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Verification of bioaccumulation models for use in environmental standards. Part C: human food chain models

Science Report – SC030197/SR4

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Steve Killeen

Head of Science

Executive summary

This report set out to verify two models for predicting human exposure to chemicals via the food chain: the EU Technical Guidance Document (TGD) and the ACC-HUMAN model.

No one model was found to make the best predictions across the whole range of endpoints considered; therefore, it is recommended that both models be used selectively, with different models for different endpoints. Recommendations for each endpoint are summarised below.

- For accumulation in fish, the recommendations in Part A of this report series should be followed.
- For accumulation in plants from air, both the ACC-HUMAN model and the TGD method give similar predictions. However, for substances that adsorb significantly onto atmospheric particulates/aerosols, the ACC-HUMAN model is recommended.
- For accumulation in plant roots from soil, only the TGD method is available. This gives reliable predictions over a relatively narrow range of $\log_{10}$ octanol-water partition coefficients (log K_{ow}) values. However, an analysis of the available data suggests that a simple equation relating the bioaccumulation factor (BAF) to log K_{ow} could be used to extend the range of applicability of the method.
- For uptake into plant leaves from soil, it is recommended that the TGD method is used. However, there are very large uncertainties associated with predictions from this method across the range of log K_{ow} values, but particularly for chemicals with log K_{ow} between four and six.
- For predictions in cattle (meat) and milk for exposure via diet, it is recommended that, in the absence of information on the rate of metabolism of a chemical in cattle, the TGD method is used for chemicals with a log K_{ow} value up to six, and the ACC-HUMAN model is used for chemicals with a log K_{ow} value greater than six. For chemicals for which a rate of metabolism in cattle is available, the ACC-HUMAN model should be used.

It was not possible to test the models for uptake into cattle and milk via drinking water and air, owing to a lack of suitable test data. However, the above conclusions would be expected to apply for exposure via feed.

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 C) outlines the verification of models and methods for the human food chain. Verification of models for the aquatic and terrestrial environments are considered in Part A and Part C of this report series respectively. Part D summarises the physico-chemical properties of the chemicals modelled in this report.

For the human food chain, the following methods and models are considered for verification.

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/).

ACC-HUMAN is a food chain model for predicting levels of lipophilic organic chemicals in humans. The model was published in a paper by Czub and McLachlan (2004a) and a computerised version of the model is available for download from the Stockholm University website (http://www.itm.su.se/research/model.php).

2 Initial comparison of the models

2.1 TGD/EUSES

The TGD (European Commission, 2003) is used for the risk assessment of new and existing chemicals within the EU, and contains a detailed description of methods to carry out an in-depth risk assessment of the exposure of aquatic organisms, wildlife and humans to a chemical through environmental pathways. For the human food chain, the method uses concentrations in air, soil and surface water to estimate the concentrations in food (root crops, leaf crops, meat, milk and fish) to which humans can be exposed; these are used, along with the estimated concentrations in air and drinking water, to determine the total daily human intake of the chemical. The TGD outlines a series of equations for carrying out these calculations and its methods are also implemented in the EUSES computer program. Concentrations of chemicals can be calculated at both the local and regional scale using methods in the TGD.

The TGD method relies on estimates of a series of partition coefficients describing the distribution of a chemical between an environmental medium (such as air, soil, water) and the food item. The main methods used for the calculations are summarised below. A more detailed description of the model is given in Environment Agency (2007).

The concentration of the chemical in fish is estimated from the concentration in surface water using a fish bioconcentration factor (BCF). The method can use an actual (experimental) BCF value, or a BCF value can be estimated from the log K_{ow} of the chemical. A detailed evaluation of this part of the method has already been undertaken in Part A of this report series and so is not considered here. However, the TGD/EUSES method for predicting concentrations in fish for human consumption does not currently include the use of a biomagnification factor (BMF, which takes into account accumulation via food as well as water) as is currently done for the assessment of exposure of fish-eating wildlife. This is considered further in Section 4.

The calculation for uptake into plants (plant roots and plant leaves) takes into account uptake from both soil (pore water) and air, and is based on the approach proposed by Trapp and Matthies (1995). The partition coefficients used in the method are outlined below.

$$K_{plant-water} = Fwater_{plant} + (Flipid_{plant} \times K_{ow}{}^{b})$$

where $K_{plant-water}$ = partition coefficient between plant tissue and water ((mg m^{-3} plant)/(mg m^{-3} water)).

$Fwater_{plant}$ = volume fraction of water in plant tissue (m^3 m^{-3}). Value assumed is 0.65 based on the properties of *Brassica oleracea* (Riederer, 1990).

$Flipid_{plant}$ = volume fraction of lipid in plant tissue (m^3 m^{-3}). Value assumed is 0.01 based on the properties of *Brassica oleracea* (Riederer, 1990).

K_{ow} = octanol-water partition coefficient (non-log value).

b = correction factor to account for differences between plant lipids and octanol. Value assumed is 0.95 taken from Trapp and Matthies (1995).

$$TSCF = 0.784 \times \left[\frac{-(\log K_{OW} - 1.78)^2}{2.44} \right]$$

where TSCF = transpiration stream concentration factor. This is the ratio between the concentration in the transpiration stream and the concentration in pore water.

log K_{ow} = octanol-water partition coefficient (log_{10} value).

$$K_{leaf-air} = Fair_{plant} + \frac{K_{plant-water}}{K_{air-water}}$$

where $K_{leaf-plant}$ = partition coefficient between plant leaves and air ($m^3\ m^{-3}$).

$Fair_{plant}$ = volume fraction of air in plant tissue ($m^3\ m^{-3}$). Value used is 0.3 based on the properties of *Brassica oleracea* (Riederer, 1990).

The method then estimates the concentration in plant roots from the soil pore water concentration using $K_{plant-water}$, and the concentration in plant leaves from both soil pore water and air using TSCF and $K_{leaf-air}$ respectively, with a one-compartment model. The model also takes into account elimination of the chemical by metabolism and/or photodegradation in the plants if data are available, and growth dilution.

The equation used to estimate TSCF was developed by Briggs *et al.* (1982) using results from a study on barley. In these experiments, the uptake by roots from solution and subsequent translocation to shoots was measured for two series of non-ionised chemicals: O-methylcarbamoyloximes and substituted phenylureas.

Translocation to the shoots was found to be a passive process and was most efficient for compounds of intermediate polarity and log K_{ow} between 1.5 and 2.0. Uptake of very lipophilic compounds (log K_{ow} greater than 4.5) was very small. A Gaussian curve was fitted to the experimental data for 17 of the 18 chemicals tested and this gave the above equation for estimating TSCF. Both series of chemicals behaved similarly and the optimum lipophilicity for maximum translocation to shoots was centered at log K_{ow} = 1.8.

The TGD recommends that the range of log K_{ow} values for which this equation can be used is between -0.5 and 4.5 and that, outside of this range, either the maximum or minimum log K_{ow} value of the range should be used.

The overall plant model calculates the concentration in plant roots and plant leaves as a result of exposure to chemicals in both soil (exposure via the soil pore water) and air (exposure via the vapour phase). If the EUSES program is used to carry out these calculations, it is relatively straight forward to estimate an overall bioaccumulation factor (BAF) that relates the concentration in either plant roots or plant leaves to the concentration in the exposure media (soil or air), by simply running the program with a nominal concentration in either the soil or air compartment. Thus, BAF can be calculated as follows (on either a wet weight soil or dry weight soil basis):

$$BAF_{root-soil} = \frac{\text{predicted concentration in root (mg kg}^{-1}\text{ wet weight)}}{\text{nominal concentration assumed in soil (mg kg}^{-1}\text{ wet weight or mg kg}^{-1}\text{ dry weight)}}$$

$$BAF_{leaf-soil} = \frac{\text{predicted concentration in leaves (mg kg}^{-1}\text{ wet weight)}}{\text{nominal concentration assumed in soil (mg kg}^{-1}\text{ wet weight or mg kg}^{-1}\text{ dry weight)}}$$

$$BAF_{leaf-air} = \frac{\text{predicted concentration in leaves (mg kg}^{-1}\text{ wet weight)}}{\text{nominal concentration assumed in air (mg m}^{-3}\text{)}}$$

BAFs of this form can then be used in the back-calculations necessary for setting standards (see Section 4).

Accumulation in meat and milk is again estimated using a series of partition coefficients. These are outlined below and are taken from the work of Travis and Arms (1988).

$$BTF_{meat} = 10^{(-7.6+\log K_{ow})}$$

where BTF_{meat} = biotransfer factor between the exposure media (air/grass/soil/drinking water) and meat ((mg kg^{-1})/(mg d^{-1})).

log K_{ow} = octanol-water partition coefficient (log_{10} value).

$$BTF_{milk} = 10^{(-8.1+\log K_{ow})}$$

where BTF_{milk} = biotransfer factor between the exposure media (air/grass/soil/drinking water) and milk ((mg kg^{-1})/(mg d^{-1})).

log K_{ow} = octanol-water partition coefficient (log_{10} value).

