,000	150,000	120,000	19,000	21,000	13,000	38,000
PCB 153	40,000	240,000	138,000	23,000	25,000	15,000	45,000
PCB 180	79,000	480,000	160,000	27,000	30,000	18,000	53,000
ΣPCB - ICES	16,000	95,000	93,000	15,000	17,000	10,000	31,000

Table B9 Bioaccumulation factors predicted by BIO v1.1 for fish in the Mersey data set

Chemical	BAF (l kg^{-1} wet weight)											
	Plaice		Flounder		Dover sole		Dab		Whiting		Cod	
	Lipid content		Lipid content		Lipid content		Lipid content		Lipid content		Lipid content	
	0.7%	8%	0.5%	8%	0.4%	8%	1.2%	8%	0.3%	8%	0.2%	8%
1,2,4,5-Tetrachloro-benzene	230	2,500	170	2,500	130	2,300	390	2,400	100	3,300	67	3,500
1,2,4-Trichloro-benzene	91	1,000	65	1,000	52	980	150	980	39	1,200	26	1,200
1,4-Dichloro-benzene	18	210	13	210	11	210	31	210	7.9	210	5.3	220
Aldrin	48,000	93,000	37,000	86,000	32,000	70,000	41,000	60,000	61,000	273,000	50,000	360,000
α- + γ-HCH	36	410	26	410	21	400	62	400	16	430	10	440
β-HCH	36	410	26	410	21	400	62	400	16	430	10	440
cis-Chlordane	21,000	61,000	15,000	56,000	13,000	46,000	21,000	41,000	18,000	170,000	13,000	220,000
trans-Chlordane	21,000	61,000	15,000	56,000	13,000	46,000	21,000	41,000	18,000	170,000	13,000	220,000
DDT – Total	23,000	63,000	17,000	58,000	15,000	48,000	23,000	42,000	20,000	180,000	15,000	230,000
Dieldrin	2,400	17,000	1,700	16,000	1,400	14,000	3,400	13,000	1,100	36,000	750	45,000
Endrin	4,200	24,000	3,000	23,000	2,500	19,000	5,500	18,000	2,200	58,000	1,500	74,000
Heptachlor	18,000	56,000	13,000	51,000	11,000	42,000	19,000	38,000	14,000	150,000	10,000	200,000
Hexachloro-benzene	3,100	20,000	2,200	19,000	1,900	16,000	4,300	16,000	1,600	46,000	1,000	58,000
Hexachloro-butadiene	380	3,900	270	3,800	220	5,600	620	3,600	170	5,600	110	6,200
Isodrin	48,000	93,000	37,000	86,000	32,000	70,000	41,000	60,000	61,000	270,000	50,000	360,000
Methoxy-chlor	990	8,800	700	8,500	580	7,500	1,500	7,600	450	16,000	250	19,000

Chemical	BAF (l kg^{-1} wet weight)											
	Plaice		Flounder		Dover sole		Dab		Whiting		Cod	
	Lipid content		Lipid content		Lipid content		Lipid content		Lipid content		Lipid content	
	0.7%	8%	0.5%	8%	0.4%	8%	1.2%	8%	0.3%	8%	0.2%	8%
Mirex	1,700	13,000	1,200	13,000	1,000	11,000	2,500	11,000	790	27,000	520	33,000
Oxychlor-dane	2,900	20,000	2,100	18,000	1,800	16,000	4,100	15,000	1,500	44,000	980	55,000
PCB 28	7,500	35,000	5,300	32,000	4,600	26,000	9,100	25,000	4,500	87,000	3,100	110,000
PCB 52	18,000	56,000	13,000	51,000	11,000	42,000	19,000	38,000	14,000	150,000	10,000	200,000
PCB 101	38,000	83,000	29,000	77,000	25,000	63,000	34,000	54,000	43,000	239,000	34,000	320,000
PCB 138	70,000	110,000	56,000	110,000	47,000	86,000	55,000	73,000	110,000	350,000	97,000	450,000
PCB 153	93,000	130,000	77,000	120,000	65,000	100,000	69,000	84,000	180,000	420,000	170,000	540,000
PCB 180	130,000	160,000	110,000	140,000	90,000	120,000	88,000	90,000	330,000	560,000	310,000	670,000
ΣPCB - ICES	48,000	93,000	37,000	86,000	32,000	70,000	41,000	60,000	61,000	273,000	50,000	360,000

Table B10 Bioaccumulation factors predicted by AQUAWEB v1.1 for plankton, crustacean and molluscs in the Mersey data set

Chemical	BAF (l kg^{-1} wet weight)						
	Phytoplankton (algae)	Zooplankton (mysid)	Hermit crab	Mussel	Worm	Shrimp	Whelk
1,2,4,5-Tetrachlorobenzene	860	1,200	2,100	550	640	490	1,000
1,2,4-Trichlorobenzene	350	470	850	220	240	180	370
1,4-Dichlorobenzene	70	94	170	45	48	37	70
Aldrin	61,000	150,000	180,000	71,000	240,000	180,000	500,000
α- and γ-HCH	140	190	340	88	95	73	140
β-HCH	140	190	340	88	95	73	140
cis-Chlordane	33,000	66,000	96,000	31,000	97,000	68,000	210,000
trans-Chlordane	33,000	66,000	96,000	31,000	97,000	68,000	210,000
DDT – Total	35,000	71,000	100,000	33,000	110,000	75,000	230,000
Dieldrin	6,700	9,900	17,000	4,600	8,200	5,900	16,000
Endrin	10,000	16,000	27,000	7,500	16,000	11,000	32,000
Heptachlor	30,000	57,000	84,000	27,000	80,000	57,000	170,000
Hexachlorobenzene	8,300	13,000	22,000	5,900	11,200	8,100	23,000
Hexachlorobutadiene	1,400	1,900	3,400	880	1,100	810	1,800
Isodrin	61,000	150,000	180,000	71,000	240,000	170,000	500,000
Methoxychlor	3,300	4,600	8,100	2,100	3,100	2,300	5,500
Mirex	5,100	7,400	13,000	3,500	5,600	4,100	11,000
Oxychlordane	8,000	12,000	21,000	5,600	11,000	7,600	21,000
PCB 28	16,000	26,000	43,000	12,000	30,000	22,000	65,000
PCB 52	30,000	57,000	84,000	27,000	80,000	57,000	170,000
PCB 101	52,000	120,000	150,000	56,000	190,000	140,000	400,000
PCB 138	83,000	240,000	240,000	110,000	370,000	270,000	720,000
PCB 153	110,000	360,000	300,000	160,000	500,000	370,000	900,000
PCB 180	140,000	600,000	340,000	250,000	650,000	510,000	1,000,000
ΣPCB - ICES	61,000	150,000	180,000	71,000	240,000	180,000	500,000

Table B11 Bioaccumulation factors predicted by AQUAWEB v1.1 for fish in the Mersey data set

Chemical	BAF (l kg^{-1} wet weight)											
	Plaice		Flounder		Dover sole		Dab		Whiting		Cod	
	Lipid content		Lipid content		Lipid content		Lipid content		Lipid content		Lipid content	
	0.7%	8%	0.5%	8%	0.4%	8%	1.2%	8%	0.3%	8%	0.2%	8%
1,2,4,5-Tetrachloro-benzene	500	3,300	430	3,400	400	3,100	660	3,000	360	4,700	320	5,300
1,2,4-Trichloro-benzene	190	1,200	160	1,200	150	1,200	250	1,100	130	1,400	120	1,500
1,4-Dichloro-benzene	36	220	31	220	29	220	49	220	26	230	24	230
Aldrin	660,000	4,300,000	540,000	5,700,000	440,000	2,400,000	580,000	1,900,000	890,000	21,000,000	980,000	42,000,000
α- + γ-HCH	72	450	62	450	57	450	97	440	52	480	47	490
β-HCH	72	450	62	450	57	450	97	440	52	480	47	490
cis-Chlordane	210,000	1,500,000	170,000	2,000,000	150,000	900,000	190,000	700,000	250,000	7,000,000	270,000	14,000,000
trans-Chlordane	210,000	1,500,000	170,000	2,000,000	150,000	900,000	190,000	700,000	250,000	7,000,000	270,000	14,000,000
DDT – Total	240,000	1,700,000	190,000	2,200,000	170,000	1,000,000	210,000	770,000	280,000	7,800,000	300,000	16,000,000
Dieldrin	8,600	63,000	7,200	73,000	6,900	50,000	9,500	40,000	6,600	190,000	6,300	310,000
Endrin	20,000	150,000	16,000	180,000	16,000	110,000	20,000	84,000	16,000	520,000	16,000	900,000
Heptachlor	170,000	1,200,000	140,000	1,600,000	120,000	730,000	150,000	570,000	190,000	5,500,000	200,000	11,000,000
Hexachloro-benzene	13,000	96,000	11,000	110,000	10,000	73,000	14,000	58,000	10,000	310,000	10,000	520,000
Hexachloro-butadiene	850	5,700	730	5,900	680	5,300	1,100	4,900	610	9,400	550	11,200
Isodrin	660,000	4,300,00	540,000	5,700,000	440,000	2,400,00	580,000	1,900,00	890,000	21,000,00	980,000	42,000,00

Chemical	BAF (l kg^{-1} wet weight)											
	Plaice		Flounder		Dover sole		Dab		Whiting		Cod	
	Lipid content		Lipid content		Lipid content		Lipid content		Lipid content		Lipid content	
	0.7%	8%	0.5%	8%	0.4%	8%	1.2%	8%	0.3%	8%	0.2%	8%
		0				0		0		0		0
Methoxy-chlor	2,700	19,000	2,300	21,000	2,200	16,000	3,200	14,000	1,900	43,000	1,800	59,000
Mirex	5,400	39,000	4,600	44,000	4,400	32,000	6,200	27,000	4,000	110,000	3,800	160,000
Oxychlor-dane	12,000	88,000	10,000	100,000	9,500	67,000	13,000	54,000	9,300	290,000	9,100	470,000
PCB 28	47,000	350,000	39,000	440,000	36,000	240,000	46,000	180,000	44,000	1,400,000	45,000	1,400,000
PCB 52	170,000	1,200,000	140,000	1,600,000	120,000	730,000	150,000	570,000	190,000	5,500,000	200,000	11,000,000
PCB 101	490,000	3,300,000	400,000	4,400,000	330,000	1,900,000	43,000	1,500,000	640,000	17,000,000	700,000	32,000,000
PCB 138	1,100,000	6,500,000	890,000	8,500,000	700,000	3,600,000	930,000	2,900,000	1,500,000	30,000,000	1,700,000	61,000,000
PCB 153	1,500,000	8,000,000	1,300,000	10,000,000	980,000	4,600,000	1,300,000	3,700,000	2,200,000	36,000,000	2,500,000	70,000,000
PCB 180	1,900,000	7,900,000	1,600,000	9,500,000	1,300,000	4,900,000	1,700,000	4,100,000	2,800,000	31,000,000	3,100,000	56,00,000
ΣPCB - ICES	660,000	4,300,000	540,000	5,700,000	440,000	2,400,000	580,000	1,900,000	890,000	21,000,000	980,000	42,000,000

1,2,4,5-Tetrachlorobenzene

The concentrations measured and predicted in several species (relative to concentration measured or predicted in plaice) for 1,2,4,5-tetrachlorobenzene are shown in **Error! Reference source not found.**. As can be seen, all three of the models appear to predict well the observed relative concentrations.

No data on the concentrations of 1,2,4,5-tetrachlorobenzene in sediment or water in the Mersey ecosystem are available and so it is not possible to compare the absolute predicted concentrations with those observed.

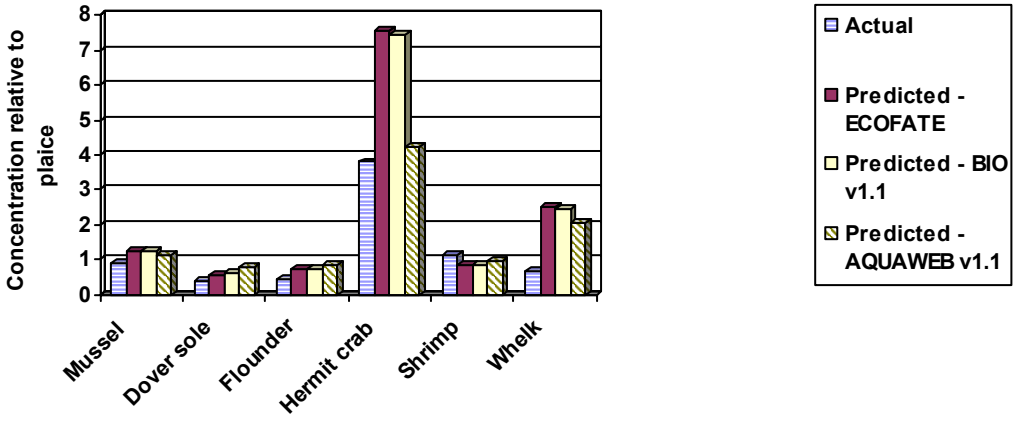

Figure B1 Predicted and actual concentration in biota relative to plaice for 1,2,4,5-tetrachlorobenzene

1,2,4-Trichlorobenzene

The relative concentrations measured and predicted for 1,2,4-trichlorobenzene are shown in Figure B2. As can be seen, all three of the models appear to predict the observed relative concentrations reasonably well for mussel and dover sole, but appear to significantly underestimate the relative concentration in shrimp.

No data on the concentrations of 1,2,4-trichlorobenzene in sediment or water in the Mersey ecosystem are available and so it is not possible to compare the absolute predicted concentrations with those observed.

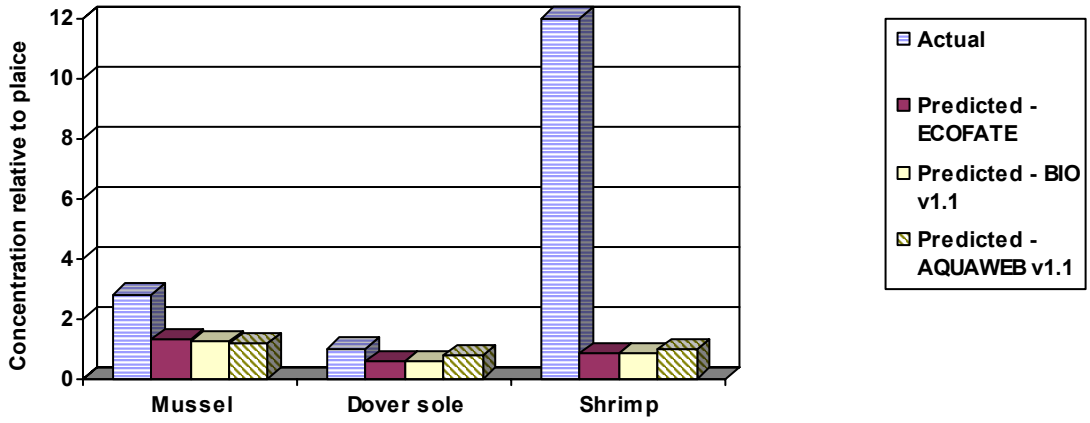

Figure B2 Predicted and actual concentration in biota relative to plaice for 1,2,4-trichlorobenzene

1,4-Dichlorobenzene

The relative concentrations measured and predicted for 1,4-dichlorobenzene are shown in Figure B4. All three of the models appear to predict the observed relative concentrations reasonably well for flounder, hermit crab and shrimp, but overpredict the relative concentrations in cod and whelk, and underpredict the relative concentrations in mussel, dab, dover sole and in particular whiting.

No data on the concentrations of 1,4-dichlorobenzene in sediment or water in the Mersey ecosystem are available and so it is not possible to compare the absolute predicted concentrations with those observed.

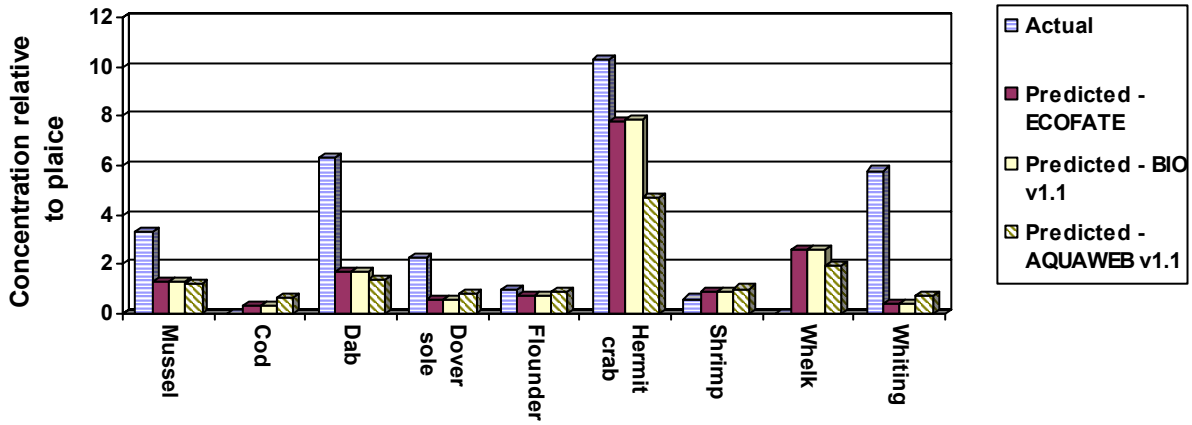

Figure B3 Predicted and actual concentration in biota relative to plaice for 1,4-dichlorobenzene

Aldrin

Aldrin was generally not detectable (concentration <0.1 µg kg^{-1} wet weight) in the aquatic biota sampled taken from the Mersey estuary and so it is not possible to carry out an analysis of the relative concentrations in biota.

The concentration of aldrin assumed to be present in the dissolved phase in water from the Mersey estuary for modelling purposes is estimated to be less than 4.3×10^{-5} µg l^{-1} (see Section B1). Predicted BAFs for aldrin in the species monitored are given below.

	Predicted BAFs (l kg^{-1} wet weight)		
	ECOFATE	BIO v1.1	AQUAWEB v1.1
Benthic invertebrates	27,000-220,000	10,000-93,000	71,000-500,000
Fish	11,000-130,000	32,000-61,000	440,000-980,000

Based on these estimated BAFs and the estimated dissolved concentration in water, the expected concentration of aldrin in biota would be around 0.4 to 22 µg kg^{-1} wet weight in benthic invertebrates and 0.5 to 42 µg kg^{-1} wet weight in fish. It is not possible to compare these data directly with the available measured data as they are all limit values.

Hexachlorocyclohexane (HCH)

The relative concentrations measured and predicted for α-HCH and γ-HCH are shown in Figure B4. All three of the models appear to predict the observed relative concentrations reasonably well for mussel, cod, dab, dover sole, flounder and whiting. The relative concentrations for hermit crab, starfish and whelk are all overpredicted slightly, but even so the relative concentration is generally within a factor of four of the observed ratio. Predictions using AQUAWEB v1.1 appear to be slightly closer to the observed ratios than predictions obtained using the other models. Overall, all predictions of the relative concentration across all species are generally within a factor of two to three of the observed ratio.

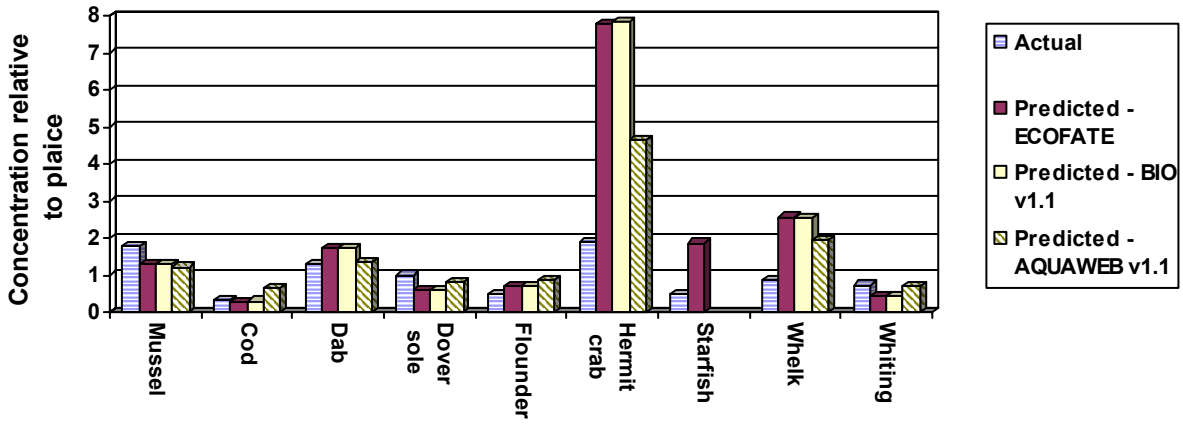

Figure B4 Predicted and actual concentration in biota relative to plaice for α- HCH and γ-HCH

The concentration of α-HCH and γ-HCH assumed to be present in the dissolved phase in water from the Mersey estuary for modelling purposes is estimated to be 0.031 μg l^{-1} (see above, Section B1). Predicted BAFs for α-HCH and γ-HCH in the edible portions of plaice were 35 l kg^{-1} wet weight using ECOFATE, 36 l kg^{-1} wet weight using BIO v1.1 and 72 l kg^{-1} wet weight using AQUAWEB v1.1

Based on these estimated BAFs and the estimated dissolved concentration in water, the expected concentration of α-HCH and γ-HCH in the edible portion of plaice would be around 1 μg kg^{-1} wet weight using the ECOFATE and BIO v1.1 estimates and around 2 μg kg^{-1} wet weight using the AQUAWEB v1.1 estimate. The actual concentration of α-HCH and γ-HCH measured in the edible portion of plaice was between 0.5 and 3.6 μg kg^{-1} wet weight, with a mean value of around 1.5 μg kg^{-1} wet weight (see above, Section B1). Therefore, there is very good agreement between the predicted and measured concentration in plaice. As there was also good agreement between predicted and observed concentrations in the other species surveyed relative to plaice, it can be concluded that concentrations in all species monitored are reasonably well predicted for α-HCH and γ-HCH.

For β-HCH, there are only very limited data available for one species of fish (flounder). Predicted BAFs for the edible portion of this species were 25 l kg^{-1} wet weight using ECOFATE, 26 l kg^{-1} wet weight using BIO v1.1 and 62 l kg^{-1} wet weight using AQUAWEB v1.1. The assumed dissolved concentration of β-HCH in water from the Mersey estuary for modelling purposes is 0.078 μg l^{-1} (see Section B1). Based on these data, the predicted concentration of β-HCH in the edible portion of flounder would be around 2 μg kg^{-1} wet weight based on the ECOFATE and BIO v1.1 estimates and 5 μg kg^{-1} wet weight based on the AQUAWEB v1.1 estimates. The observed concentration in the edible portion of flounder was 360 μg kg^{-1} wet weight. Predicted concentrations are therefore around two orders of magnitude lower than observed. However, it should be noted that for β-HCH, the data base of measured levels is very small and so it is not clear how representative the measured sample is.

cis-Chlordane

The relative concentrations measured and predicted for cis-chlordane are shown in Figure B5. All three of the models appear to predict the observed relative concentrations reasonably well for dab, dover sole, shrimp, whelk and whiting, but overpredict the relative concentrations in cod and starfish, and underpredict the relative concentrations in mussel, flounder and hermit crab. Overall, with the exception of mussel, starfish and hermit crab, predictions for the relative concentration across all species are generally in agreement with the observed ratios to within a factor of two to three, often much lower than this.

No data on the concentrations of cis-chlordane in sediment or water in the Mersey ecosystem are available and so it is not possible to compare the absolute predicted concentrations with those observed.

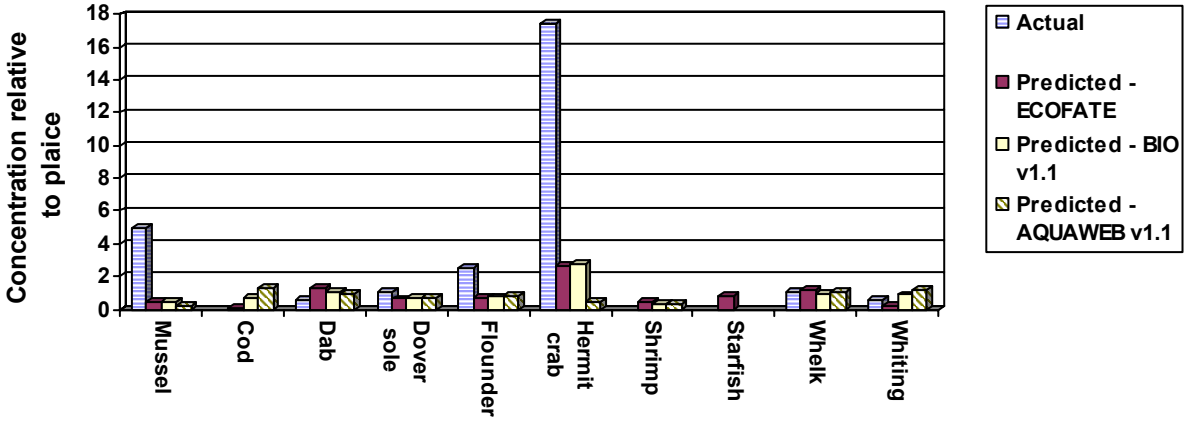

Figure B5 Predicted and actual concentration in biota relative to plaice for cis-chlordane

trans-Chlordane

The relative concentrations measured and predicted for trans-chlordane are shown inFigure B6. Similar to the case with cis-chlordane, all three of the models appear to predict the observed relative concentrations well for dab, dover sole, shrimp and whiting, but overpredict the relative concentrations in cod and starfish, and underpredict the relative concentrations in mussel and to a lesser extent flounder and whelk. For hermit crab, both ECOFATE and BIO v1.1 appear to slightly overestimate the relative concentration in hermit crab, but AQUAWEB v1.1 appears to slightly underestimate the relative concentration in hermit crab. Overall, with the exception of mussel and cod, the relative concentrations across all species appear to be predicted to within a factor of two to three (often much better than this).

No data on the concentrations of trans-chlordane in sediment or water in the Mersey ecosystem are available and so it is not possible to compare the absolute predicted concentrations with those observed.

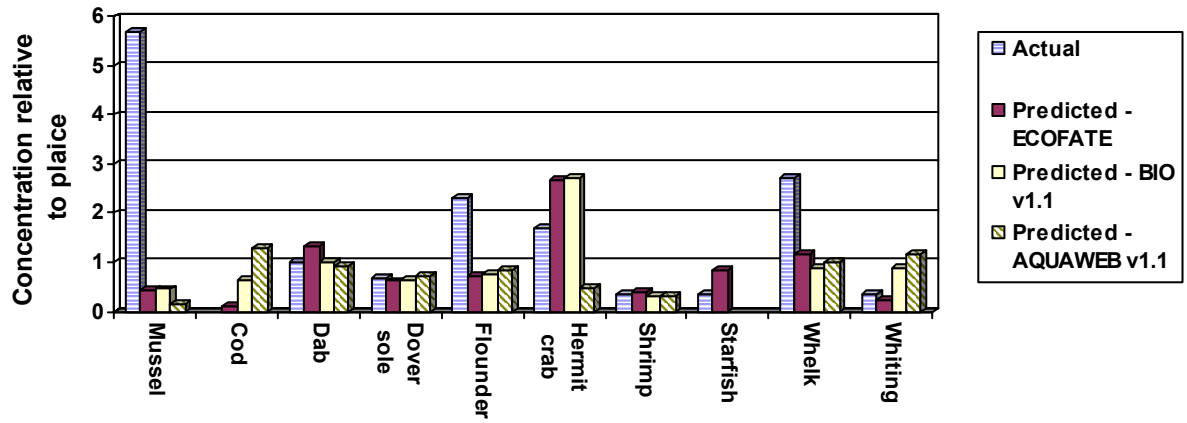

Figure B6 Predicted and actual concentration in biota relative to plaice for trans-chlordane

DDT Total

The relative concentrations measured and predicted for total DDT are shown in Figure B7. All three of the models appear to predict the observed relative concentrations reasonably well for dab, dover sole and in some cases cod, hermit crab and whiting. Relative concentrations in mussel, flounder, whelk, and in some cases hermit crab all appear to be underpredicted to some extent. Some of the methods also appear to slightly overpredict the relative concentration in cod and whiting. Overall, with the exception of mussel, cod and whelk, most predictions of the relative concentration across all species are generally within a factor of two to three of the observed ratio.

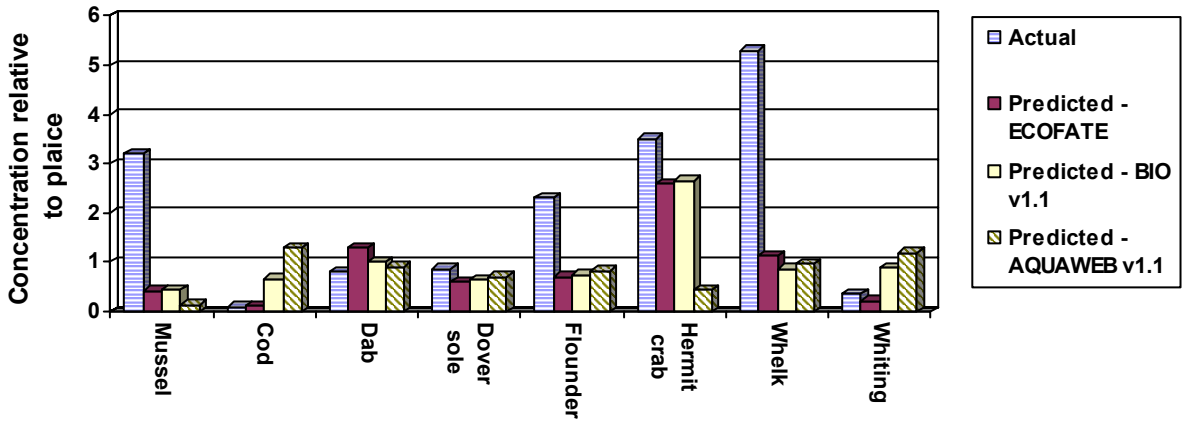

Figure B7 Predicted and actual concentration in biota relative to plaice for DDT – Total

The concentration of total DDT assumed to be present in the dissolved phase in water from the Mersey estuary for modelling purposes is estimated to be 0.022 µg l^{-1} (see above, Section B1). Predicted BAFs for total DDT in the edible portions of plaice were 38,000 l kg^{-1} wet weight using ECOFATE, 23,000 l kg^{-1} wet weight using BIO v1.1 and 240,000 l kg^{-1} wet weight using AQUAWEB v1.1

Based on these estimated BAFs and the estimated dissolved concentration in water, the expected concentration of total DDT in the edible portion of plaice would be around 840 µg kg^{-1} wet weight using the ECOFATE estimate, 510 µg kg^{-1} wet weight using BIO v1.1 estimate and around 5,300 µg kg^{-1} wet weight using the AQUAWEB v1.1 estimate. The actual concentration of total DDT measured in the edible portion of plaice was between 5.3 and 14 µg kg^{-1} wet weight, with a mean value of around 9.5 µg kg^{-1} wet weight (see above, Section B1). Therefore, predicted concentrations were around 50 to 500 times higher than observed concentrations. As there was a reasonable agreement between predicted and observed concentrations in the other species surveyed relative to plaice (see above), it can be concluded that the models would provide a similar level of overprediction of the observed concentration for all the other species to that found for plaice.

Dieldrin

No measured data were available for plaice and so it was not possible to carry out a comparison of the actual and predicted concentrations relative to plaice for this substance. However, measured data were available for several other species.

The concentration of dieldrin assumed to be present in the dissolved phase in water from the Mersey estuary for modelling purposes is estimated to be less than 3.4×10^{-4} µg l^{-1}. Predicted BAFs for dieldrin in the species monitored are summarised below.

	Predicted BAFs (l kg^{-1} wet weight)		
	ECOFATE	BIO v1.1	AQUAWEB v1.1
Benthic invertebrates	1,800-14,000	1,400-13,000	4,600-17,000
Fish	530-3,800	750-3,400	6,300-9,500

Based on these estimated BAFs and the estimated dissolved concentration in water, the expected concentration of aldrin in biota would be around 0.5 to 6 µg kg^{-1} wet weight in benthic invertebrates and 0.2 to 3 µg kg^{-1} wet weight in fish. The mean measured levels for dieldrin ranged between 0.8 and 13 µg kg^{-1} wet weight in benthic invertebrates and 0.4 and 2.3 µg kg^{-1} wet weight in fish (see above, Section B1). As the concentration in water used for this simulation is a limit value, it is not possible to draw any firm conclusions from these data, but the upper limit of the predictions are reasonably consistent with the available measurements.

Endrin

Endrin was generally not detected (concentration <0.1 µg kg^{-1} wet weight) in the biota samples taken from the Mersey estuary. In addition. there was no estimate available for the likely concentration of endrin in water or sediment in the Mersey estuary at the time of sampling and so it was not possible to carry out a further analysis of the predictions for this chemical.

Heptachlor

Heptachlor was generally not detected (concentration <0.1 µg kg^{-1} wet weight) in the biota samples taken from the Mersey estuary and so it was not possible to carry out a comparison of the predicted and relative concentrations in the various species.

The concentration of heptachlor assumed to be present in the dissolved phase in water from the Mersey estuary for modelling purposes is estimated to be 1.4×10^{-3} µg l^{-1} (see above, Section B1). The predicted BAFs for heptachlor in the species monitored are summarised below.

	Predicted BAFs (l kg^{-1} wet weight)		
	ECOFATE	BIO v1.1	AQUAWEB v1.1
Benthic invertebrates	11,000-78,000	5,600-52,000	27,000-170,000
Fish	3,500-36,000	10,000-19,000	120,000-200,000

Based on these estimated BAFs and the estimated dissolved concentration in water, the expected concentration of aldrin in biota would be around 8 to 240 μg kg^{-1} wet weight in benthic invertebrates and 5 to 280 μg kg^{-1} wet weight in fish. For comparison, heptachlor was not detected (concentration <0.1 μg kg^{-1} wet weight) in any of the samples of benthic invertebrates or fish analysed from the Mersey estuary. On this basis, the models appear to significantly overestimate the concentrations found.

Hexachlorobenzene

The relative concentrations measured and predicted for hexachlorobenzene are shown in Figure B8. All three of the models appear to predict the observed relative concentrations reasonably well for dab, shrimp, starfish and whelk. There is a small underprediction of the relative concentrations for mussel, flounder, shrimp and whiting, and an overprediction of the relative concentration for cod and dover sole. Overall, predictions for most of the species are within a factor of four of the observed relative concentrations, and are often much closer than this.

No data on the concentrations of hexachlorobenzene in sediment or water in the Mersey ecosystem are available and so it is not possible to compare the absolute predicted concentrations with those observed.

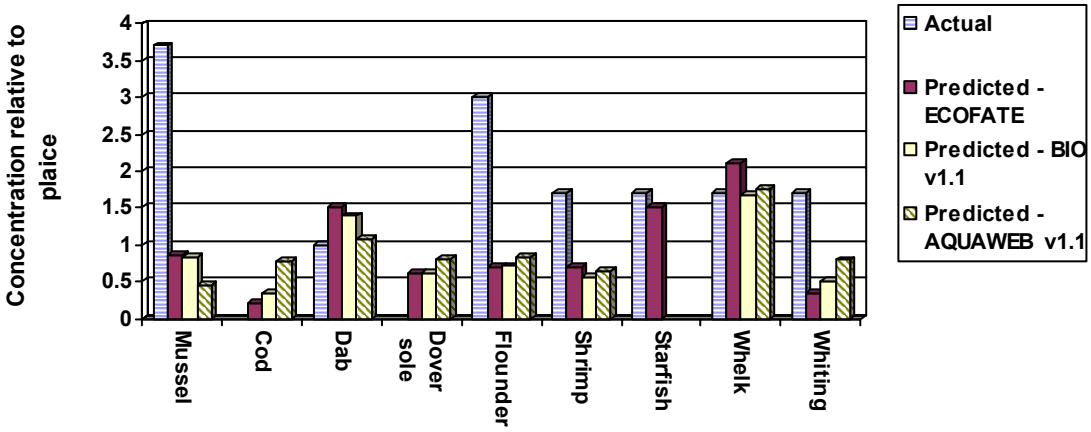

Figure B8 Predicted and actual concentration in biota relative to plaice for hexachlorobenzene

Hexachlorobutadiene

The relative concentrations measured and predicted for hexachlorobutadiene are shown in Figure B9. All three of the models appear to predict the observed relative concentrations reasonably well for dab. There is an underprediction of the relative concentrations for mussel, flounder, shrimp and whiting, and an overprediction of the relative concentrations for hermit crab, starfish and whelk.

No data on the concentrations of hexachlorobutadiene in sediment or water in the Mersey ecosystem are available and so it is not possible to compare the absolute predicted concentrations with those observed.

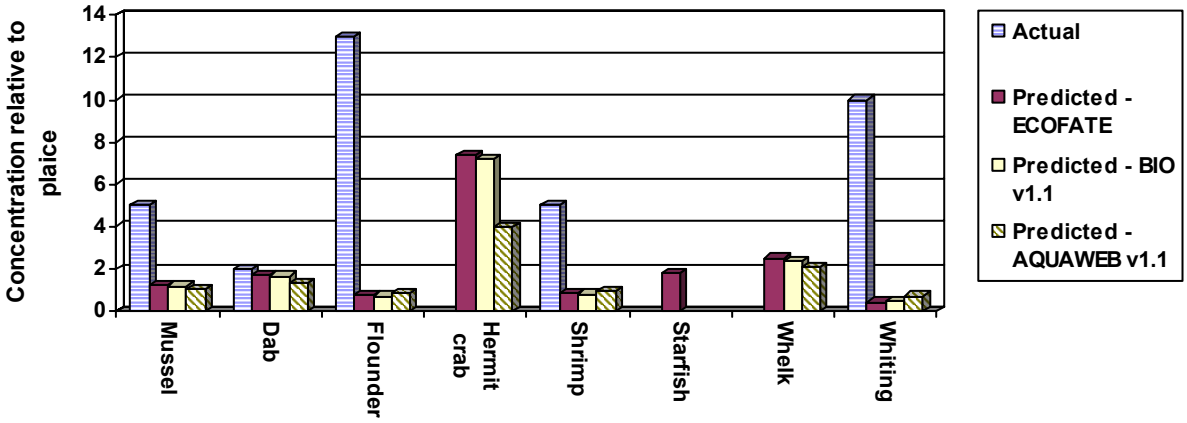

Figure B9 Predicted and actual concentration in biota relative to plaice for hexachlorobutadiene

Isodrin

Isodrin was generally not detected (concentration <0.1 µg kg^{-1} wet weight) in the biota samples taken from the Mersey estuary. In addition, there was no estimate available on the likely concentration of isodrin in water or sediment in the Mersey estuary at the time of sampling and so it was not possible to carry out a further analysis of the predictions for this chemical.