The resulting concentration in meat and milk can be estimated by summing the contributions from air, soil, grass and drinking water as follows:

$$C_{meat} = BTF_{meat} \times \sum C_i \times IC_i$$

and

$$C_{milk} = BTF_{milk} \times \sum C_i \times IC_i$$

where C_i = concentration in exposure medium i (i = grass, soil, air and drinking water) (mg kg^{-1} wet weight or mg m^{-3} or mg l^{-1}).

IC_i = daily intake of exposure medium i (kg wet weight day^{-1}, m^3 day^{-1} or l day^{-1}).

C_{meat} = concentration in meat (mg kg^{-1} wet weight)

C_{milk} = concentration in milk (mg kg^{-1} whole milk).

From these equations, it is relatively straight forward to estimate the biomagnification factor (BMF) for uptake into meat or milk via diet (feed) alone, as shown below. BMFs of this form are used later to test this method against experimental/field data.

$$BMF_{meat-feed} = \frac{C_{meat}}{C_{feed(grass)}} = BTF_{meat} \times IC_{feed(grass)}$$

$$BMF_{milk-feed} = \frac{C_{milk}}{C_{feed(grass)}} = BTF_{milk} \times IC_{feed(grass)}$$

The Travis and Arms (1988) study investigated biotransfer factors for organic compounds (mainly chlorinated pesticides) in beef and milk. The data used for the study were taken from a number of sources including Kenaga (1980), Radeleff *et al.* (1952), Fries *et al.* (1973), Crayford *et al.* (1976), MacDougall (1972), Clark *et al.* (1975), Fries *et al.* (1969), Fries and Marrow (1976), Oehler and Ivie (1980), Potter *et al.* (1974), Beck *et al.* (1966), Claborn *et al.* (1960), Radeleff and Polen (1963), Borzelleca *et al.* (1971), Adler *et al.* (1972), Pasarela *et al.* (1962), Guardigli *et al.* (1976), Geissbühler *et al.* (1971), Claborn *et al.* (1953), Saha (1969), Dorough and Hemken (1973), St. John Jr and Lisk (1973), McKellar *et al.* (1976), Bjerke *et al.* (1972), Whiting *et al.* (1973), Wilson and Cook (1972), Baldwin *et al.* (1976), Johnson Jr and Bowman (1972), Wszolek *et al.* (1980), Bruce *et al.* (1965), Dorough and Ivie (1974), Eisele *et al.* (1983) and Jensen and Hummel (1982).

For beef, a total of 36 chemicals were used in the study and Travis and Arms (1988) found that the biotransfer factors were directly proportional to the octanol-water partition coefficient. The log K_{ow} range of the chemicals considered was 1.34 to 6.98 and the geometric mean regression of the data was as follows:

$$\log BTF_{meat} = -7.735 + 1.033 \log K_{ow} \qquad n = 36, r = 0.81$$

Constraining the slope in this equation to be one and refitting the data yielded the following equation:

$$\log BTF_{meat} = -7.6 + \log K_{ow} \qquad n = 36, r = 0.81.$$

A similar analysis for 28 chemicals in milk led to the following regression equation. The log K_{ow} range of the chemicals considered for milk was between 2.81 and 6.89.

$$\log BTF_{milk} = -8.056 + 0.992 \log K_{ow} \qquad n = 28, r = 0.74$$

Or constraining the slope to be one:

$$\log BTF_{milk} = -8.10 + \log K_{ow} \qquad n = 28, r = 0.74$$

The authors noted that the fresh weight biotransfer for meat was 3.2 times larger than that for milk. On a lipid basis, the biotransfer factor for milk was 21.5 times larger than that for meat. However, the uncertainty in this estimation was considerable.

The TGD recommends that the estimation methods for meat and milk can be used fro substances with a log K_{ow} of between 1.5 and 6.5. Outside of this range, the TGD suggests that the maximum or minimum of this range should be used for substances with log K_{ow} values higher or lower than this.

Similar to the case with plants, it is relatively straightforward to estimate a BAF for meat and milk related to the concentration in soil, drinking water or air if EUSES is used with a nominal concentration in air, water or soil only (on a wet weight soil or dry weight soil basis):

$$BAF_{meat-soil} = \frac{\text{predicted concentration in meat (mg kg}^{-1}\text{ wet weight)}}{\text{nominal concentration assumed in soil (mg kg}^{-1}\text{ wet weight or mg kg}^{-1}\text{ dry weight)}}$$

$$BAF_{milk-soil} = \frac{\text{predicted concentration in milk (mg kg}^{-1}\text{ wet weight)}}{\text{nominal concentration assumed in soil (mg kg}^{-1}\text{ wet weight or mg kg}^{-1}\text{ dry weight)}}$$

$$BAF_{meat-air} = \frac{\text{predicted concentration in meat (mg kg}^{-1}\text{ wet weight)}}{\text{nominal concentration assumed in air (mg m}^{-3}\text{)}}$$

$$BAF_{milk-air} = \frac{\text{predicted concentration in meat (mg kg}^{-1}\text{ wet weight)}}{\text{nominal concentration assumed in air (mg m}^{-3}\text{)}}$$

$$BAF_{meat-water} = \frac{\text{predicted concentration in meat (mg kg}^{-1}\text{ wet weight)}}{\text{nominal concentration assumed in drinking water (mg l}^{-1}\text{)}}$$

$$BAF_{milk-water} = \frac{\text{predicted concentration in meat (mg kg}^{-1}\text{ wet weight)}}{\text{nominal concentration assumed in drinking water (mg l}^{-1}\text{)}}$$

These BAFs integrate several routes of exposure into an overall BAF; that is, they take account of the exposure of plants either by soil and air, and the subsequent ingestion of the plants, ingestion of soil and drinking water or inhalation of air.

For drinking water, the TGD assumes that drinking water is produced from both surface water and groundwater. The model is based on Hrubec and Toet (1992) and assumes a complete removal of suspended particles from surface water or groundwater. Treatment processes used for the purification of groundwater are not generally designed to remove organic pollutants, and so the effects of these processes are ignored in the method. There are two different treatment systems assumed for surface water depending on the type of storage. System 1 includes storage in open reservoirs and system 2 includes dune recharge. Removal of dissolved fractions of chemicals from the surface water is modelled by purification factors which take into account Henry's law constant, log K_{ow} and the aerobic biodegradation rate in days. These factors are multiplied to give the purification factor for each system. The concentration in drinking water is then calculated using the following equation:

$$C_{drw} = \text{maximum } (C_{water} \times F_{pur} \text{ or } C_{grw})$$

where C_{drw} = concentration in drinking water (mg l^{-1}),

C_{water} = dissolved concentration in surface water (mg l^{-1}),

F_{pur} = worst-case purification factor for surface water from either system 1 or 2.

C_{grw} = groundwater concentration (mg l^{-1}).

The total daily intake for humans is then calculated by summing the daily dose through inhalation, intake of drinking water, fish, plant leaves, plant root, meat and milk as shown below. In the method, the concentration in milk is used as a surrogate for all dairy products. Similarly, the concentration in leaf crops is used as a surrogate for fruit and cereals. Calculations also take into account the bioavailability of the chemical through inhalation.

$$DOSE_i = \frac{C_i \times IH_i}{BW}$$

where $DOSE_i$ = daily human dose through intake of i (i =, fish, plant leaves, plant roots, meat milk, drinking water) (mg kg^{-1} bw day^{-1}).

C_i = concentration of chemical in medium i (mg kg^{-1} wet weight or mg l^{-1}).

IH_i = daily human intake of medium i (kg wet weight day^{-1} or l day^{-1}).

The values assumed are 0.115 kg wet weight day^{-1} for fish, 1.2 kg wet weight day^{-1} for leaf crops (including fruit and cereals), 0.384 kg wet weight day^{-1} for root crops, 0.301 kg wet weight day^{-1} for meat, 0.561 kg wet weight day^{-1} for milk/dairy products and 2.0 l day^{-1} for drinking water.

BW = body weight of human. This is taken to be 70 kg.

$$DOSE_{air} = \frac{C_{air} \times IH_{air}}{BW} \times \frac{BIO_{inh}}{BIO_{oral}}$$

where $DOSE_{air}$ = daily human dose through inhalation (mg kg^{-1} bw day^{-1}).

IH_i = daily human intake of air (m^3 day^{-1}). The value assumed is 20 m^3 day^{-1}.

BIO_{inh} = bioavailability of chemical through inhalation. The value assumed by default is 0.75.

BIO_{oral} = bioavailability of chemical through oral route. The value assumed by default is one.