Methoxychlor

Methoxychlor was generally not detected (concentration <0.1 µg kg^{-1} wet weight) in the biota samples taken from the Mersey estuary. In addition, there was no estimate available on the likely concentration of methoxychlor in water or sediment in the Mersey estuary at the time of sampling and so it was not possible to carry out a further analysis of the predictions for this chemical.

Mirex

Mirex was generally not detected (concentration <0.1 µg kg^{-1} wet weight) in the biota samples taken from the Mersey estuary. In addition, there was no estimate available on the likely concentration of mirex in water or sediment in the Mersey estuary at the time of sampling and so it was not possible to carry out a further analysis of the predictions for this chemical.

Oxychlordane

Oxychlordane was generally not detected (concentration <0.1 µg kg^{-1} wet weight) in the biota samples taken from the Mersey estuary. In addition, there was no estimate available on the likely concentration of oxychlordane in water or sediment in the Mersey estuary at the time of

sampling and so it was not possible to carry out a further analysis of the predictions for this chemical.

PCB 28

The relative concentrations measured and predicted for PCB 28 are shown in Figure B10. All three of the models appear to predict the observed relative concentrations reasonably well for starfish and whelk. Relative concentrations in dab and to a lesser extent dover sole appear to be overpredicted to some extent, and the relative concentration in flounder appears to be underpredicted. Overall with the exception of dab, predictions of the relative concentration across all species are generally within a factor of two to three of the observed ratio.

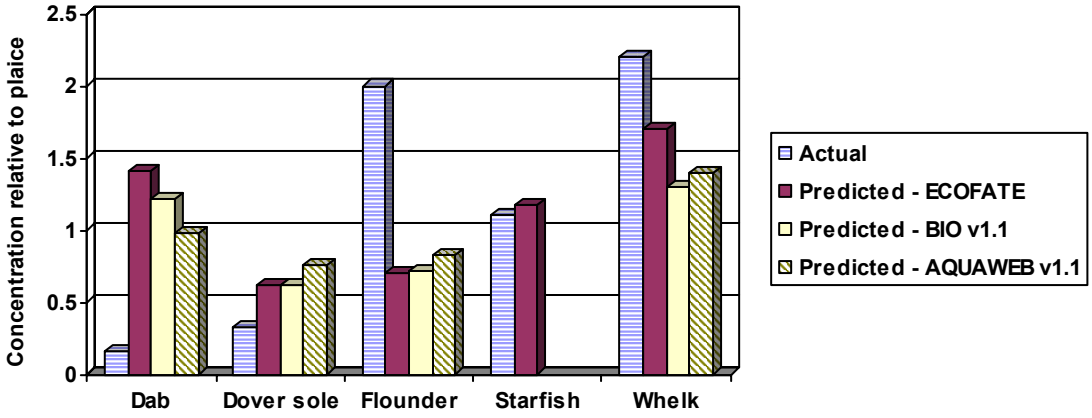

Figure B10 Predicted and actual concentration in biota relative to plaice for PCB 28

The concentration of PCB 28 assumed to be present in the dissolved phase in water from the Mersey estuary for modelling purposes is estimated to be 3.2×10^{-3} µg l^{-1} (see above, Section B1). The predicted BAFs for PCB 28 in the edible portions of plaice were 9,300 l kg^{-1} wet weight using ECOFATE, 7,500 l kg^{-1} wet weight using BIO v1.1 and 47,000 l kg^{-1} wet weight using AQUAWEB v1.1

Based on these estimated BAFs and the estimated dissolved concentration in water, the expected concentration of PCB 28 in the edible portion of plaice would be around 30 µg kg^{-1} wet weight using the ECOFATE estimate, 24 µg kg^{-1} wet weight using BIO v1.1 estimate and around 150 µg kg^{-1} wet weight using the AQUAWEB v1.1 estimate. The actual concentration of PCB 28 measured in the edible portion of plaice was 0.55 µg kg^{-1} wet weight (see above, Section B1). Therefore, predicted concentrations were around 45 to 300 times higher than observed concentrations. As there was reasonable agreement between predicted and observed concentrations in the other species surveyed relative to the concentration in plaice (see above), it can be concluded that the models would provide a similar level of overprediction of the observed concentration for all the other species to that found for plaice.

PCB 52

The relative concentrations measured and predicted for PCB 52 are shown inFigure B11. All three of the models appear to well predict the observed relative concentrations for dover sole, starfish and whelk. The relative concentrations in dab appear to be overpredicted to some extent, and the relative concentration in flounder appears to be underpredicted. Overall, with the exception of dab, predictions of the relative concentration across all species are generally within a factor of two to three of the observed ratio.

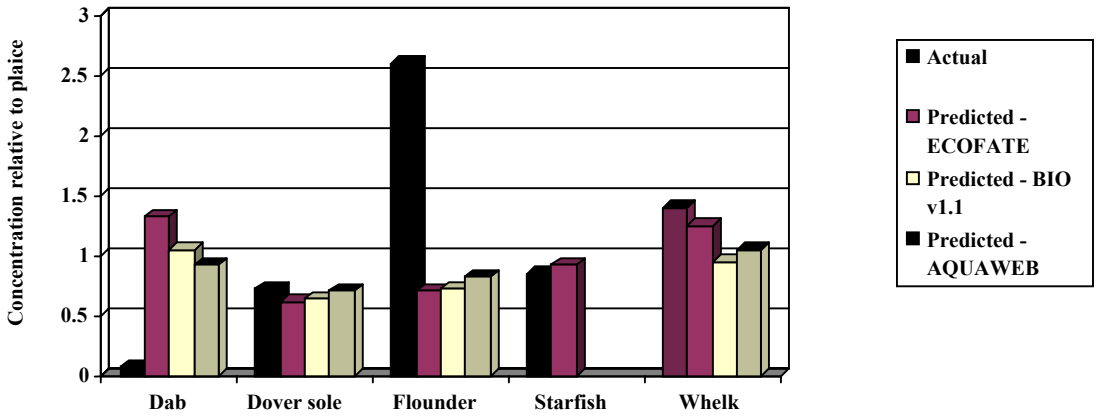

Figure B11 Predicted and actual concentration in biota relative to plaice for PCB 52

The concentration of PCB 52 assumed to be present in the dissolved phase in water from the Mersey estuary for modelling purposes is estimated to be 4.6×10^{-3} µg l^{-1} (see above, Section B1). The predicted BAFs for PCB 52 in the edible portions of plaice were 27,000 l kg^{-1} wet weight using ECOFATE, 18,000 l kg^{-1} wet weight using BIO v1.1 and 170,000 l kg^{-1} wet weight using AQUAWEB v1.1

Based on these estimated BAFs and the estimated dissolved concentration in water, the expected concentration of PCB 52 in the edible portion of plaice would be around 120 µg kg^{-1} wet weight using the ECOFATE estimate, 80 µg kg^{-1} wet weight using BIO v1.1 estimate and around 800 µg kg^{-1} wet weight using the AQUAWEB v1.1 estimate. The actual concentration of PCB 52 measured in the edible portion of plaice was 0.71 µg kg^{-1} wet weight (see above, Section B1). Therefore, predicted concentrations were around 100 to 1,000 times higher than observed concentrations. As there was reasonable agreement between predicted and observed concentrations in the other species surveyed relative to the concentration in plaice (see above), it can be concluded that the models would provide a similar level of overprediction of the observed concentration for all the other species to that found for plaice.

PCB 101

The relative concentrations measured and predicted for PCB 101 are shown in Figure B12. All three of the models appear to well predict the observed relative concentrations for starfish and whelk. The relative concentrations in dab appear to be overpredicted to some extent, and the relative concentrations in dover sole and flounder appear to be underpredicted. Overall, predictions of the relative concentration across all species are generally within a factor of two to three of the observed ratio.

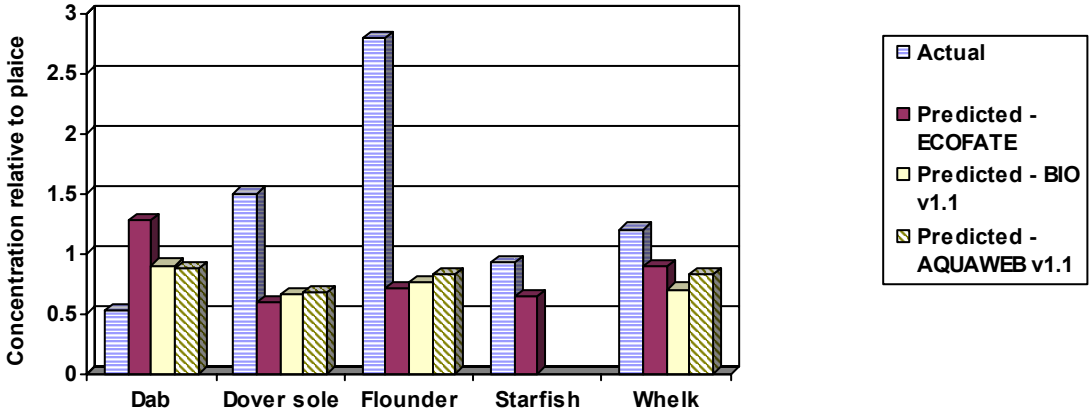

Figure B12 Predicted and actual concentration in biota relative to plaice for PCB 101

The concentration of PCB 101 assumed to be present in the dissolved phase in water from the Mersey estuary for modelling purposes is estimated to be 2.6×10^{-3} µg l^{-1} (see above, Section B1). The predicted BAFs for PCB 101 in the edible portions of plaice were 77,000 l kg^{-1} wet weight using ECOFATE, 38,000 l kg^{-1} wet weight using BIO v1.1 and 490,000 l kg^{-1} wet weight using AQUAWEB v1.1

Based on these estimated BAFs and the estimated dissolved concentration in water, the expected concentration of PCB 101 in the edible portion of plaice would be around 200 µg kg^{-1} wet weight using the ECOFATE estimate, 100 µg kg^{-1} wet weight using BIO v1.1 estimate and around 1,300 µg kg^{-1} wet weight using the AQUAWEB v1.1 estimate. The actual concentration of PCB 101 measured in the edible portion of plaice was 1.3 µg kg^{-1} wet weight (see above, Section B1). Therefore, predicted concentrations were around 80 to 1,000 times higher than observed concentrations. As there was reasonable agreement between predicted and observed concentrations in the other species surveyed relative to the concentration in plaice (see above), it can be concluded that the models would provide a similar level of overprediction of the observed concentration for all the other species to that found for plaice.

PCB 138

The relative concentrations measured and predicted for PCB 138 are shown in Figure B13. All three of the models appear to well predict the observed relative concentrations for dab and dover sole. The relative concentrations in flounder, starfish and in particular whelk appear to be underpredicted. Overall, with the exception of whelk, predictions of the relative concentration across all species are generally within a factor of two of the observed ratio.

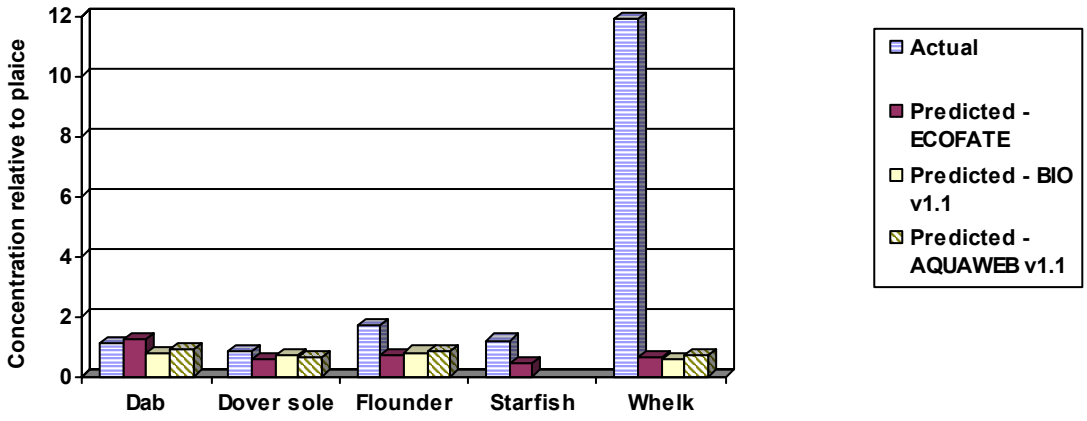

Figure B13 Predicted and actual concentration in biota relative to plaice for PCB 138

The concentration of PCB 138 assumed to be present in the dissolved phase in water from the Mersey estuary for modelling purposes is estimated to be 1.8×10^{-3} µg l^{-1} (see above, Section B1). Predicted BAFs for PCB 138 in the edible portions of plaice were 180,000 l kg^{-1} wet weight using ECOFATE, 70,000 l kg^{-1} wet weight using BIO v1.1 and 1,100,000 l kg^{-1} wet weight using AQUAWEB v1.1

Based on these estimated BAFs and the estimated dissolved concentration in water, the expected concentration of PCB 138 in the edible portion of plaice would be around 320 µg kg^{-1} wet weight using the ECOFATE estimate, 130 µg kg^{-1} wet weight using BIO v1.1 estimate and around 2,000 µg kg^{-1} wet weight using the AQUAWEB v1.1 estimate. The actual concentration of PCB 138 measured in the edible portion of plaice was 2.7 µg kg^{-1} wet weight (see above, Section B1). Therefore, predicted concentrations were around 50 to 700 times higher than the observed concentration. As there was reasonable agreement between predicted and observed concentrations in the other species surveyed relative to the concentration in plaice (see above), it can be concluded that the models would provide a similar level of overprediction of the observed concentration for all the other species to that found for plaice.

PCB 153

The relative concentrations measured and predicted for PCB 153 are shown in Figure B14. All three of the models appear to well predict the observed relative concentrations for dab. Relative concentrations in dover sole, flounder, starfish and in particular whelk appear to be underpredicted. Overall, with the exception of whelk, predictions of the relative concentration across all species are generally within a factor of two of the observed ratio.

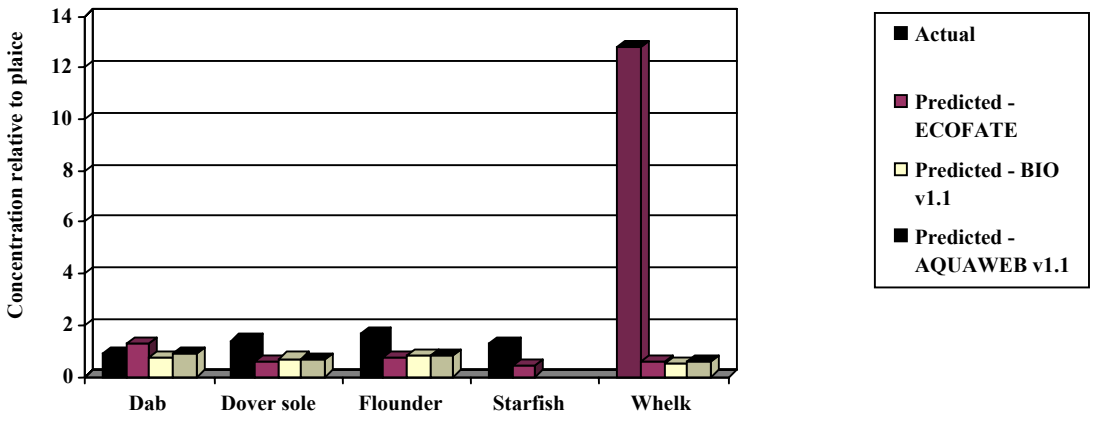

Figure B14 Predicted and actual concentration in biota relative to plaice for PCB 153

The concentration of PCB 153 assumed to be present in the dissolved phase in water from the Mersey estuary for modelling purposes is estimated to be 1.0×10^{-3} µg l^{-1} (see above, Section B1). Predicted BAFs for PCB 153 in the edible portions of plaice were 270,000 l kg^{-1} wet weight using ECOFATE, 93,000 l kg^{-1} wet weight using BIO v1.1 and 1,500,000 l kg^{-1} wet weight using AQUAWEB v1.1

Based on these estimated BAFs and the estimated dissolved concentration in water, the expected concentration of PCB 153 in the edible portion of plaice would be around 270 µg kg^{-1} wet weight using the ECOFATE estimate, 90 µg kg^{-1} wet weight using BIO v1.1 estimate and around 1,500 µg kg^{-1} wet weight using the AQUAWEB v1.1 estimate. The actual concentration of PCB 153 measured in the edible portion of plaice was 2.9 µg kg^{-1} wet weight (see above, Section B1). Therefore, predicted concentrations were around 30 to 500 times higher than the observed concentration. As there was reasonable agreement between predicted and observed concentrations in the other species surveyed relative to the concentration in plaice (see above), it can be concluded that the models would provide a similar level of overprediction of the observed concentration for all the other species to that found for plaice.

PCB 180

The relative concentrations measured and predicted for PCB 180 are shown Figure B15. All three of the models appear to well predict the observed relative concentrations for dab, dover sole, flounder and starfish. The relative concentration in whelk appears to be underpredicted. Overall, with the exception of whelk, predictions of the relative concentration across all species are generally within a factor of two of the observed ratio.

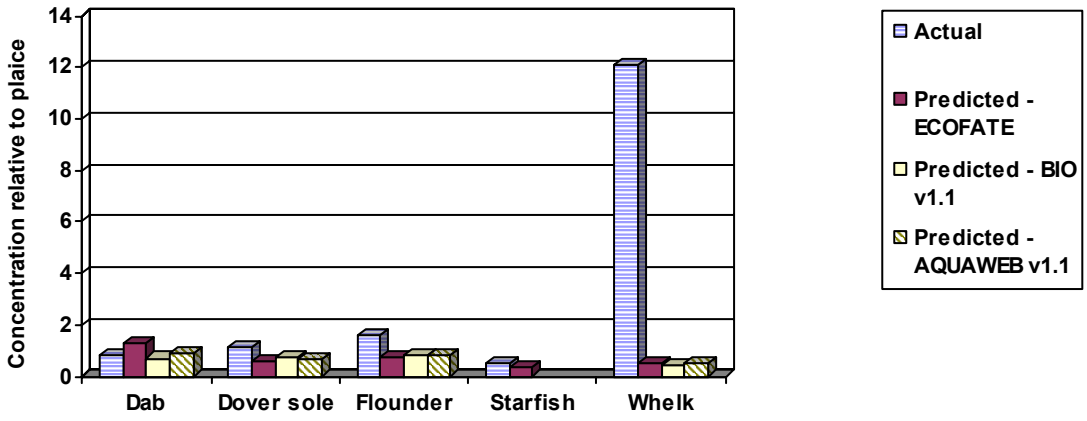

Figure B15 Predicted and actual concentration in biota relative to plaice for PCB 180

The concentration of PCB 180 assumed to be present in the dissolved phase in water from the Mersey estuary for modelling purposes is estimated to be 3.5×10^{-4} µg l^{-1} (see above, Section B1). Predicted BAFs for PCB 180 in the edible portions of plaice were 410,000 l kg^{-1} wet weight using ECOFATE, 130,000 l kg^{-1} wet weight using BIO v1.1 and 1,900,000 l kg^{-1} wet weight using AQUAWEB v1.1

Based on these estimated BAFs and the estimated dissolved concentration in water, the expected concentration of PCB 180 in the edible portion of plaice would be around 140 µg kg^{-1} wet weight using the ECOFATE estimate, 45 µg kg^{-1} wet weight using BIO v1.1 estimate and around 670 µg kg^{-1} wet weight using the AQUAWEB v1.1 estimate. The actual concentration of PCB 180 measured in the edible portion of plaice was 1.4 µg kg^{-1} wet weight (see above, Section B1). Therefore, predicted concentrations were around 30 to 500 times higher than observed concentrations. As there was reasonable agreement between predicted and observed concentrations in the other species surveyed relative to the concentration in plaice (see above), it can be concluded that the models would provide a similar level of overprediction of the observed concentration for all the other species to that found for plaice.

ΣPCBs - ICES

The relative concentrations measured and predicted for ΣPCBs are shown Figure B16. All three of the models appear to well predict the observed relative concentrations for dab, dover sole, flounder, and in one case cod and whiting. Relative concentrations in cod and whiting in some cases appear to be overpredicted to some extent, and the relative concentration in mussel, hermit crab, shrimp and whelk appears to be underpredicted.

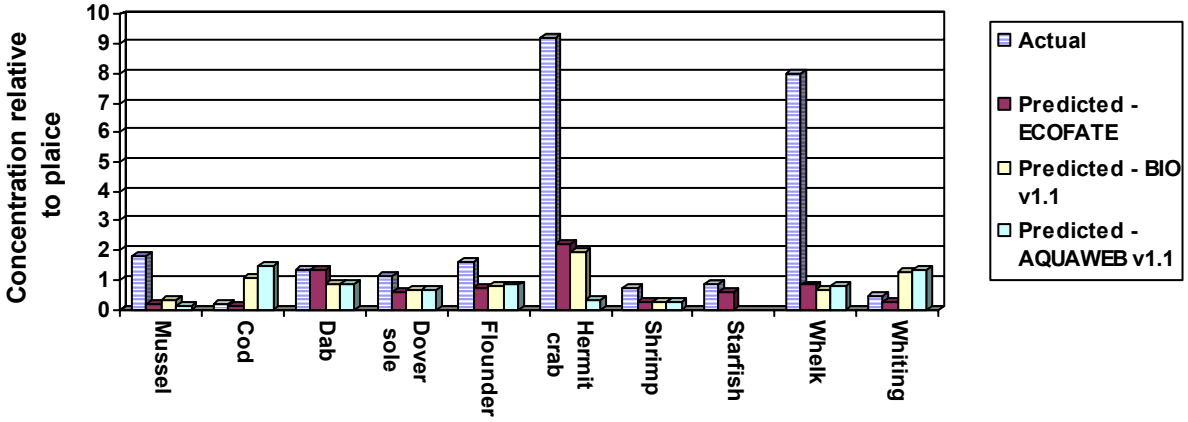

Figure B16 Predicted and actual concentration in biota relative to plaice for ΣPCBs - ICES

The concentration of ΣPCBs assumed to be present in the dissolved phase in water from the Mersey estuary for modelling purposes is estimated to be 0.016 µg l^{-1} (see above, Section B1). Predicted BAFs for ΣPCBs in the edible portions of plaice were 100,000 l kg^{-1} wet weight using ECOFATE, 48,000 l kg^{-1} wet weight using BIO v1.1 and 660,000 l kg^{-1} wet weight using AQUAWEB v1.1

Based on these estimated BAFs and the estimated dissolved concentration in water, the expected concentration of ΣPCBs in the edible portion of plaice would be around 1,600 µg kg^{-1} wet weight using the ECOFATE estimate, 770 µg kg^{-1} wet weight using BIO v1.1 estimate and around 10,500 µg kg^{-1} wet weight using the AQUAWEB v1.1 estimate. The actual concentration of ΣPCBs measured in the edible portion of plaice was between 7.9 and 18.9 µg kg^{-1} wet weight, with a mean value of 11.4 µg kg^{-1} wet weight (see Section B1). Therefore, predicted concentrations were around 70 to 1,000 times higher than observed concentrations. As there was reasonable agreement between predicted and observed concentrations in the other species surveyed relative to the concentration in plaice (see above), it can be concluded that the models would provide a similar level of overprediction of the observed concentration for all the other species to that found for plaice.

Appendix C – BAF data set used in Section 6

As discussed in the main report, Voutsas *et al.* (2002) tabulated a large number of BAF values from literature sources. The data from Oliver and Niimi (1988) are considered in Section 4 of this report. This appendix outlines the other BAFs used in development and testing of the Voutsas *et al.* (2002) method. These data covered a number of species but were separated by Voutsas *et al.* (2002) into four general trophic levels, and this classification has been used here.

Trophic level 1:	Plankton (see Table C1; the TGD method does not provide estimates for this trophic level)
Trophic level 2:	Benthic invertebrates (see Table C2; the TGD method does not provide estimates for this trophic level)
Trophic level 3:	Planktivorous fish (See table C3)
Trophic level 4:	Piscivorous fish (see table C4)

The data used by Voutsas *et al.* (2002) were taken from the following sources: Metcalfe and Metcalfe (1997), Morrison *et al.* (1996), Burkhard *et al.* (1997), van Hattum *et al.* (1998), Kidd *et al.* (1998) and Pereira *et al.* (1988).

The tables of data also list predicted BAF values using the TGD, AQUAWEB and BIO models. These are followed by a full analysis of the predicted results, a subset of which is included in the main report.

Table C1 Experimental and predicted BAFs for trophic level 1

Substance	log K_{ow}[g]	Experimental BAF (l kg^{-1} lipid)		Predicted BAF											
		log BAF_t	log BAF_{fd}	Original Voutsas et al. (2002) method		AQUAWEB v1.1								BIO v1.1[a]	
				log BAF_t	log BAF_{fd}	log BAF_{fd}								log BAF_{fd}	
						a		b		c		d		d	
						Phyt[e]	Zoo[f]	Phyt[e]	Zoo[f]	Phyt[e]	Zoo[f]	Phyt[e]	Zoo[f]	Phyt[e]	Zoo[f]
PCB 18	5.24	6.30	6.35	6.36	6.17	5.96	5.45	5.97	5.46	5.96	5.45	5.97	5.46	5.24	5.24
PCB 28/31	5.60	6.56	6.68	6.60	6.57	6.30	5.82	6.32	5.84	6.30	5.82	6.32	5.84	5.60	5.60
PCB 31	5.67	6.66	6.79	6.64	6.64	6.37	5.90	6.38	5.91	6.37	5.90	6.38	5.91	5.67	5.67
PCB 42	5.60	6.62	6.74	6.60	6.57	6.30	5.82	6.32	5.84	6.30	5.82	6.32	5.84	5.60	5.60
PCB 44	5.75	6.63	6.78	6.69	6.73	6.44	5.98	6.46	6.00	6.44	5.98	6.46	6.00	5.75	5.75
	6.00	6.50	6.75	6.81	6.98	6.65	6.24	6.69	6.28	6.65	6.24	6.69	6.28	6.00	6.00
PCB 49	5.85	6.20	6.39	6.74	6.83	6.52	6.08	6.55	6.11	6.52	6.08	6.55	6.11	5.85	5.85
	6.10	6.40	6.69	6.84	7.07	6.73	6.34	6.77	6.39	6.73	6.34	6.77	6.39	6.10	6.10
PCB 52	5.84	6.47	6.65	6.73	6.82	6.52	6.07	6.54	6.10	6.52	6.07	6.54	6.10	5.84	5.84
	6.10	6.39	6.69	6.84	7.07	6.73	6.34	6.77	6.39	6.73	6.34	6.77	6.39	6.10	6.10
PCB 60	5.90	6.76	6.96	6.76	6.88	6.57	6.14	6.60	6.17	6.57	6.14	6.60	6.17	5.90	5.90
PCB 64	6.10	6.75	7.05	6.84	7.07	6.73	6.34	6.77	6.39	6.73	6.34	6.77	6.39	6.10	6.10
PCB 66	6.20	6.63	6.97	6.88	7.17	6.80	6.44	6.86	6.50	6.80	6.44	6.86	6.50	6.20	6.20
PCB 66/95	5.80	6.76	6.93	6.71	6.78	6.48	6.03	6.50	6.06	6.48	6.03	6.50	6.06	5.80	5.80
PCB 70	5.90	6.42	6.63	6.76	6.88	6.57	6.14	6.60	6.17	6.57	6.14	6.60	6.17	5.90	5.90
PCB 74	6.10	6.66	6.95	6.84	7.07	6.73	6.34	6.77	6.39	6.73	6.34	6.77	6.39	6.10	6.10
PCB 77	6.36	6.26	6.70	6.92	7.31	6.90	6.60	6.98	6.68	6.90	6.60	6.98	6.68	6.36	6.36
PCB 81	6.36	6.19	6.62	6.92	7.31	6.90	6.60	6.98	6.68	6.90	6.60	6.98	6.68	6.36	6.36
PCB 87	6.29	6.48	6.87	6.90	7.25	6.86	6.53	6.93	6.60	6.86	6.53	6.93	6.60	6.29	6.29
	6.50	6.74	7.27	6.95	7.43	6.98	6.72	7.09	6.83	6.98	6.72	7.09	6.83	6.50	6.50
PCB 97	6.60	6.92	7.53	6.97	7.51	7.03	6.80	7.16	6.93	7.03	6.80	7.16	6.93	6.60	6.60
PCB 99	6.39	6.54	6.99	6.93	7.34	6.92	6.63	7.01	6.71	6.92	6.63	7.01	6.71	6.39	6.39

Substance	log K_{ow}[g]	Experimental BAF (l kg^{-1} lipid)		Predicted BAF											
		log BAF_t	log BAF_{fd}	Original Voutsas et al. (2002) method		AQUAWEB v1.1								BIO v1.1[a]	
				log BAF_t	log BAF_{fd}	log BAF_{fd}								log BAF_{fd}	
						a		b		c		d		d	
						Phyt[e]	Zoo[f]	Phyt[e]	Zoo[f]	Phyt[e]	Zoo[f]	Phyt[e]	Zoo[f]	Phyt[e]	Zoo[f]
	6.60	6.90	7.50	6.97	7.51	7.03	6.80	7.16	6.93	7.03	6.80	7.16	6.93	6.60	6.60
PCB 101	6.38	6.49	6.94	6.93	7.33	6.92	6.62	7.00	6.70	6.92	6.62	7.00	6.70	6.38	6.38
	6.40	6.89	7.36	6.93	7.34	6.93	6.64	7.01	6.72	6.93	6.64	7.01	6.72	6.40	6.40
PCB 105	6.40	7.27	7.73	6.93	7.34	6.93	6.64	7.01	6.72	6.93	6.64	7.01	6.72	6.40	6.40
	6.65	6.63	7.27	6.97	7.55	7.04	6.84	7.19	6.99	7.04	6.84	7.19	6.99	6.65	6.65
PCB 110	6.48	6.45	6.97	6.95	7.41	6.97	6.71	7.07	6.81	6.97	6.71	7.07	6.81	6.48	6.48
	6.50	7.05	7.58	6.95	7.43	6.98	6.72	7.09	6.83	6.98	6.72	7.09	6.83	6.50	6.50
PCB 118	6.40	6.95	7.41	6.93	7.34	6.93	6.64	7.01	6.72	6.93	6.64	7.01	6.72	6.40	6.40
	6.74	6.29	7.00	6.98	7.62	7.07	6.90	7.24	7.07	7.07	6.90	7.24	7.07	6.74	6.74
PCB 126	6.89	6.46	7.29	6.99	7.74	7.10	6.99	7.32	7.21	7.10	6.99	7.32	7.21	6.89	6.89
PCB 138	6.83	6.44	7.23	6.99	7.69	7.09	6.96	7.29	7.16	7.09	6.96	7.29	7.16	6.83	6.83
	7.00	7.43	8.36	6.98	7.82	7.10	7.03	7.37	7.31	7.10	7.03	7.37	7.31	7.00	7.00
PCB 146	6.90	7.59	8.44	6.99	7.74	7.10	6.99	7.33	7.22	7.10	6.99	7.33	7.22	6.90	6.90
PCB 149	6.80	7.48	8.24	6.99	7.67	7.08	6.94	7.28	7.13	7.08	6.94	7.28	7.13	6.80	6.80
PCB 151	6.64	6.29	6.92	6.97	7.54	7.04	6.83	7.18	6.98	7.04	6.83	7.18	6.98	6.64	6.64
	6.90	7.44	8.29	6.99	7.74	7.10	6.99	7.33	7.22	7.10	6.99	7.33	7.22	6.90	6.90
PCB 153	6.90	7.51	8.36	6.99	7.74	7.10	6.99	7.33	7.22	7.10	6.99	7.33	7.22	6.90	6.90
	6.92	6.44	7.30	6.99	7.76	7.10	7.00	7.34	7.24	7.10	7.00	7.34	7.24	6.92	6.92
PCB 156	7.18	6.55	7.64	6.97	7.94	7.08	7.08	7.44	7.45	7.08	7.08	7.44	7.45	7.18	7.18
PCB 169	7.42	7.05	8.37	6.92	8.09	6.99	7.09	7.51	7.61	6.99	7.09	7.51	7.61	7.42	7.42
PCB 170	7.27	6.41	7.58	6.95	8.00	7.05	7.09	7.47	7.51	7.05	7.09	7.47	7.51	7.27	7.27
PCB 170/190	7.30	7.70	8.91	6.95	8.02	7.04	7.09	7.48	7.53	7.04	7.09	7.48	7.53	7.30	7.30
PCB 174	7.00	7.78	8.71	6.98	7.82	7.10	7.03	7.37	7.31	7.10	7.03	7.37	7.31	7.00	7.00
PCB 180	7.36	6.40	7.66	6.94	8.05	7.02	7.09	7.50	7.57	7.02	7.09	7.50	7.57	7.36	7.36
	7.40	7.57	8.87	6.93	8.08	7.00	7.09	7.51	7.60	7.00	7.09	7.51	7.60	7.40	7.40
PCB 182/187	7.20	7.69	8.81	6.97	7.95	7.07	7.08	7.45	7.46	7.07	7.08	7.45	7.46	7.20	7.20
PCB 183	7.00	7.63	8.57	6.98	7.82	7.10	7.03	7.37	7.31	7.10	7.03	7.37	7.31	7.00	7.00

Substance	log K_{ow}[g]	Experimental BAF (l kg^{-1} lipid)		Predicted BAF											
		log BAF_t	log BAF_{fd}	Original Voutsas et al. (2002) method		AQUAWEB v1.1								BIO v1.1[a]	
				log BAF_t	log BAF_{fd}	log BAF_{fd}								log BAF_{fd}	
						a		b		c		d		d	
						Phyt[e]	Zoo[f]	Phyt[e]	Zoo[f]	Phyt[e]	Zoo[f]	Phyt[e]	Zoo[f]	Phyt[e]	Zoo[f]
PCB 194	7.80	6.10	7.78	6.80	8.30	6.75	7.01	7.57	7.82	6.75	7.01	7.57	7.82	7.80	7.80
PCB 195	7.56	6.24	7.70	6.88	8.17	6.91	7.07	7.54	7.70	6.91	7.07	7.54	7.70	7.56	7.56
PCB 199	7.20	6.33	7.44	6.97	7.95	7.07	7.08	7.45	7.46	7.07	7.08	7.45	7.46	7.20	7.20
PCB 201	7.50	7.21	8.61	6.90	8.14	6.95	7.08	7.53	7.66	6.95	7.08	7.53	7.66	7.50	7.50
PCB 209	8.18	6.66	8.71	6.61	8.47	6.44	6.83	7.60	7.98	6.44	6.83	7.60	7.98	8.18	8.18

a) Simulation assuming the TGD default QSAR for K_{oc} and the water properties relevant to the Great Lakes.

b) Simulation assuming the TGD default QSAR for K_{oc} and the water properties from the TGD.

c) Simulation assuming the TGD QSAR for predominantly hydrophobics for K_{oc} and the water properties relevant to the Great Lakes.

d) Simulation assuming the TGD QSAR for predominantly hydrophobics for K_{oc} and the water properties from the TGD.

e) Phyt = Predictions for phytoplankton.

f) Zoo = Predictions for zooplankton.

g) As explained in the main text, Voutsas et al. (2002) reports different log K_{ow} values for the same chemicals. The analysis carried out here uses the same log K_{ow} values as Voutsas et al. (2002) in order that the estimates can be compared directly with those using the Voutsas et al. (2002) method.

Table C2 Experimental and predicted BAFs for trophic level 2

Substance	log K_{ow}[g]	Experimental BAF (l kg^{-1} lipid)		Predicted BAF											
		log BAF_t	log BAF_{fd}	Original Voutsas et al. (2002) method		AQUAWEB v1.1								BIO v1.1	
				log BAF_t	log BAF_{fd}	log BAF_{fd}								log BAF_{fd}	
						a		b		c		d		d	
						Zeb[e]	May[f]	Zeb[e]	May[f]	Zeb[e]	May[f]	Zeb[e]	May[f]	Zeb[e]	May[f]
Anthracene	4.54	5.40	5.41	5.12	5.17	4.72	4.66	4.72	4.66	4.73	4.67	4.73	4.68	4.08	4.08
Benzo[a]anthracene	5.61	5.70	5.82	6.45	6.54	5.85	5.72	5.81	5.74	5.87	5.79	5.83	5.81	4.95	4.95
Benzo[b]fluoranthene	5.98	5.90	6.14	6.76	6.96	6.27	6.07	6.21	6.11	6.30	6.19	6.23	6.22	5.25	5.25
Benzo[k]fluoranthene	6.04	6.00	6.26	6.80	7.02	6.34	6.13	6.27	6.17	6.37	6.26	6.29	6.29	5.29	5.29
Benzo[a]pyrene	6.35	6.00	6.43	6.98	7.35	6.67	6.39	6.61	6.47	6.71	6.59	6.63	6.64	5.55	5.55
Chrysene	5.61	5.90	6.02	6.45	6.54	5.85	5.72	5.81	5.74	5.87	5.79	5.83	5.81	4.95	4.95
DDE (p,p'-isomer)	6.51	6.08	6.64	7.05	7.51	6.82	6.51	6.78	6.61	6.86	6.75	6.80	6.82	5.68	5.68
	6.51	5.91	6.47	7.05	7.51	6.82	6.51	6.78	6.61	6.86	6.75	6.80	6.82	5.68	5.68
1,2-Dichlorobenzene	3.43	4.46	4.46	3.02	3.52	3.62	3.56	3.63	3.57	3.63	3.57	3.63	3.58	3.20	3.20
1,3-Dichlorobenzene	3.53	3.86	3.86	3.24	3.68	3.72	3.66	3.73	3.67	3.72	3.67	3.73	3.68	3.28	3.28
1,4-Dichlorobenzene	3.44	4.53	4.53	3.05	3.53	3.63	3.57	3.64	3.58	3.64	3.58	3.64	3.59	3.21	3.21
Fluoranthene	5.22	5.60	5.65	6.05	6.07	5.42	5.33	5.40	5.34	5.44	5.37	5.42	5.38	4.63	4.63
Hexachlorobenzene	5.73	6.71	7.03	6.56	6.68	5.99	5.84	5.94	5.86	6.01	5.92	5.95	5.94	5.04	5.04
Hexachlorobutadiene	4.84	4.53	4.74	5.56	5.58	5.03	4.96	5.02	4.96	5.04	4.98	5.03	4.99	4.32	4.32
	5.60	5.07	5.74	6.44	6.53	5.84	5.71	5.80	5.73	5.86	5.78	5.81	5.79	4.94	4.94
	5.60	4.89	5.56	6.44	6.53	5.84	5.71	5.80	5.73	5.86	5.78	5.81	5.79	4.94	4.94
	5.60	5.84	6.51	6.44	6.53	5.84	5.71	5.80	5.73	5.86	5.78	5.81	5.79	4.94	4.94
	5.60	5.09	5.76	6.44	6.53	5.84	5.71	5.80	5.73	5.86	5.78	5.81	5.79	4.94	4.94
	5.60	6.21	6.88	6.44	6.53	5.84	5.71	5.80	5.73	5.86	5.78	5.81	5.79	4.94	4.94
trans-Nonachlor	6.35	5.71	6.16	6.98	7.35	6.67	6.39	6.61	6.47	6.71	6.59	6.63	6.64	5.55	5.55
	6.35	5.57	6.02	6.98	7.35	6.67	6.39	6.61	6.47	6.71	6.59	6.63	6.64	5.55	5.55
PCB 18	5.24	5.71	5.76	6.07	6.09	5.45	5.35	5.42	5.36	5.46	5.39	5.44	5.40	4.65	4.65
	5.24	5.71	5.77	6.07	6.09	5.45	5.35	5.42	5.36	5.46	5.39	5.44	5.40	4.65	4.65

Substance	log K_{ow}[g]	Experimental BAF (l kg^{-1} lipid)		Predicted BAF											
		log BAF_t	log BAF_{fd}	Original Voutsas et al. (2002) method		AQUAWEB v1.1								BIO v1.1	
				log BAF_t	log BAF_{fd}	log BAF_{fd}								log BAF_{fd}	
						a		b		c		d		d	
						Zeb[e]	May[f]	Zeb[e]	May[f]	Zeb[e]	May[f]	Zeb[e]	May[f]	Zeb[e]	May[f]
	5.24	5.35	5.41	6.07	6.09	5.45	5.35	5.42	5.36	5.46	5.39	5.44	5.40	4.65	4.65
PCB 28/31	5.60	6.60	6.71	6.44	6.53	5.84	5.71	5.80	5.73	5.86	5.78	5.81	5.79	4.94	4.94
	5.60	6.62	6.73	6.44	6.53	5.84	5.71	5.80	5.73	5.86	5.78	5.81	5.79	4.94	4.94
	5.60	6.43	6.55	6.44	6.53	5.84	5.71	5.80	5.73	5.86	5.78	5.81	5.79	4.94	4.94
	5.60	6.46	6.57	6.44	6.53	5.84	5.71	5.80	5.73	5.86	5.78	5.81	5.79	4.94	4.94
PCB 31	5.67	6.08	6.21	6.51	6.61	5.92	5.78	5.87	5.80	5.94	5.85	5.89	5.87	4.99	4.99
	5.67	6.34	6.47	6.51	6.61	5.92	5.78	5.87	5.80	5.94	5.85	5.89	5.87	4.99	4.99
	5.67	5.87	6.00	6.51	6.61	5.92	5.78	5.87	5.80	5.94	5.85	5.89	5.87	4.99	4.99
PCB 42	5.60	6.60	6.72	6.44	6.53	5.84	5.71	5.80	5.73	5.86	5.78	5.81	5.79	4.94	4.94
	5.60	6.73	6.85	6.44	6.53	5.84	5.71	5.80	5.73	5.86	5.78	5.81	5.79	4.94	4.94
PCB 44	5.75	6.31	6.46	6.58	6.70	6.01	5.85	5.96	5.88	6.03	5.94	5.98	5.96	5.06	5.06
	5.75	6.46	6.61	6.58	6.70	6.01	5.85	5.96	5.88	6.03	5.94	5.98	5.96	5.06	5.06
	5.75	5.96	6.12	6.58	6.70	6.01	5.85	5.96	5.88	6.03	5.94	5.98	5.96	5.06	5.06
	6.00	6.62	6.87	6.77	6.98	6.29	6.09	6.23	6.13	6.32	6.21	6.25	6.25	5.26	5.26
	6.00	6.67	6.92	6.77	6.98	6.29	6.09	6.23	6.13	6.32	6.21	6.25	6.25	5.26	5.26
	6.00	6.76	7.01	6.77	6.98	6.29	6.09	6.23	6.13	6.32	6.21	6.25	6.25	5.26	5.26
	6.00	5.81	6.05	6.77	6.98	6.29	6.09	6.23	6.13	6.32	6.21	6.25	6.25	5.26	5.26
PCB 49	5.85	6.32	6.50	6.66	6.81	6.12	5.95	6.07	5.98	6.15	6.05	6.08	6.07	5.14	5.14
	5.85	6.39	6.58	6.66	6.81	6.12	5.95	6.07	5.98	6.15	6.05	6.08	6.07	5.14	5.14
	5.85	5.45	5.63	6.66	6.81	6.12	5.95	6.07	5.98	6.15	6.05	6.08	6.07	5.14	5.14
	6.10	6.55	6.84	6.84	7.09	6.41	6.18	6.34	6.23	6.44	6.32	6.36	6.36	5.34	5.34
	6.10	6.61	6.91	6.84	7.09	6.41	6.18	6.34	6.23	6.44	6.32	6.36	6.36	5.34	5.34
	6.10	6.60	6.89	6.84	7.09	6.41	6.18	6.34	6.23	6.44	6.32	6.36	6.36	5.34	5.34
	6.10	6.04	6.33	6.84	7.09	6.41	6.18	6.34	6.23	6.44	6.32	6.36	6.36	5.34	5.34
PCB 52	5.84	5.96	6.14	6.65	6.80	6.11	5.94	6.06	5.97	6.14	6.04	6.07	6.06	5.13	5.13
	5.84	6.18	6.36	6.65	6.80	6.11	5.94	6.06	5.97	6.14	6.04	6.07	6.06	5.13	5.13
	5.84	5.85	6.03	6.65	6.80	6.11	5.94	6.06	5.97	6.14	6.04	6.07	6.06	5.13	5.13
	6.10	6.54	6.84	6.84	7.09	6.41	6.18	6.34	6.23	6.44	6.32	6.36	6.36	5.34	5.34
	6.10	6.61	6.90	6.84	7.09	6.41	6.18	6.34	6.23	6.44	6.32	6.36	6.36	5.34	5.34
	6.10	6.55	6.85	6.84	7.09	6.41	6.18	6.34	6.23	6.44	6.32	6.36	6.36	5.34	5.34

Substance	log K_{ow}[g]	Experimental BAF (l kg^{-1} lipid)		Predicted BAF											
		log BAF_t	log BAF_{fd}	Original Voutsas et al. (2002) method		AQUAWEB v1.1								BIO v1.1	
				log BAF_t	log BAF_{fd}	log BAF_{fd}								log BAF_{fd}	
						a		b		c		d		d	
						Zeb[e]	May[f]	Zeb[e]	May[f]	Zeb[e]	May[f]	Zeb[e]	May[f]	Zeb[e]	May[f]
	6.10	6.14	6.43	6.84	7.09	6.41	6.18	6.34	6.23	6.44	6.32	6.36	6.36	5.34	5.34
PCB 60	5.90	6.85	7.05	6.70	6.87	6.18	6.00	6.12	6.03	6.21	6.10	6.14	6.13	5.18	5.18
	5.90	6.85	7.06	6.70	6.87	6.18	6.00	6.12	6.03	6.21	6.10	6.14	6.13	5.18	5.18
	5.90	6.68	6.88	6.70	6.87	6.18	6.00	6.12	6.03	6.21	6.10	6.14	6.13	5.18	5.18
PCB 64	6.10	6.94	7.23	6.84	7.09	6.41	6.18	6.34	6.23	6.44	6.32	6.36	6.36	5.34	5.34
	6.10	7.02	7.31	6.84	7.09	6.41	6.18	6.34	6.23	6.44	6.32	6.36	6.36	5.34	5.34
	6.10	6.58	6.87	6.84	7.09	6.41	6.18	6.34	6.23	6.44	6.32	6.36	6.36	5.34	5.34
PCB 66	6.20	6.69	7.03	6.90	7.19	6.52	6.27	6.45	6.32	6.55	6.43	6.47	6.47	5.42	5.42
	6.20	6.91	7.25	6.90	7.19	6.52	6.27	6.45	6.32	6.55	6.43	6.47	6.47	5.42	5.42
	6.20	5.98	6.32	6.90	7.19	6.52	6.27	6.45	6.32	6.55	6.43	6.47	6.47	5.42	5.42
PCB 66/95	5.80	6.71	6.88	6.62	6.76	6.07	5.90	6.01	5.93	6.09	6.00	6.03	6.02	5.10	5.10
	5.80	6.82	6.99	6.62	6.76	6.07	5.90	6.01	5.93	6.09	6.00	6.03	6.02	5.10	5.10
	5.80	6.67	6.84	6.62	6.76	6.07	5.90	6.01	5.93	6.09	6.00	6.03	6.02	5.10	5.10
	5.80	6.39	6.56	6.62	6.76	6.07	5.90	6.01	5.93	6.09	6.00	6.03	6.02	5.10	5.10
PCB 70	5.90	6.42	6.63	6.70	6.87	6.18	6.00	6.12	6.03	6.21	6.10	6.14	6.13	5.18	5.18
	5.90	6.57	6.78	6.70	6.87	6.18	6.00	6.12	6.03	6.21	6.10	6.14	6.13	5.18	5.18
	5.90	6.45	6.66	6.70	6.87	6.18	6.00	6.12	6.03	6.21	6.10	6.14	6.13	5.18	5.18
	5.90	5.70	5.90	6.70	6.87	6.18	6.00	6.12	6.03	6.21	6.10	6.14	6.13	5.18	5.18
PCB 74	6.10	6.90	7.19	6.84	7.09	6.41	6.18	6.34	6.23	6.44	6.32	6.36	6.36	5.34	5.34
	6.10	6.93	7.22	6.84	7.09	6.41	6.18	6.34	6.23	6.44	6.32	6.36	6.36	5.34	5.34
	6.10	7.07	7.36	6.84	7.09	6.41	6.18	6.34	6.23	6.44	6.32	6.36	6.36	5.34	5.34
	6.10	6.66	6.95	6.84	7.09	6.41	6.18	6.34	6.23	6.44	6.32	6.36	6.36	5.34	5.34
PCB 81	6.36	5.96	6.40	6.98	7.36	6.68	6.40	6.62	6.48	6.72	6.60	6.64	6.65	5.55	5.55

Substance	log K_{ow}[g]	Experimental BAF (l kg^{-1} lipid)		Predicted BAF											
		log BAF_t	log BAF_{fd}	Original Voutsas et al. (2002) method		AQUAWEB v1.1								BIO v1.1	
				log BAF_t	log BAF_{fd}	log BAF_{fd}								log BAF_{fd}	
						a		b		c		d		d	
						Zeb[e]	May[f]	Zeb[e]	May[f]	Zeb[e]	May[f]	Zeb[e]	May[f]	Zeb[e]	May[f]
PCB 87	6.29	6.25	6.64	6.95	7.29	6.61	6.34	6.55	6.41	6.65	6.53	6.57	6.58	5.50	5.50
	6.29	6.29	6.68	6.95	7.29	6.61	6.34	6.55	6.41	6.65	6.53	6.57	6.58	5.50	5.50
	6.29	5.91	6.30	6.95	7.29	6.61	6.34	6.55	6.41	6.65	6.53	6.57	6.58	5.50	5.50
	6.50	6.76	7.29	7.05	7.50	6.81	6.50	6.77	6.61	6.85	6.74	6.79	6.81	5.67	5.67
	6.50	6.94	7.47	7.05	7.50	6.81	6.50	6.77	6.61	6.85	6.74	6.79	6.81	5.67	5.67
	6.50	6.95	7.48	7.05	7.50	6.81	6.50	6.77	6.61	6.85	6.74	6.79	6.81	5.67	5.67
	6.50	6.56	7.09	7.05	7.50	6.81	6.50	6.77	6.61	6.85	6.74	6.79	6.81	5.67	5.67
PCB 97	6.60	6.95	7.55	7.08	7.60	6.89	6.57	6.86	6.69	6.94	6.83	6.89	6.91	5.75	5.75
	6.60	7.08	7.69	7.08	7.60	6.89	6.57	6.86	6.69	6.94	6.83	6.89	6.91	5.75	5.75
	6.60	7.01	7.62	7.08	7.60	6.89	6.57	6.86	6.69	6.94	6.83	6.89	6.91	5.75	5.75
	6.60	6.74	7.35	7.08	7.60	6.89	6.57	6.86	6.69	6.94	6.83	6.89	6.91	5.75	5.75
PCB 99	6.39	6.39	6.84	7.00	7.39	6.71	6.42	6.65	6.50	6.75	6.63	6.67	6.69	5.58	5.58
	6.39	6.71	7.16	7.00	7.39	6.71	6.42	6.65	6.50	6.75	6.63	6.67	6.69	5.58	5.58
	6.39	5.97	6.42	7.00	7.39	6.71	6.42	6.65	6.50	6.75	6.63	6.67	6.69	5.58	5.58
	6.60	7.13	7.73	7.08	7.60	6.89	6.57	6.86	6.69	6.94	6.83	6.89	6.91	5.75	5.75
	6.60	7.19	7.80	7.08	7.60	6.89	6.57	6.86	6.69	6.94	6.83	6.89	6.91	5.75	5.75
	6.60	7.28	7.88	7.08	7.60	6.89	6.57	6.86	6.69	6.94	6.83	6.89	6.91	5.75	5.75
	6.60	7.09	7.70	7.08	7.60	6.89	6.57	6.86	6.69	6.94	6.83	6.89	6.91	5.75	5.75
PCB 101	6.38	6.29	6.73	6.99	7.38	6.70	6.41	6.64	6.50	6.74	6.62	6.66	6.68	5.57	5.57
	6.38	6.41	6.85	6.99	7.38	6.70	6.41	6.64	6.50	6.74	6.62	6.66	6.68	5.57	5.57
	6.38	5.85	6.29	6.99	7.38	6.70	6.41	6.64	6.50	6.74	6.62	6.66	6.68	5.57	5.57
	6.40	6.90	7.36	7.00	7.40	6.72	6.43	6.66	6.51	6.76	6.64	6.68	6.70	5.59	5.59
	6.40	7.09	7.55	7.00	7.40	6.72	6.43	6.66	6.51	6.76	6.64	6.68	6.70	5.59	5.59
	6.40	7.11	7.57	7.00	7.40	6.72	6.43	6.66	6.51	6.76	6.64	6.68	6.70	5.59	5.59

Substance	log K_{ow}[g]	Experimental BAF (l kg^{-1} lipid)		Predicted BAF											
		log BAF_t	log BAF_{fd}	Original Voutsas et al. (2002) method		AQUAWEB v1.1								BIO v1.1	
				log BAF_t	log BAF_{fd}	log BAF_{fd}								log BAF_{fd}	
						a		b		c		d		d	
						Zeb[e]	May[f]	Zeb[e]	May[f]	Zeb[e]	May[f]	Zeb[e]	May[f]	Zeb[e]	May[f]
	6.40	6.80	7.26	7.00	7.40	6.72	6.43	6.66	6.51	6.76	6.64	6.68	6.70	5.59	5.59
PCB 105	6.40	7.41	7.87	7.00	7.40	6.72	6.43	6.66	6.51	6.76	6.64	6.68	6.70	5.59	5.59
	6.40	7.62	8.08	7.00	7.40	6.72	6.43	6.66	6.51	6.76	6.64	6.68	6.70	5.59	5.59
	6.40	7.34	7.80	7.00	7.40	6.72	6.40	6.66	6.51	6.76	6.64	6.68	6.70	5.59	5.59
	6.40	7.07	7.54	7.00	7.40	6.72	6.43	6.66	6.51	6.76	6.64	6.68	6.70	5.59	5.59
	6.65	6.49	7.12	7.10	7.65	6.93	6.60	6.91	6.74	6.98	6.88	6.94	6.96	5.79	5.79
	6.65	6.92	7.56	7.10	7.65	6.93	6.60	6.91	6.74	6.98	6.88	6.94	6.96	5.79	5.79
	6.65	6.22	6.86	7.10	7.65	6.93	6.60	6.91	6.74	6.98	6.88	6.94	6.96	5.79	5.79
PCB 110	6.48	6.36	6.87	7.04	7.48	6.79	6.49	6.74	6.59	6.83	6.72	6.77	6.78	5.65	5.65
	6.48	6.46	6.98	7.04	7.48	6.79	6.49	6.74	6.59	6.83	6.72	6.77	6.78	5.65	5.65
	6.48	6.02	6.53	7.04	7.48	6.79	6.49	6.74	6.59	6.83	6.72	6.77	6.78	5.65	5.65
	6.50	7.14	7.67	7.05	7.50	6.81	6.50	6.77	6.61	6.85	6.74	6.79	6.81	5.67	5.67
	6.50	7.20	7.73	7.05	7.50	6.81	6.50	6.77	6.61	6.85	6.74	6.79	6.81	5.67	5.67
	6.50	6.98	7.51	7.05	7.50	6.81	6.50	6.77	6.61	6.85	6.74	6.79	6.81	5.67	5.67
	6.50	6.48	7.01	7.05	7.50	6.81	6.50	6.77	6.61	6.85	6.74	6.79	6.81	5.67	5.67
PCB 118	6.40	7.33	7.79	7.00	7.40	6.72	6.43	6.66	6.51	6.76	6.64	6.68	6.70	5.59	5.59
	6.40	7.37	7.84	7.00	7.40	6.72	6.43	6.66	6.51	6.76	6.64	6.68	6.70	5.59	5.59
	6.40	7.60	8.07	7.00	7.40	6.72	6.43	6.66	6.51	6.76	6.64	6.68	6.70	5.59	5.59
	6.40	7.28	7.74	7.00	7.40	6.72	6.43	6.66	6.51	6.76	6.64	6.68	6.70	5.59	5.59
	6.74	6.19	6.90	7.13	7.73	6.99	6.64	7.00	6.81	7.04	6.96	7.02	7.05	5.86	5.86
	6.74	6.16	6.87	7.13	7.73	6.99	6.64	7.00	6.81	7.04	6.96	7.02	7.05	5.86	5.86
	6.74	5.74	6.45	7.13	7.73	6.99	6.64	7.00	6.81	7.04	6.96	7.02	7.05	5.86	5.86
PCB 126	6.89	5.70	6.53	7.16	7.87	7.06	6.71	7.12	6.92	7.13	7.07	7.15	7.18	5.98	5.98

Substance	log K_{ow}[g]	Experimental BAF (l kg^{-1} lipid)		Predicted BAF											
		log BAF_t	log BAF_{fd}	Original Voutsas et al. (2002) method		AQUAWEB v1.1								BIO v1.1	
				log BAF_t	log BAF_{fd}	log BAF_{fd}								log BAF_{fd}	
						a		b		c		d		d	
						Zeb[e]	May[f]	Zeb[e]	May[f]	Zeb[e]	May[f]	Zeb[e]	May[f]	Zeb[e]	May[f]
	6.89	5.61	6.44	7.16	7.87	7.06	6.71	7.12	6.92	7.13	7.07	7.15	7.18	5.98	5.98
PCB 138	6.83	6.51	7.29	7.15	7.82	7.03	6.69	7.07	6.88	7.10	7.03	7.10	7.13	5.93	5.93
	6.83	6.54	7.32	7.15	7.82	7.03	6.69	7.07	6.88	7.10	7.03	7.10	7.13	5.93	5.93
	6.83	6.07	6.85	7.15	7.82	7.03	6.69	7.07	6.88	7.10	7.03	7.10	7.13	5.93	5.93
	7.00	7.73	8.67	7.17	7.97	7.09	6.74	7.20	7.00	7.17	7.15	7.23	7.27	6.07	6.07
	7.00	7.83	8.77	7.17	7.97	7.09	6.74	7.20	7.00	7.17	7.15	7.23	7.27	6.07	6.07
	7.00	7.89	8.82	7.17	7.97	7.09	6.74	7.20	7.00	7.17	7.15	7.23	7.27	6.07	6.07
	7.00	7.68	8.61	7.17	7.97	7.09	6.74	7.20	7.00	7.17	7.15	7.23	7.27	6.07	6.07
PCB 146	6.90	7.90	8.75	7.16	7.88	7.06	6.71	7.13	6.93	7.13	7.08	7.16	7.19	5.99	5.99
	6.90	7.99	8.84	7.16	7.88	7.06	6.71	7.13	6.93	7.13	7.08	7.16	7.19	5.99	5.99
	6.90	8.26	9.10	7.16	7.88	7.06	6.71	7.13	6.93	7.13	7.08	7.16	7.19	5.99	5.99
	6.90	7.86	8.70	7.16	7.88	7.06	6.71	7.13	6.93	7.13	7.08	7.16	7.19	5.99	5.99
PCB 149	6.80	7.51	8.27	7.14	7.79	7.02	6.67	7.05	6.86	7.08	7.00	7.07	7.10	5.91	5.91
	6.80	7.65	8.42	7.14	7.79	7.02	6.67	7.05	6.86	7.08	7.00	7.07	7.10	5.91	5.91
	6.80	7.55	8.32	7.14	7.79	7.02	6.67	7.05	6.86	7.08	7.00	7.07	7.10	5.91	5.91
	6.80	7.17	7.94	7.14	7.79	7.02	6.67	7.05	6.86	7.08	7.00	7.07	7.10	5.91	5.91
PCB 151	6.64	6.33	6.96	7.10	7.64	6.92	6.59	6.90	6.73	6.97	6.87	6.93	6.95	5.78	5.78
	6.64	6.39	7.03	7.10	7.64	6.92	6.59	6.90	6.73	6.97	6.87	6.93	6.95	5.78	5.78
	6.64	5.67	6.30	7.10	7.64	6.92	6.59	6.90	6.73	6.97	6.87	6.93	6.95	5.78	5.78
	6.90	7.53	8.38	7.16	7.88	7.06	6.71	7.13	6.93	7.13	7.08	7.16	7.19	5.99	5.99
	6.90	7.61	8.46	7.16	7.88	7.06	6.71	7.13	6.93	7.13	7.08	7.16	7.19	5.99	5.99
	6.90	7.58	8.42	7.16	7.88	7.06	6.71	7.13	6.93	7.13	7.08	7.16	7.19	5.99	5.99
	6.90	7.27	8.12	7.16	7.88	7.06	6.71	7.13	6.93	7.13	7.08	7.16	7.19	5.99	5.99
PCB 153	6.90	7.83	8.68	7.16	7.88	7.06	6.71	7.13	6.93	7.13	7.08	7.16	7.19	5.99	5.99
	6.90	7.96	8.80	7.16	7.88	7.06	6.71	7.13	6.93	7.13	7.08	7.16	7.19	5.99	5.99
	6.90	8.01	8.86	7.16	7.88	7.06	6.71	7.13	6.93	7.13	7.08	7.16	7.19	5.99	5.99
	6.90	7.79	8.63	7.16	7.88	7.06	6.71	7.13	6.93	7.13	7.08	7.16	7.19	5.99	5.99
	6.92	6.46	7.32	7.16	7.90	7.07	7.07	7.14	6.94	7.14	7.10	7.17	7.21	6.01	6.01
	6.92	6.48	7.34	7.16	7.90	7.07	7.07	7.14	6.94	7.14	7.10	7.17	7.21	6.01	6.01

Substance	log K_{ow}[g]	Experimental BAF (l kg^{-1} lipid)		Predicted BAF											
		log BAF_t	log BAF_{fd}	Original Voutsas et al. (2002) method		AQUAWEB v1.1								BIO v1.1	
				log BAF_t	log BAF_{fd}	log BAF_{fd}								log BAF_{fd}	
						a		b		c		d		d	
						Zeb[e]	May[f]	Zeb[e]	May[f]	Zeb[e]	May[f]	Zeb[e]	May[f]	Zeb[e]	May[f]
	6.92	5.98	6.84	7.16	7.90	7.07	7.07	7.14	6.94	7.14	7.10	7.17	7.21	6.01	6.01
PCB 156	7.18	6.33	7.42	7.18	8.13	7.11	6.77	7.32	7.11	7.21	7.25	7.35	7.40	6.22	6.22
	7.18	6.50	7.59	7.18	8.13	7.11	6.77	7.32	7.11	7.21	7.25	7.35	7.40	6.22	6.22
	7.18	5.87	6.96	7.18	8.13	7.11	6.77	7.32	7.11	7.21	7.25	7.35	7.40	6.22	6.22
PCB 169	7.42	6.22	7.53	7.17	8.33	7.06	6.75	7.44	7.22	7.22	7.35	7.47	7.53	6.41	6.41
PCB 170	7.27	6.28	7.45	7.18	8.21	7.10	6.77	7.37	7.15	7.22	7.30	7.40	7.45	6.29	6.29
	7.27	6.58	7.76	7.18	8.21	7.10	6.77	7.37	7.15	7.22	7.30	7.40	7.45	6.29	6.29
	7.27	6.02	7.20	7.18	8.21	7.10	6.77	7.37	7.15	7.22	7.30	7.40	7.45	6.29	6.29
PCB 170/190	7.30	8.16	9.37	7.18	8.23	7.09	6.77	7.38	7.17	7.22	7.31	7.42	7.47	6.31	6.31
	7.30	8.24	9.45	7.18	8.23	7.09	6.77	7.38	7.17	7.22	7.31	7.42	7.47	6.31	6.31
	7.30	8.30	9.51	7.18	8.23	7.09	6.77	7.38	7.17	7.22	7.31	7.42	7.47	6.31	6.31
	7.30	8.02	9.23	7.18	8.23	7.09	6.77	7.38	7.17	7.22	7.31	7.42	7.47	6.31	6.31
PCB 174	7.00	8.03	8.96	7.17	7.97	7.09	6.74	7.20	7.00	7.17	7.15	7.23	7.27	6.07	6.07
	7.00	8.17	9.10	7.17	7.97	7.09	6.74	7.20	7.00	7.17	7.15	7.23	7.27	6.07	6.07
	7.00	8.07	9.01	7.17	7.97	7.09	6.74	7.20	7.00	7.17	7.15	7.23	7.27	6.07	6.07
	7.00	7.81	8.75	7.17	7.97	7.09	6.74	7.20	7.00	7.17	7.15	7.23	7.27	6.07	6.07
PCB 180	7.36	6.39	7.65	7.18	8.28	7.08	6.76	7.41	7.20	7.22	7.33	7.44	7.50	6.36	6.36
	7.36	6.48	7.74	7.18	8.28	7.08	6.76	7.41	7.20	7.22	7.33	7.44	7.50	6.36	6.36
	7.36	6.14	7.40	7.18	8.28	7.08	6.76	7.41	7.20	7.22	7.33	7.44	7.50	6.36	6.36
	7.40	8.03	9.34	7.17	8.31	7.07	6.76	7.43	7.21	7.22	7.35	7.46	7.52	6.39	6.39
	7.40	8.12	9.42	7.17	8.31	7.07	6.76	7.43	7.21	7.22	7.35	7.46	7.52	6.39	6.39
	7.40	8.21	9.51	7.17	8.31	7.07	6.76	7.43	7.21	7.22	7.35	7.46	7.52	6.39	6.39
	7.40	7.99	9.30	7.17	8.31	7.07	6.76	7.43	7.21	7.22	7.35	7.46	7.52	6.39	6.39
PCB 182/187	7.20	8.08	9.19	7.18	8.15	7.11	6.77	7.33	7.12	7.21	7.26	7.36	7.41	6.23	6.23
	7.20	8.17	9.29	7.18	8.15	7.11	6.77	7.33	7.12	7.21	7.26	7.36	7.41	6.23	6.23
	7.20	8.26	9.38	7.18	8.15	7.11	6.77	7.33	7.12	7.21	7.26	7.36	7.41	6.23	6.23

Substance	log K_{ow}[g]	Experimental BAF (l kg^{-1} lipid)		Predicted BAF											
		log BAF_t	log BAF_{fd}	Original Voutsas et al. (2002) method		AQUAWEB v1.1								BIO v1.1	
				log BAF_t	log BAF_{fd}	log BAF_{fd}								log BAF_{fd}	
						a		b		c		d		d	
						Zeb[e]	May[†]	Zeb[e]	May[†]	Zeb[e]	May[†]	Zeb[e]	May[†]	Zeb[e]	May[†]
	7.20	8.04	9.16	7.18	8.15	7.11	6.77	7.33	7.12	7.21	7.26	7.36	7.41	6.23	6.23
PCB 183	7.00	7.98	8.91	7.17	7.97	7.09	6.74	7.20	7.00	7.17	7.15	7.23	7.27	6.07	6.07
	7.00	8.11	9.04	7.17	7.97	7.09	6.74	7.20	7.00	7.17	7.15	7.23	7.27	6.07	6.07
	7.00	8.24	9.18	7.17	7.97	7.09	6.74	7.20	7.00	7.17	7.15	7.23	7.27	6.07	6.07
	7.00	7.79	8.73	7.17	7.97	7.09	6.74	7.20	7.00	7.17	7.15	7.23	7.27	6.07	6.07
PCB 194	7.80	6.03	7.71	7.07	8.62	6.85	6.63	7.55	7.34	7.17	7.43	7.59	7.66	6.72	6.72
	7.80	6.40	8.08	7.07	8.62	6.85	6.63	7.55	7.34	7.17	7.43	7.59	7.66	6.72	6.72
	7.80	6.12	7.80	7.07	8.62	6.85	6.63	7.55	7.34	7.17	7.43	7.59	7.66	6.72	6.72
PCB 195	7.56	6.12	7.57	7.14	8.44	7.00	6.72	7.49	7.27	7.21	7.40	7.52	7.59	6.53	6.53
	7.56	6.61	8.06	7.14	8.44	7.00	6.72	7.49	7.27	7.21	7.40	7.52	7.59	6.53	6.53
	7.56	6.22	7.67	7.14	8.44	7.00	6.72	7.49	7.27	7.21	7.40	7.52	7.59	6.53	6.53
PCB 199	7.20	6.20	7.31	7.18	8.15	7.11	6.77	7.33	7.12	7.21	7.26	7.36	7.41	6.23	6.23
	7.20	6.44	7.55	7.18	8.15	7.11	6.77	7.33	7.12	7.21	7.26	7.36	7.41	6.23	6.23
	7.20	6.02	7.13	7.18	8.15	7.11	6.77	7.33	7.12	7.21	7.26	7.36	7.41	6.23	6.23
PCB 201	7.50	7.59	8.99	7.15	8.39	7.03	6.74	7.47	7.25	7.21	7.38	7.50	7.57	6.48	6.48
	7.50	7.72	9.12	7.15	8.39	7.03	6.74	7.47	7.25	7.21	7.38	7.50	7.57	6.48	6.48
	7.50	7.72	9.12	7.15	8.39	7.03	6.74	7.47	7.25	7.21	7.38	7.50	7.57	6.48	6.48
	7.50	7.54	8.94	7.15	8.39	7.03	6.74	7.47	7.25	7.21	7.38	7.50	7.57	6.48	6.48
PCB 209	8.18	6.24	8.30	6.89	8.89	6.55	6.42	7.60	7.40	7.09	7.44	7.64	7.70	7.03	7.03
	8.18	6.54	8.60	6.89	8.89	6.55	6.42	7.60	7.40	7.09	7.44	7.64	7.70	7.03	7.03
	8.18	6.61	8.67	6.89	8.89	6.55	6.42	7.60	7.40	7.09	7.44	7.64	7.70	7.03	7.03
Pentachlorobenzene	5.11	4.91	5.25	5.92	5.93	5.31	5.23	5.29	5.23	5.32	5.26	5.30	5.27	4.54	4.54
	5.11	5.00	5.34	5.92	5.93	5.31	5.23	5.29	5.23	5.32	5.26	5.30	5.27	4.54	4.54
	5.11	4.97	5.31	5.92	5.93	5.31	5.23	5.29	5.23	5.32	5.26	5.30	5.27	4.54	4.54
	5.11	5.82	6.17	5.92	5.93	5.31	5.23	5.29	5.23	5.32	5.26	5.30	5.27	4.54	4.54
	5.11	4.89	5.24	5.92	5.93	5.31	5.23	5.29	5.23	5.32	5.26	5.30	5.27	4.54	4.54
	5.11	5.62	5.96	5.92	5.93	5.31	5.23	5.29	5.23	5.32	5.26	5.30	5.27	4.54	4.54

Substance	log K_{ow}[g]	Experimental BAF (l kg^{-1} lipid)		Predicted BAF											
		log BAF_t	log BAF_{fd}	Original Voutsas et al. (2002) method		AQUAWEB v1.1								BIO v1.1	
				log BAF_t	log BAF_{fd}	log BAF_{fd}								log BAF_{fd}	
						a		b		c		d		d	
						Zeb[e]	May[f]	Zeb[e]	May[f]	Zeb[e]	May[f]	Zeb[e]	May[f]	Zeb[e]	May[f]
	5.18	6.12	6.23	6.00	6.02	5.38	5.30	5.36	5.30	5.40	5.33	5.38	5.34	4.60	4.60
	4.54	4.84	4.96	5.12	5.17	4.72	4.66	4.72	4.66	4.73	4.67	4.73	4.68	4.08	4.08
E-Pentachloro butadiene	4.54	4.51	4.63	5.12	5.17	4.72	4.66	4.72	4.66	4.73	4.67	4.73	4.68	4.08	4.08
Phenanthrene	4.57	5.20	5.21	5.17	5.22	4.75	4.69	4.75	4.69	4.76	4.76	4.76	4.71	4.11	4.11
Pyrene	5.18	5.80	5.85	6.00	6.02	5.38	5.30	5.36	5.30	5.40	5.33	5.38	5.34	4.60	4.60
Tetrachlorobenzene (mixture of isomers)	4.60	4.69	4.83	5.21	5.26	4.78	4.72	4.78	4.72	4.79	4.73	4.79	4.74	4.13	4.13
	4.60	4.82	4.96	5.21	5.26	4.78	4.72	4.78	4.72	4.79	4.73	4.79	4.74	4.13	4.13
	4.60	4.91	5.04	5.21	5.26	4.78	4.72	4.78	4.72	4.79	4.73	4.79	4.74	4.13	4.13
	4.60	5.59	5.73	5.21	5.26	4.78	4.72	4.78	4.72	4.79	4.73	4.79	4.74	4.13	4.13
	4.60	4.73	4.86	5.21	5.26	4.78	4.72	4.78	4.72	4.79	4.73	4.79	4.74	4.13	4.13
	4.60	5.08	5.22	5.21	5.26	4.78	4.72	4.78	4.72	4.79	4.73	4.79	4.74	4.13	4.13
1,2,3,4-Tetrachloro benzene	4.59	4.66	4.79	5.20	5.24	4.77	4.71	4.77	4.71	4.78	4.72	4.78	4.73	4.12	4.12
	4.59	4.82	4.95	5.20	5.24	4.77	4.71	4.77	4.71	4.78	4.72	4.78	4.73	4.12	4.12
	4.59	4.92	5.06	5.20	5.24	4.77	4.71	4.77	4.71	4.78	4.72	4.78	4.73	4.12	4.12
	4.59	5.54	5.67	5.20	5.24	4.77	4.71	4.77	4.71	4.78	4.72	4.78	4.73	4.12	4.12
	4.59	4.58	4.72	5.20	5.24	4.77	4.71	4.77	4.71	4.78	4.72	4.78	4.73	4.12	4.12
	4.59	5.14	5.27	5.20	5.24	4.77	4.71	4.77	4.71	4.78	4.72	4.78	4.73	4.12	4.12
1,2,3,5-Tetrachloro benzene	4.62	5.20	5.23	5.24	5.28	4.80	4.74	4.80	4.74	4.81	4.75	4.81	4.76	4.15	4.15
1,2,4,5-Tetrachloro benzene	4.64	5.70	5.74	5.27	5.31	4.82	4.76	4.82	4.76	4.83	4.77	4.83	4.78	4.16	4.16
Z-1,1,2,4-Tetrachloro butadiene	4.23	4.61	4.67	4.61	4.74	4.41	4.35	4.41	4.35	4.42	4.36	4.42	4.37	3.83	3.83
	4.23	4.33	4.40	4.61	4.74	4.41	4.35	4.41	4.35	4.42	4.36	4.42	4.37	3.83	3.83
1,1,4,4-Tetrachloro butadiene	4.29	4.36	4.43	4.71	4.82	4.47	4.41	4.47	4.41	4.48	4.42	4.48	4.43	3.88	3.88
	4.29	4.72	4.79	4.71	4.82	4.47	4.41	4.47	4.41	4.48	4.42	4.48	4.43	3.88	3.88

Substance	log K_{ow}[g]	Experimental BAF (l kg^{-1} lipid)		Predicted BAF											
		log BAF_t	log BAF_{fd}	Original Voutsas et al. (2002) method		AQUAWEB v1.1								BIO v1.1	
				log BAF_t	log BAF_{fd}	log BAF_{fd}								log BAF_{fd}	
						a		b		c		d		d	
						Zeb[e]	May[f]	Zeb[e]	May[f]	Zeb[e]	May[f]	Zeb[e]	May[f]	Zeb[e]	May[f]
	4.29	4.48	4.55	4.71	4.82	4.47	4.41	4.47	4.41	4.48	4.42	4.48	4.43	3.88	3.88
1,2,3-Trichloro benzene	4.09	4.29	4.34	4.36	4.53	4.27	4.21	4.27	4.22	4.28	4.22	4.28	4.23	3.72	3.72
	4.09	4.51	4.56	4.36	4.53	4.27	4.21	4.27	4.22	4.28	4.22	4.28	4.23	3.72	3.72
	4.09	4.70	4.75	4.36	4.53	4.27	4.21	4.27	4.22	4.28	4.22	4.28	4.23	3.72	3.72
	4.09	5.09	5.14	4.36	4.53	4.27	4.21	4.27	4.22	4.28	4.22	4.28	4.23	3.72	3.72
	4.09	4.33	4.38	4.36	4.53	4.27	4.21	4.27	4.22	4.28	4.22	4.28	4.23	3.72	3.72
	4.09	4.76	4.81	4.36	4.53	4.27	4.21	4.27	4.22	4.28	4.22	4.28	4.23	3.72	3.72
	4.14	4.77	4.78	4.45	4.60	4.32	4.26	4.32	4.26	4.33	4.27	4.33	4.28	3.76	3.76
1,2,4-Trichloro benzene	4.02	4.90	4.91	4.23	4.43	4.20	4.14	4.20	4.15	4.21	4.15	4.21	4.16	3.66	3.66
	4.02	4.13	4.17	4.23	4.43	4.20	4.14	4.20	4.15	4.21	4.15	4.21	4.16	3.66	3.66
	4.02	4.39	4.43	4.23	4.43	4.20	4.14	4.20	4.15	4.21	4.15	4.21	4.16	3.66	3.66
	4.02	4.79	4.83	4.23	4.43	4.20	4.14	4.20	4.15	4.21	4.15	4.21	4.16	3.66	3.66
	4.02	5.19	5.23	4.23	4.43	4.20	4.14	4.20	4.15	4.21	4.15	4.21	4.16	3.66	3.66
	4.02	4.18	4.22	4.23	4.43	4.20	4.14	4.20	4.15	4.21	4.15	4.21	4.16	3.66	3.66
	4.02	4.77	4.81	4.23	4.43	4.20	4.14	4.20	4.15	4.21	4.15	4.21	4.16	3.66	3.66
1,3,5-Trichloro benzene	4.19	4.45	4.46	4.54	4.68	4.37	4.31	4.37	4.31	4.38	4.32	4.38	4.33	3.80	3.80

a) Simulation assuming the TGD default QSAR for K_{oc} and the water properties relevant to the Great Lakes.
b) Simulation assuming the TGD default QSAR for K_{oc} and the water properties from the TGD.
c) Simulation assuming the TGD QSAR for predominantly hydrophobics for K_{oc} and the water properties relevant to the Great Lakes.
d) Simulation assuming the TGD QSAR for predominantly hydrophobics for K_{oc} and the water properties from the TGD.
e) Zeb = Predictions for zebra mussel.
f) May = Predictions for mayfly larvae.
g) As explained in the main text, Voutsas et al. (2002) reports different log K_{ow} values for the same chemicals. The analysis carried out here uses the same log K_{ow} values as Voutsas et al. (2002) in order that the estimates can be compared directly with those using the Voutsas et al. (2002) method.