BW = body weight of human. This is taken to be 70 kg.

$$DOSE_{total} = (\sum DOSE_i) + DOSE_{air}$$

where $DOSE_{total}$ = total daily intake for humans (mg kg^{-1} bw day^{-1}).

2.2 ACC-HUMAN

ACC-HUMAN is a fugacity-based, non-steady state, mechanistic model which was developed to predict human tissue levels of lipophilic organic pollutants starting from concentrations in air, water and soil. It focuses on the primary background human exposure to persistent lipophilic contaminants in fish, dairy products and beef. The model was published in a paper by Czub and McLachlan (2004a) and is described in detail in an Environment Agency report (2007).

The model is subdivided into an agricultural and a marine system, each consisting of one food chain. The agricultural food chain is represented by grass, milk, cows and beef cattle. A simple pelagic food chain consisting of zooplankton, planktivorous fish and piscivorous fish was chosen for the marine system. Humans are the top predator linking both systems. Contaminants enter the food chains via uptake from air, water and soil. They are transferred to higher trophic levels via predator-prey interactions. In addition to ingestion, uptake mechanisms including gill ventilation (fish), atmospheric deposition and root uptake (grass), ingestion of soil with feed (cattle), and inhalation and drinking (humans). Contaminants are eliminated via egestion, urination, exhalation, gill ventilation, lactation, percutaneous excretion and metabolism. Although this structure was chosen to reflect the primary pathways of human exposure to persistent bioaccumulating pollutants in Northern Europe, it can be adapted to other regions.

The fish bioaccumulation model in ACC-HUMAN is based on a non-steady state model developed by Gobas *et al.* (1988). This model is very similar in principle to the ECOFATE/Food Chain Bioaccumulation/AQUAWEB models that are tested and validated in Part A of this report series. Therefore, little further verification work on the fish bioaccumulation model in ACC-HUMAN has been carried out here. The findings from Part A are likely to be relevant to ACC-HUMAN.

A mass-balance approach is used to describe uptake into grass from pasture. Atmospheric deposition onto plant leaves from both gaseous and particle-bound contaminants are taken into account. Gaseous uptake is based on a two-resistance model developed by Riederer (1990). The deposition of aerosol-associated chemicals is calculated using an average net deposition velocity. Root uptake into plants is treated as an inflow of soil pore water equally to the grass' transpiration rate, which is corrected for the transpiration stream concentration factor based on the work of Briggs *et al.* (1982). Therefore, the part of the model dealing with uptake into plant leaves from soil is essentially identical to the approach used in the TGD method.

The milk cow model is based on McLachlan (1994), where the milk-cow is treated as two compartments, the digestive tract and the cow itself, and is assumed to be at steady state. The beef cattle model is similar to the milk-cow model, except that steady-state behaviour is not assumed.

The main chemical-related properties needed by the model are the log K_{ow}, the log air-water partition coefficient (log K_{aw}, also known as the dimensionless Henry's law constant) and the log octanol-air partition coefficient (log K_{oa}, which can be estimated by the program from the log K_{ow} and log K_{aw} if unknown). The model can also take into account metabolism rate constants for fish, milk cattle, beef cattle and grass. The model uses a heat of phase transfer for octanol-water, air-water and octanol-water (units of J $mole^{-1}$). The values given in the program are relevant for the example chemicals provided in the program (mainly PCBs) and these were not altered for this work.

Due to their high bioaccumulation potential, persistent lipophilic organic pollutants were the primary target of the model. The predictive ability of the model was evaluated using polychlorinated biphenyls (PCB 52, 101, 118, 138, 153 and 180) in the Swedish environment

as a case study. These data were used in the evaluation, and model parameterization is discussed in detail in Czub and McLachlan (2004a).

The model predicted PCB concentrations as a function of time in each of the trophic levels, and predictions were compared with measurements in biota. The resulting model prediction of PCB concentrations in fish, milk, beef and in human tissue, discussed in detail in Environment Agency (2007), were found to be in good agreement with measured concentrations from Swedish monitoring programs.

The formulation of ACC-HUMAN means that it is not so straightforward to outline simple equations with which to estimate BAFs for various parts of the food chains. However, it is possible to estimate overall BAFs (in a similar way as suggested in Section 2.1 for TGD/EUSES) by running the program with a nominal concentration in one of water, soil or air. The resulting predicted concentrations can then be used to derive an overall BAF as follows:

$$BAF_{feed/grass-soil} = \frac{\text{predicted concentration in feed/grass (mg kg}^{-1}\text{ wet weight)}}{\text{nominal concentration assumed in soil (mg kg}^{-1}\text{ wet weight or mg kg}^{-1}\text{ dry weight)}}$$

$$BAF_{feed/grass-air} = \frac{\text{predicted concentration in feed/grass (mg kg}^{-1}\text{ wet weight)}}{\text{nominal concentration assumed in air (mg m}^{-3}\text{)}}$$

$$BAF_{meat-soil} = \frac{\text{predicted concentration in meat (mg kg}^{-1}\text{ wet weight)}}{\text{nominal concentration assumed in soil (mg kg}^{-1}\text{ wet weight or mg kg}^{-1}\text{ dry weight)}}$$

$$BAF_{milk-soil} = \frac{\text{predicted concentration in milk (mg kg}^{-1}\text{ wet weight)}}{\text{nominal concentration assumed in soil (mg kg}^{-1}\text{ wet weight or mg kg}^{-1}\text{ dry weight)}}$$

$$BAF_{meat-air} = \frac{\text{predicted concentration in meat (mg kg}^{-1}\text{ wet weight)}}{\text{nominal concentration assumed in air (mg m}^{-3}\text{)}}$$

$$BAF_{milk-air} = \frac{\text{predicted concentration in milk (mg kg}^{-1}\text{ wet weight)}}{\text{nominal concentration assumed in air (mg m}^{-3}\text{)}}$$

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$$BAF_{milk-water} = \frac{\text{predicted concentration in milk (mg kg}^{-1}\text{ wet weight)}}{\text{nominal concentration assumed in drinking water (mg l}^{-1}\text{)}}$$

From these BAFs, it is possible to estimate BAFs for uptake into meat or milk from feed. BAFs of this type are used later in the verification of this model against field/experimental data.

$$BAF_{meat-feed} = \frac{\text{concentration in meat (mg kg}^{-1}\text{ wet weight)}}{\text{concentration in feed (mg kg}^{-1}\text{ wet weight)}} = \frac{BAF_{meat-soil}}{BAF_{feed/grass-soil}}$$

$$BAF_{milk-feed} = \frac{\text{concentration in milk (mg kg}^{-1}\text{ wet weight)}}{\text{concentration in feed (mg kg}^{-1}\text{ wet weight)}} = \frac{BAF_{milk-soil}}{BAF_{feed/grass-soil}}$$

The input concentrations used in ACC-HUMAN are all in g m^{-3}. In order to make the calculations comparable with the units more normally used for soil (such as mg kg^{-1}), it is necessary to use a density of soil. For this analysis, a bulk density of soil of 1,700 kg m^{-3} was used (the default value from the TGD).

Concentrations in milk and meat estimated by ACC-HUMAN are given on a lipid weight basis. In order to compare these with values on a whole milk or wet weight meat basis (as given in the TGD method), a lipid content of around three to four per cent for milk and around 25 per cent for meat was generally assumed in this analysis.

ACC-HUMAN calculates the concentration in both grass (pasture) and feed. In the version of the program used in this analysis (v1.1), only the concentration in feed was given in the output (the concentration predicted in grass was always zero). As Czub and McLachlan (2004a) indicate that the concentration in feed is assumed to be equal to the concentration in grass in the model, this assumption was used here.

2.3 Comparison of predictions using a hypothetical test set

Predictions from the two methods were first compared by carrying out a series of calculations for a set of hypothetical chemicals with increasing log K_{ow} values. Both methods essentially use log K_{ow} as the starting point for predicting accumulation in the food chain, but ACC-HUMAN also used log K_{aw}[1].

Our approach investigated the effects of varying the log K_{ow} (and in the case of ACC-HUMAN, log K_{aw}) on the predicted uptake for a single exposure media (such as air, water or soil) in turn. This allowed any obvious patterns or trends to be identified.

[1] The K_{aw} value is also used in the TGD method (calculated from vapour pressure and water solubility), but this only significantly affects the predicted concentrations in plant leaves and grass using the approach taken here. A constant vapour pressure (1 Pa) and water solubility (1 mg l^{-1}), and hence constant K_{aw}, was assumed in the simulations here.

2.3.1 TGD method/EUSES

Input data used for the model simulations in EUSES v2.03 are summarised in Table 2.1.