Table C3 Experimental and predicted BAFs for trophic level 3

Substance	log K_{ow}[g]	Experimental BAF (l kg^{-1} lipid)		Predicted BAF (l kg^{-1} lipid)										
		log BAF_t	log BAF_{fd}	Original Voutsas et al. (2002) method		TGD method[h]				AQUAWEB v1.1[a]				BIO v1.1[a]
				log BAF_t	log BAF_{fd}	log BAF_t		log BAF_{fd}		log BAF_{fd}				log BAF_{fd}
						BMF_1[e]	BMF_2[f]	BMF_1[e]	BMF_2[f]	a	b	c	d	d
DDE (p,p'-isomer)	6.51	7.13	7.54	7.30	7.69	6.64	7.64	6.77	7.77	6.91	7.02	6.91	7.02	6.31
	6.51	6.78	7.20	7.30	7.69	6.64	7.64	6.77	7.77	6.91	7.02	6.91	7.02	6.31
1,2-Dichlorobenzene	3.43	3.94	3.94	2.88	3.34	3.35	3.35	3.35	3.35	3.47	3.47	3.47	3.47	3.44
1,3-Dichlorobenzene	3.53	3.60	3.60	3.10	3.51	3.43	3.43	3.43	3.43	3.57	3.57	3.57	3.57	3.54
1,4-Dichlorobenzene	3.44	3.91	3.91	2.90	3.36	3.35	3.35	3.35	3.35	3.48	3.48	3.48	3.48	3.45
Hexachlorobenzene	5.73	6.42	6.74	6.66	6.77	6.27	7.27	6.30	7.30	6.03	6.05	6.03	6.05	5.61
	4.84	5.43	5.64	5.54	5.56	4.84	5.14	4.85	5.15	4.94	4.95	4.94	4.95	4.81
	4.84	6.06	6.28	5.54	5.56	4.84	5.14	4.85	5.15	4.94	4.95	4.94	4.95	4.81
	4.84	5.47	5.69	5.54	5.56	4.84	5.14	4.85	5.15	4.94	4.95	4.94	4.95	4.81
	4.84	6.66	6.88	5.54	5.56	4.84	5.14	4.85	5.15	4.94	4.95	4.94	4.95	4.81
	4.84	4.91	5.13	5.54	5.56	4.84	5.14	4.85	5.15	4.94	4.95	4.94	4.95	4.81
	4.84	5.97	6.19	5.54	5.56	4.84	5.14	4.85	5.15	4.94	4.95	4.94	4.95	4.81
	4.84	4.64	4.86	5.54	5.56	4.84	5.14	4.85	5.15	4.94	4.95	4.94	4.95	4.81
	4.84	5.66	5.88	5.54	5.56	4.84	5.14	4.85	5.15	4.94	4.95	4.94	4.95	4.81
	4.84	5.29	5.51	5.54	5.56	4.84	5.14	4.85	5.15	4.94	4.95	4.94	4.95	4.81
	4.84	5.68	5.89	5.54	5.56	4.84	5.14	4.85	5.15	4.94	4.95	4.94	4.95	4.81
	5.60	5.07	5.74	6.53	6.60	6.16	7.16	6.19	7.19	5.87	5.88	5.87	5.88	5.50
	5.60	5.38	6.05	6.53	6.60	6.16	7.16	6.19	7.19	5.87	5.88	5.87	5.88	5.50
	5.60	5.20	5.87	6.53	6.60	6.16	7.16	6.19	7.19	5.87	5.88	5.87	5.88	5.50
	5.60	6.68	7.35	6.53	6.60	6.16	7.16	6.19	7.19	5.87	5.88	5.87	5.88	5.50
	5.60	5.28	5.95	6.53	6.60	6.16	7.16	6.19	7.19	5.87	5.88	5.87	5.88	5.50
	5.60	6.32	6.99	6.53	6.60	6.16	7.16	6.19	7.19	5.87	5.88	5.87	5.88	5.50
	5.60	6.22	6.90	6.53	6.60	6.16	7.16	6.19	7.19	5.87	5.88	5.87	5.88	5.50
	5.60	5.65	6.33	6.53	6.60	6.16	7.16	6.19	7.19	5.87	5.88	5.87	5.88	5.50

Substance	log K_{ow}[g]	Experimental BAF (l kg^{-1} lipid)		Predicted BAF (l kg^{-1} lipid)										
		log BAF_t	log BAF_{fd}	Original Voutsas et al. (2002) method		TGD method[h]				AQUAWEB v1.1[a]				BIO v1.1[a]
				log BAF_t	log BAF_{fd}	log BAF_t		log BAF_{fd}		log BAF_{fd}				log BAF_{fd}
						BMF_1[e]	BMF_2[f]	BMF_1[e]	BMF_2[f]	a	b	c	d	d
	5.60	6.58	7.26	6.53	6.60	6.16	7.16	6.19	7.19	5.87	5.88	5.87	5.88	5.50
Hexachloroethane	4.14	4.26	4.31	4.35	4.51	3.95	3.95	3.95	3.95	4.19	4.19	4.19	4.19	4.14
	4.14	4.45	4.50	4.35	4.51	3.95	3.95	3.95	3.95	4.19	4.19	4.19	4.19	4.14
	4.14	4.26	4.31	4.35	4.51	3.95	3.95	3.95	3.95	4.19	4.19	4.19	4.19	4.14
	4.14	5.29	5.34	4.35	4.51	3.95	3.95	3.95	3.95	4.19	4.19	4.19	4.19	4.14
	4.14	3.90	3.95	4.35	4.51	3.95	3.95	3.95	3.95	4.19	4.19	4.19	4.19	4.14
	4.14	4.71	4.76	4.35	4.51	3.95	3.95	3.95	3.95	4.19	4.19	4.19	4.19	4.14
	4.14	4.08	4.13	4.35	4.51	3.95	3.95	3.95	3.95	4.19	4.19	4.19	4.19	4.14
	4.14	4.04	4.09	4.35	4.51	3.95	3.95	3.95	3.95	4.19	4.19	4.19	4.19	4.14
	4.14	4.49	4.55	4.35	4.51	3.95	3.95	3.95	3.95	4.19	4.19	4.19	4.19	4.14
trans-Nonachlor	6.35	6.95	7.28	7.19	7.51	6.64	7.64	6.75	7.75	6.77	6.84	6.77	6.84	6.16
	6.35	6.89	7.21	7.19	7.51	6.64	7.64	6.75	7.75	6.77	6.84	6.77	6.84	6.16
PCB 18	5.24	5.64	5.69	6.10	6.12	5.87	6.87	5.88	6.88	5.41	5.42	5.41	5.42	5.18
	5.24	6.32	6.37	6.10	6.12	5.87	6.87	5.88	6.88	5.41	5.42	5.41	5.42	5.18
	5.24	6.38	6.43	6.10	6.12	5.87	6.87	5.88	6.88	5.41	5.42	5.41	5.42	5.18
PCB 31	5.67	5.85	5.98	6.60	6.69	6.22	7.22	6.25	7.25	5.96	5.97	5.96	5.97	5.56
	5.67	6.36	6.49	6.60	6.69	6.22	7.22	6.25	7.25	5.96	5.97	5.96	5.97	5.56
	5.67	6.49	6.62	6.60	6.69	6.22	7.22	6.25	7.25	5.96	5.97	5.96	5.97	5.56
PCB 44	5.75	7.23	7.38	6.68	6.79	6.28	7.28	6.32	7.32	6.06	6.08	6.06	6.08	5.62
	5.75	7.01	7.17	6.68	6.79	6.28	7.28	6.32	7.32	6.06	6.08	6.06	6.08	5.62
	5.75	7.12	7.28	6.68	6.79	6.28	7.28	6.32	7.32	6.06	6.08	6.06	6.08	5.62
PCB 49	5.85	6.67	6.85	6.78	6.92	6.36	7.36	6.40	7.40	6.18	6.21	6.18	6.21	5.71
	5.85	6.69	6.88	6.78	6.92	6.36	7.36	6.40	7.40	6.18	6.21	6.18	6.21	5.71
	5.85	6.65	6.83	6.78	6.92	6.36	7.36	6.40	7.40	6.18	6.21	6.18	6.21	5.71
PCB 52	5.84	6.80	6.98	6.77	6.90	6.35	7.35	6.39	7.39	6.17	6.20	6.17	6.20	5.70
	5.84	6.81	6.99	6.77	6.90	6.35	7.35	6.39	7.39	6.17	6.20	6.17	6.20	5.70
	5.84	6.89	7.07	6.77	6.90	6.35	7.35	6.39	7.39	6.17	6.20	6.17	6.20	5.70
PCB 66	6.20	7.46	7.80	7.08	7.34	6.63	7.63	6.71	7.71	6.61	6.66	6.61	6.66	6.02
	6.20	7.59	7.93	7.08	7.34	6.63	7.63	6.71	7.71	6.61	6.66	6.61	6.66	6.02

Substance	log K_{ow}[g]	Experimental BAF (l kg^{-1} lipid)		Predicted BAF (l kg^{-1} lipid)										
		log BAF_t	log BAF_{fd}	Original Voutsas et al. (2002) method		TGD method[h]				AQUAWEB v1.1[a]				BIO v1.1[a]
				log BAF_t	log BAF_{fd}	log BAF_t		log BAF_{fd}		log BAF_{fd}				log BAF_{fd}
						BMF_1[e]	BMF_2[f]	BMF_1[e]	BMF_2[f]	a	b	c	d	d
	6.20	7.74	8.08	7.08	7.34	6.63	7.63	6.71	7.71	6.61	6.66	6.61	6.66	6.02
PCB 77	6.36	5.99	6.43	7.20	7.52	6.64	7.64	6.75	7.75	6.78	6.86	6.78	6.86	6.17
	6.36	6.25	6.68	7.20	7.52	6.64	7.64	6.75	7.75	6.78	6.86	6.78	6.86	6.17
	6.36	6.13	6.56	7.20	7.52	6.64	7.64	6.75	7.75	6.78	6.86	6.78	6.86	6.17
PCB 81	6.36	6.22	6.66	7.20	7.52	6.64	7.64	6.75	7.75	6.78	6.86	6.78	6.86	6.17
	6.36	6.03	6.46	7.20	7.52	6.64	7.64	6.75	7.75	6.78	6.86	6.78	6.86	6.17
PCB 87	6.29	6.98	7.37	7.15	7.44	6.64	7.64	6.73	7.73	6.70	6.77	6.70	6.77	6.10
	6.29	7.20	7.59	7.15	7.44	6.64	7.64	6.73	7.73	6.70	6.77	6.70	6.77	6.10
	6.29	7.27	7.67	7.15	7.44	6.64	7.64	6.73	7.73	6.70	6.77	6.70	6.77	6.10
PCB 99	6.39	7.45	7.90	7.22	7.56	6.64	7.64	6.75	7.75	6.81	6.89	6.81	6.89	6.19
	6.39	7.37	7.82	7.22	7.56	6.64	7.64	6.75	7.75	6.81	6.89	6.81	6.89	6.19
	6.39	7.29	7.74	7.22	7.56	6.64	7.64	6.75	7.75	6.81	6.89	6.81	6.89	6.19
PCB 101	6.38	7.09	7.53	7.21	7.55	6.64	7.64	6.75	7.75	6.80	6.88	6.80	6.88	6.18
	6.38	7.29	7.74	7.21	7.55	6.64	7.64	6.75	7.75	6.80	6.88	6.80	6.88	6.18
	6.38	7.30	7.75	7.21	7.55	6.64	7.64	6.75	7.75	6.80	6.88	6.80	6.88	6.18
PCB 105	6.65	7.80	8.43	7.38	7.85	6.62	7.62	6.79	7.79	7.02	7.16	7.02	7.16	6.44
	6.65	7.61	8.25	7.38	7.85	6.62	7.62	6.79	7.79	7.02	7.16	7.02	7.16	6.44
	6.65	7.79	8.43	7.38	7.85	6.62	7.62	6.79	7.79	7.02	7.16	7.02	7.16	6.44
PCB 110	6.48	6.94	7.45	7.28	7.66	6.64	7.64	6.77	7.77	6.89	6.99	6.89	6.99	6.28
	6.48	7.19	7.71	7.28	7.66	6.64	7.64	6.77	7.77	6.89	6.99	6.89	6.99	6.28
	6.48	7.27	7.78	7.28	7.66	6.64	7.64	6.77	7.77	6.89	6.99	6.89	6.99	6.28
PCB 118	6.74	6.76	7.47	7.42	7.94	6.60	7.60	6.79	7.79	7.07	7.24	7.07	7.24	6.52
	6.74	7.17	7.88	7.42	7.94	6.60	7.60	6.79	7.79	7.07	7.24	7.07	7.24	6.52
	6.74	7.19	7.90	7.42	7.94	6.60	7.60	6.79	7.79	7.07	7.24	7.07	7.24	6.52
PCB 126	6.89	6.23	7.07	7.49	8.10	6.56	7.56	6.79	7.79	7.13	7.36	7.13	7.36	6.66
	6.89	6.35	7.19	7.49	8.10	6.56	7.56	6.79	7.79	7.13	7.36	7.13	7.36	6.66
	6.89	6.29	7.12	7.49	8.10	6.56	7.56	6.79	7.79	7.13	7.36	7.13	7.36	6.66
PCB 138	6.83	7.48	8.27	7.46	8.04	6.58	7.58	6.80	7.80	7.11	7.32	7.11	7.32	6.61
	6.83	7.59	8.37	7.46	8.04	6.58	7.58	6.80	7.80	7.11	7.32	7.11	7.32	6.61

Substance	log K_{ow}[g]	Experimental BAF (l kg^{-1} lipid)		Predicted BAF (l kg^{-1} lipid)										
		log BAF_t	log BAF_{fd}	Original Voutsas et al. (2002) method		TGD method[h]				AQUAWEB v1.1[a]				BIO v1.1[a]
				log BAF_t	log BAF_{fd}	log BAF_t		log BAF_{fd}		log BAF_{fd}				log BAF_{fd}
						BMF_1[e]	BMF_2[f]	BMF_1[e]	BMF_2[f]	a	b	c	d	d
	6.83	7.58	8.37	7.46	8.04	6.58	7.58	6.80	7.80	7.11	7.32	7.11	7.32	6.61
PCB 151	6.64	6.99	7.62	7.37	7.84	6.62	7.62	6.79	7.79	7.01	7.15	7.01	7.15	6.43
	6.64	7.14	7.77	7.37	7.84	6.62	7.62	6.79	7.79	7.01	7.15	7.01	7.15	6.43
	6.64	7.09	7.72	7.37	7.84	6.62	7.62	6.79	7.79	7.01	7.15	7.01	7.15	6.43
PCB 153	6.92	7.47	8.33	7.50	8.13	6.55	7.55	6.79	7.79	7.14	7.38	7.14	7.38	6.69
	6.92	7.57	8.43	7.50	8.13	6.55	7.55	6.79	7.79	7.14	7.38	7.14	7.38	6.69
	6.92	7.59	8.45	7.50	8.13	6.55	7.55	6.79	7.79	7.14	7.38	7.14	7.38	6.69
PCB 156	7.18	7.25	8.35	7.58	8.40	6.42	7.42	6.77	7.77	7.15	7.52	7.15	7.51	6.94
	7.18	7.43	8.52	7.58	8.40	6.42	7.42	6.77	7.77	7.15	7.52	7.15	7.52	6.94
	7.18	7.54	8.63	7.58	8.40	6.42	7.42	6.77	7.77	7.15	7.52	7.15	7.52	6.94
PCB 169	7.42	6.76	8.07	7.62	8.63	6.26	7.26	6.73	7.73	7.06	7.58	7.06	7.58	7.17
	7.42	6.93	8.25	7.62	8.63	6.26	7.26	6.73	7.73	7.06	7.58	7.06	7.58	7.17
	7.42	6.71	8.03	7.62	8.63	6.26	7.26	6.73	7.73	7.06	7.58	7.06	7.58	7.17
PCB 170	7.27	7.52	8.69	7.60	8.48	6.37	7.37	6.76	7.76	7.12	7.55	7.12	7.55	7.03
	7.27	7.67	8.85	7.60	8.48	6.37	7.37	6.76	7.76	7.12	7.55	7.12	7.55	7.03
	7.27	7.56	8.74	7.60	8.48	6.37	7.37	6.76	7.76	7.12	7.55	7.12	7.55	7.03
PCB 180	7.36	7.44	8.70	7.61	8.57	6.31	7.31	6.74	7.74	7.09	7.57	7.09	7.57	7.11
	7.36	7.61	8.87	7.61	8.57	6.31	7.31	6.74	7.74	7.09	7.57	7.09	7.57	7.11
	7.36	7.56	8.82	7.61	8.57	6.31	7.31	6.74	7.74	7.09	7.57	7.09	7.57	7.11
PCB 194	7.80	7.37	9.05	7.62	8.97	5.92	6.92	6.61	7.61	6.74	7.56	6.74	7.56	7.51
	7.80	7.38	9.06	7.62	8.97	5.92	6.92	6.61	7.61	6.74	7.56	6.74	7.56	7.51
	7.80	7.32	9.00	7.62	8.97	5.92	6.92	6.61	7.61	6.74	7.56	6.74	7.56	7.51
PCB 195	7.56	7.74	9.19	7.63	8.76	6.15	7.15	6.69	7.69	6.96	7.58	6.96	7.58	7.30
	7.56	7.83	9.28	7.63	8.76	6.15	7.15	6.69	7.69	6.96	7.58	6.96	7.58	7.30
	7.56	7.53	8.98	7.63	8.76	6.15	7.15	6.69	7.69	6.96	7.58	6.96	7.58	7.30
PCB 199	7.20	7.32	8.43	7.58	8.42	6.41	7.41	6.77	7.77	7.14	7.52	7.14	7.52	6.96
	7.20	7.60	8.71	7.58	8.42	6.41	7.41	6.77	7.77	7.14	7.52	7.14	7.52	6.96
	7.20	7.53	8.64	7.58	8.42	6.41	7.41	6.77	7.77	7.14	7.52	7.14	7.52	6.96
PCB 209	8.18	8.01	10.07	7.55	9.28	4.97	5.44	5.92	6.40	6.27	7.42	6.27	7.42	7.82
	8.18	7.80	9.86	7.55	9.28	4.97	5.44	5.92	6.40	6.27	7.42	6.27	7.42	7.82

Substance	log K_{ow}[g]	Experimental BAF (l kg^{-1} lipid)		Predicted BAF (l kg^{-1} lipid)										
		log BAF_t	log BAF_{fd}	Original Voutsas et al. (2002) method		TGD method[h]				AQUAWEB v1.1[a]				BIO v1.1[a]
				log BAF_t	log BAF_{fd}	log BAF_t		log BAF_{fd}		log BAF_{fd}				log BAF_{fd}
						BMF_1[e]	BMF_2[f]	BMF_1[e]	BMF_2[f]	a	b	c	d	d
	8.18	7.65	9.71	7.55	9.28	5.49	6.49	6.44	7.44	6.27	7.42	6.27	7.42	7.82
Pentachlorobenzene	5.11	5.42	5.76	5.93	5.94	5.76	6.76	5.77	6.77	5.26	5.26	5.26	5.26	5.06
	5.11	5.52	5.86	5.93	5.94	5.76	6.76	5.77	6.77	5.26	5.26	5.26	5.26	5.06
	5.11	5.50	5.84	5.93	5.94	5.76	6.76	5.77	6.77	5.26	5.26	5.26	5.26	5.06
	5.11	6.52	6.86	5.93	5.94	5.76	6.76	5.77	6.77	5.26	5.26	5.26	5.26	5.06
	5.11	5.14	5.48	5.93	5.94	5.76	6.76	5.77	6.77	5.26	5.26	5.26	5.26	5.06
	5.11	6.12	6.47	5.93	5.94	5.76	6.76	5.77	6.77	5.26	5.26	5.26	5.26	5.06
	5.11	4.89	5.23	5.93	5.94	5.76	6.76	5.77	6.77	5.26	5.26	5.26	5.26	5.06
	5.11	5.87	6.21	5.93	5.94	5.76	6.76	5.77	6.77	5.26	5.26	5.26	5.26	5.06
	5.11	5.49	5.83	5.93	5.94	5.76	6.76	5.77	6.77	5.26	5.26	5.26	5.26	5.06
	5.11	6.05	6.39	5.93	5.94	5.76	6.76	5.77	6.77	5.26	5.26	5.26	5.26	5.06
	5.18	5.93	6.04	6.02	6.04	5.82	6.82	5.83	6.83	5.34	5.35	5.34	5.35	5.12
E-Pentachloro butadiene	4.54	4.47	4.59	5.06	5.12	4.59	4.89	4.59	4.89	4.61	4.62	4.61	4.62	4.53
	4.54	4.50	4.62	5.06	5.12	4.59	4.89	4.59	4.89	4.61	4.62	4.61	4.62	4.53
	4.54	4.94	5.06	5.06	5.12	4.59	4.89	4.59	4.89	4.61	4.62	4.61	4.62	4.53
	4.54	5.28	5.40	5.06	5.12	4.59	4.89	4.59	4.89	4.61	4.62	4.61	4.62	4.53
	4.54	4.38	4.50	5.06	5.12	4.59	4.89	4.59	4.89	4.61	4.62	4.61	4.62	4.53
	4.54	4.66	4.78	5.06	5.12	4.59	4.89	4.59	4.89	4.61	4.62	4.61	4.62	4.53
	4.54	4.43	4.56	5.06	5.12	4.59	4.89	4.59	4.89	4.61	4.62	4.61	4.62	4.53
	4.54	4.93	5.05	5.06	5.12	4.59	4.89	4.59	4.89	4.61	4.62	4.61	4.62	4.53
	4.54	5.21	5.33	5.06	5.12	4.59	4.89	4.59	4.89	4.61	4.62	4.61	4.62	4.53
	4.54	5.72	5.84	5.06	5.12	4.59	4.89	4.59	4.89	4.61	4.62	4.61	4.62	4.53
Z-Pentachloro butadiene	4.54	4.28	4.41	5.06	5.12	4.59	4.89	4.59	4.89	4.61	4.62	4.61	4.62	4.53
	4.54	4.82	4.94	5.06	5.12	4.59	4.89	4.59	4.89	4.61	4.62	4.61	4.62	4.53
	4.54	4.99	5.11	5.06	5.12	4.59	4.89	4.59	4.89	4.61	4.62	4.61	4.62	4.53
	4.54	4.52	4.64	5.06	5.12	4.59	4.89	4.59	4.89	4.61	4.62	4.61	4.62	4.53
	4.54	4.43	4.55	5.06	5.12	4.59	4.89	4.59	4.89	4.61	4.62	4.61	4.62	4.53

Substance	log K_{ow}[g]	Experimental BAF (l kg^{-1} lipid)		Predicted BAF (l kg^{-1} lipid)										
		log BAF_t	log BAF_{fd}	Original Voutsas et al. (2002) method		TGD method[h]				AQUAWEB v1.1[a]				BIO v1.1[a]
				log BAF_t	log BAF_{fd}	log BAF_t		log BAF_{fd}		log BAF_{fd}				log BAF_{fd}
						BMF_1[e]	BMF_2[f]	BMF_1[e]	BMF_2[f]	a	b	c	d	d
	4.54	5.17	5.29	5.06	5.12	4.59	4.89	4.59	4.89	4.61	4.61	4.61	4.62	4.53
Tetrachlorobenzene (mixture of isomers)	4.60	5.12	5.26	5.16	5.21	4.64	4.94	4.64	4.94	4.68	4.68	4.68	4.68	4.58
	4.60	5.33	5.47	5.16	5.21	4.64	4.94	4.64	4.94	4.68	4.68	4.68	4.68	4.58
	4.60	4.99	5.12	5.16	5.21	4.64	4.94	4.64	4.94	4.68	4.68	4.68	4.68	4.58
	4.60	4.67	4.81	5.16	5.21	4.64	4.94	4.64	4.94	4.68	4.68	4.68	4.68	4.58
	4.60	5.50	5.64	5.16	5.21	4.64	4.94	4.64	4.94	4.68	4.68	4.68	4.68	4.58
	4.60	4.24	4.37	5.16	5.21	4.64	4.94	4.64	4.94	4.68	4.68	4.68	4.68	4.58
	4.60	4.90	5.04	5.16	5.21	4.64	4.94	4.64	4.94	4.68	4.68	4.68	4.68	4.58
	4.60	4.88	5.02	5.16	5.21	4.64	4.94	4.64	4.94	4.68	4.68	4.68	4.68	4.58
	4.60	5.15	5.28	5.16	5.21	4.64	4.94	4.64	4.94	4.68	4.68	4.68	4.80	4.58
1,2,3,4-Tetrachloro benzene	4.59	4.95	5.08	5.15	5.20	4.63	4.93	4.63	4.93	4.67	4.67	4.67	4.67	4.57
	4.59	5.04	5.17	5.15	5.20	4.63	4.93	4.63	4.93	4.67	4.67	4.67	4.67	4.57
	4.59	5.05	5.18	5.15	5.20	4.63	4.93	4.63	4.93	4.67	4.67	4.67	4.67	4.57
	4.59	5.72	5.85	5.15	5.20	4.63	4.93	4.63	4.93	4.67	4.67	4.67	4.67	4.57
	4.59	4.59	4.72	5.15	5.20	4.63	4.93	4.63	4.93	4.67	4.67	4.67	4.67	4.57
	4.59	5.31	5.44	5.15	5.20	4.63	4.93	4.63	4.93	4.67	4.67	4.67	4.67	4.57
	4.59	4.48	4.62	5.15	5.20	4.63	4.93	4.63	4.93	4.67	4.67	4.67	4.67	4.57
	4.59	5.09	5.23	5.15	5.20	4.63	4.93	4.63	4.93	4.67	4.67	4.67	4.67	4.57
	4.59	5.03	5.16	5.15	5.20	4.63	4.93	4.63	4.93	4.67	4.67	4.67	4.67	4.57
	4.59	5.42	5.55	5.15	5.20	4.63	4.93	4.63	4.93	4.67	4.67	4.67	4.67	4.57
1,2,3,5-Tetrachloro benzene	4.62	5.05	5.08	5.19	5.24	4.65	4.96	4.66	4.96	4.70	4.70	4.70	4.70	4.57
1,2,4,5-Tetrachloro benzene	4.64	5.46	5.50	5.23	5.27	4.67	4.97	4.68	4.98	4.72	4.72	4.72	4.72	4.62

Substance	log K_{ow}[g]	Experimental BAF (l kg^{-1} lipid)		Predicted BAF (l kg^{-1} lipid)										
		log BAF_t	log BAF_{fd}	Original Voutsas et al. (2002) method		TGD method[h]				AQUAWEB v1.1[a]				BIO v1.1[a]
				log BAF_t	log BAF_{fd}	log BAF_t		log BAF_{fd}		log BAF_{fd}				log BAF_{fd}
						BMF_1[e]	BMF_2[f]	BMF_1[e]	BMF_2[f]	a	b	c	d	d
Z-1,1,2,4-Tetrachloro butadiene	4.23	4.02	4.09	4.52	4.65	4.02	4.02	4.03	4.03	4.29	4.29	4.29	4.29	4.22
	4.23	3.83	3.89	4.52	4.65	4.02	4.02	4.03	4.03	4.29	4.29	4.29	4.29	4.22
	4.23	4.26	4.33	4.52	4.65	4.02	4.02	4.03	4.03	4.29	4.29	4.29	4.29	4.22
	4.23	4.51	4.57	4.52	4.65	4.02	4.02	4.03	4.03	4.29	4.29	4.29	4.29	4.22
	4.23	4.02	4.09	4.52	4.65	4.02	4.02	4.03	4.03	4.29	4.29	4.29	4.29	4.22
	4.23	3.81	3.88	4.52	4.65	4.02	4.02	4.03	4.03	4.29	4.29	4.29	4.29	4.22
	4.23	4.24	4.30	4.52	4.65	4.02	4.02	4.03	4.03	4.29	4.29	4.29	4.29	4.22
	4.23	4.37	4.43	4.52	4.65	4.02	4.02	4.03	4.03	4.29	4.29	4.29	4.29	4.22
	4.23	4.95	5.02	4.52	4.65	4.02	4.02	4.03	4.03	4.29	4.29	4.29	4.29	4.22
1,1,4,4-Tetrachloro butadiene	4.29	4.23	4.30	4.63	4.74	4.07	4.07	4.08	4.08	4.35	4.35	4.35	4.35	4.28
	4.29	4.26	4.33	4.63	4.74	4.07	4.07	4.08	4.08	4.35	4.35	4.35	4.35	4.28
	4.29	4.39	4.46	4.63	4.74	4.07	4.07	4.08	4.08	4.35	4.35	4.35	4.35	4.28
	4.29	4.75	4.82	4.63	4.74	4.07	4.07	4.08	4.08	4.35	4.35	4.35	4.35	4.28
	4.29	4.51	4.59	4.63	4.74	4.07	4.07	4.08	4.08	4.35	4.35	4.35	4.35	4.28
	4.29	3.94	4.01	4.63	4.74	4.07	4.07	4.08	4.08	4.35	4.35	4.35	4.35	4.28
	4.29	4.31	4.39	4.63	4.74	4.07	4.07	4.08	4.08	4.35	4.35	4.35	4.35	4.28
	4.29	4.27	4.34	4.63	4.74	4.07	4.07	4.08	4.08	4.35	4.35	4.35	4.35	4.28
	4.29	5.01	5.09	4.63	4.74	4.07	4.07	4.08	4.08	4.35	4.35	4.35	4.35	4.28
1,2,3-Trichloro benzene	4.09	4.47	4.52	4.26	4.43	3.91	3.91	3.91	3.91	4.14	4.14	4.14	4.14	4.09
	4.09	4.72	4.77	4.26	4.43	3.91	3.91	3.91	3.91	4.14	4.14	4.14	4.14	4.09
	4.09	4.63	4.67	4.26	4.43	3.91	3.91	3.91	3.91	4.14	4.14	4.14	4.14	4.09
	4.09	5.11	5.16	4.26	4.43	3.91	3.91	3.91	3.91	4.14	4.14	4.14	4.14	4.09
	4.09	4.05	4.10	4.26	4.43	3.91	3.91	3.91	3.91	4.14	4.14	4.14	4.14	4.09
	4.09	4.77	4.82	4.26	4.43	3.91	3.91	3.91	3.91	4.14	4.14	4.14	4.14	4.09
	4.09	4.18	4.23	4.26	4.43	3.91	3.91	3.91	3.91	4.14	4.14	4.14	4.14	4.09
	4.09	4.56	4.60	4.26	4.43	3.91	3.91	3.91	3.91	4.14	4.14	4.14	4.14	4.09

Substance	log K_{ow}[g]	Experimental BAF (l kg^{-1} lipid)		Predicted BAF (l kg^{-1} lipid)										
		log BAF_t	log BAF_{fd}	Original Voutsas et al. (2002) method		TGD method[h]				AQUAWEB v1.1[a]				BIO v1.1[a]
				log BAF_t	log BAF_{fd}	log BAF_t		log BAF_{fd}		log BAF_{fd}				log BAF_{fd}
						BMF_1[e]	BMF_2[f]	BMF_1[e]	BMF_2[f]	a	b	c	d	d
	4.09	4.70	4.74	4.26	4.43	3.91	3.91	3.91	3.91	4.14	4.14	4.14	4.14	4.09
	4.09	4.96	5.01	4.26	4.43	3.91	3.91	3.91	3.91	4.14	4.14	4.14	4.14	4.09
	4.14	4.54	4.55	4.35	4.51	3.95	3.95	3.95	3.95	4.19	4.19	4.19	4.19	4.14
1,2,4-Trichloro benzene	4.02	4.76	4.77	4.12	4.32	3.85	3.85	3.85	3.85	4.07	4.07	4.07	4.07	4.02
	4.02	4.55	4.59	4.12	4.32	3.85	3.85	3.85	3.85	4.07	4.07	4.07	4.07	4.02
	4.02	4.67	4.71	4.12	4.32	3.85	3.85	3.85	3.85	4.07	4.07	4.07	4.07	4.02
	4.02	4.72	4.76	4.12	4.32	3.85	3.85	3.85	3.85	4.07	4.07	4.07	4.07	4.02
	4.02	5.63	5.67	4.12	4.32	3.85	3.85	3.85	3.85	4.07	4.07	4.07	4.07	4.02
	4.02	4.01	4.05	4.12	4.32	3.85	3.85	3.85	3.85	4.07	4.07	4.07	4.07	4.02
	4.02	4.86	4.90	4.12	4.32	3.85	3.85	3.85	3.85	4.07	4.07	4.07	4.07	4.02
	4.02	4.18	4.22	4.12	4.32	3.85	3.85	3.85	3.85	4.07	4.07	4.07	4.07	4.02
	4.02	4.57	4.61	4.12	4.32	3.85	3.85	3.85	3.85	4.07	4.07	4.07	4.07	4.02
	4.02	4.63	4.67	4.12	4.32	3.85	3.85	3.85	3.85	4.07	4.07	4.07	4.07	4.02
	4.02	5.03	5.07	4.12	4.32	3.85	3.85	3.85	3.85	4.07	4.07	4.07	4.07	4.02
1,3,5-Trichloro benzene	4.19	4.40	4.41	4.45	4.59	3.99	3.99	3.99	3.99	4.25	4.25	4.25	4.25	4.19

a) Simulation assuming the TGD default QSAR for K_{oc} and the water properties relevant to the Great Lakes.
b) Simulation assuming the TGD default QSAR for K_{oc} and the water properties from the TGD.
c) Simulation assuming the TGD QSAR for predominantly hydrophobics for K_{oc} and the water properties relevant to the Great Lakes.
d) Simulation assuming the TGD QSAR for predominantly hydrophobics for K_{oc} and the water properties from the TGD.
e) Estimates using the BMF_1 value as recommended in the TGD for freshwater food chains.
f) Estimates using the BMF_1 and BMF_2 values as recommended in the TGD for marine food chains.
g) As explained in the main text, Voutsas et al. (2002) reports different log K_{ow} values for the same chemicals. The analysis carried out here uses the same log K_{ow} values as Voutsas et al. (2002) in order that the estimates can be compared directly with those using the Voutsas et al. (2002) method.
h) The TGD method calculates BAF values on a wet weight fish basis. These have been converted here to a lipid weight basis by assuming a lipid content of 7.4 per cent for fish in trophic level 3 (in line with the AQUAWEB model).