Table 2.1 Input data used for the simulations with EUSES v2.03

Parameter	Value	Comment
Molecular weight	500 g mol^{-1}	Value used not important for this simulation.
Melting point	200	Value used not important for this simulation.
Boiling point	100	Value used not important for this simulation.
Vapour pressure at 25°C	1 Pa	Value used not important for this simulation.
Water solubility at 25°C	1 mg l^{-1}	Value used not important for this simulation.
Log K_{ow}	Range from 0 to 10 in steps of 0.5	
Local PEC surface water during emission episode (dissolved). Average local PEC in surface water (dissolved).	1 μg l^{-1} 1 μg l^{-1}	All other local PECs set to zero.
Annual average local PEC in air (total)	1 μg m^{-3}	All other local PECs set to zero.
Local PEC in agricultural soil (total) averaged over 30 days. Local PEC in agricultural soil (total) averaged over 180 days. Local PEC in grassland (total) averaged over 180 days.	1 μg kg^{-1} wet weight 1 μg kg^{-1} wet weight 1 μg kg^{-1} wet weight	All other local PEC_S set to zero Note: EUSES generates values for local PECs in pore water of agricultural soil and grassland.
Method used to estimate the soil organic carbon partition coefficient (K_{oc})	Non-hydrophobics (the TGD default QSAR).	Affects the partitioning behaviour between soil and soil pore water. This will affect the predicted concentrations in the simulations based on a constant soil concentration.

Figure 2.1 shows a plot of predicted concentration (mg l^{-1} or mg kg^{-1} wet weight) in fish, drinking water, milk and meat against log K_{ow} for the TGD method. Calculations were carried out using the EUSES model. A constant dissolved concentration of one μg l^{-1} in surface water (during the emission episode) was assumed for this series of calculations and the substance was assumed to be not readily biodegradable. All other concentrations in exposure media (such as soil and air) were set to zero. As seen from the plot, the concentration in wet fish is predicted to increase to a maximum at log K_{ow} of around seven and then decrease with increasing log K_{ow} (a more detailed analysis of this part of the model is given in report Part A). The concentration in drinking water remains relatively constant between a log K_{ow} of zero and four, then decreases in a step-wise fashion over a log K_{ow} between four and six, and becomes constant again between a log K_{ow} of six and ten. In meat, predicted concentrations are relatively constant at low log K_{ow} (of less than two), increase with increasing log K_{ow} until around six and then become constant at log K_{ow} greater than six. A similar pattern is evident in the predicted concentration in milk, but here the concentration is constant at log K_{ow} lower than four. Concentrations predicted in other parts of the human food chain were all zero in this simulation, as exposure was via drinking water only.

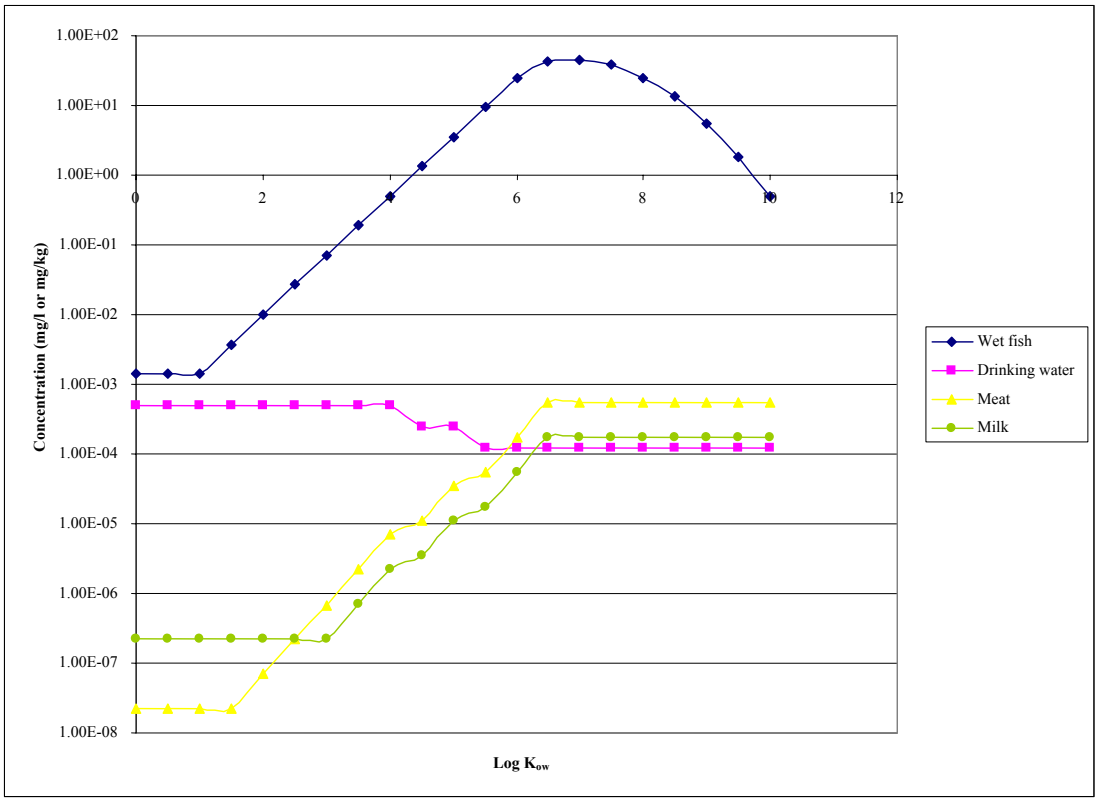

Figure 2.1 Plot of predicted concentration against log K_{ow} for TGD method for exposure via water only

For the second series of simulations using the TGD method/EUSES, the concentration in air was assumed to be constant (1×10^{-6} g m^{-3}) and concentrations in all other exposure media were set to zero. Again, no degradation was assumed in the model. A plot of predicted concentrations in grass, plant leaves, meat and milk (mg kg^{-1} wet weight) against log K_{ow} is shown in Figure 2.2. As seen from the plot, the concentrations in grass and plant leaves increase with increasing log K_{ow} (sigmoidal curve), reaching a maximum at log K_{ow} of around 10. Predicted concentrations in grass and plant leaves are the same. In meat and milk, predicted concentrations remain constant at low log K_{ow} (log K_{ow} of zero to 1.5 and log K_{ow} of zero to three respectively), and then increase with increasing log K_{ow} to a maximum at a log K_{ow} of around 10 (sigmoidal curve). Concentrations predicted in other parts of the human food chain (such as fish, plant roots and drinking water) were zero in this simulation.

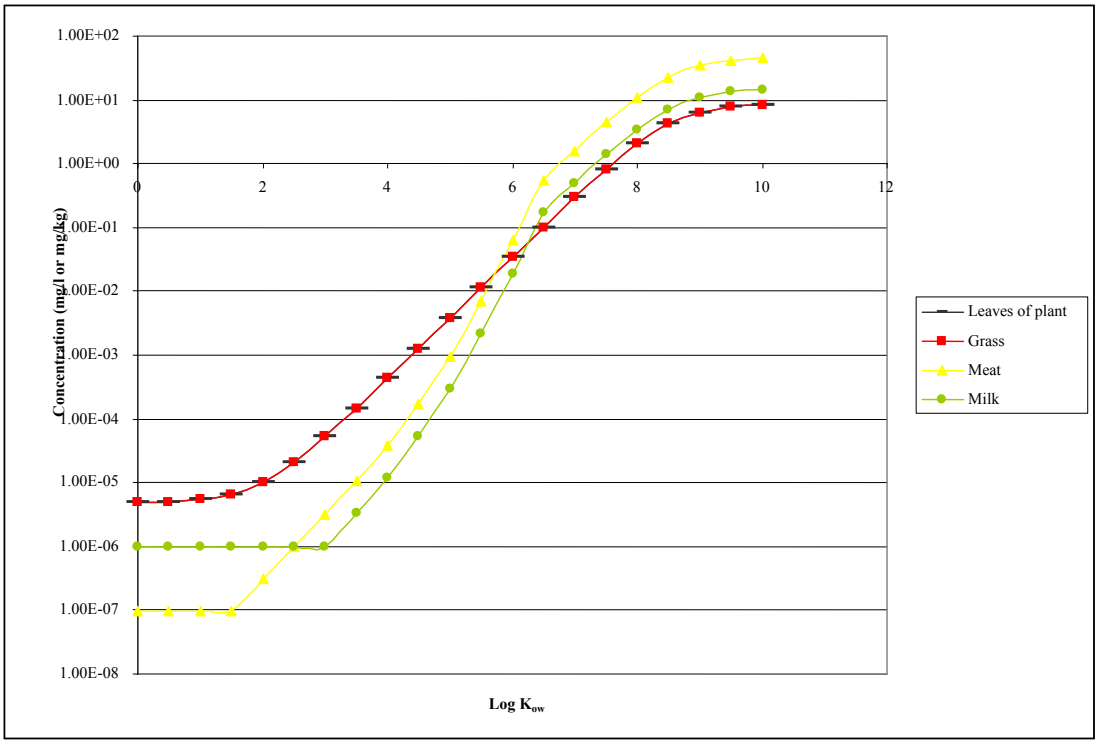

Figure 2.2 Plot of predicted concentration against log K_{ow} for TGD method for exposure via air only

In Figure 2.3, predicted concentrations in plant leaves, root tissue, grass, drinking water, meat and milk resulting from exposure via soil only are shown (mg l^{-1} or mg kg^{-1} wet weight). For this set of simulations, the local concentrations in agricultural soil (total) averaged over 30 days and 180 days, and the concentrations in grassland (total) averaged over 180 days were set to 1×10^{-6} g kg^{-1} wet weight. Concentrations in other exposure media (air and surface water) were set to zero. As can be seen from Figure 2.3, the concentration predicted in drinking water decreases with increasing log K_{ow} across the entire log K_{ow} range. For plant roots, the predicted concentration decreases at low log K_{ow} (between zero and two), reaching a minimum at log K_{ow} of two, and then increases with increasing log K_{ow}. The predicted concentrations in plant leaves and grass similarly decrease, reaching a minimum at log K_{ow} of around five, and then increase to a maximum at log K_{ow} of around 8.5, and then decrease again. In meat and milk, predicted concentrations decrease to a minimum at a log K_{ow} of around 1.5 and three respectively, increase to a maximum at log K_{ow} of around six and then remain fairly constant (slight decrease) at higher log K_{ow} values. The concentrations predicted in other parts of the food chain (such as fish) were zero in this simulation.

Calculations for the simulation, assuming a constant total soil concentration, are dependent on the soil organic carbon-water partition coefficient (K_{oc}). EUSES contains several methods for estimating K_{oc}, depending on the type of chemical in question, but for this simulation the method for non-hydrophobics (the TGD default method) was used. The overall pattern in the variation of predicted concentration with log K_{ow} would be expected to be similar if other methods for estimating log K_{ow} were used, but there would undoubtedly be some differences in the details of the concentrations predicted and possibly the exact variation with log K_{ow}.

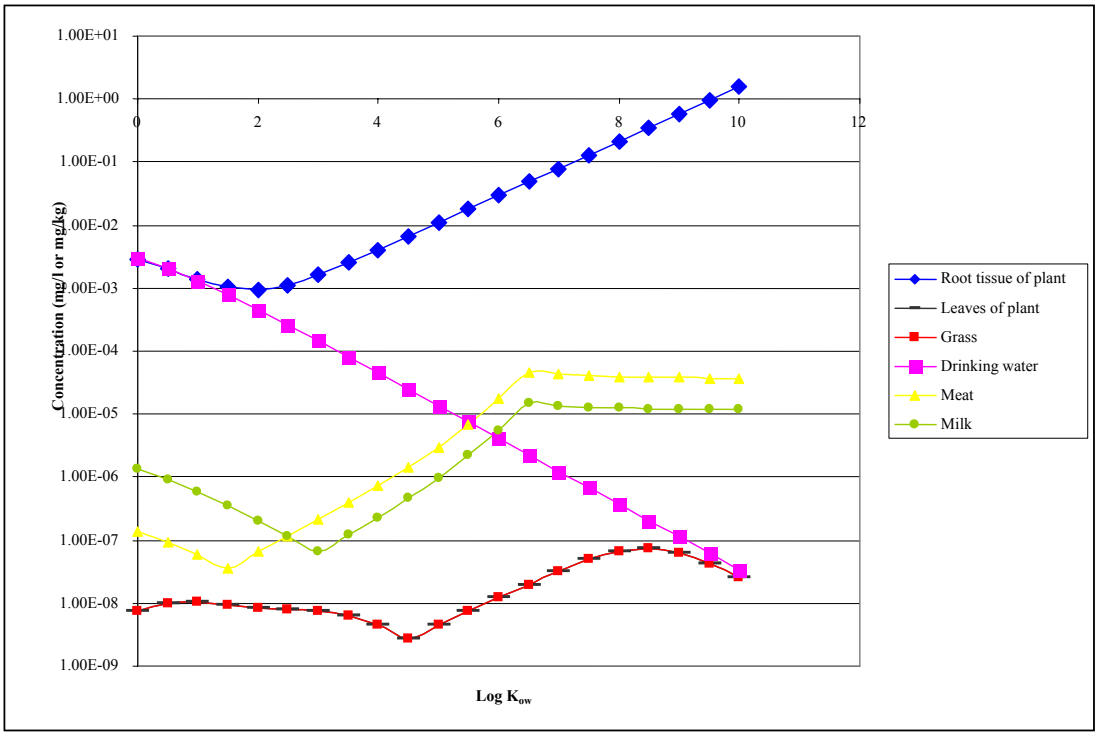

Figure 2.3 Plot of predicted concentration against log K_{ow} for TGD method for exposure via soil only

2.3.2 ACC-HUMAN

The input data used for the model simulations in ACC-HUMAN v1.1 are summarised in Table 2.2.

Using the ACC-HUMAN method, predicted concentrations for a set of hypothetical chemicals were calculated for grass/feed, soil in feed, milk, milk cattle, beef (0-1 year old and 1-2 year old) and humans (female 0-10, 30 to 40 and 70-80 year old and male 0-10, 30-40 and 70-80 year old)[2]. For this simulation, the log K_{ow} value was increased from two to 10 in intervals of one log unit and log K_{aw} was increased from -5 to +5 in steps of one log unit. The partition coefficient log K_{oa} (log K_{oa} = log K_{ow} – log K_{aw}) [3] is calculated by the program and simulations were performed for the combinations of log K_{ow} and log K_{aw} where log K_{oa} was greater than four. Only selected results are shown here; additional plots are included in Appendix 1.

[2] The program will also generate data for other age ranges of humans if required.

[3] The allowable range of values that can be used by the program are a log K_{ow} value between two and 10, a log K_{aw} value between -10 to 10 and a log K_{oa} value between zero and 12. The program will not work if values outside of this range are input and so this limits the combinations of log K_{ow} and log K_{aw} that can be tested.

Table 2.2 Input data used for the simulations with ACC-HUMAN v1.1

Parameter	Value	Comment
Molecular weight	500 g mol^{-1}	Value used not important for this simulation
Log K_{ow} (log K_{aw} + log K_{ow})	Range from 2 to 10 in steps of 1	Range of log K_{ow} values input for each value of log K_{aw} where log K_{ow} – log K_{aw} ≥ 4
Log K_{aw} (log K_{aw} + log K_{oa})	Range from -5 to +5 in steps of 1	See above
Log K_{oa} (log K_{ow} + log K_{oa})	≥ 4	Calculated by the program for varying combinations of log K_{ow} and log K_{aw}
dU_P (dU_{aw} + dU_P)	-20,000 J mol^{-1}	Heat of phase transfer taken from Czub and Mclachlan (2004b)
dU_{aw} (dU_{aw} + dU_{oa})	60,000 J mol^{-1}	As above
dU_{oa} (dU_P + dU_{oa})	-80,000 J mol^{-1}	As above
Constant concentration in air	1×10^{-6} g m^{-3}	Concentration in freshwater, seawater and soil set to zero
Constant concentration in fresh water	1×10^{-6} g m^{-3}	Concentration in freshwater, seawater and soil set to zero
Constant concentration in soil	1×10^{-6} g m^{-3}	Concentration in freshwater, seawater and soil set to zero
Temperature of sea water	280 K	Calculated by program
Terrestrial environment	290 K	
Metabolism rate constant (human, milk cattle, beef cattle, grass, fish)	1×10^{-10} 1 h^{-1}	
Faeces/blood partition coefficient (human)	2×10^{-8}	
Model conditions	100 year (876,000 h)	
Time step for simulation	24 h	

For the first series of calculations, the concentration in fresh water was assumed to be constant at 1×10^{-6} g m^{-3}. Concentrations in air, soil and sea water were set to zero. Figure 2.4 shows a plot of concentration (pg g^{-1} lipid or ng g^{-1} in humans) against log K_{ow} with a constant log K_{aw} of minus four. As seen from this plot, concentration increases between a log K_{ow} of two and four, remains constant between a log K_{ow} of four to seven and then starts to decrease at higher log K_{ow} values. Predicted concentrations are higher in milk cows, beef cattle (0-1 and 1-2 year old) and beef (upper series of curves) than in humans (the lower series of curves). The results obtained for the simulation with log K_{aw} of minus five were very similar. As exposure was via water only, the concentrations in grass/feed were zero.