Table C4 Experimental and predicted BAFs for trophic level 4

Substance	log K_{ow}[d]	Experimental BAF (l kg^{-1} lipid)		Predicted BAF (l kg^{-1} lipid)										
		log BAF_t	log BAF_{fd}	Original Voutsas et al. (2002) method		TGD method[a e]				AQUAWEB v1.1[a]				BIO v1.1[a]
				log BAF_t	log BAF_{fd}	log BAF_t		log BAF_{fd}		log BAF_{fd}				log BAF_{fd}
						BMF_1[b]	BMF_2[c]	BMF_1[b]	BMF_2[c]	a	b	c	d	d
Hexachlorobutadiene	4.84	5.66	5.87	5.74	5.77	4.83	5.13	4.84	5.14	5.22	5.22	5.22	5.22	5.00
	4.84	5.76	5.97	5.74	5.77	4.83	5.13	4.84	5.14	5.22	5.22	5.22	5.22	5.00
	4.84	5.18	5.39	5.74	5.77	4.83	5.13	4.84	5.14	5.22	5.22	5.22	5.22	5.00
	5.60	6.88	7.55	6.72	6.81	6.16	7.16	6.18	7.18	6.45	6.47	6.45	6.47	5.88
	5.60	6.19	6.86	6.72	6.81	6.16	7.16	6.18	7.18	6.45	6.47	6.45	6.47	5.88
	5.60	5.74	6.41	6.72	6.81	6.16	7.16	6.18	7.18	6.45	6.47	6.45	6.47	5.88
Hexachloroethane	4.14	4.55	4.61	4.63	4.78	3.94	3.94	3.94	3.94	4.27	4.27	4.27	4.27	4.19
	4.14	4.74	4.79	4.63	4.78	3.94	3.94	3.94	3.94	4.27	4.27	4.27	4.27	4.19
	4.14	4.25	4.30	4.63	4.78	3.94	3.94	3.94	3.94	4.27	4.27	4.27	4.27	4.19
PCB 18	5.24	6.37	6.42	6.29	6.32	5.86	6.86	5.88	6.88	5.86	5.86	5.86	5.86	5.48
PCB 31	5.67	7.01	7.14	6.80	6.91	6.21	7.21	6.24	7.24	6.57	6.58	6.57	6.58	5.96
PCB 44	5.75	7.31	7.46	6.89	7.01	6.28	7.28	6.31	7.31	6.69	6.71	6.69	6.71	6.04
PCB 49	5.85	6.57	6.75	6.99	7.15	6.35	7.35	6.40	7.40	6.85	6.87	6.85	6.87	6.14
PCB 52	5.84	7.19	7.37	6.98	7.14	6.35	7.35	6.39	7.39	6.83	6.86	6.83	6.86	6.13
PCB 66	6.20	7.93	8.27	7.33	7.61	6.63	7.63	6.70	7.70	7.33	7.39	7.33	7.39	6.49
PCB 77	6.36	6.45	6.89	7.47	7.82	6.64	7.64	6.74	7.74	7.52	7.60	7.52	7.60	6.64
PCB 81	6.36	6.80	7.24	7.47	7.82	6.64	7.64	6.74	7.74	7.52	7.60	7.52	7.60	6.64
PCB 87	6.29	7.19	7.59	7.41	7.73	6.64	7.64	6.73	7.73	7.44	7.51	7.44	7.51	6.29
PCB 99	6.39	8.15	8.60	7.49	7.86	6.64	7.64	6.75	7.75	7.55	7.63	7.55	7.63	6.67
PCB 101	6.38	7.53	7.97	7.49	7.85	6.64	7.64	6.75	7.75	7.54	7.62	7.54	7.62	6.66
PCB 105	6.65	8.07	8.70	7.69	8.20	6.62	7.62	6.78	7.78	7.76	7.91	7.76	7.91	6.92
PCB 110	6.48	7.47	7.98	7.57	7.98	6.64	7.64	6.76	7.76	7.63	7.74	7.63	7.74	6.76
PCB 118	6.74	7.77	8.48	7.76	8.31	6.60	7.60	6.79	7.79	7.81	7.98	7.81	7.98	7.01
PCB 126	6.89	7.20	8.04	7.85	8.51	6.55	7.55	6.79	7.79	7.86	8.09	7.86	8.09	7.15

Substance	log K_{ow}[d]	Experimental BAF (l kg^{-1} lipid)		Predicted BAF (l kg^{-1} lipid)										
		log BAF_t	log BAF_{fd}	Original Voutsas et al. (2002) method		TGD method[a e]				AQUAWEB v1.1[a]				BIO v1.1[a]
				log BAF_t	log BAF_{fd}	log BAF_t		log BAF_{fd}		log BAF_{fd}				log BAF_{fd}
						BMF_1[b]	BMF_2[c]	BMF_1[b]	BMF_2[c]	a	b	c	d	d
PCB 138	6.83	8.17	8.95	7.82	8.43	6.57	7.57	6.79	7.79	7.85	8.05	7.85	8.05	7.10
PCB 151	6.64	6.67	7.30	7.69	8.19	6.62	7.62	6.78	7.78	7.76	7.90	7.76	7.90	6.91
PCB 153	6.92	8.18	9.04	7.87	8.55	6.54	7.54	6.79	7.79	7.86	8.10	7.86	8.10	7.18
PCB 156	7.18	8.23	9.32	8.01	8.88	6.42	7.42	6.77	7.77	7.82	8.19	7.82	8.19	7.43
PCB 169	7.42	7.58	8.90	8.12	9.18	6.26	7.26	6.72	7.72	7.65	8.17	7.65	8.17	7.64
PCB 170	7.27	8.18	9.35	8.06	8.99	6.36	7.36	6.75	7.75	7.77	8.19	7.77	8.19	7.51
PCB 180	7.36	8.22	9.48	8.10	9.10	6.30	7.30	6.74	7.74	7.70	8.18	7.70	8.18	7.59
PCB 194	7.80	8.21	9.90	8.24	9.65	5.92	6.92	6.61	7.61	7.16	7.97	7.16	7.97	7.96
PCB 195	7.56	8.45	9.91	8.17	9.35	6.14	7.14	6.69	7.69	7.50	8.12	7.50	8.12	7.77
PCB 199	7.20	8.22	9.33	8.02	8.90	6.41	7.41	6.76	7.76	7.81	8.19	7.81	8.19	7.44
PCB 209	8.18	8.37	10.43	8.31	10.11	4.96	5.44	5.91	6.39	6.44	7.60	6.44	7.60	8.20
Pentachlorobenzene	5.11	6.25	6.59	6.11	6.15	5.76	6.76	5.77	6.77	5.64	5.65	5.64	5.65	5.32
	5.11	6.10	6.44	6.11	6.15	5.76	6.76	5.77	6.77	5.64	5.65	5.64	5.65	5.32
	5.11	5.61	5.95	6.11	6.15	5.76	6.76	5.77	6.77	5.64	5.65	5.64	5.65	5.32
E-Pentachloro butadiene	4.54	5.75	5.87	5.29	5.35	4.58	4.88	4.58	4.89	4.78	4.78	4.78	4.78	4.64
	4.54	5.71	5.83	5.29	5.35	4.58	4.88	4.58	4.89	4.78	4.78	4.78	4.78	4.64
	4.54	5.33	5.45	5.29	5.35	4.58	4.88	4.58	4.89	4.78	4.78	4.78	4.78	4.64
Z-Pentachloro butadiene	4.54	5.53	5.65	5.29	5.35	4.58	4.88	4.58	4.89	4.78	4.78	4.78	4.78	4.64
	4.54	5.40	5.52	5.29	5.35	4.58	4.88	4.58	4.89	4.78	4.78	4.78	4.78	4.64
	4.54	4.51	4.63	5.29	5.35	4.58	4.88	4.58	4.89	4.78	4.78	4.78	4.78	4.64
Tetrachlorobenzene (mixture of isomers)	4.60	5.20	5.33	5.38	5.44	4.63	4.93	4.64	4.94	4.87	4.87	4.87	4.87	4.71
	4.60	5.27	5.40	5.38	5.44	4.63	4.93	4.64	4.94	4.87	4.87	4.87	4.87	4.71
	4.60	4.90	5.04	5.38	5.44	4.63	4.93	4.64	4.94	4.87	4.87	4.87	4.87	4.71
1,2,3,4-Tetrachlorobenzene	4.59	5.51	5.65	5.36	5.42	4.62	4.92	4.63	4.93	4.85	4.85	4.85	4.85	4.70
	4.59	5.51	5.64	5.36	5.42	4.62	4.92	4.63	4.93	4.85	4.85	4.85	4.85	4.70
	4.59	5.05	5.18	5.36	5.42	4.62	4.92	4.63	4.93	4.85	4.85	4.85	4.85	4.70

Substance	log K_{ow}[d]	Experimental BAF (l kg^{-1} lipid)		Predicted BAF (l kg^{-1} lipid)										
		log BAF_t	log BAF_{fd}	Original Voutsas et al. (2002) method		TGD method[a e]				AQUAWEB v1.1[a]				BIO v1.1[a]
				log BAF_t	log BAF_{fd}	log BAF_t		log BAF_{fd}		log BAF_{fd}				log BAF_{fd}
						BMF_1[b]	BMF_2[c]	BMF_1[b]	BMF_2[c]	a	b	c	d	d
Z-1,1,2,4-Tetrachloro butadiene	4.23	4.91	4.97	4.78	4.91	4.02	4.02	4.02	4.02	4.38	4.38	4.38	4.38	4.29
	4.23	4.79	4.86	4.78	4.91	4.02	4.02	4.02	4.02	4.38	4.38	4.38	4.38	4.29
	4.23	4.36	4.42	4.78	4.91	4.02	4.02	4.02	4.02	4.38	4.38	4.38	4.38	4.29
1,1,4,4-Tetrachloro butadiene	4.29	4.95	5.02	4.88	5.00	4.07	4.07	4.07	4.07	4.46	4.46	4.46	4.46	4.36
	4.29	4.83	4.90	4.88	5.00	4.07	4.07	4.07	4.07	4.46	4.46	4.46	4.46	4.36
	4.29	4.33	4.40	4.88	5.00	4.07	4.07	4.07	4.07	4.46	4.46	4.46	4.46	4.36
1,2,3-Trichlorobenzene	4.09	4.92	4.97	4.54	4.71	3.90	3.90	3.90	3.90	4.21	4.21	4.21	4.21	4.14
	4.09	4.91	4.96	4.54	4.71	3.90	3.90	3.90	3.90	4.21	4.21	4.21	4.21	4.14
	4.09	4.59	4.64	4.54	4.71	3.90	3.90	3.90	3.90	4.21	4.21	4.21	4.21	4.14
1,2,4-Trichlorobenzene	4.02	5.00	5.04	4.42	4.61	3.84	3.84	3.84	3.84	4.13	4.13	4.13	4.13	4.06
	4.02	5.03	5.07	4.42	4.61	3.84	3.84	3.84	3.84	4.13	4.13	4.13	4.13	4.06
	4.02	4.62	4.66	4.42	4.61	3.84	3.84	3.84	3.84	4.13	4.13	4.13	4.13	4.06

a) Simulation assuming the TGD default QSAR for K_{oc} and the water properties relevant to the Great Lakes.
b) Simulation assuming the TGD default QSAR for K_{oc} and the water properties from the TGD.
c) Simulation assuming the TGD QSAR for predominantly hydrophobics for K_{oc} and the water properties relevant to the Great Lakes.
d) Simulation assuming the TGD QSAR for predominantly hydrophobics for K_{oc} and the water properties from the TGD.
e) Estimates using the BMF_1 value as recommended in the TGD for freshwater food chains.
f) Estimates using the BMF_1 and BMF_2 values as recommended in the TGD for marine food chains.
g) As explained in the main text, Voutsas et al. (2002) reports different log K_{ow} values for the same chemicals. The analysis carried out here uses the same log K_{ow} values as Voutsas et al. (2002) in order that the estimates can be compared directly with those using the Voutsas et al. (2002) method.
h) The TGD method calculates BAF values on a wet weight fish basis. These have been converted here to a lipid weight basis by assuming a lipid content of 7.4 per cent for fish in trophic level 3 (in line with the AQUAWEB model).

Comparisons of predicted and field BAFs for Section 6

This part of Appendix C presents a more extensive comparison of measured and field BAF values based on the analysis described in Section 6 of the main report. As noted in Section 6, the main comparison here involves the AQUAWEB and TGD methods. Plots of the residuals found using the Voutsas *et al.* (2002) equations are also included here; as noted in Section 6, comparing these to the results of other methods is not an equal comparison, as many of these data were used in the development of the Voutsas *et al*. equations.

For trophic level 1, plots comparing the predicted BAF_{fd} obtained from AQUAWEB v1.1 with the actual BAF_{fd} are shown in Figure C1 (using the Great Lakes water properties) and Figure C2 (using the TGD water properties). The corresponding residuals in the prediction are shown in Figure C3 and Figure C4 respectively. For comparison, the residuals in the prediction obtained using the Voutsas *et al.* (2002) method are shown in Figure C5.

As can be seen from these plots, the field data show a more or less linear increase in the log BAF_{fd} with log K_{ow} (as was found by Voutsas *et al.* (2002)). The predicted log BAF_{fd} depends on the water properties used (the dissolved organic carbon concentration). For simulations using the Great Lakes water properties (where the dissolved organic carbon content was set to 2.2×10^{-6} kg l^{-1}), the predicted log BAF shows a maximum value at a log K_{ow} of around seven and then decreases with increasing log K_{ow}. For simulations carried out using the TGD water properties (where the dissolved organic carbon content was set to zero), the log BAF shows an increasing trend with increasing log K_{ow} across the entire data set, but appears to tend to a maximum value of log BAF at very high log K_{ow} values (around nine to ten). As discussed previously, the model adjusts the bioavailable fraction of the chemical in water to take account of the association with dissolved organic carbon and this explains the different patterns seen in the two sets of simulations. Only when the dissolved organic carbon content is set to zero will the predicted BAF reflect the BAF on a true dissolved concentration in water.

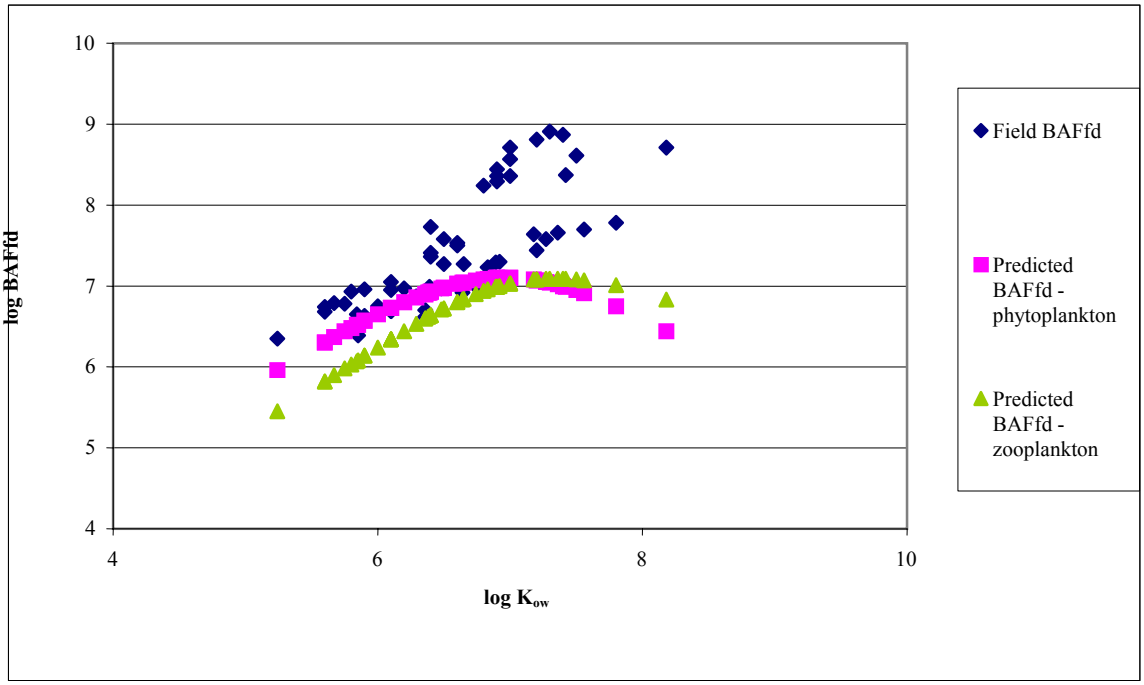

Figure C1 Predicted BAF_{fd} for trophic level 1 using AQUAWEB (Great Lakes water properties and QSAR for predominantly hydrophobics)

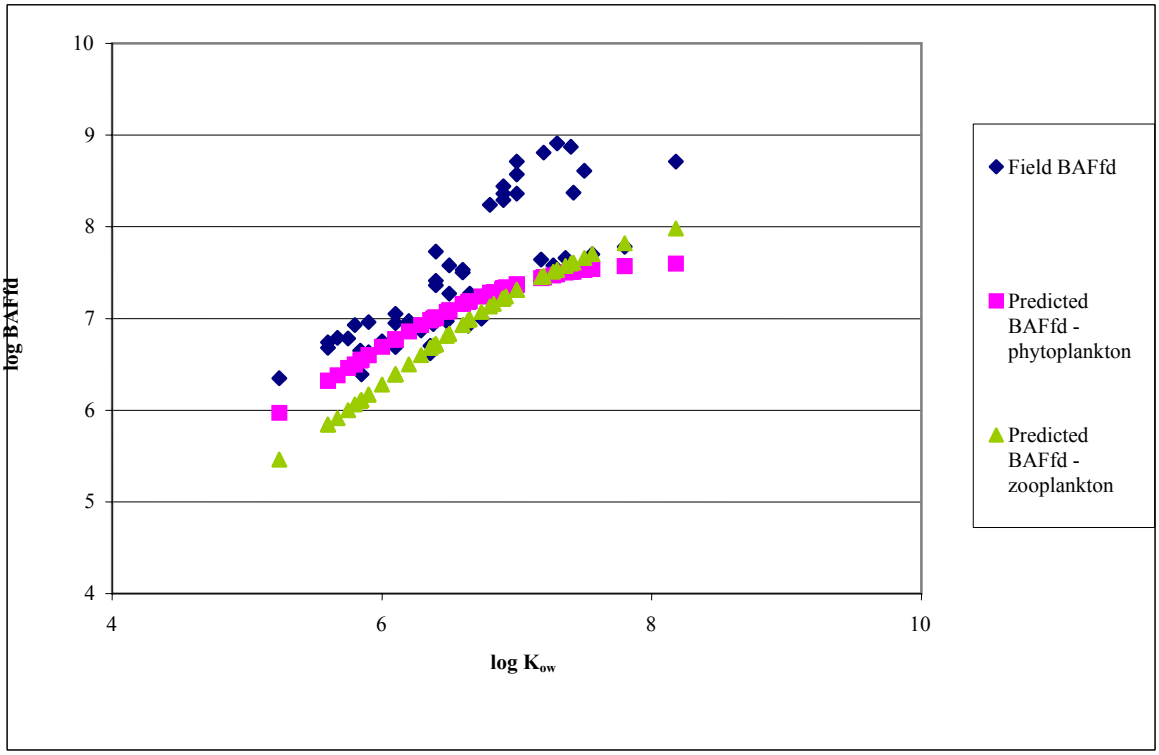

Figure C2 Predicted BAF_{fd} for trophic level 1 using AQUAWEB (TGD water properties and QSAR for predominantly hydrophobics)

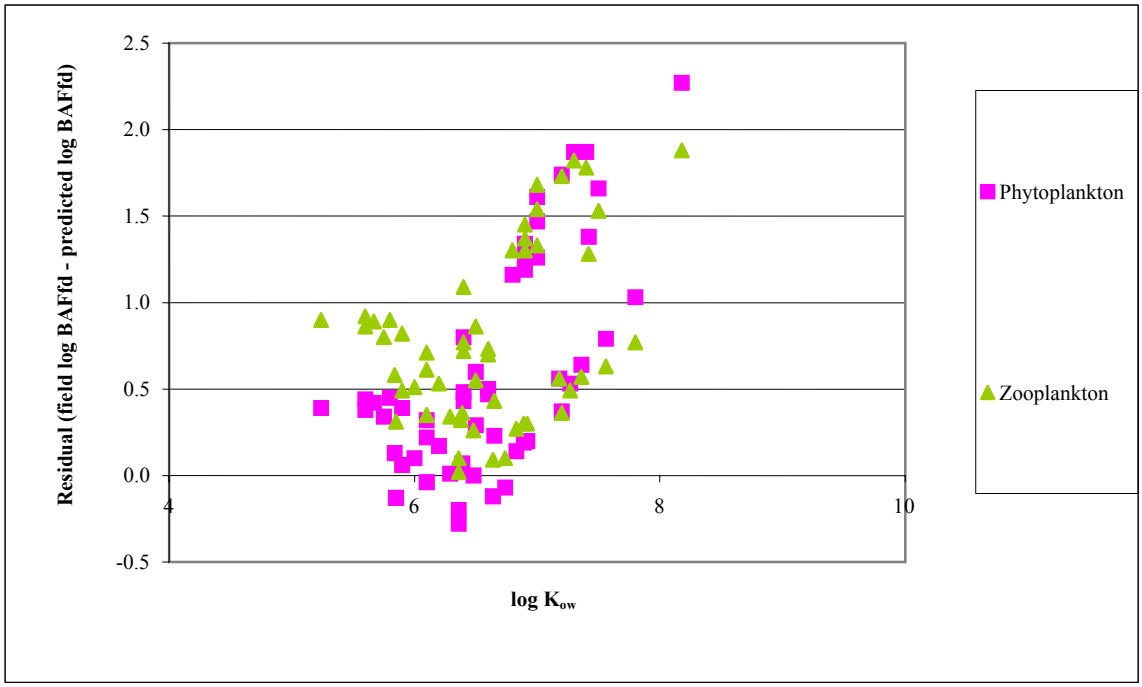

Figure C3 Residual in the prediction in log BAF_{fd} for trophic level 1 using AQUAWEB v1.1 (Great Lakes water properties and QSAR for predominantly hydrophobics)

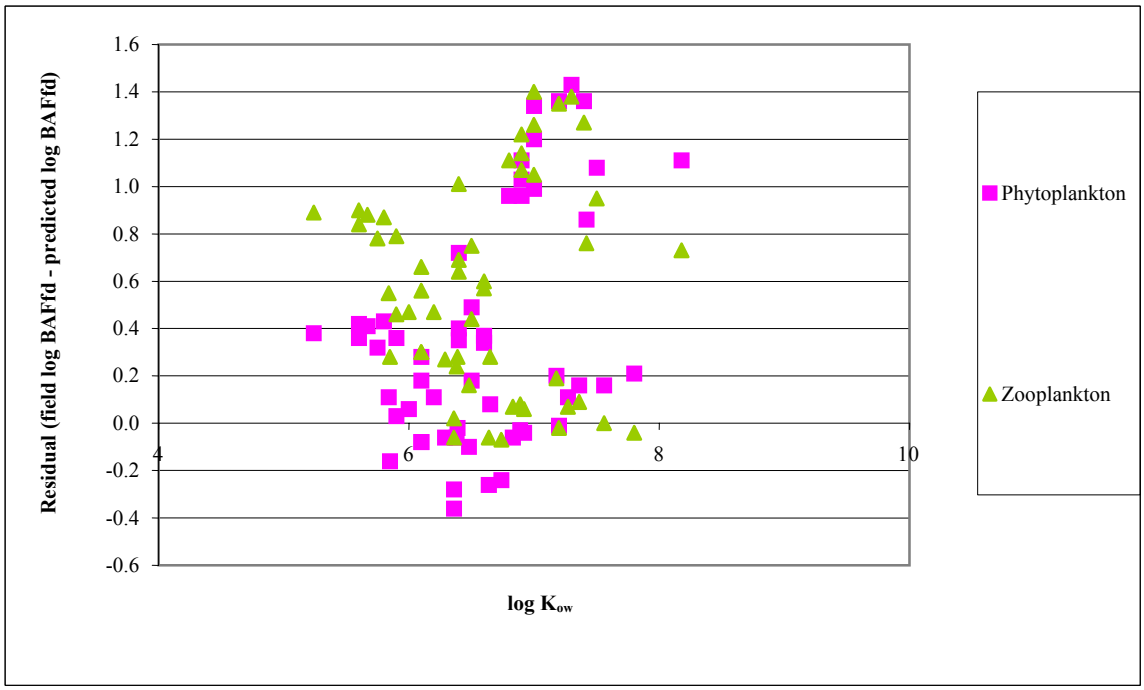

Figure C4 Residual in the prediction in log BAF_{fd} for trophic level 1 using AQUAWEB v1.1 (TGD water properties and QSAR for predominantly hydrophobics)

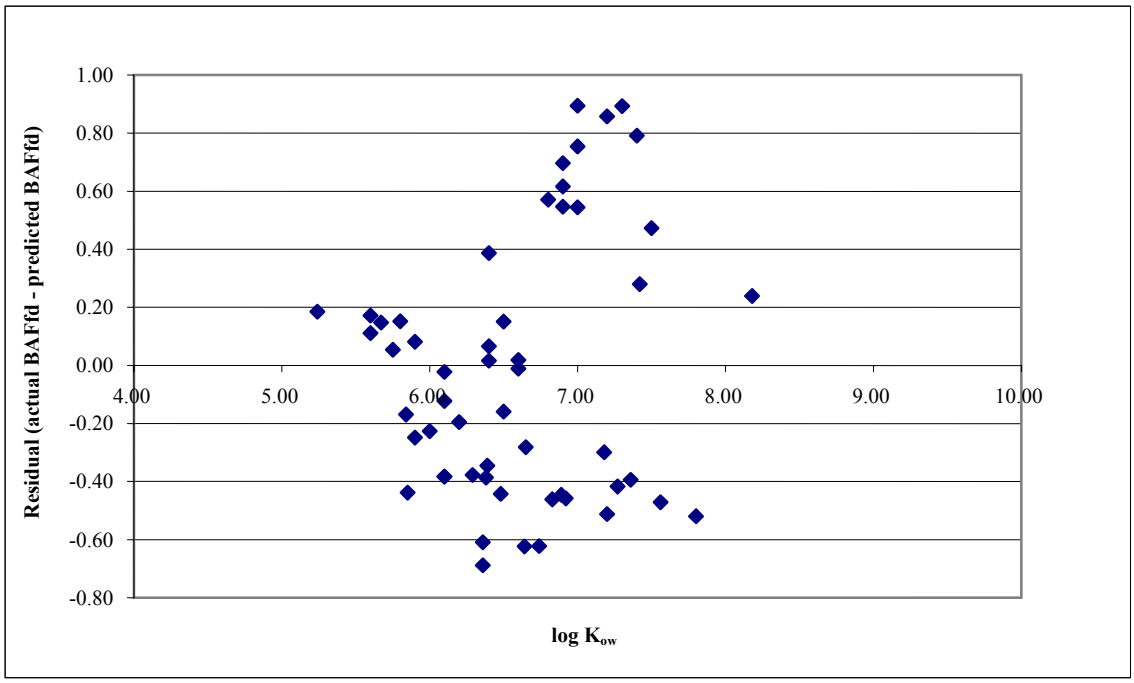

Figure C5 Residual in the prediction in log BAF_{fd} for trophic level 1 using the Voutsas *et al.* (2002) method

The analysis of the residuals (see Table in the main report) shows that the Voutsas *et al.* (2002) method appears to perform best for this trophic level, with a mean residual of -0.02, a mean absolute residual of 0.38 and the 95th percentile absolute residual of 0.81. In addition, the plot of the residuals against log K_{ow} Figure C5 shows no systematic over or underprediction that is log K_{ow} dependent. The mean absolute residual of 0.38 translates to a mean over- or underprediction of the actual BAF_{fd} of a factor of 2.4, and the 95th percentile absolute residual means that 95 per cent of the predictions are within a factor of 6.5 of the actual value. The analysis of the residuals generally shows that the AQUAWEB v1.1 model performs better than the BIO v1.1 model for this test set.

BAF_{fd} data values presented by Voutsas *et al.* (2002) were converted from BAF_t values (lipid-normalized bioaccumulation factors on a total concentration in water) to a freely dissolved basis by assuming an equilibrium partitioning approach. Details of how this was carried out are given in Voutsas *et al.* (2002). In order to test if this data conversion could account for the difference between the predicted and actual BAF_{fd} seen here, a comparison was made between the predicted BAF_t using the Great Lakes water properties and the BAF_t data set. This is shown in Figure C6 and Figure C7. Here the predicted log BAF_t shows a maximum at a log K_{ow} of around seven. The scatter in the actual log BAF_t data set is quite large but it appears to show a similar maximum at a log K_{ow} of around seven. Statistics for the analysis of the residuals (Table in the main report) shows that, although the Voutsas *et al.* (2002) method appears to perform better than the AQUAWEB v1.1 method against this data set, the difference in performance is less marked than found for the analysis of the log BAF_{fd}. For example, the mean and 95th percentile of the absolute residual from the Voutsas *et al.* (2002) method for the log BAFft is 0.38 and 0.73 respectively,

compared with a mean and 95th percentile for the AQUAWEB predictions for phytoplankton of 0.40 and 1.20 respectively.

Thus, it is possible that the assumptions made by Voutsas *et al.* (2002) in converting the data set to BAF_{fd} values may have introduced further uncertainties into the data set, particularly at log K_{ow} values greater than seven. This may relate to general problems in estimating the freely dissolved or bioavailable fraction in water for highly lipophilic substances.

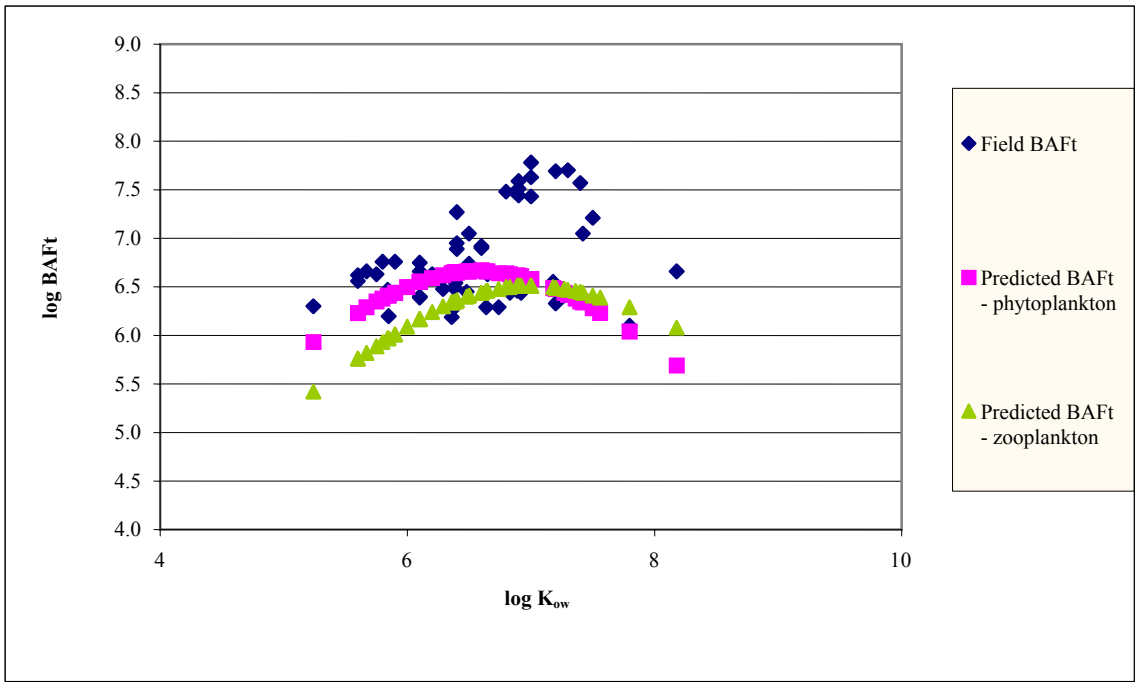

Figure C6 Predicted BAF_t for trophic level 1 using AQUAWEB (Great Lakes water properties and QSAR for predominantly hydrophobics)

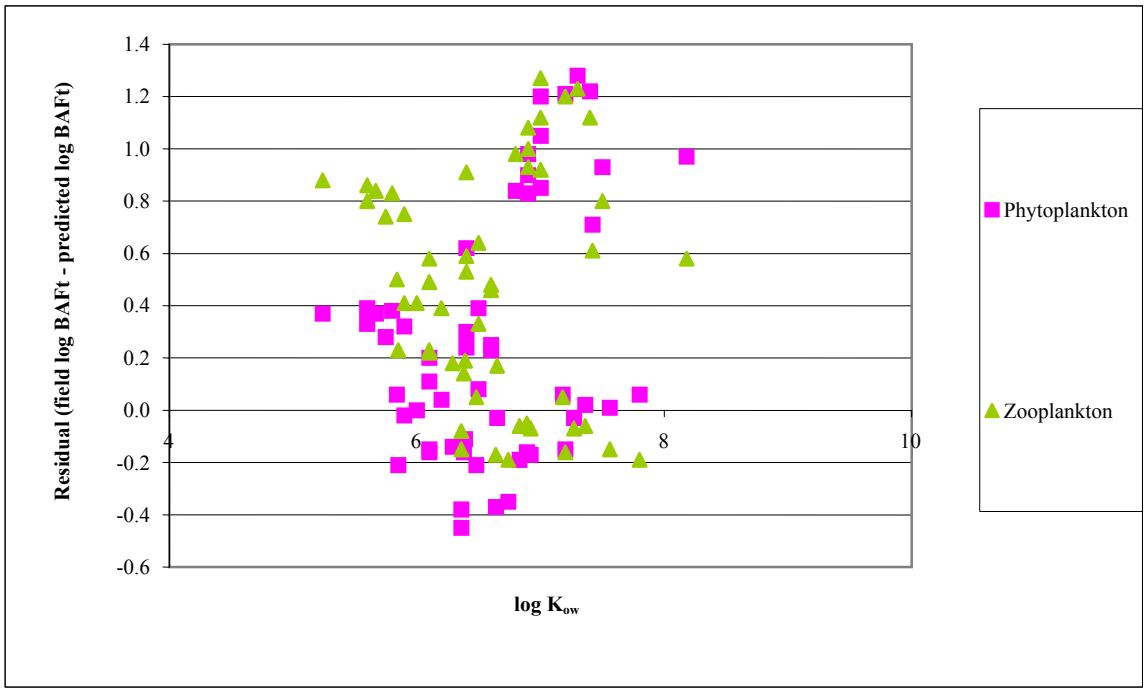

Figure C7 Residual in the prediction in log BAF_t for trophic level 1 using AQUAWEB v1.1 (Great Lakes water properties and QSAR for predominantly hydrophobics)

Trophic level 2

For trophic level 2, plots comparing the BAF_{fd} estimated using AQUAWEB v1.1 with the actual BAF_{fd} are shown in Figure C8 (using the Great Lakes water properties) and Figure C9 (using the TGD water properties). The corresponding residuals in the prediction are shown in Figure C10 and Figure C11 respectively. For comparison, the residuals in the prediction obtained using the Voutsas *et al.* (2002) method are shown in Figure C12.

As can be seen from these plots, the field data again show a more or less linear increase in the log BAF_{fd} with log K_{ow}. The predicted log BAF_{fd} appears to follow this increase well up to a log K_{ow} of around seven, and then tends to a maximum value of log BAF_{fd} at log K_{ow} values of around eight to nine (depending on the assumptions made over the dissolved organic carbon content of the water). This is broadly similar to the pattern seen in the predictions for trophic level 1.

Analysis of the residuals shows that the Voutsas *et al.* (2002) method again appears to perform best for this trophic level, with a mean residual of -0.08, a mean absolute residual of 0.53 and a 95th percentile residual of 1.18. The mean absolute residual of 0.53 translates to a mean over- or underprediction of the actual BAF_{fd} of a factor of 3.4, and the 95th percentile absolute residual means that 95 per cent of the predictions are within a factor of 15 of the actual value.