As the value of log K_{aw} is increased, the curvature of plots of predicted concentrations in cattle show a more pronounced peak, with the maximum value being attained for a shorter range of log K_{ow} values. This is illustrated in Figure 2.5 for log K_{aw} of minus one. The maximum value reached here is virtually the same as for lower values of log K_{aw}. Higher values of log K_{aw} lead to a reduction in the maximum concentration reached, and an increase in the value of log K_{ow} at which this maximum is reached. The maximum concentration in humans remains the same as log K_{aw} is increased, but tends to be reached at higher log K_{ow} values.

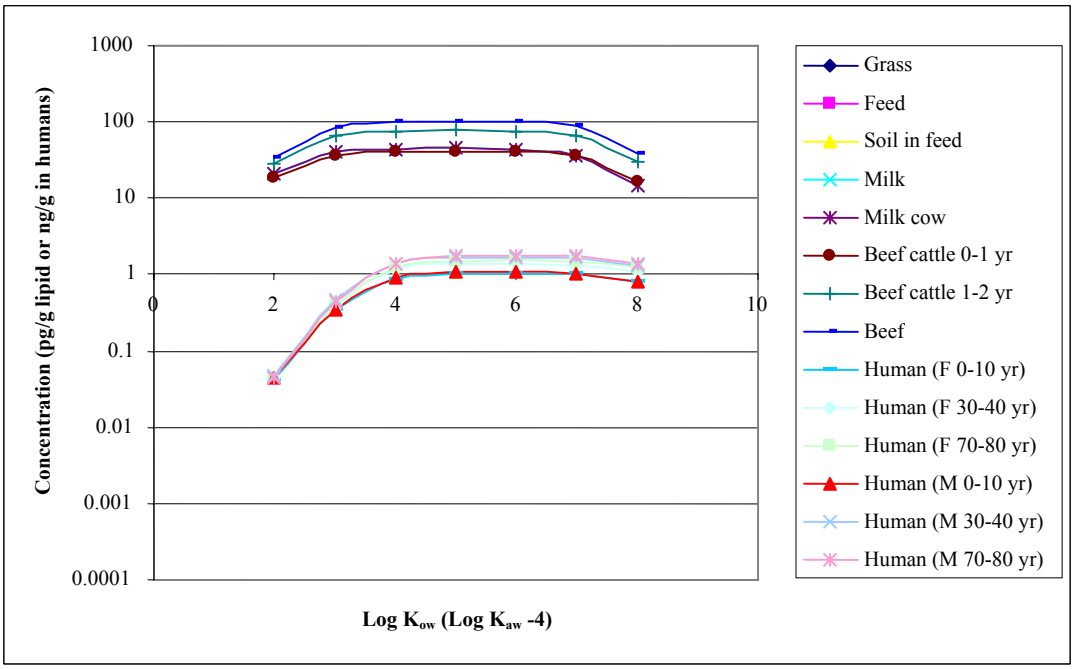

Figure 2.4 Plot of predicted concentration against log K_{ow} (log K_{aw} of minus four) for ACC-HUMAN method (fresh water)

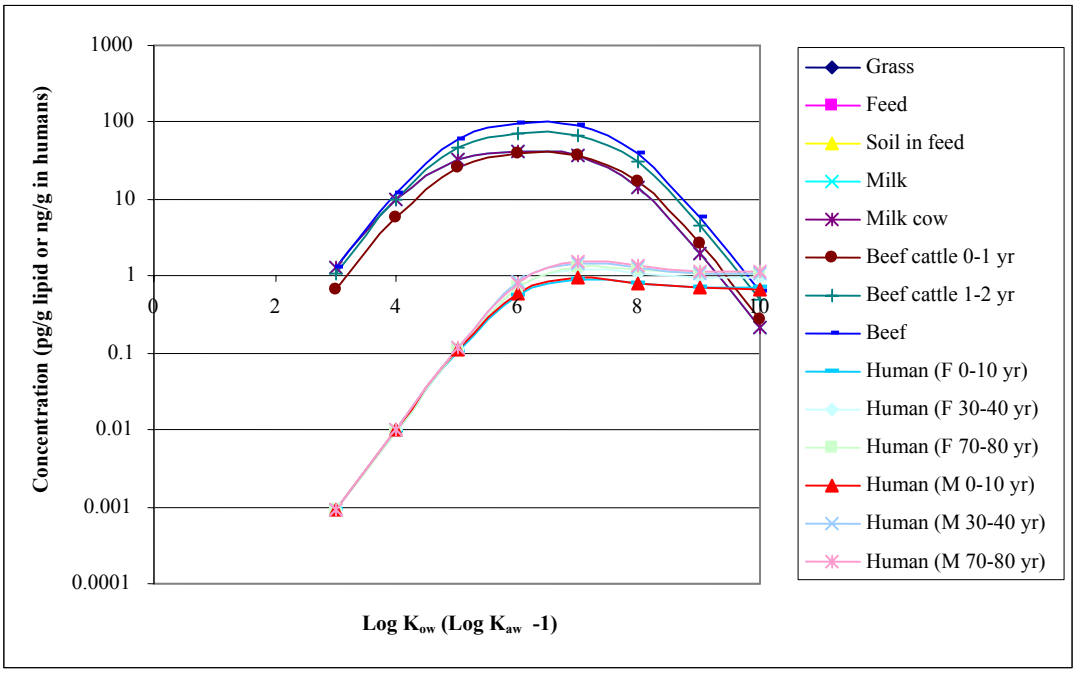

Figure 2.5 Plot of predicted concentration against log K_{ow} (log K_{aw} of minus one) for ACC-HUMAN method (fresh water)

Predicted concentrations for grass, feed and soil in feed are zero for all values of log K_{ow} and log K_{aw} in these simulations (exposure via surface water/drinking water only).

For the next series of simulations, the concentration in soil was assumed to be constant at 1×10^{-6} g m^{-3}, and concentrations in air, soil and sea water were set to zero. As seen from the plots shown in Figure 2.6 and Figure 2.7, predicted concentrations for feed, milk, milk cattle, beef cattle 0-1 year old, beef cattle 1-2 year old, beef (the upper series of curves) and in humans (the lower series of curves) decrease with increasing log K_{ow}. Predicted concentrations also decrease with increasing log K_{aw}. Although simulations were performed for log K_{aw} values ranging from -5 to +5, only selected plots are shown since the same trend was observed for the range of log K_{aw} values.

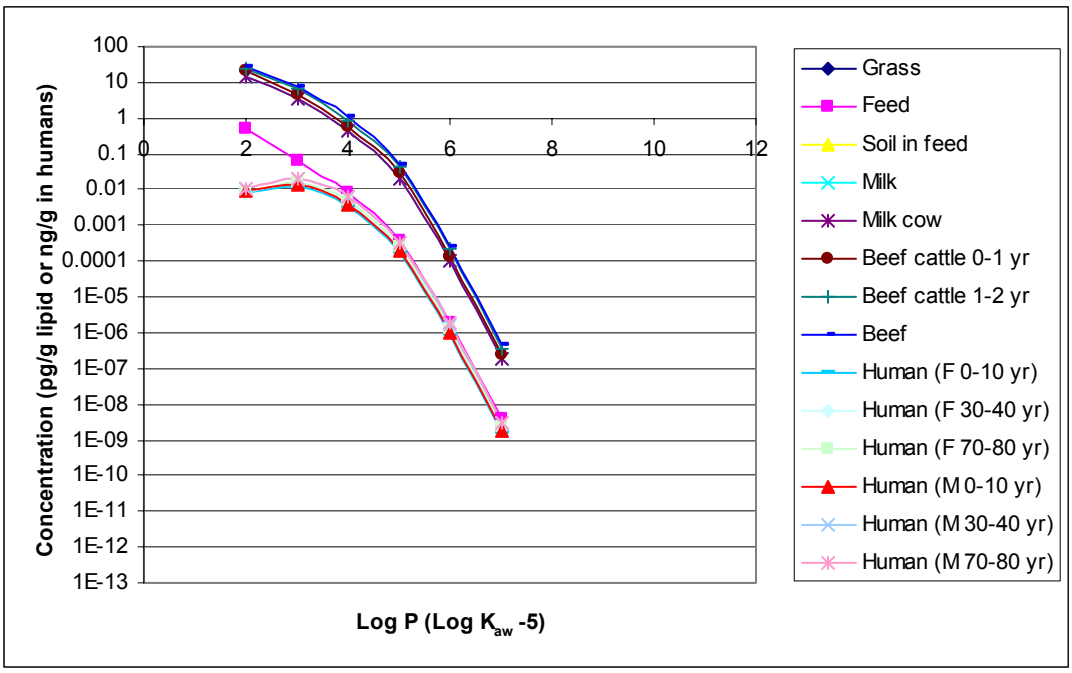

Figure 2.6 Plot of predicted concentration against log K_{ow} (log K_{aw} of minus five) for ACC-HUMAN method (soil)

For the final set of simulations, the concentration in air was set to 1×10^{-6} g m^{-3} and concentrations in air, soil and sea water were set to zero. As seen from the plot shown in Figure 2.8 (log K_{aw} of minus five), predicted concentrations for grass/feed, milk/cattle/beef (upper series of curves) and in humans (the lower series of curves) increase with increasing log K_{ow}.