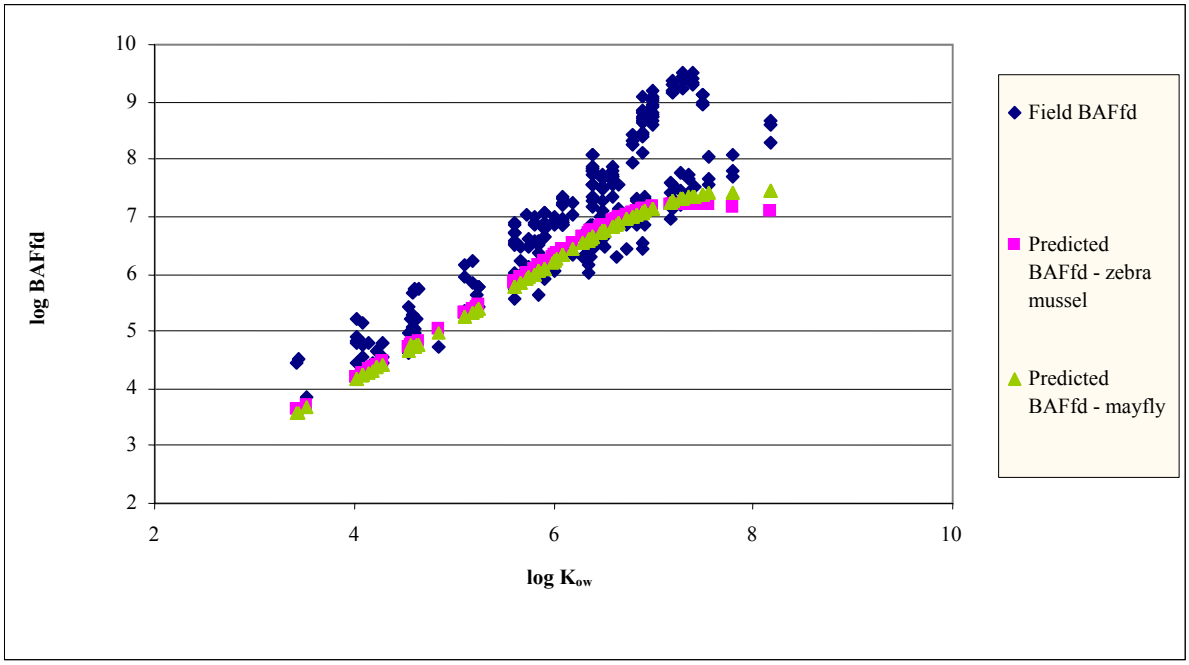

Figure C8 Predicted BAF_{fd} for trophic level 2 using AQUAWEB (Great Lakes water properties and QSAR for predominantly hydrophobics)

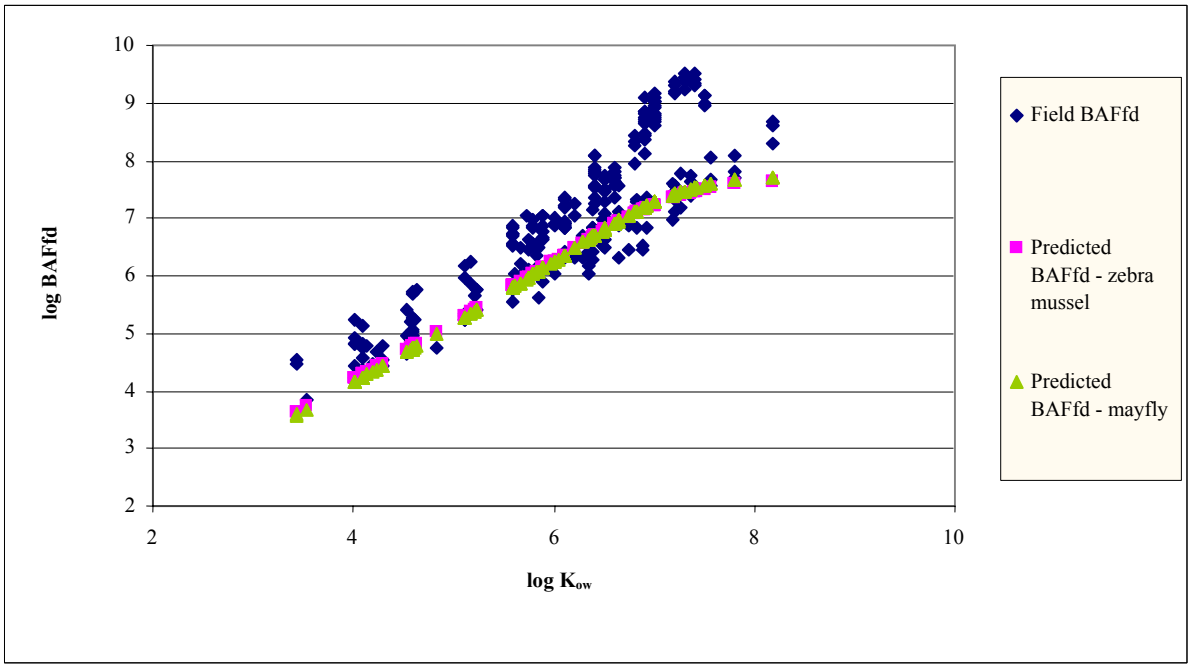

Figure C9 Predicted BAF_{fd} for trophic level 2 using AQUAWEB (TGD water properties and QSAR for predominantly hydrophobics)

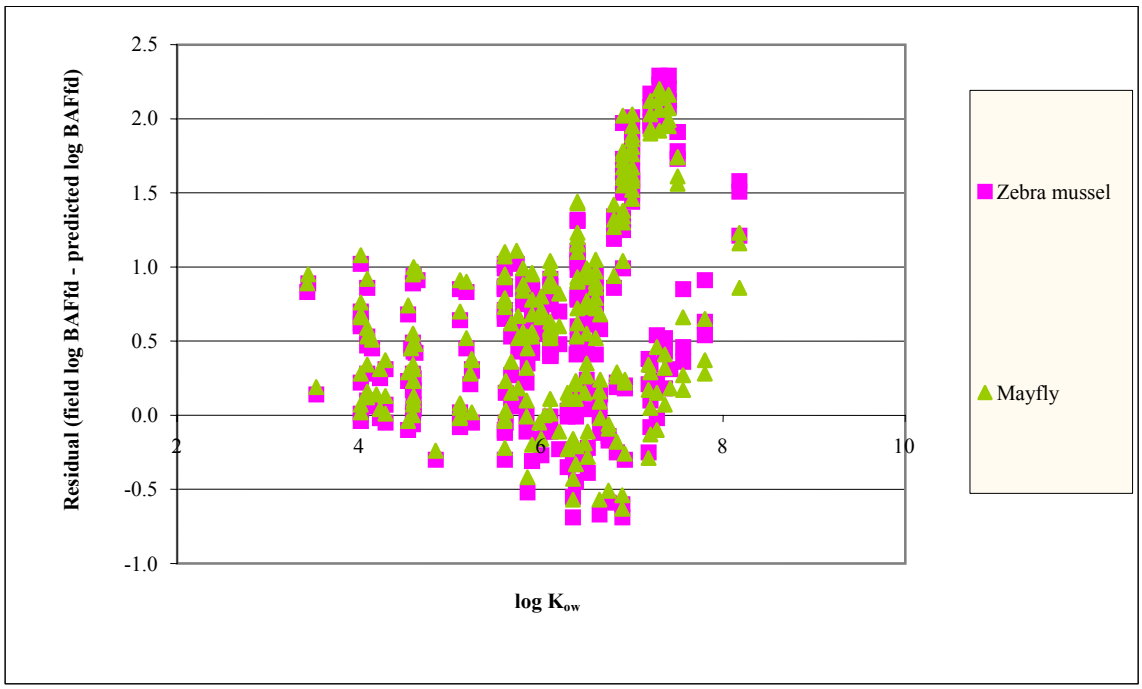

Figure C10 Residual in the prediction in log BAF_{fd} for trophic level 2 using AQUAWEB v1.1 (Great Lakes water properties and QSAR for predominantly hydrophobics)

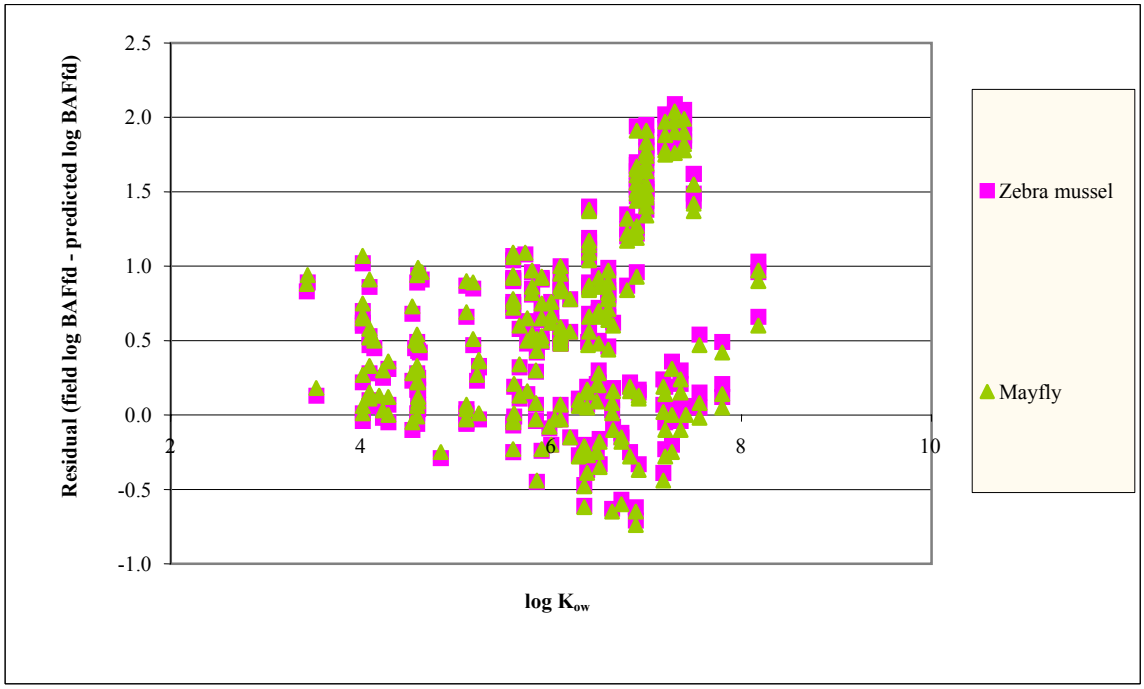

Figure C11 Residual in the prediction in log BAF_{fd} for trophic level 2 using AQUAWEB v1.1 (TGD water properties and QSAR for predominantly hydrophobics)

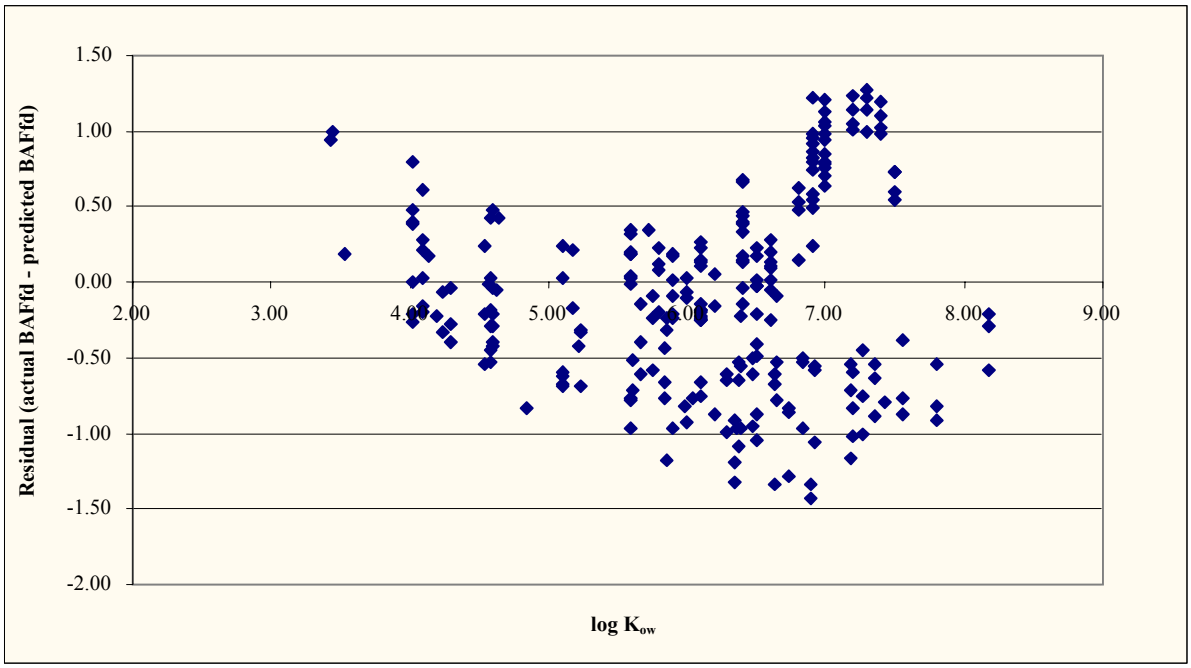

Figure C12 Residual in the prediction in log BAF_{fd} for trophic level 2 using the Voutsas *et al.* (2002) method

Similar to trophic level 1, BAF_{fd} data presented by Voutsas *et al.* (2002) were converted from BAF_t. To see if this conversion could account for some of the difference between predicted and actual BAF_{fd} values outlined above, a comparison was made between the predicted and actual BAF_t values. This is shown in Figure C13 for AQUAWEB using the Great Lakes water properties. Figure C14 shows the corresponding residuals in the prediction. As can be seen from the plots, the AQUAWEB v1.1 model appears to perform reasonably well against this data set. This can also be seen in the analysis of the residuals given in Table of the main report. Although the Voutsas *et al.* (2002) method still appears to perform better against this data set than the AQUAWEB v1.1 model, the difference in performance is relatively small (for example the mean residual, mean absolute residual and 95th percentile residual for the predictions using the Voutsas *et al.* (2002) method are -0.16, 0.55 and 1.21 respectively, compared with 0.19, 0.57 and 1.12 respectively obtained using the AQUAWEB v1.1 model for mayfly larvae). Analysis of the residuals again shows that the AQUAWEB v1.1 model performs better than the BIO v1.1 model for this test set.

Again, it is possible that the assumptions made by Voutsas *et al.* (2002) in converting the data set to BAF_{fd} values may have introduced further uncertainties into the data set, particularly at log K_{ow} values greater than seven. When the BAF_t data are analysed, both the Voutsas *et al.* (2002) method and the AQUAWEB v1.1 model appear to perform similarly.

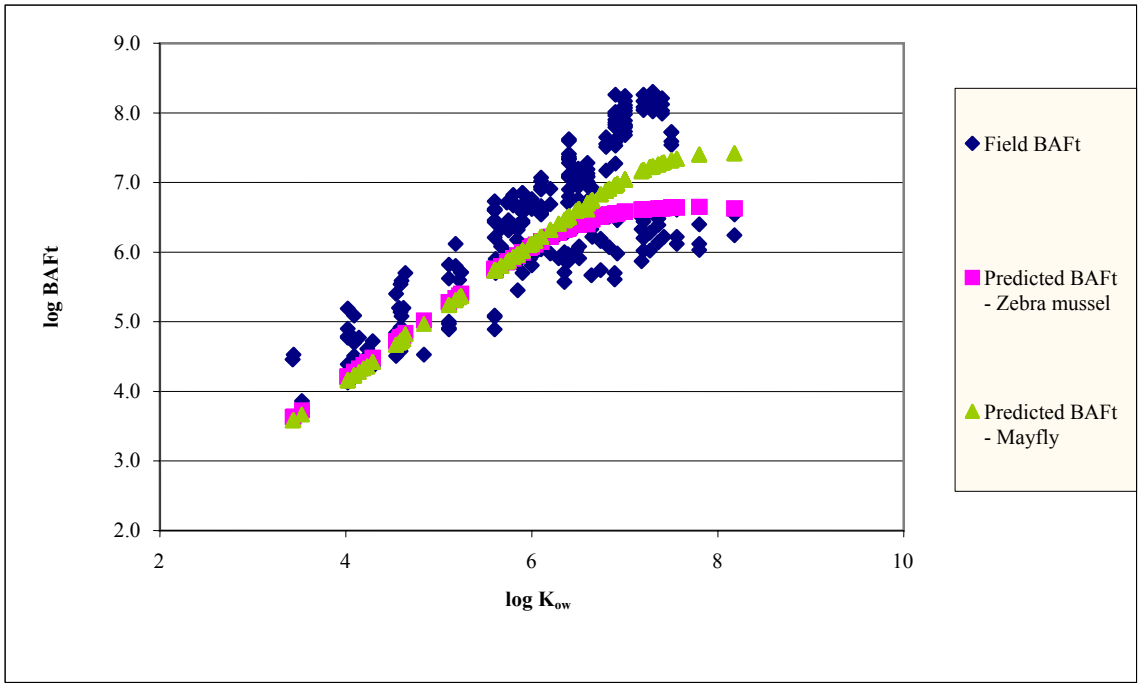

Figure C13 Predicted BAF_t for trophic level 2 using AQUAWEB (Great Lakes water properties and QSAR for predominantly hydrophobics)

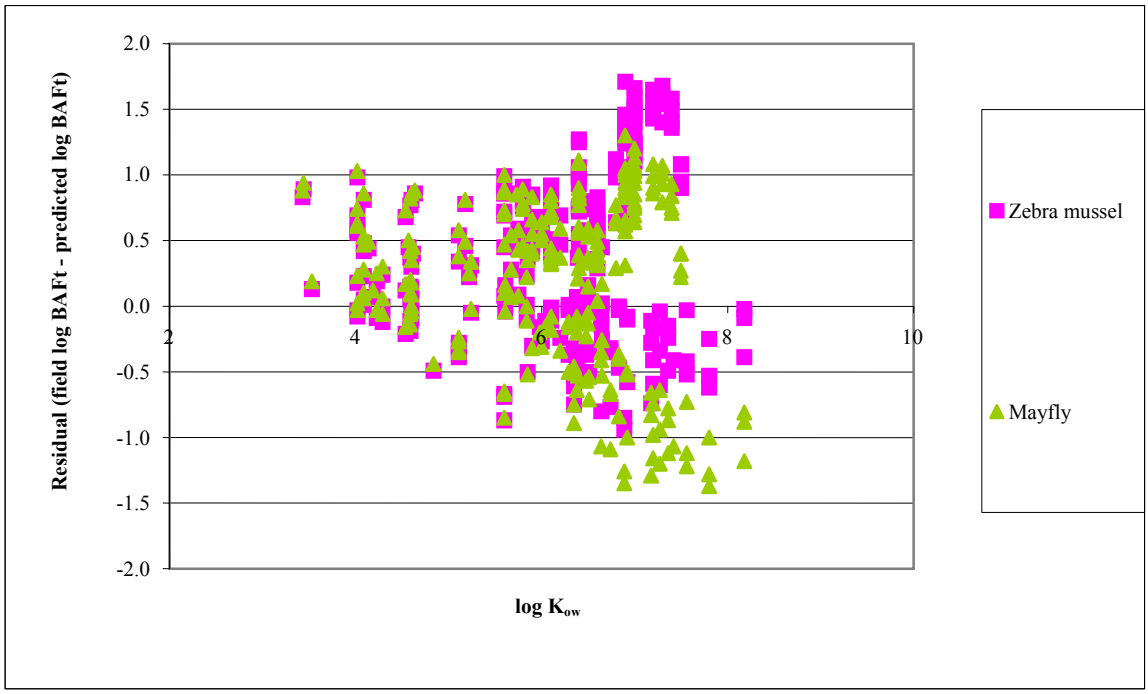

Figure C14 Residual in the prediction in log BAF_t for trophic level 2 using AQUAWEB v1.1 (Great Lakes water properties and QSAR for predominantly hydrophobics)

Trophic level 3

For trophic level 3, plots comparing the BAF_{fd} estimated using AQUAWEB v1.1 with the actual BAF_{fd} are shown in Figure C15 (using the Great Lakes water properties) and Figure C16 (using the TGD water properties). The equivalent plot for BAF_{fd} estimated using the TGD method is shown in Figure C17. Plots of the residual in the prediction are shown in Figure C18 (AQUAWEB v1.1 using the Great Lakes water properties), Figure C19 (AQUAWEB v1.1 using the TGD water properties) and Figure C20 (the TGD method). For reference, a plot of the residual obtained using the Voutsas *et al.* (2002) method is shown in Figure C21.

As can be seen from these plots, the field data show a linear increase of log BAF_{fd} with increasing log K_{ow} values. Predictions obtained using AQUAWEB v1.1 appear to follow this increase reasonably well at lower log K_{ow} values but reach a maximum in the log BAF_{fd} at a log K_{ow} value of around seven or eight (depending on the assumptions made of the dissolved organic carbon content of water). A similar pattern is also evident in the TGD predictions, with a maximum on the predicted BAF_{fd} occurring at a log K_{ow} of around seven.

Analysis of the residuals shows that the Voutsas *et al.* (2002) method appears to perform best for this trophic level, with a mean residual of 0.00, a mean absolute residual of 0.36 and a 95th percentile residual of 0.86. The mean absolute residual of 0.36 corresponds to a mean over- or underprediction of the actual BAF_{fd} of a factor of 2.3, and the 95th percentile absolute residual means that 95 per cent of the predictions are within a factor of 7.2 of the actual BAF_{fd}. Analysis of the residuals shows that the AQUAWEB v1.1 model performs better than the BIO v1.1 model for this test set.

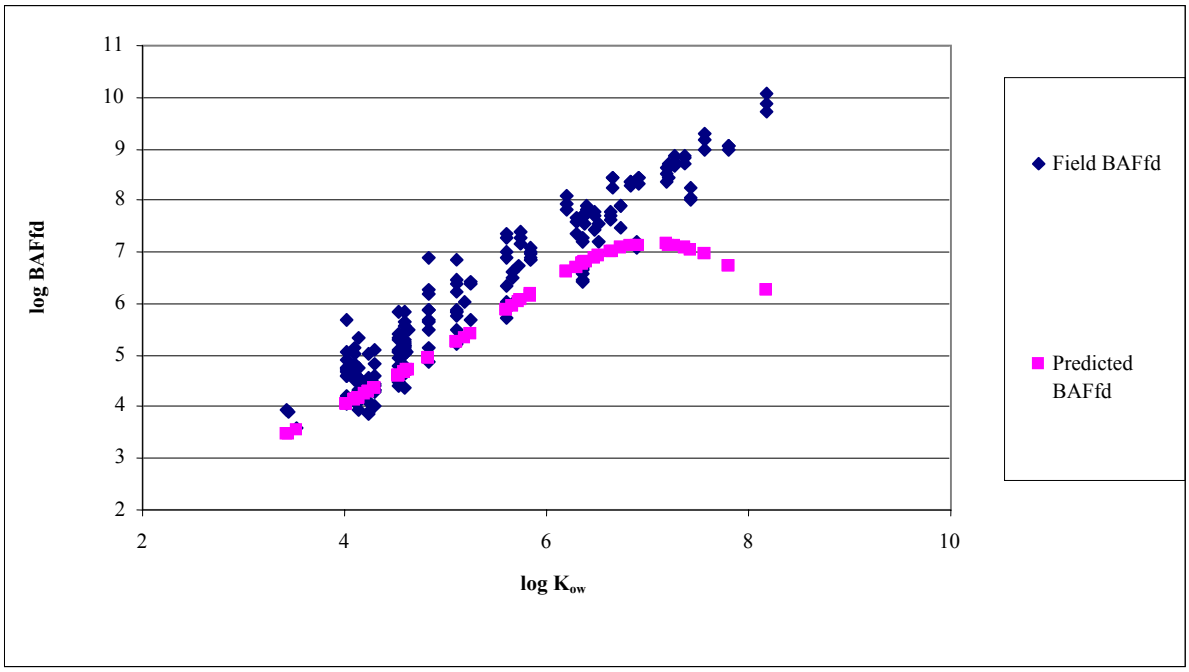

Figure C15 Predicted BAF_{fd} for trophic level 3 using AQUAWEB v1.1 (Great Lakes water properties and QSAR for predominantly hydrophobics)

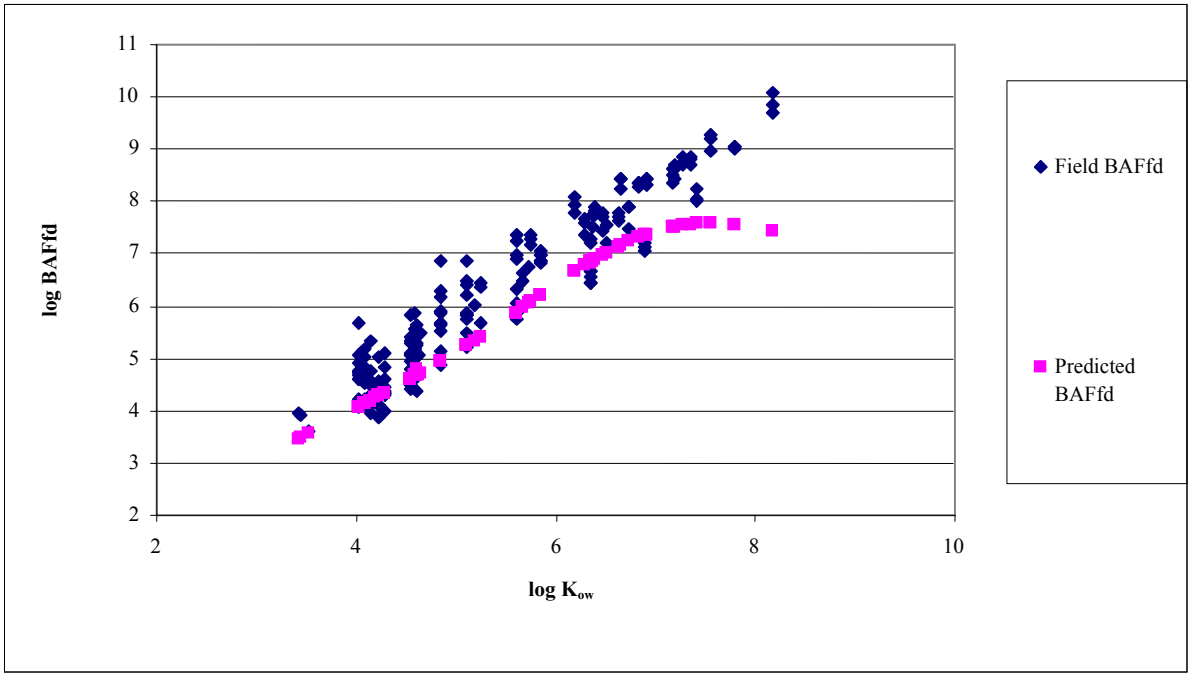

Figure C16 Predicted BAF_{fd} for trophic level 3 using AQUAWEB v1.1 (TGD water properties and QSAR for predominantly hydrophobics)

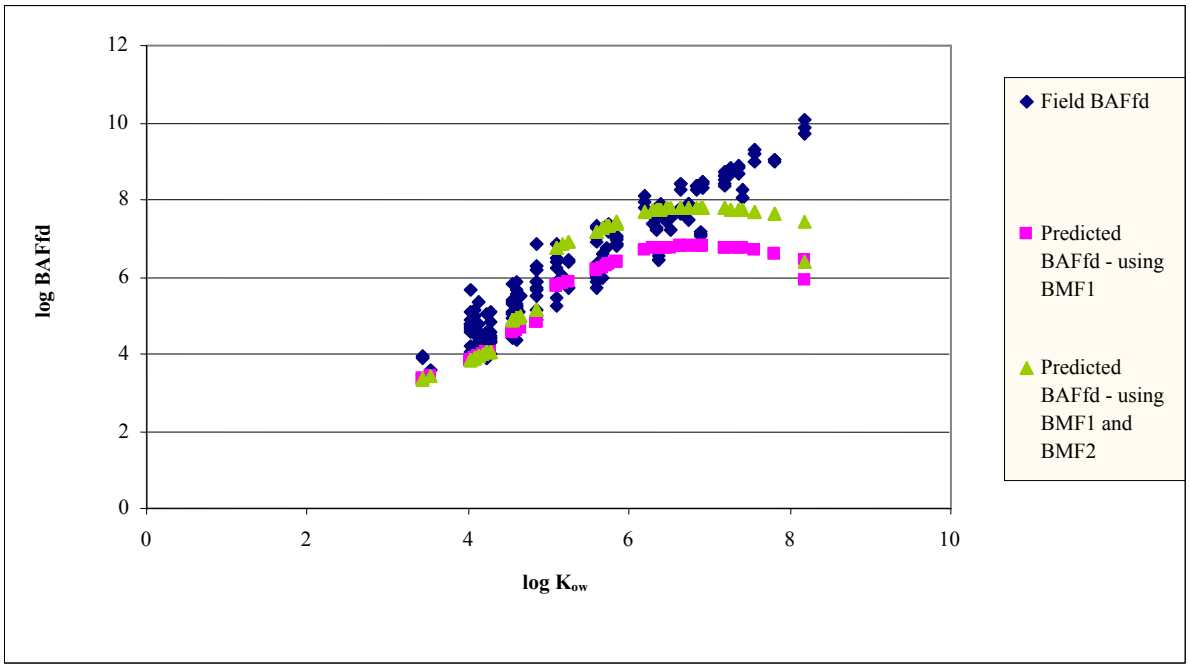

Figure C17 Predicted BAF_{fd} for trophic level 3 using the TGD method

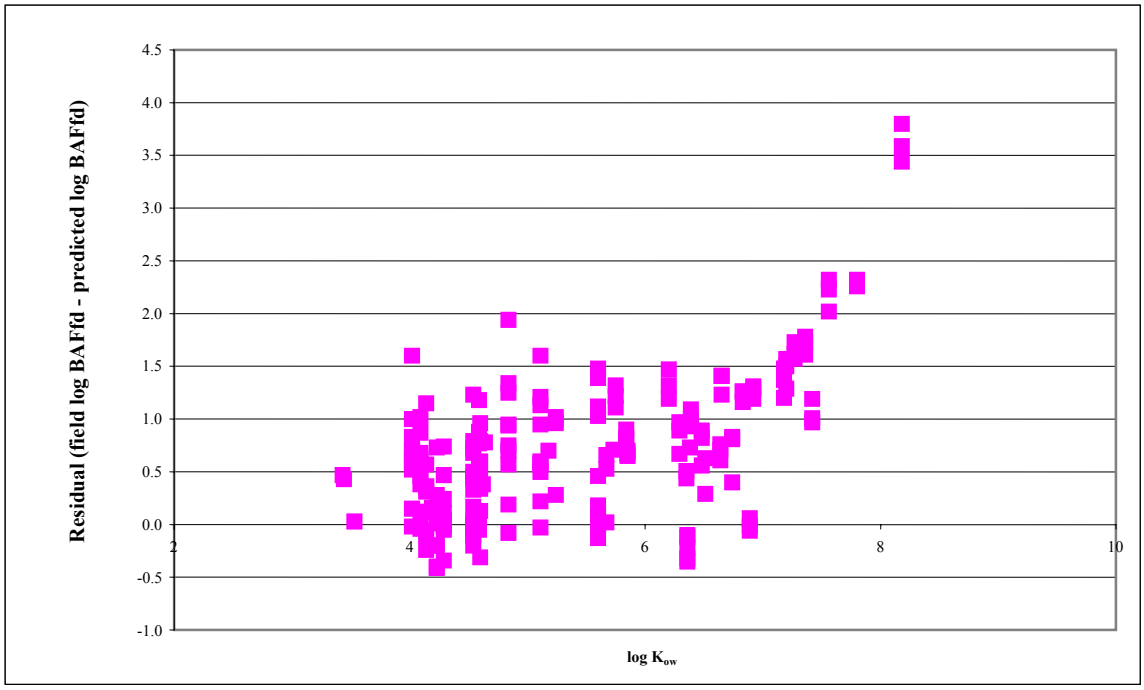

Figure C18 Residual in the prediction in log BAF_{fd} for trophic level 3 using AQUAWEB v1.1 (Great Lakes water properties and QSAR for predominantly hydrophobics)

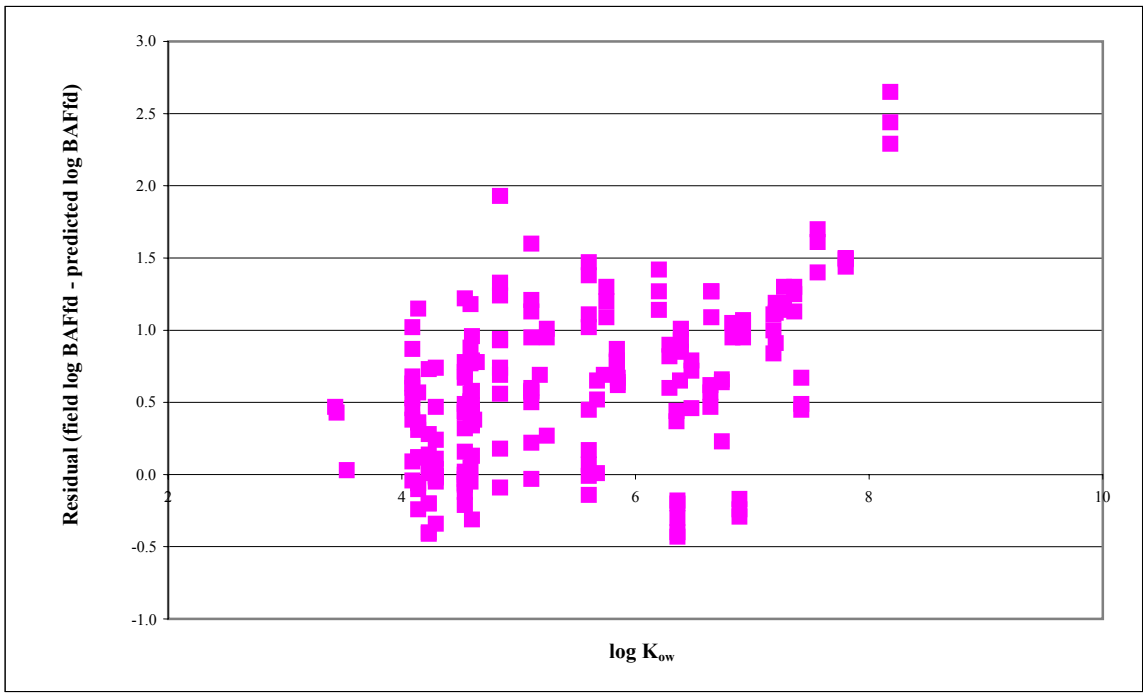

Figure C19 Residual in the prediction in log BAF_{fd} for trophic level 3 using AQUAWEB v1.1 (TGD water properties and QSAR for predominantly hydrophobics)

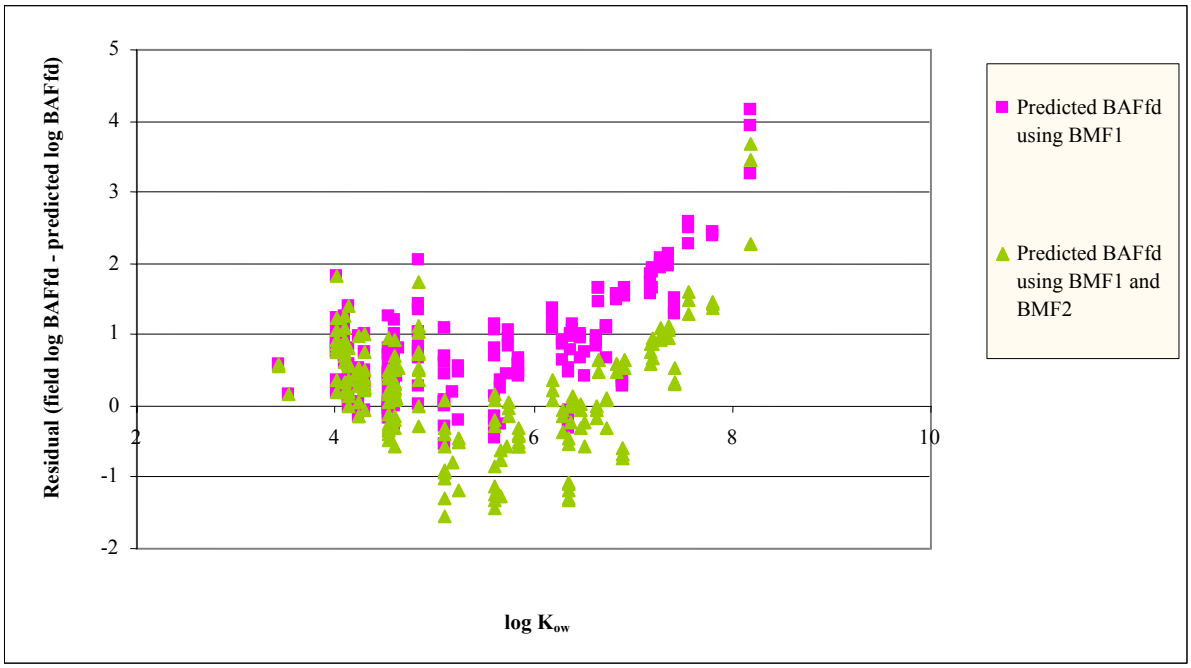

Figure C20 Residual in the prediction in log BAF_{fd} for trophic level 3 using the TGD method

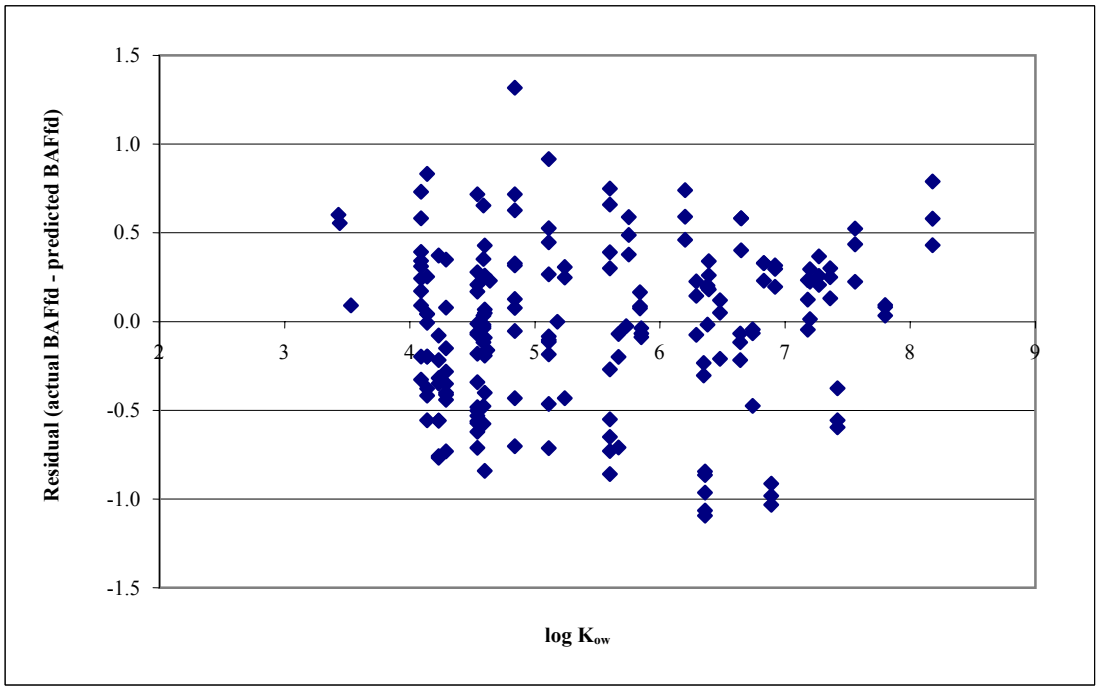

Figure C21 Residual in the prediction in log BAF_{fd} for trophic level 3 using the Voutsas *et al.* (2002) method

Similar to the preceding trophic levels, an analysis of predicted BAF_t values was carried out to test if the conversion applied by Voutsas *et al.* (2002) when deriving BAF_{fd} values could account for the differences seen between actual and predicted

values. Plots showing the predicted BAF_t and actual BAF_t are given in Figure C22 (AQUAWEB v1.1 using the Great Lakes water properties) Figure C23 (TGD method). The corresponding plots for residuals are given in Figure C24 and C25 respectively.