However, at higher log K_{aw} values (as illustrated in Figure 2.9 for log K_{aw} of minus three), predicted concentrations increase with increasing log K_{ow} to a maximum at around seven, before decreasing. The exception is the predicted concentration in feed which continues to increase as log K_{ow} increases. The trend continues for log K_{aw} values from three and minus two. Predicted concentrations increase with increasing log K_{ow} to a maximum, before decreasing. However, the value of log K_{ow} at which the maximum predicted concentration occurs also increases with increasing log K_{aw}. Predicted concentrations for the same log K_{ow} value also decrease with increasing log K_{aw}.

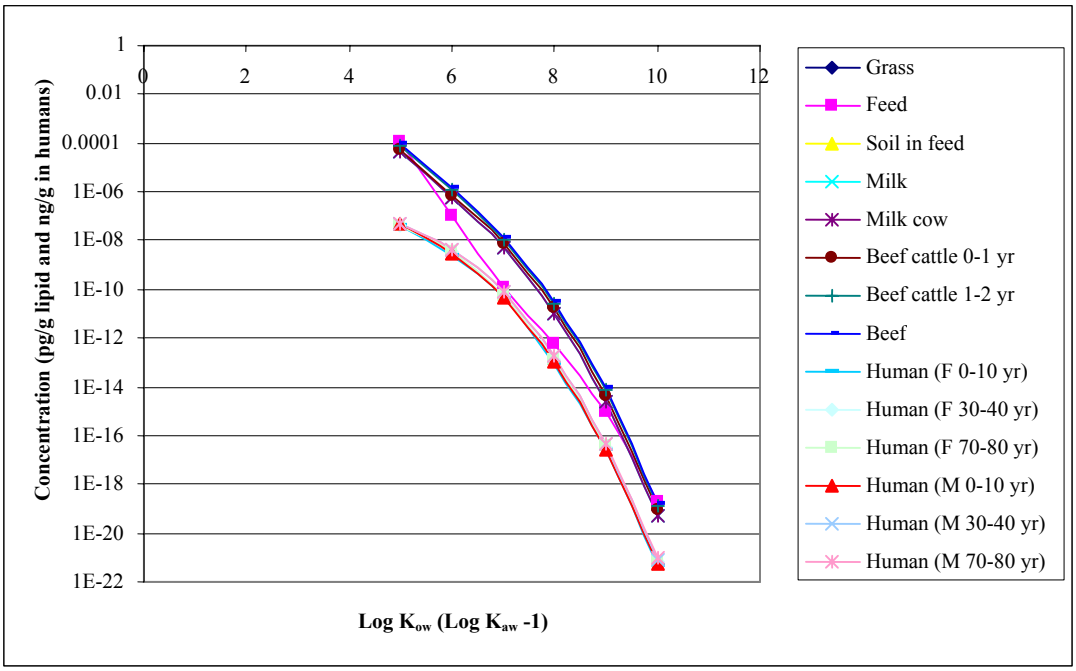

Figure 2.7 Plot of predicted concentration against log K_{ow} (log K_{aw} of minus one) for ACC-HUMAN method (soil)

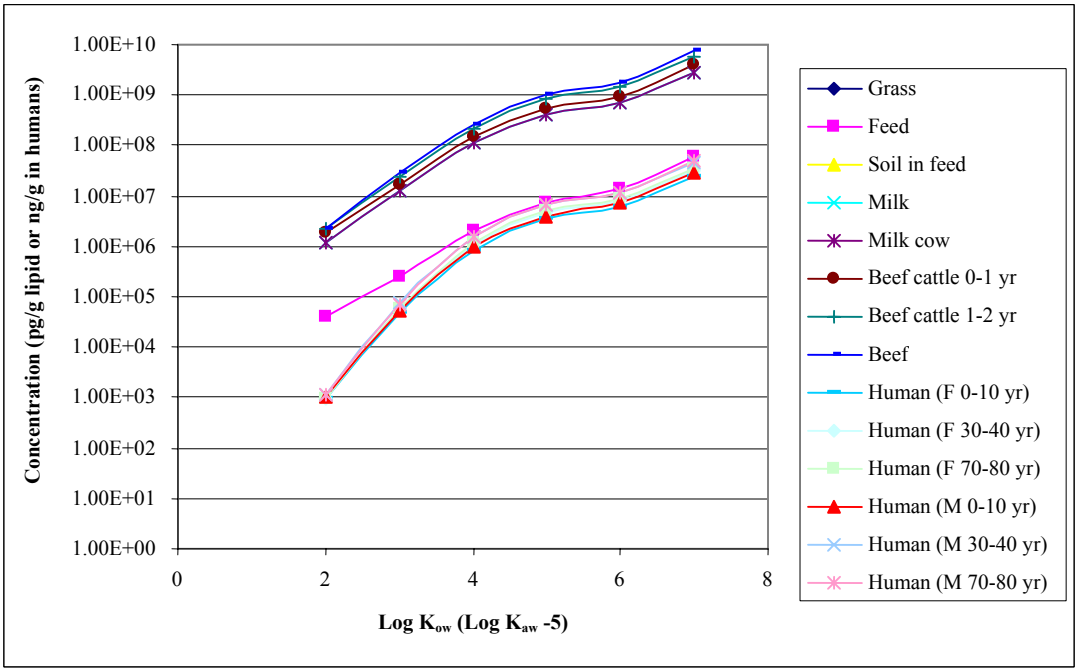

Figure 2.8 Plot of predicted concentration against log K_{ow} (log K_{aw} of minus five) for ACC-HUMAN method (air)

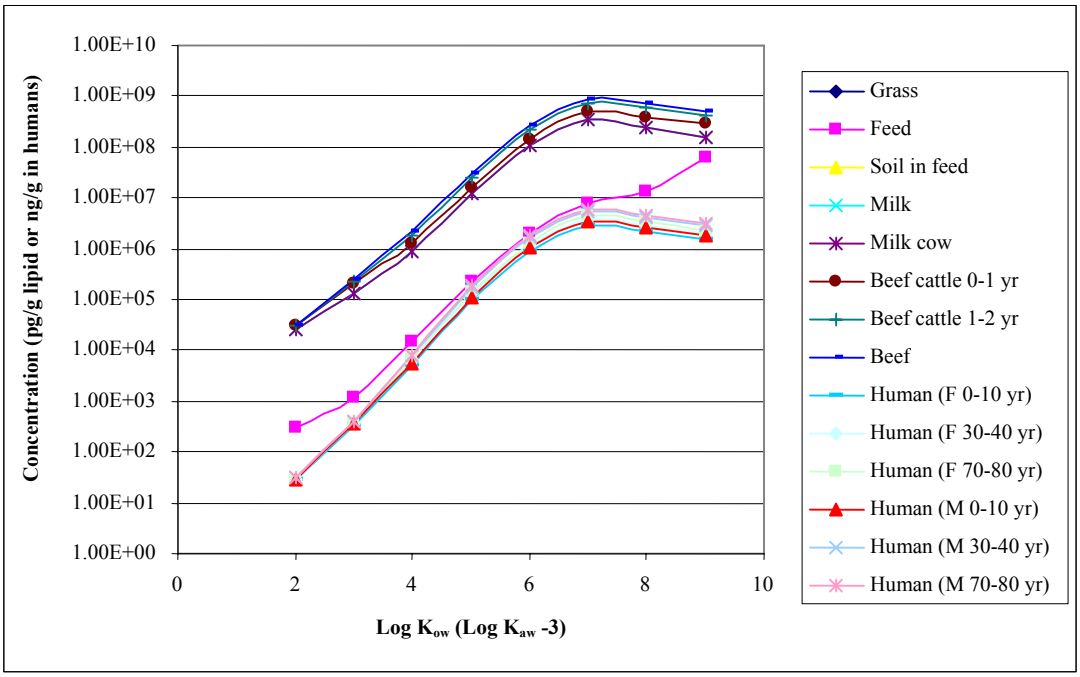

Figure 2.9 Plot of predicted concentration against log K_{ow} (log K_{aw} of minus three) for ACC-HUMAN method (air)

2.4 Comparison of the two methods

In order to better compare predictions from the two methods, concentrations predicted using the TGD approach (for log K_{ow} between two and 10) and the ACC-HUMAN model (log K_{ow} between two and 10, log K_{aw} between -5 and +5 and log K_{oa} greater than four) were converted into bioaccumulation factors in beef, milk and grass/feed. Comparisons were made between three exposure media: water, air and soil.