As can be seen from the plots, both methods predict a maximum log BAF_t at a log K_{ow} of six to seven. The available data set of actual BAF_t values shows a large degree of scatter, but appears to show an increasing trend in the log BAF_t with increasing log K_{ow} (although there is some suggestion of a leveling off of the log BAF_t value at log K_{ow} values above seven). Based on the analysis of residuals given in Table 6.2 of the main report, overall the Voutsas *et al.* (2002) method still appears to perform best against this data set, although the AQUAWEB v1.1 and TGD method (using both a BMF_1 and BMF_2 value) are much closer in performance to the Voutsas *et al.* (2002) method than was found for the BAF_{fd} data set. For example, the 95th percentile values for the absolute residuals are 1.12 for the Voutsas *et al.* (2002) method compared with 1.30 obtained using the AQUAWEB v1.1 model and 1.61 obtained using the TGD method with a BMF_1 and BMF_2 value.

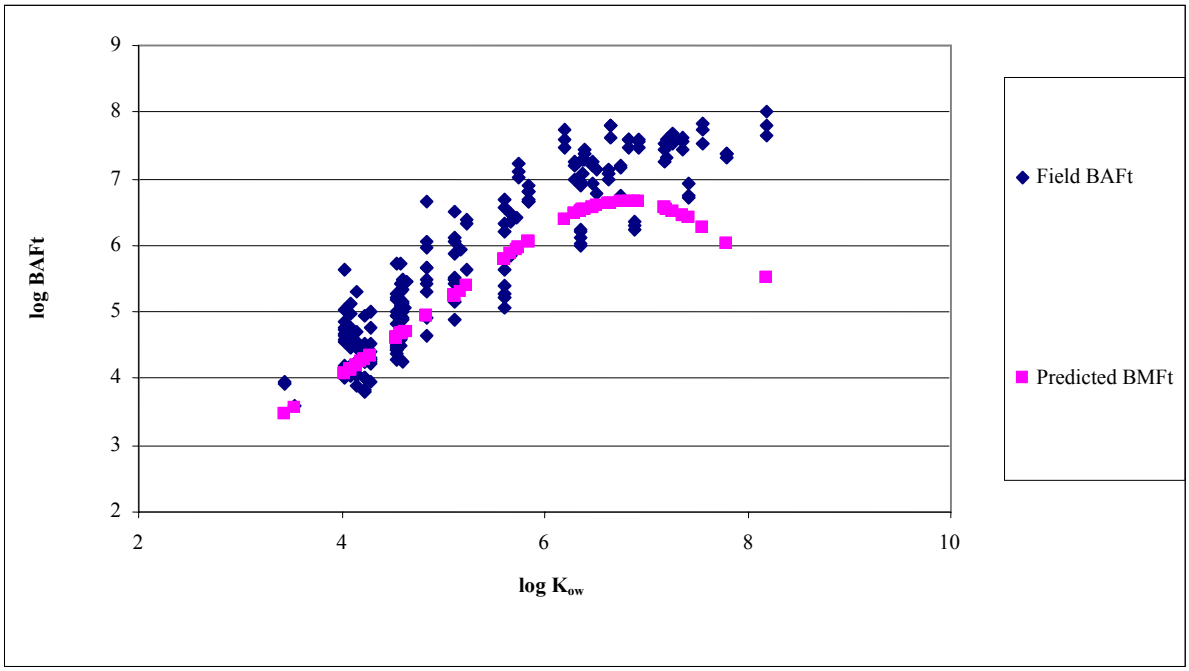

Figure C22 Predicted BAF_t for trophic level 3 using AQUAWEB (Great Lakes water properties and QSAR for predominantly hydrophobics)

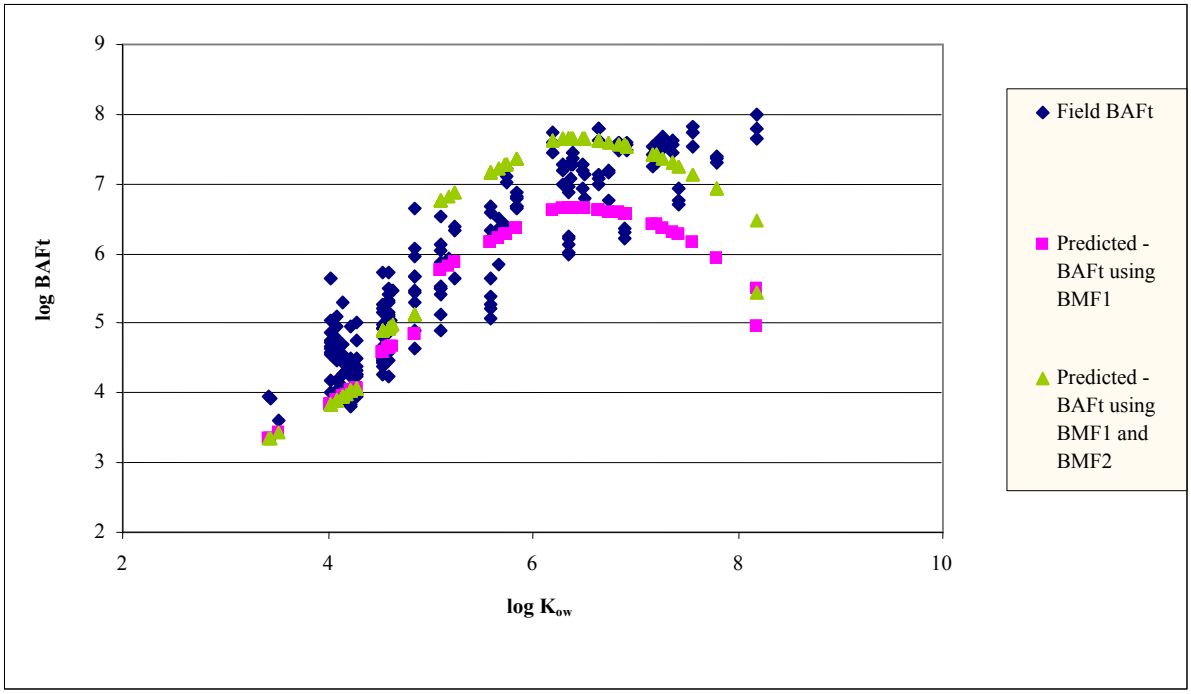

Figure C23 Predicted BAF_t for trophic level 3 using the TGD method

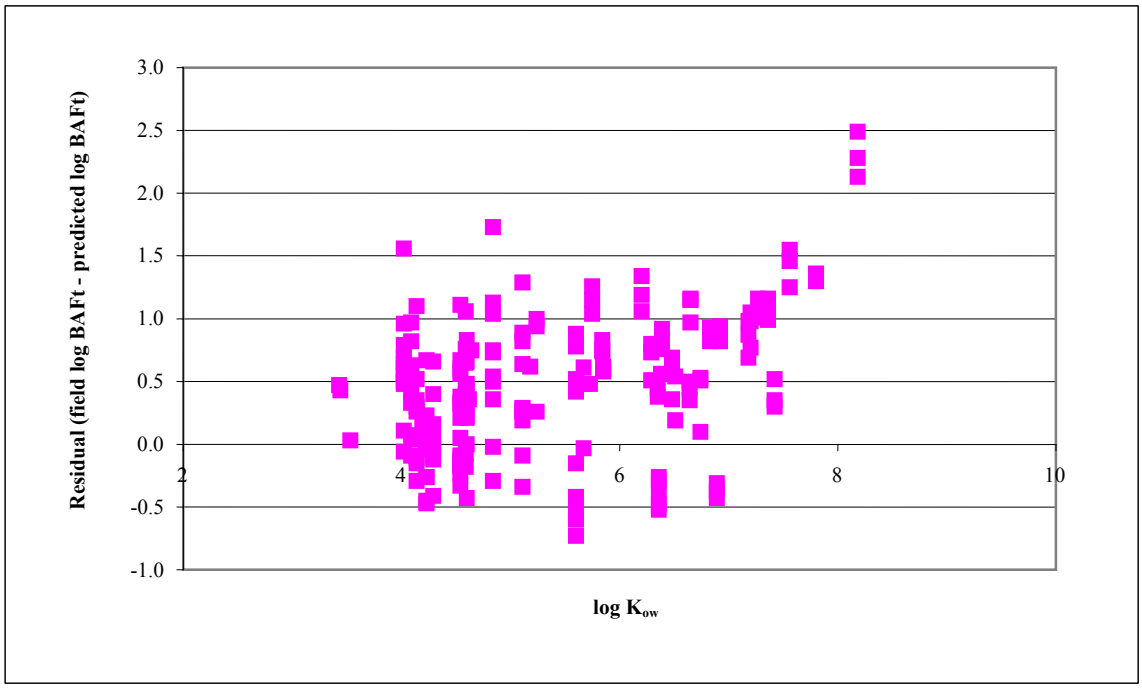

Figure C24 Residual in the prediction in log BAF_t for trophic level 3 using AQUAWEB v1.1 (Great Lakes water properties and QSAR for predominantly hydrophobics)

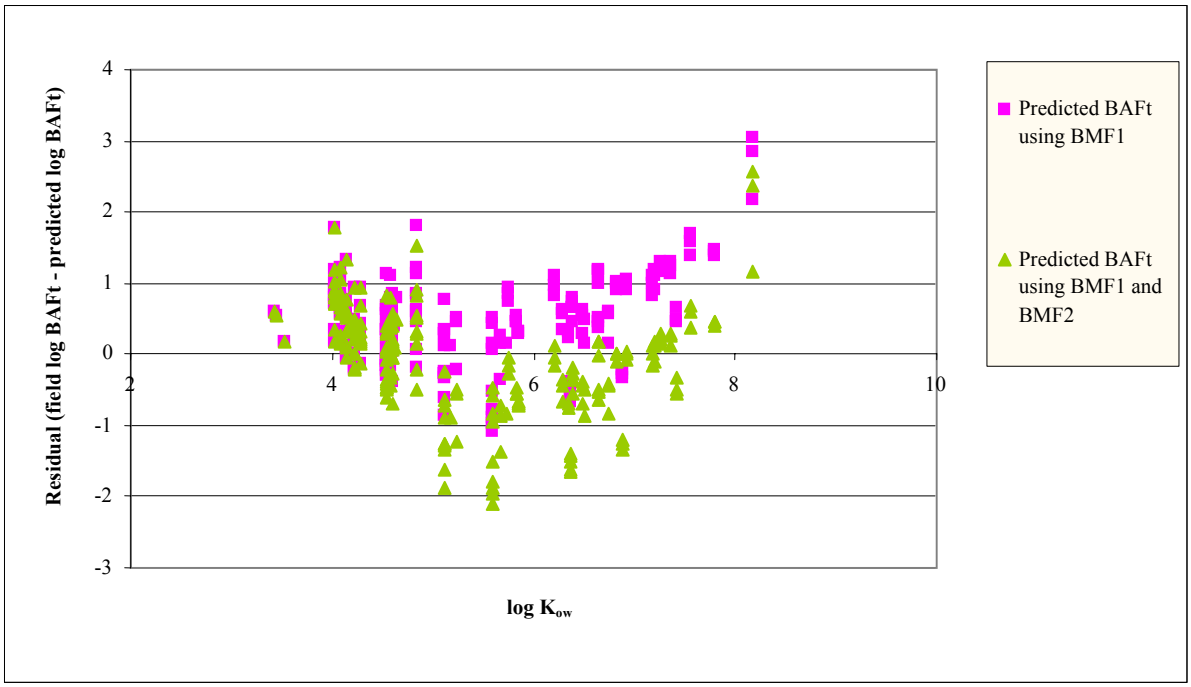

Figure C25 Residual in the prediction in log BAF_t for trophic level 3 using the TGD method

Again, it is possible that the assumptions made by Voutsas *et al.* (2002) in converting the data set to BAF_{fd} values may have introduced further uncertainties into the data set, particularly at log K_{ow} values greater than seven.

The TGD method using both a BMF_1 and BMF_2 value (as is currently recommended for extended marine food chains) appears to perform better against this freshwater data set than the TGD method employing a single BMF_1 value (as is currently recommended for freshwater food chains).

Trophic level 4

The findings for trophic level 4 are very similar to those for trophic level 3. Plots comparing the estimated BAF_{fd} with the actual BAF_{fd} are shown in Figure C26 (AQUAWEB v1.1 using the Great Lakes water properties), Figure C27 (AQUAWEB v1.1 using the TGD water properties) and Figure C28 (the TGD method). The corresponding residuals in the predictions are displayed in Figure C29 (AQUAWEB v1.1 using Great Lakes water properties), Figure C30 (AQUAWEB v1.1 using TGD water properties) and Figure C31 (the TGD method). Figure C32 shows the residuals in the prediction obtained using the Voutsas *et al.* (2002) method for reference.

Again, the plots reveal that the field data show a linear increase in log BAF_{fd} with increasing log K_{ow} across the range of log K_{ow} values studied, but both the AQUAWEB v1.1 model and the TGD method predict a maximum in the log BAF_{fd} at a log K_{ow} of around seven to eight.

From the analysis of the residuals in Table in the main report, it can be seen that the Voutsas *et al.* (2002) method performs well against this data set, with a mean residual, a mean absolute residual and a 95th percentile residual of 0.07, 0.33 and 0.74 respectively. The mean absolute residual of 0.33 corresponds to a mean over- or underprediction of the actual BAF_{fd} of a factor of 2.1, and the 95th percentile absolute residual means that 95 per cent of the predictions are within a factor of 5.5 of the actual BAF_{fd}. Both the AQUAWEB v1.1 and TGD methods appear to work reasonably well against this data set for a log K_{ow} up to around six (TGD method using a single BMF_1) or seven (AQUAWEB v1.1 and TGD method using both a BMF_1 and BMF_2). Analysis of the residuals shows that the AQUAWEB v1.1 model performs better than the BIO v1.1 model for this test set.

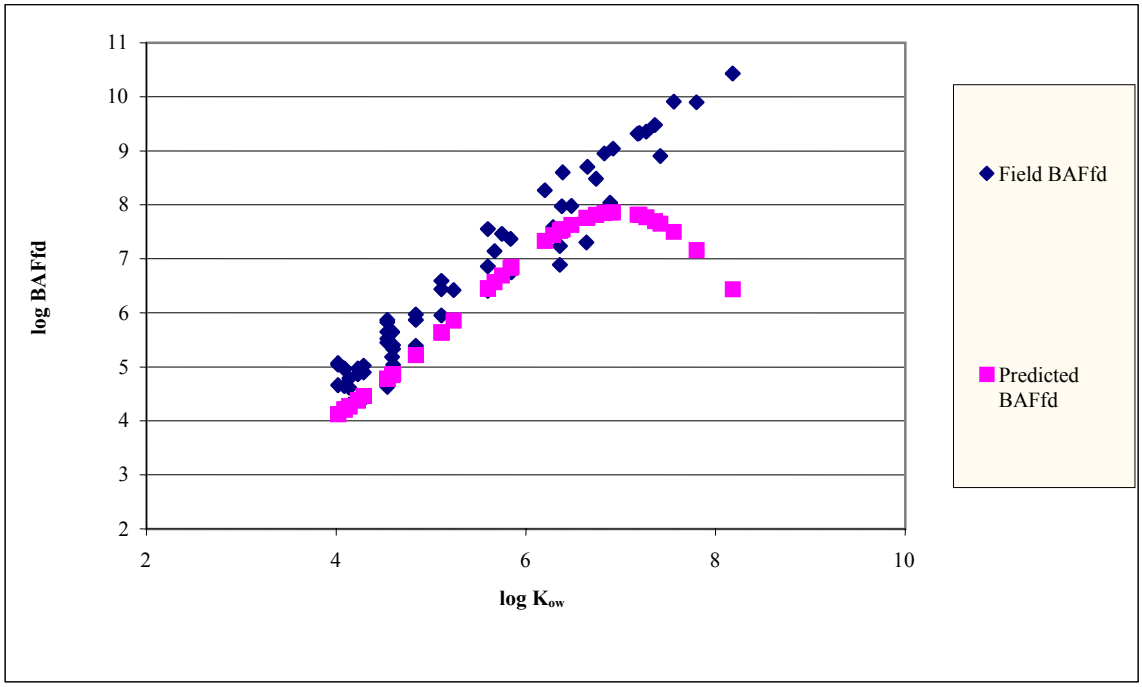

Figure C26 Predicted BAF_{fd} for trophic level 4 using AQUAWEB (Great Lakes water properties and QSAR for predominantly hydrophobics)

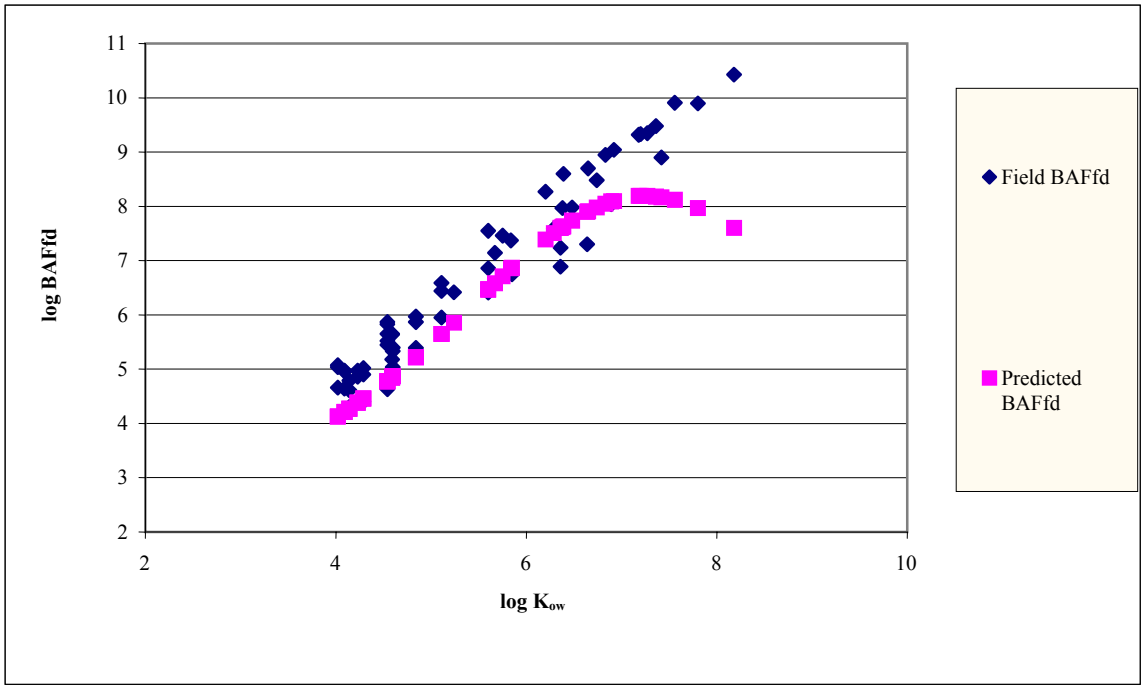

Figure C27 Predicted BAF_{fd} for trophic level 4 using AQUAWEB (TGD water properties and QSAR for predominantly hydrophobics)

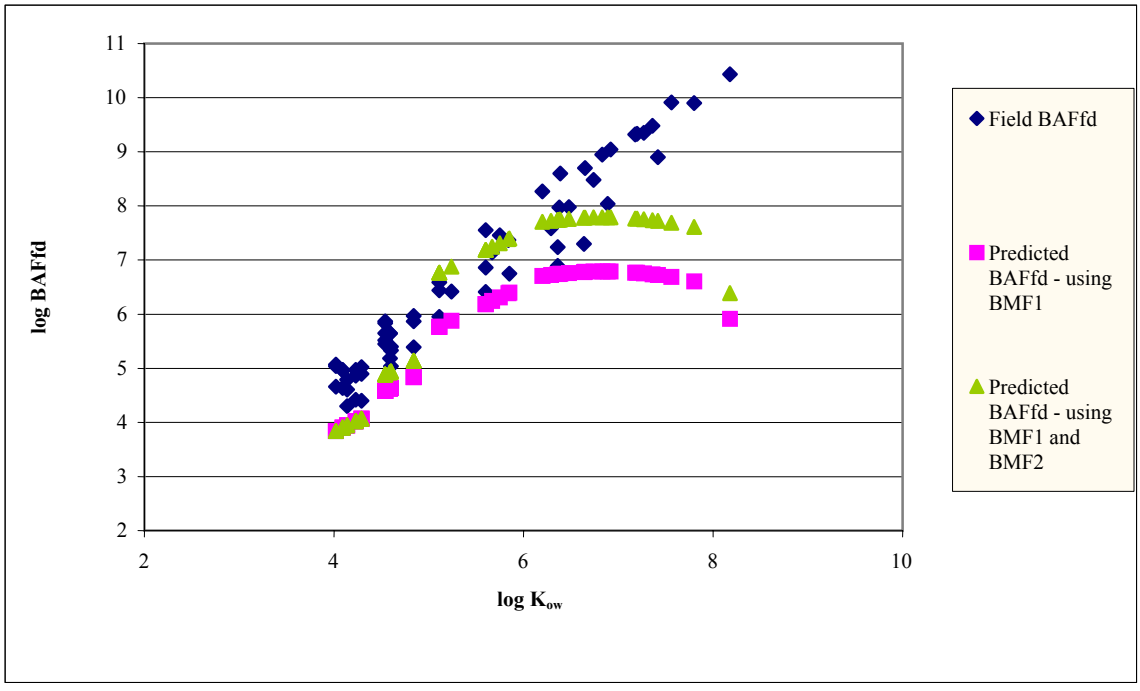

Figure C28 Predicted BAF_{fd} for trophic level 4 using the TGD method

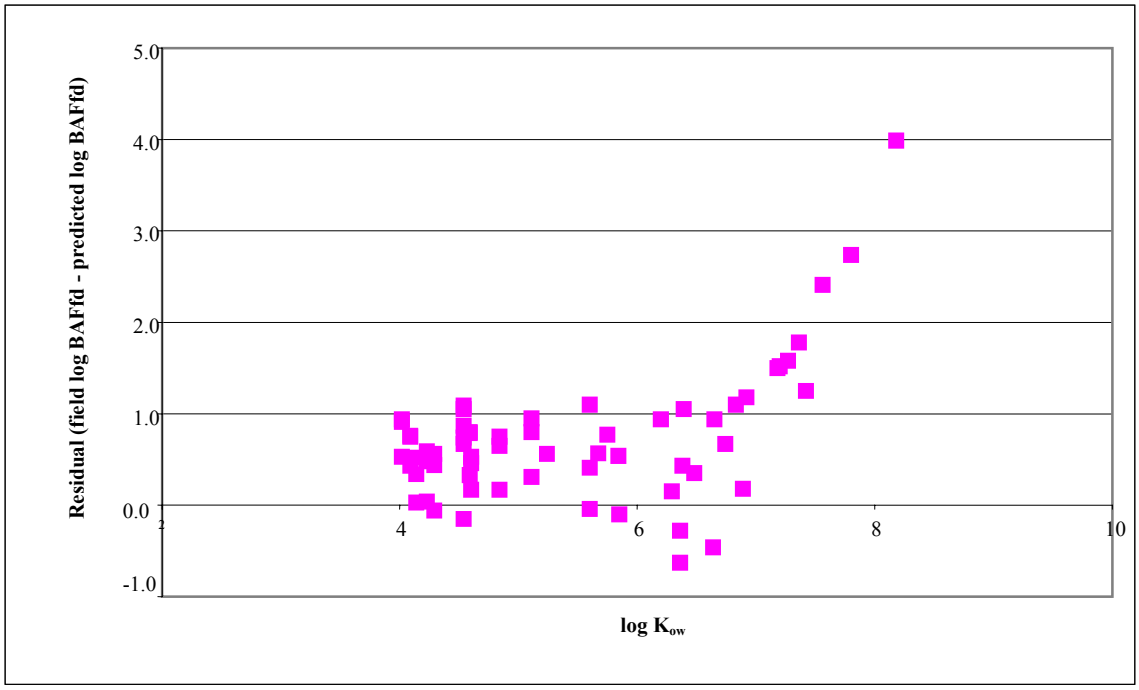

Figure C29 Residual in the prediction in log BAF_{fd} for trophic level 4 using AQUAWEB v1.1 (Great Lakes water properties and QSAR for predominantly hydrophobics)

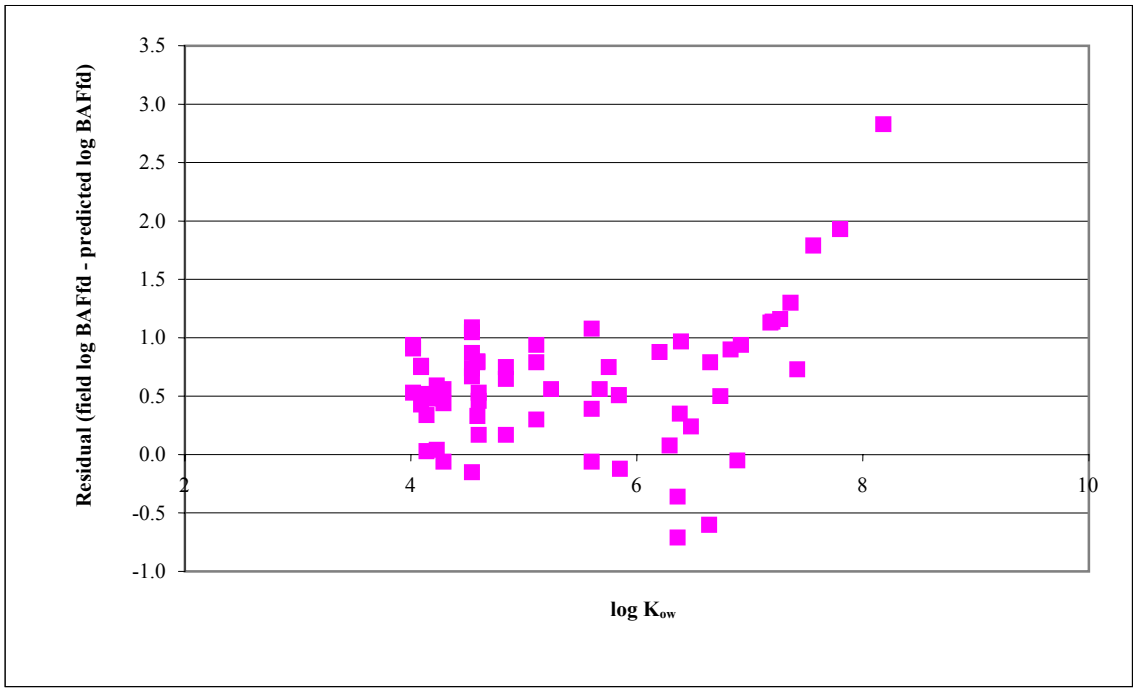

Figure C30 Residual in the prediction in log BAF_{fd} for trophic level 4 using AQUAWEB v1.1 (TGD water properties and QSAR for predominantly hydrophobics)

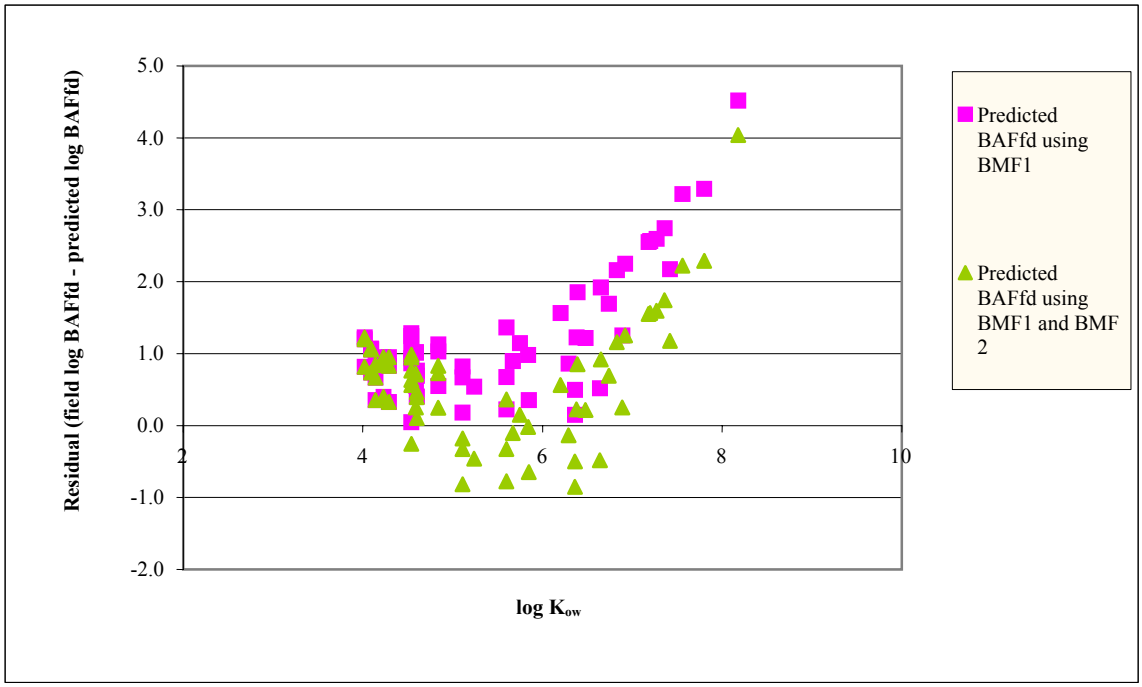

Figure C31 Residual in the prediction in log BAF_{fd} for trophic level 4 using the TGD method

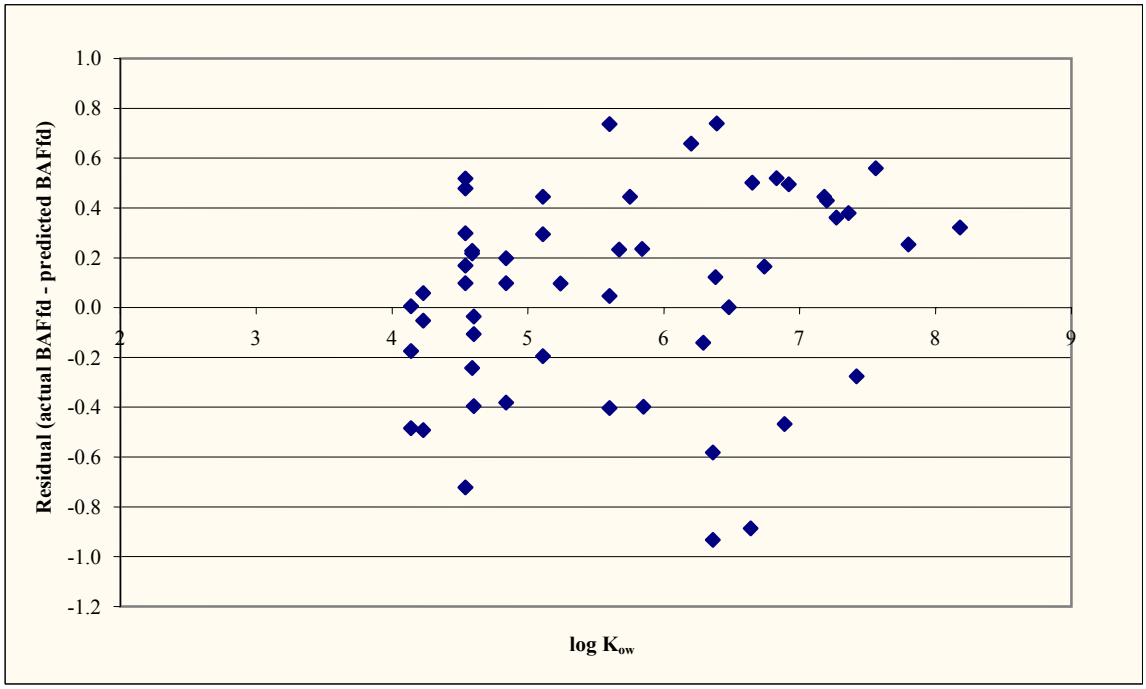

Figure C32 Residual in the prediction in log BAF_{fd} for trophic level 4 using the Voutsas *et al.* (2002) method

Plots showing the predicted BAF_t and actual BAF_t are given in Figure C33 (AQUAWEB v1.1 using Great Lakes water properties) Figure C34 (TGD method).

The corresponding plots for the residuals are given in Figure C35 and Figure C36 respectively.

Similar to the case with trophic level 3, both methods predict a maximum BAF_t at a log K_{ow} of around seven. The data set of actual BAF_t values reveals some scatter, but appears to show an increasing trend in log BAF_t with increasing log K_{ow}. Based on the analysis of residuals given in Table 6.2 in the main report, overall the Voutsas *et al.* (2002) method again appears to perform best against this data set, although the AQUAWEB v1.1 and TGD method (using both a BMF_1 and BMF_2 value) are much closer in performance to the Voutsas *et al.* (2002) method than was found for the BAF_{fd} data set. For example, the 95th percentile values for the absolute residuals are 0.77 for the Voutsas *et al.* (2002) method compared with 1.14 obtained using the AQUAWEB v1.1 model and 1.29 obtained using the TGD method with a BMF_1 and BMF_2 value. Again, the analysis indicates that the TGD method using both a BMF_1 and BMF_2 value appears to perform better against this data set than the TGD method using a single BMF_1 value.

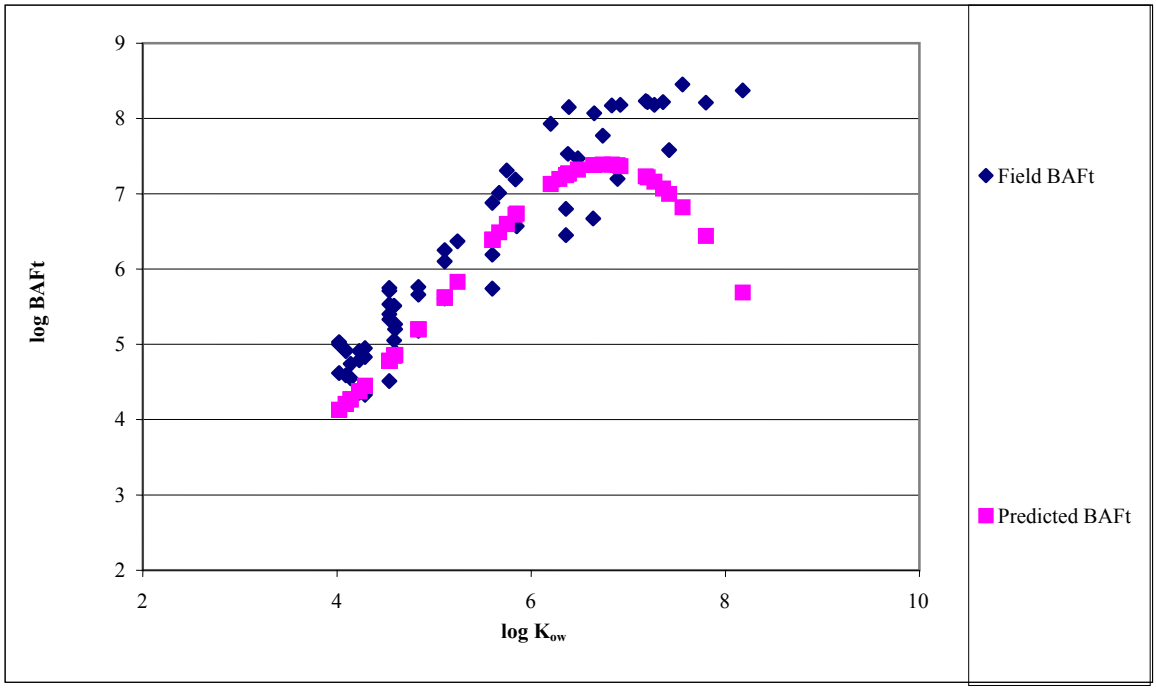

Figure C33 Predicted BAF_t for trophic level 4 using AQUAWEB (Great Lakes water properties and QSAR for predominantly hydrophobics)

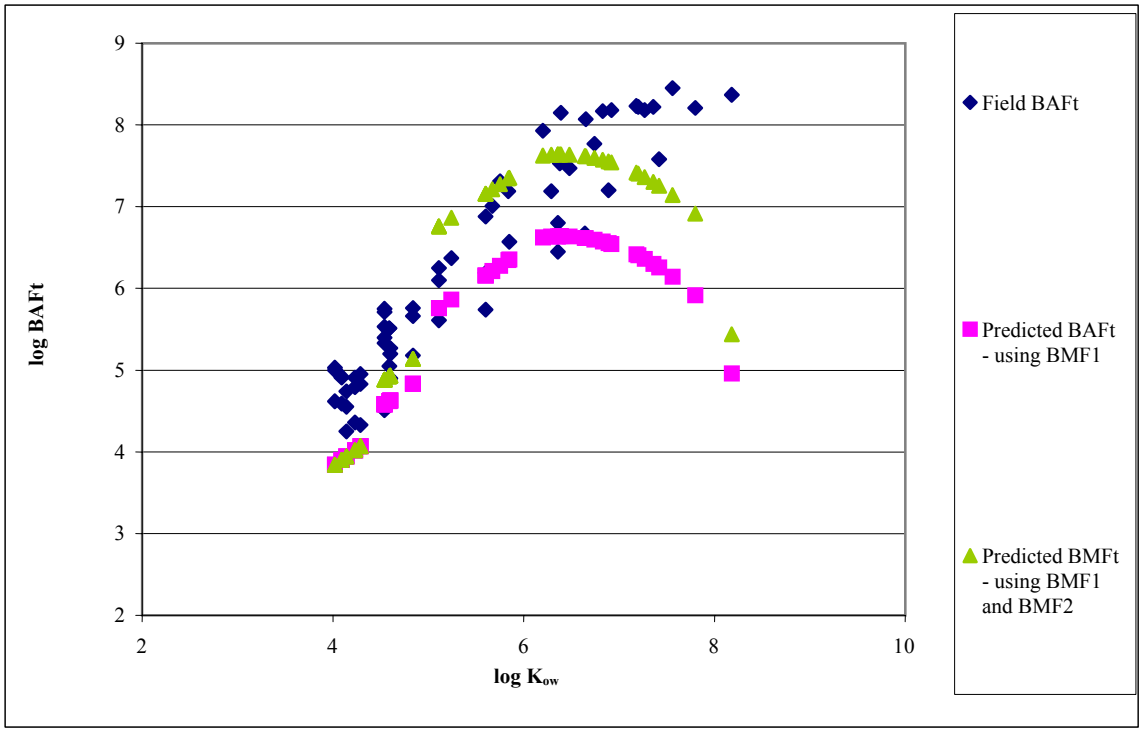

Figure C34 Predicted BAF_t for trophic level 4 using the TGD method

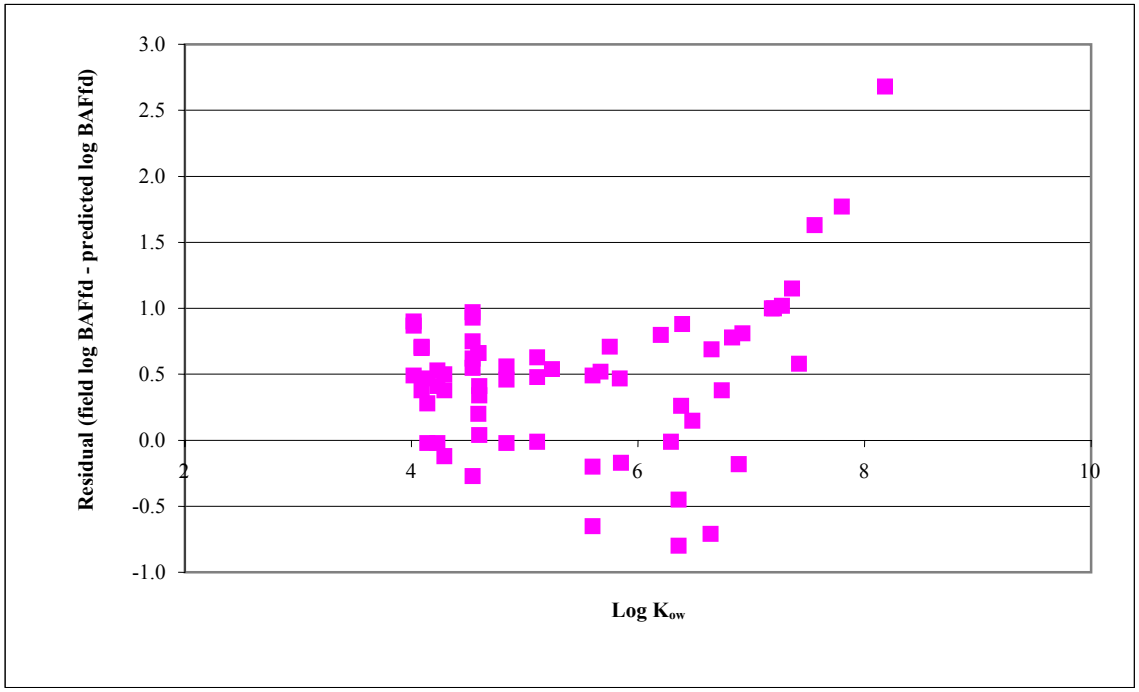

Figure C35 Residual in the prediction in log BAF_t for trophic level 4 using AQUAWEB v1.1 (Great Lakes water properties and QSAR for predominantly hydrophobics)

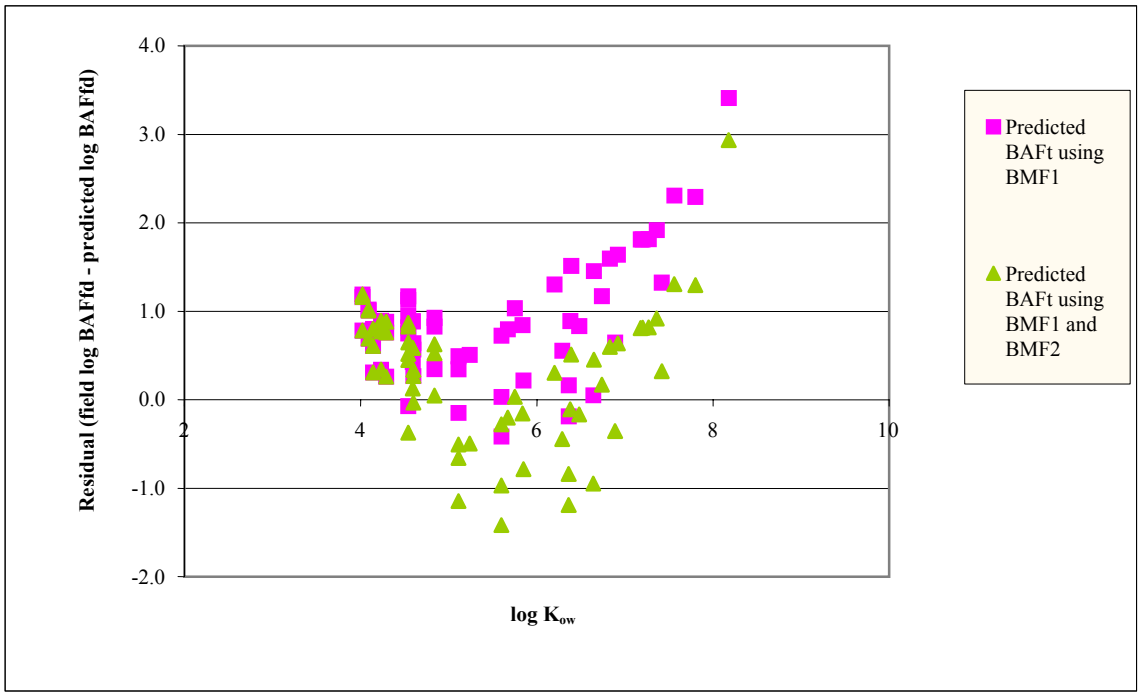

Figure C36 Residual in the prediction in log BAF_t for trophic level 4 using the TGD method

Appendix D – Re-evaluation of Voutsas *et al.* data and equations

As described in Section 2.2 of this report, Voutsas *et al*. (2002) derived a series of equations to predict BAF values from the log K_{ow}. These are based on measured values taken from a number of sources. As described in Section 2.4, the equations for trophic levels 3 and 4 show BAF values continuing to increase at log K_{ow} values of nine or higher. This is in contrast to the other two methods considered in this report, which have the BAF value peaking and then decreasing. Although this report concludes that there are currently no methods suitable for predicting BAF values for log K_{ow} values above seven, in view of this difference it was decided to look more closely at the data used in developing the equations for trophic levels 3 and 4.

BAF values for high log K_{ow} substances come largely from two studies, Metcalfe and Metcalfe (1997) and Oliver and Niimi (1988). These and the other studies used are considered to be reliable, and the data have been used in testing and developing models in this area.

Conversion between total and dissolved concentrations

As discussed in the main report, the conversion of BAF values from a total concentration basis to a dissolved concentration basis has an impact on the assessment of the method. This aspect has therefore been examined in more detail.

The conversion between total and dissolved concentrations was carried out using the following equation:

$$\frac{C_{wd}}{C_{wt}} = \frac{1}{1 + K_{DOC}DOC + K_{POC}POC}$$

where C_{wd} = dissolved concentration in water (mg/l)

C_{wt} = total concentration in water (mg/l)

K_{DOC} = dissolved organic carbon-water partition coefficient (l/kg)

K_{POC} = particulate organic carbon-water partition coefficient (l/kg)

DOC = concentration of dissolved organic carbon (kg/l)

POC = concentration of particulate organic carbon (kg/l)

There are few values available for the K_{DOC} and K_{POC} and so these were estimated as 0.1 x K_{ow} and K_{ow} respectively. Hence the equation can be expressed as

$$\frac{C_{wd}}{C_{wt}} = \frac{1}{1 + K_{OW}(0.1DOC + POC)}$$

The two sources of data on high log K_{ow} substances do not include specific data on the levels of DOC or POC in the waters sampled. Metcalfe and Metcalfe (1997) mention suspended solids levels of 0.6 to 1.3 mg/l, but do not mention DOC. Comparing the total and free dissolved BAF values in Voutsas *et al*. (2002), the conversion they employed used a value for (0.1DOC+POC) of 0.75 mg/l. This is applied to the total concentrations in water reported by Metcalfe and Metcalfe (1997). The paper did present concentrations of substances as dissolved and on suspended solids, but commented that the filtration employed in the sample preparation may not have separated the dissolved and particulate phases effectively and so combined concentrations were also presented.

Oliver and Niimi (1988) also did not include information on the specific DOC and POC levels in the water samples. They included a value of 2 mg/l for DOC as representative for Lake Ontario. The water samples were centrifuged to remove particulates before measurement of the levels in water. The conversion applied to their data in Voutsas *et al.* (2002) uses a value for (0.1DOC+POC) of 0.2 mg/l, so presumably applying the representative DOC value and assuming that all of the POC was removed.

There may therefore be some uncertainty over the conversions from total concentrations to dissolved concentrations, which will be more important for substances with higher log K_{ow} values.

Data check

Papers from which the data in Voutsas *et al*. (2002) were taken were obtained and checked against the data appearing in Voutsas *et al*. Two relatively important mistakes appear to have been made in extracting the data.

The first relates to the data taken from Metcalfe and Metcalfe (1997). The data used in Voutsas *et al.* (2002) for trophic level 4, which should be for piscivorous fish, is actually the data for levels in gulls' eggs.

The second relates to data taken from Burkhard *et al.* (1997), where the data for one sampling location have had the conversion from total to dissolved concentrations applied twice.

The data set included in this appendix has these two areas corrected. Regression analyses were carried out on the revised data set, and the results are compared with those in the original paper in Table D1.

Table D1 Equation coefficients

		$(\log K_{ow})^2$	$\log K_{ow}$	Constant	R^2	Maximum[a]
BAF_{fd}						
Trophic level 3	Original	-0.0977	2.2855	-3.693	0.912	11.7 (9.80)
	Revised	-0.0968	2.3855	-3.73	0.912	12.3 (11)
Trophic level 4	Original	-0.0278	1.6604	-1.6135	0.929	30 (24)
	Revised	-0.099	2.3176	-3.1551	0.912	11.7 (10.4)
BAF_t						
Trophic level 3	Original	-0.2707	4.1253	-8.0866	0.857	7.6 (7.6)
	Revised	-0.2693	4.1192	-8.1161	0.860	7.6 (7.6)
Trophic level 4	Original	-0.2029	3.4112	-6.0182	0.897	8.4 (8.3)
	Revised	-0.2739	4.0688	-7.5704	0.822	7.4 (7.5)

a) log K_{ow} value at which maximum BAF is predicted (maximum log BAF value in parentheses)

Changes in the trophic level 3 equations are small in both cases. The changes to the equations for trophic level 4 are more notable. For both BAF_{fd} and BAF_t, the revised level 4 equations are much more similar to those for trophic level 3. In particular, changes to the BAF_{fd} equation for trophic level 4 lead to a maximum predicted BAF value at a much lower log K_{ow} value (and a much lower predicted BAF). Log K_{ow} values giving the maximum predicted BAF value are still higher than those from the other two methods assessed in the main report when considering the values based on dissolved concentrations. Equations derived using the total concentrations in water give maximum values at similar log K_{ow} values to the other methods.

The changes made to the data set do not have a great impact on the results.

References

The numbers relate to the data tables following.

1. METCALFE, T.L. AND METCALFE, C.D., 1997. The trophodynamics of PCBs, including mono and non-ortho congeners, in the food web of North-Central Lake Ontario. Science of the Total Environment, 201, 245-272.

3. OLIVER, B.G. AND NIIMI, A.J., 1988. Trophodynamic analysis of polychlorinated biphenyl congeners and other chlorinated hydrocarbons in the Lake Ontario ecosystem. Environmental Science and Technology, 22, 388-397.

4. BURKHARD, L.P., SHEEDY, B.R., MCCAULEY, D.J. AND DEGRAEVE, G.M., 1997. Bioaccumulation factors for chlorinated benzenes, chlorinated

butadienes and hexachloroethane. Environmental Toxicology and Chemistry, 16, 1677-1686.

6. KIDD, K.A., HESSLEIN, R.H., ROSS, B.J., KOCZANSKI, K., STEPHENS, G.R. AND MUIR, C.G., 1998. Bioaccumulation of organochlorines through a remote freshwater food web in the Canadian Arctic. Environmental Pollution, 102, 91-103.

Revised data set for Voutsas *et al*. (2002)

Training set for trophic level 3

Compound	log K_{ow}	log BAF_t	log BAF_{fd}	Reference
Hexachloroethane	4.14	4.26	4.31	4
Z-1,1,2,4-Tetrachlorobutadiene	4.23	4.02	4.09	4
1,1,4,4-Tetrachlorobutadiene	4.29	4.23	4.30	4
E-Pentachlorobutadiene	4.54	4.47	4.59	4
Hexachlorobutadiene	4.84	5.43	5.64	4
1,2,3-Trichlorobenzene	4.09	4.47	4.52	4
1,2,4-Trichlorobenzene	4.02	4.55	4.59	4
Tetrachlorobenzene mix.	4.60	5.12	5.26	4
1,2,3,4-Tetrachlorobenzene	4.59	4.95	5.08	4
Pentachlorobenzene	5.11	5.42	5.76	4
Hexachlorobenzene	5.60	5.52	6.23	4
Hexachloroethane	4.14	4.45	4.50	4
Z-1,1,2,4-Tetrachlorobutadiene	4.23	3.83	3.89	4
1,1,4,4-Tetrachlorobutadiene	4.29	4.26	4.33	4
E-Pentachlorobutadiene	4.54	4.50	4.62	4
Z-Pentachlorobutadiene	4.54	4.28	4.41	4
Hexachlorobutadiene	4.84	5.76	5.90	4
1,2,3-Trichlorobenzene	4.09	4.72	4.77	4
1,2,4-Trichlorobenzene	4.02	4.67	4.71	4
Tetrachlorobenzene mix.	4.60	5.33	5.47	4
1,2,3,4-Tetrachlorobenzene	4.59	5.04	5.17	4
Pentachlorobenzene	5.11	5.52	5.86	4
Hexachlorobenzene	5.60	5.38	6.05	4
Hexachloroethane	4.14	4.26	4.31	4
Z-1,1,2,4-Tetrachlorobutadiene	4.23	4.26	4.33	4
1,1,4,4-Tetrachlorobutadiene	4.29	4.39	4.46	4
E-Pentachlorobutadiene	4.54	4.94	5.06	4
Z-Pentachlorobutadiene	4.54	4.82	4.94	4
Hexachlorobutadiene	4.84	5.47	5.69	4
1,2,3-Trichlorobenzene	4.09	4.63	4.67	4
1,2,4-Trichlorobenzene	4.02	4.72	4.76	4
Tetrachlorobenzene mix.	4.60	4.99	5.12	4
1,2,3,4-Tetrachlorobenzene	4.59	5.05	5.18	4
Pentachlorobenzene	5.11	5.50	5.84	4
Hexachlorobenzene	5.60	5.20	5.87	4
Hexachloroethane	4.14	5.29	5.34	4
Z-1,1,2,4-Tetrachlorobutadiene	4.23	4.51	4.57	4
1,1,4,4-Tetrachlorobutadiene	4.29	4.75	4.82	4
E-Pentachlorobutadiene	4.54	5.28	5.40	4
Z-Pentachlorobutadiene	4.54	4.99	5.11	4
Hexachlorobutadiene	4.84	6.66	6.88	4
1,2,3-Trichlorobenzene	4.09	5.11	5.16	4
1,2,4-Trichlorobenzene	4.02	5.63	5.67	4
1,2,3,4-Tetrachlorobenzene	4.59	5.72	5.85	4
Pentachlorobenzene	5.11	6.52	6.86	4
Hexachlorobenzene	5.60	6.68	7.35	4
Hexachloroethane	4.14	3.90	3.95	4

Compound	log K_{ow}	log BAF_t	log BAF_{fd}	Reference
E-Pentachlorobutadiene	4.54	4.38	4.50	4
Hexachlorobutadiene	4.84	4.91	5.13	4
1,2,3-Trichlorobenzene	4.09	4.05	4.10	4
1,2,4-Trichlorobenzene	4.02	4.01	4.05	4
Tetrachlorobenzene mix.	4.60	4.67	4.81	4
1,2,3,4-Tetrachlorobenzene	4.59	4.59	4.72	4
Pentachlorobenzene	5.11	5.14	5.48	4
Hexachlorobenzene	5.60	5.28	5.95	4
Hexachloroethane	4.14	4.64	4.71	4
Z-1,1,2,4-Tetrachlorobutadiene	4.23	3.99	4.02	4
1,1,4,4-Tetrachlorobutadiene	4.29	4.43	4.51	4
E-Pentachlorobutadiene	4.54	4.51	4.66	4
Z-Pentachlorobutadiene	4.54	4.38	4.52	4
Hexachlorobutadiene	4.84	5.72	5.97	4
1,2,3-Trichlorobenzene	4.09	4.72	4.77	4
1,2,4-Trichlorobenzene	4.02	4.81	4.86	4
Tetrachlorobenzene mix.	4.60	5.34	5.50	4
1,2,3,4-Tetrachlorobenzene	4.59	5.15	5.31	4
Pentachlorobenzene	5.11	5.73	6.12	4
Hexachlorobenzene	5.60	5.58	6.32	4
Z-1,1,2,4-Tetrachlorobutadiene	4.23	3.81	3.88	4
1,1,4,4-Tetrachlorobutadiene	4.29	3.94	4.01	4
E-Pentachlorobutadiene	4.54	4.43	4.56	4
Hexachlorobutadiene	4.84	4.64	4.86	4
1,2,3-Trichlorobenzene	4.09	4.18	4.23	4
1,2,4-Trichlorobenzene	4.02	4.18	4.22	4
Tetrachlorobenzene mix.	4.60	4.24	4.37	4
1,2,3,4-Tetrachlorobenzene	4.59	4.48	4.62	4
Pentachlorobenzene	5.11	4.89	5.23	4
Hexachloroethane	4.14	4.08	4.13	4
Z-1,1,2,4-Tetrachlorobutadiene	4.23	4.24	4.30	4
1,1,4,4-Tetrachlorobutadiene	4.29	4.31	4.39	4
E-Pentachlorobutadiene	4.54	4.93	5.05	4
Z-Pentachlorobutadiene	4.54	4.43	4.55	4
Hexachlorobutadiene	4.84	5.66	5.88	4
1,2,3-Trichlorobenzene	4.09	4.56	4.60	4
1,2,4-Trichlorobenzene	4.02	4.57	4.61	4
Tetrachlorobenzene mix.	4.60	4.90	5.04	4
1,2,3,4-Tetrachlorobenzene	4.59	5.09	5.23	4
Pentachlorobenzene	5.11	5.87	6.21	4
Hexachlorobenzene	5.60	6.22	6.90	4
Hexachloroethane	4.14	4.04	4.09	4
Z-1,1,2,4-Tetrachlorobutadiene	4.23	4.37	4.43	4
1,1,4,4-Tetrachlorobutadiene	4.29	4.27	4.34	4
E-Pentachlorobutadiene	4.54	5.21	5.33	4
Hexachlorobutadiene	4.84	5.29	5.51	4
1,2,3-Trichlorobenzene	4.09	4.70	4.74	4
1,2,4-Trichlorobenzene	4.02	4.63	4.67	4
Tetrachlorobenzene mix.	4.60	4.88	5.02	4
1,2,3,4-Tetrachlorobenzene	4.59	5.03	5.16	4
Pentachlorobenzene	5.11	5.49	5.83	4
Hexachlorobenzene	5.60	5.65	6.33	4
Hexachloroethane	4.14	4.43	4.49	4

Compound	log K_{ow}	log BAF_t	log BAF_{fd}	Reference
Z-1,1,2,4-Tetrachlorobutadiene	4.23	4.88	4.95	4
1,1,4,4-Tetrachlorobutadiene	4.29	4.93	5.01	4
E-Pentachlorobutadiene	4.54	5.58	5.72	4
Z-Pentachlorobutadiene	4.54	5.02	5.17	4
Hexachlorobutadiene	4.84	5.43	5.68	4
1,2,3-Trichlorobenzene	4.09	4.9	4.96	4
1,2,4-Trichlorobenzene	4.02	4.98	5.03	4
Tetrachlorobenzene mix.	4.60	4.98	5.15	4
1,2,3,4-Tetrachlorobenzene	4.59	5.26	5.42	4
Pentachlorobenzene	5.11	5.66	6.05	4
Hexachlorobenzene	5.60	5.84	6.58	4
p,p'-DDE	6.51	7.13	7.54	6
trans-Nonachlor	6.35	6.95	7.28	6
p,p'-DDE	6.51	6.78	7.20	6
trans-Nonachlor	6.35	6.89	7.21	6
PCB 18	5.24	5.64	5.69	1
PCB 31	5.67	5.85	5.98	1
PCB 52	5.84	6.80	6.98	1
PCB 49	5.85	6.67	6.85	1
PCB 44	5.75	7.23	7.38	1
PCB 101	6.38	7.09	7.53	1
PCB 87	6.29	6.98	7.37	1
PCB 99	6.39	7.45	7.90	1
PCB 110	6.48	6.94	7.45	1
PCB 151	6.64	6.99	7.62	1
PCB 153	6.92	7.47	8.33	1
PCB 138	6.83	7.48	8.27	1
PCB 180	7.36	7.44	8.70	1
PCB 170	7.27	7.52	8.69	1
PCB 199	7.20	7.32	8.43	1
PCB 195	7.56	7.74	9.19	1
PCB 194	7.80	7.37	9.05	1
PCB 209	8.18	8.01	10.07	1
PCB 66	6.20	7.46	7.80	1
PCB 105	6.65	7.80	8.43	1
PCB 118	6.74	6.76	7.47	1
PCB 156	7.18	7.25	8.35	1
PCB 81	6.36	6.22	6.66	1
PCB 77	6.36	5.99	6.43	1
PCB 126	6.89	6.23	7.07	1
PCB 169	7.42	6.76	8.07	1
PCB 18	5.24	6.32	6.37	1
PCB 31	5.67	6.36	6.49	1
PCB 52	5.84	6.81	6.99	1
PCB 49	5.85	6.69	6.88	1
PCB 44	5.75	7.01	7.17	1
PCB 101	6.38	7.29	7.74	1
PCB 87	6.29	7.20	7.59	1
PCB 99	6.39	7.37	7.82	1
PCB 110	6.48	7.19	7.71	1
PCB 151	6.64	7.14	7.77	1
PCB 153	6.92	7.57	8.43	1
PCB 138	6.83	7.59	8.37	1

Compound	log K_{ow}	log BAF_t	log BAF_{fd}	Reference
PCB 180	7.36	7.61	8.87	1
PCB 170	7.27	7.67	8.85	1
PCB 199	7.20	7.60	8.71	1
PCB 195	7.56	7.83	9.28	1
PCB 194	7.80	7.38	9.06	1
PCB 209	8.18	7.80	9.86	1
PCB 66	6.20	7.59	7.93	1
PCB 105	6.65	7.61	8.25	1
PCB 118	6.74	7.17	7.88	1
PCB 156	7.18	7.43	8.52	1
PCB 81	6.36	6.03	6.46	1
PCB 77	6.36	6.25	6.68	1
PCB 126	6.89	6.35	7.19	1
PCB 169	7.42	6.93	8.25	1
PCB 18	5.24	6.38	6.43	1
PCB 31	5.67	6.49	6.62	1
PCB 52	5.84	6.89	7.07	1
PCB 49	5.85	6.65	6.83	1
PCB 44	5.75	7.12	7.28	1
PCB 101	6.38	7.30	7.75	1
PCB 87	6.29	7.27	7.67	1
PCB 99	6.39	7.29	7.74	1
PCB 110	6.48	7.27	7.78	1
PCB 151	6.64	7.09	7.72	1
PCB 153	6.92	7.59	8.45	1
PCB 138	6.83	7.58	8.37	1
PCB 180	7.36	7.56	8.82	1
PCB 170	7.27	7.56	8.74	1
PCB 199	7.20	7.53	8.64	1
PCB 195	7.56	7.53	8.98	1
PCB 194	7.80	7.32	9.00	1
PCB 209	8.18	7.65	9.71	1
PCB 66	6.20	7.74	8.08	1
PCB 105	6.65	7.79	8.43	1
PCB 118	6.74	7.19	7.90	1
PCB 156	7.18	7.54	8.63	1
PCB 77	6.36	6.13	6.56	1
PCB 126	6.89	6.29	7.12	1
PCB 169	7.42	6.71	8.03	1
PCB 28/31	5.67	6.33	6.37	3
PCB 18	5.24	5.96	5.97	3
PCB 66	6.20	7.33	7.45	3
PCB 70/76	6.17	6.95	7.06	3
PCB 50/60/81	6.03	7.37	7.45	3
PCB 52	5.84	6.74	6.80	3
PCB 47/48	5.82	6.10	6.15	3
PCB 74	6.20	7.18	7.30	3
PCB 49	5.85	6.72	6.77	3
PCB 64	5.95	7.09	7.16	3
PCB 42	5.76	7.03	7.07	3
PCB 101	6.38	7.13	7.30	3
PCB 84	6.04	7.96	8.05	3
PCB 118	6.74	7.54	7.86	3

Compound	log K_{ow}	log BAF_t	log BAF_{fd}	Reference
PCB 110	6.48	7.24	7.44	3
PCB 87/97	6.29	7.40	7.54	3
PCB 105	6.65	7.54	7.82	3
PCB 95	6.13	6.87	6.98	3
PCB 85	6.30	7.35	7.50	3
PCB 92	6.35	7.54	7.70	3
PCB 82	6.20	7.48	7.60	3
PCB 91	6.13	6.34	6.44	3
PCB 153	6.92	7.63	8.05	3
PCB 138	6.83	7.69	8.06	3
PCB 149	6.67	7.00	7.28	3
PCB 146	6.89	8.09	8.49	3
PCB 141	6.82	7.75	8.11	3
PCB 151	6.64	8.06	8.34	3
PCB 132	6.58	7.17	7.41	3
PCB 136	6.22	7.01	7.13	3
PCB 180	7.36	7.71	8.45	3
PCB 187/182	7.19	7.46	8.07	3
PCB 203/196	7.65	8.14	9.14	3
PCB 194	7.80	7.38	8.52	3
PCB 28/31	5.67	6.64	6.68	3
PCB 66	6.20	7.45	7.57	3
PCB 70/76	6.17	7.20	7.31	3
PCB 50/60/81	6.03	7.67	7.76	3
PCB 52	5.84	6.79	6.84	3
PCB 47/48	5.82	6.80	6.85	3
PCB 74	6.20	7.23	7.35	3
PCB 49	5.85	6.92	6.98	3
PCB 64	5.95	7.23	7.30	3
PCB 42	5.76	7.34	7.38	3
PCB 101	6.38	7.08	7.25	3
PCB 84	6.04	7.81	7.90	3
PCB 118	6.74	7.39	7.71	3
PCB 110	6.48	7.31	7.51	3
PCB 87/97	6.29	7.75	7.89	3
PCB 105	6.65	7.44	7.72	3
PCB 95	6.13	7.04	7.14	3
PCB 85	6.30	7.52	7.67	3
PCB 92	6.35	7.76	7.93	3
PCB 82	6.20	7.74	7.86	3
PCB 91	6.13	6.63	6.74	3
PCB 99	6.39	7.19	7.37	3
PCB 153	6.92	7.39	7.82	3
PCB 138	6.83	7.52	7.89	3
PCB 149	6.67	7.46	7.75	3
PCB 146	6.89	7.90	8.30	3
PCB 141	6.82	7.60	7.96	3
PCB 151	6.64	7.90	8.17	3
PCB 132	6.58	7.20	7.45	3
PCB 136	6.22	7.13	7.25	3
PCB 180	7.36	7.40	8.15	3
PCB 187/182	7.19	7.38	7.99	3
PCB 203/196	7.65	7.82	8.82	3

Compound	log K_{ow}	log BAF_t	log BAF_{fd}	Reference
PCB 184	7.80	7.09	8.22	3
PCB 28/31	5.67	6.53	6.57	3
PCB 66	6.20	7.34	7.46	3
PCB 70/76	6.17	7.21	7.32	3
PCB 50/60/81	6.03	7.62	7.70	3
PCB 52	5.84	6.48	6.54	3
PCB 47/48	5.82	6.68	6.73	3
PCB 74	6.20	7.19	7.31	3
PCB 49	5.85	6.40	6.46	3
PCB 64	5.95	7.07	7.14	3
PCB 42	5.76	7.13	7.18	3
PCB 101	6.38	6.88	7.05	3
PCB 84	6.04	7.81	7.90	3
PCB 118	6.74	7.43	7.76	3
PCB 110	6.48	7.20	7.41	3
PCB 87/97	6.29	7.64	7.79	3
PCB 105	6.65	7.43	7.71	3
PCB 95	6.13	6.72	6.83	3
PCB 85	6.30	7.26	7.41	3
PCB 92	6.35	7.01	7.17	3
PCB 82	6.20	7.65	7.77	3
PCB 91	6.13	6.30	6.40	3
PCB 153	6.92	7.51	7.93	3
PCB 138	6.83	7.49	7.87	3
PCB 149	6.67	7.34	7.63	3
PCB 146	6.89	7.90	8.30	3
PCB 141	6.82	7.48	7.84	3
PCB 151	6.64	7.47	7.74	3
PCB 132	6.58	6.81	7.06	3
PCB 180	7.36	7.43	8.18	3
PCB 187/182	7.19	7.40	8.01	3
PCB 203/196	7.65	7.80	8.79	3
PCB 194	7.80	7.11	8.24	3
PCB 28/31	5.67	6.88	6.92	3
PCB 66	6.20	7.76	7.88	3
PCB 70/76	6.17	7.60	7.71	3
PCB 50/60/81	6.03	8.00	8.09	3
PCB 52	5.84	6.85	6.91	3
PCB 47/48	5.82	7.17	7.22	3
PCB 74	6.20	7.54	7.66	3
PCB 49	5.85	6.97	7.03	3
PCB 64	5.95	7.47	7.54	3
PCB 42	5.76	7.59	7.63	3
PCB 101	6.38	7.18	7.35	3
PCB 84	6.04	8.20	8.29	3
PCB 118	6.74	7.81	8.13	3
PCB 110	6.48	7.60	7.81	3
PCB 87/97	6.29	7.91	8.06	3
PCB 105	6.65	7.83	8.11	3
PCB 95	6.13	7.06	7.17	3
PCB 85	6.30	7.70	7.85	3
PCB 92	6.35	7.64	7.80	3
PCB 82	6.20	8.02	8.14	3

Compound	log K_{ow}	log BAF_t	log BAF_{fd}	Reference
PCB 91	6.13	6.80	6.90	3
PCB 99	6.39	7.23	7.40	3
PCB 153	6.92	7.81	8.24	3
PCB 138	6.83	7.85	8.22	3
PCB 149	6.67	7.71	7.99	3
PCB 146	6.89	8.25	8.66	3
PCB 141	6.82	7.80	8.17	3
PCB 151	6.64	8.01	8.28	3
PCB 132	6.58	7.42	7.67	3
PCB 180	7.36	7.71	8.45	3
PCB 187/182	7.19	7.73	8.34	3
PCB 203/196	7.65	8.13	9.13	3
PCB 194	7.80	7.37	8.50	3

Training set for trophic level 4

Compound	log K_{ow}	log BAF_t	log BAF_{fd}	Reference
Hexachloroethane	4.14	4.49	4.55	4
Z-1,1,2,4-Tetrachlorobutadiene	4.23	4.83	4.91	4
1,1,4,4-Tetrachlorobutadiene	4.29	4.86	4.95	4
E-Pentachlorobutadiene	4.54	5.61	5.75	4
Z-Pentachlorobutadiene	4.54	5.38	5.53	4
Hexachlorobutadiene	4.84	5.41	5.66	4
1,2,3-Trichlorobenzene	4.09	4.87	4.92	4
1,2,4-Trichlorobenzene	4.02	4.95	5.00	4
Tetrachlorobenzene mix.	4.60	5.03	5.20	4
1,2,3,4-Tetrachlorobenzene	4.59	5.35	5.51	4
Pentachlorobenzene	5.11	5.86	6.25	4
Hexachlorobenzene	5.60	6.14	6.88	4
Hexachloroethane	4.14	4.74	4.79	4
Z-1,1,2,4-Tetrachlorobutadiene	4.23	4.79	4.86	4
1,1,4,4-Tetrachlorobutadiene	4.29	4.83	4.90	4
E-Pentachlorobutadiene	4.54	5.71	5.83	4
Z-Pentachlorobutadiene	4.54	5.40	5.52	4
Hexachlorobutadiene	4.84	5.76	5.97	4
1,2,3-Trichlorobenzene	4.09	4.91	4.96	4
1,2,4-Trichlorobenzene	4.02	5.03	5.07	4
Tetrachlorobenzene mix.	4.60	5.27	5.40	4
1,2,3,4-Tetrachlorobenzene	4.59	5.51	5.64	4
Pentachlorobenzene	5.11	6.10	6.44	4
Hexachlorobenzene	5.60	6.19	6.86	4
Hexachloroethane	4.14	4.25	4.30	4
Z-1,1,2,4-Tetrachlorobutadiene	4.23	4.36	4.42	4
1,1,4,4-Tetrachlorobutadiene	4.29	4.33	4.40	4
E-Pentachlorobutadiene	4.54	5.33	5.45	4
Z-Pentachlorobutadiene	4.54	4.51	4.63	4
Hexachlorobutadiene	4.84	5.18	5.39	4
1,2,3-Trichlorobenzene	4.09	4.59	4.64	4
1,2,4-Trichlorobenzene	4.02	4.62	4.66	4
Tetrachlorobenzene mix.	4.60	4.90	5.04	4
1,2,3,4-Tetrachlorobenzene	4.59	5.05	5.18	4
Pentachlorobenzene	5.11	5.61	5.95	4
Hexachlorobenzene	5.60	5.74	6.41	4
PCB 28/31	5.67	6.85	6.89	3
PCB 18	5.24	5.73	5.75	3
PCB 22	5.58	6.36	6.39	3
PCB 16	5.16	5.90	5.92	3
PCB 17	5.25	5.51	5.52	3
PCB 24/27	5.40	6.74	6.76	3
PCB 66	6.20	7.67	7.79	3
PCB 70/76	6.17	7.45	7.56	3
PCB 50/60/81	6.03	7.84	7.93	3
PCB 52	5.84	6.95	7.01	3
PCB 47/48	5.82	7.12	7.18	3
PCB 74	6.20	7.54	7.66	3
PCB 49	5.85	7.07	7.13	3
PCB 64	5.95	7.44	7.51	3
PCB 42	5.76	7.44	7.49	3

Compound	log K_{ow}	log BAF_t	log BAF_{fd}	Reference
PCB 53	5.62	6.47	6.51	3
PCB 40	5.66	6.52	6.55	3
PCB 101	6.38	7.28	7.45	3
PCB 84	6.04	8.20	8.28	3
PCB 118	6.74	7.83	8.15	3
PCB 110	6.48	7.58	7.79	3
PCB 87/97	6.29	7.94	8.08	3
PCB 105	6.65	7.85	8.13	3
PCB 95	6.13	7.15	7.25	3
PCB 85	6.30	7.75	7.89	3
PCB 92	6.35	7.95	8.11	3
PCB 82	6.20	8.01	8.13	3
PCB 91	6.13	6.82	6.92	3
PCB 99	6.39	7.22	7.39	3
PCB 153	6.92	7.89	8.32	3
PCB 138	6.83	7.93	8.30	3
PCB 149	6.67	7.71	7.99	3
PCB 146	6.89	8.32	8.73	3
PCB 141	6.82	7.96	8.32	3
PCB 151	6.64	8.23	8.51	3
PCB 132	6.58	7.32	7.56	3
PCB 136	6.22	7.25	7.37	3
PCB 180	7.36	7.83	8.58	3
PCB 187/182	7.19	7.82	8.43	3
PCB 203/196	7.65	8.26	9.26	3
PCB 194	7.80	7.43	8.56	3
PCB 18	5.24	6.16	6.22	1
PCB 31	5.67	6.23	6.37	1
PCB 52	5.84	6.63	6.81	1
PCB 49	5.85	6.47	6.65	1
PCB 44	5.75	6.94	7.09	1
PCB 101	6.38	6.98	7.43	1
PCB 87	6.29	6.97	7.36	1
PCB 99	6.39	7.33	7.78	1
PCB 110	6.48	6.90	7.41	1
PCB 151	6.64	6.80	7.43	1
PCB 153	6.92	7.26	8.12	1
PCB 138	6.83	7.30	8.08	1
PCB 180	7.36	7.30	8.56	1
PCB 170	7.27	7.30	8.48	1
PCB 199	7.20	7.24	8.35	1
PCB 195	7.56	7.46	8.91	1
PCB 194	7.80	7.12	8.80	1
PCB 209	8.18	7.41	9.47	1
PCB 66	6.20	7.38	7.72	1
PCB 105	6.65	7.30	7.93	1
PCB 118	6.74	6.95	7.66	1
PCB 156	7.18	7.12	8.21	1
PCB 81	6.36	6.15	6.59	1
PCB 77	6.36	5.83	6.26	1
PCB 126	6.89	5.98	6.81	1
PCB 169	7.42	6.31	7.63	1

We are The Environment Agency. It's our job to look after your environment and make it **a better place** – for you, and for future generations.

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