Figure 2.10 and Figure 2.11 show plots of log BAF against log K_{ow} in the water compartment for beef and milk, respectively. Bioaccumulation factors were calculated by dividing the predicted concentrations calculated in EUSES (mg kg^{-1} wet weight) and ACC-HUMAN (ng kg^{-1} lipid) by the concentration of the hypothetical chemical in water used to generate the predicted concentration. In the TGD approach, a local PEC in surface water during the emission episode of 1,000 ng l^{-1} was used. For the ACC-HUMAN method, a constant concentration of hypothetical chemical of one ng l^{-1} was assumed. The concentrations predicted in EUSES were converted to a lipid basis, assuming a lipid fraction (by volume) in beef cattle at the time of slaughter of 0.15, and a lipid volume in milk cattle of 0.1 (Czub and McLachlan, 2004a).

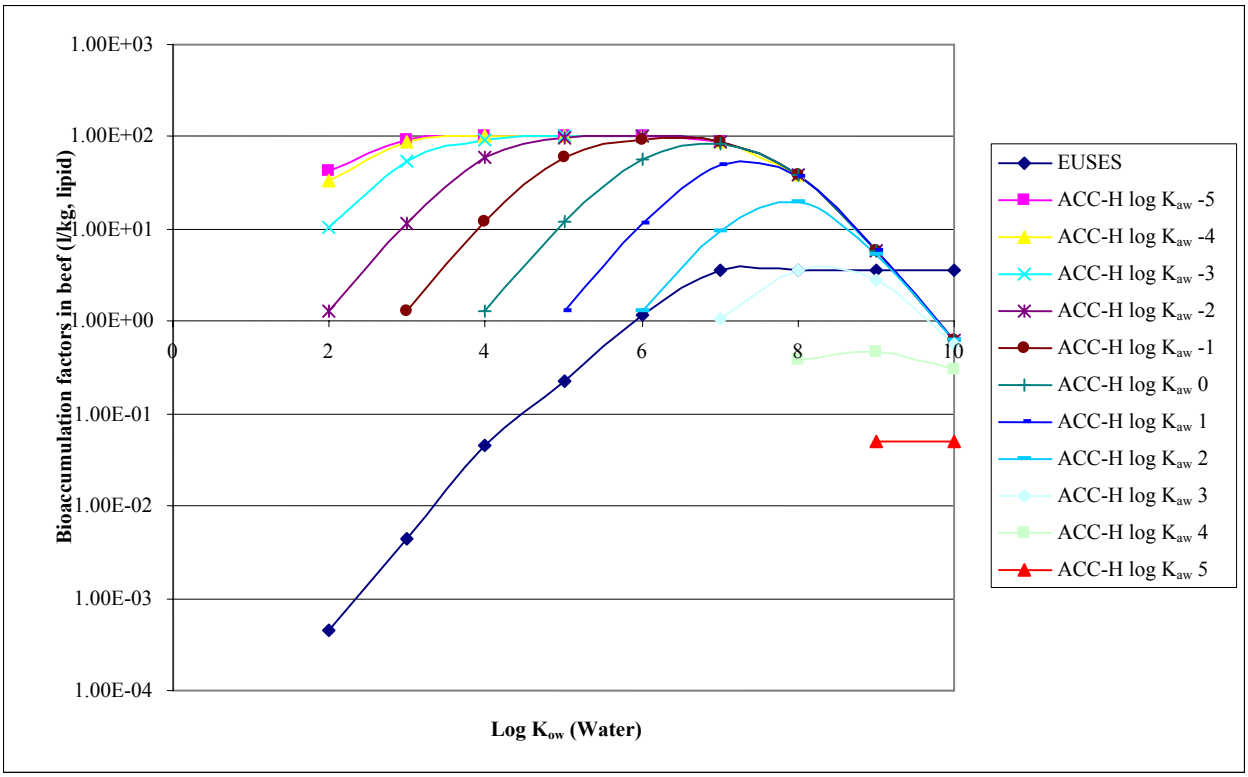

Figure 2.10 Plot of log BAF in beef against log K_{ow} using the TGD approach and the ACC-HUMAN method (water) ($BAF_{meat-water}$)

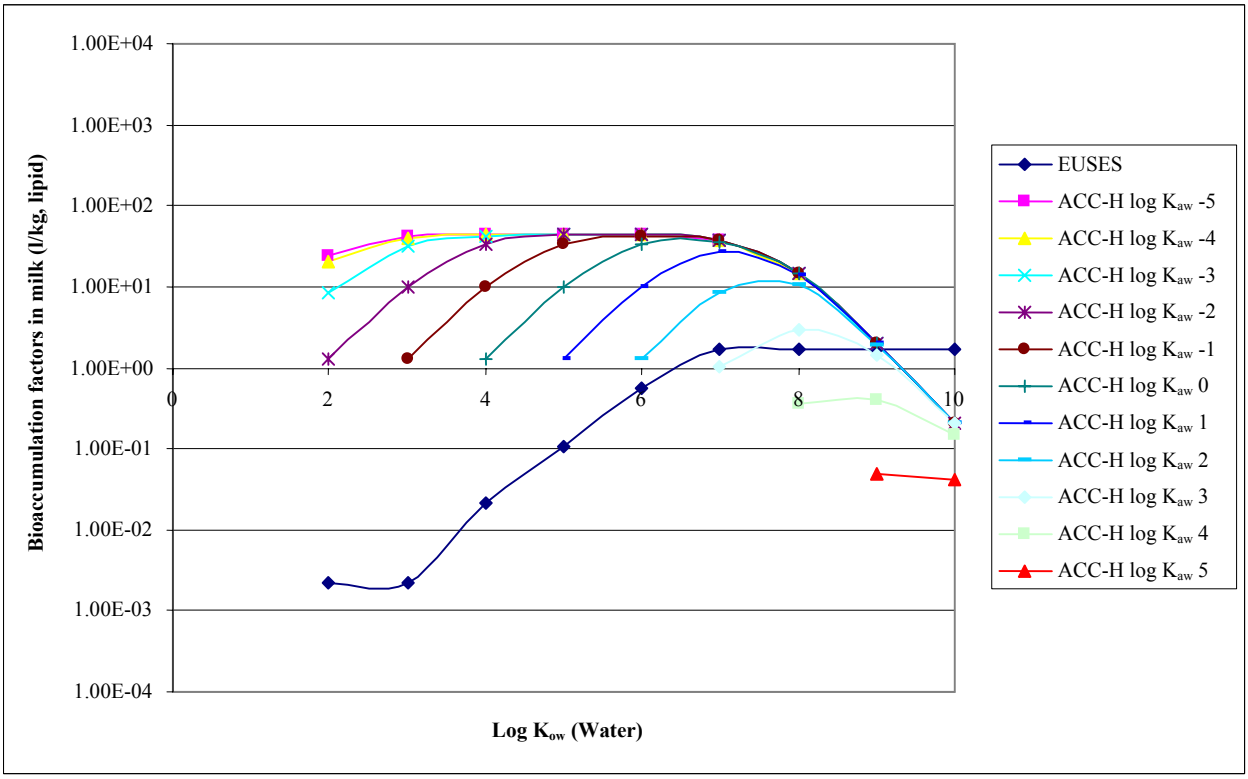

Figure 2.11 Plot of log BAF in milk against log K_{ow} using the TGD approach and the ACC-HUMAN method (water) ($BAF_{milk-water}$)

As seen from these figures, bioaccumulation factors predicted using the TGD approach increase with increasing log K_{ow}, until a log K_{ow} of around seven. Between log K_{ow} values of seven and 10, the predicted BAFs remain constant. Bioaccumulation factors predicted using ACC-HUMAN for a log K_{aw} of three show the greatest similarity to those predicted using EUSES/TGD method. BAFs predicted in ACC-HUMAN (where log K_{aw} is between -5 and +2) are higher than those predicted using EUSES, and tend to increase with increasing values of log K_{ow} to a maximum value and then decrease with further increases in log K_{ow}. It is clear from these plots that the bioaccumulation factors predicted using the ACC-HUMAN method are also dependent on the value of log K_{aw} (and hence log K_{oa}) used in the calculation. When log K_{aw} is four or five, the predicted BAFs in ACC-HUMAN are lower than those in EUSES.

Plots of predicted bioaccumulation factors in beef, milk and grass/feed (EUSES and ACC-HUMAN) for exposure via air versus log K_{ow} are shown in Figure 2.12 to Figure 2.13. Similarities in the predicted bioaccumulation factors using EUSES and ACC-HUMAN (where log K_{aw} is minus one) are seen in beef and milk, and particularly in feed/grass. BAFs predicted using both programs tend to increase with increasing log K_{ow}. Again, it is clear that the BAFs predicted using ACC-HUMAN are dependent on the value of log K_{aw} used in the calculation.

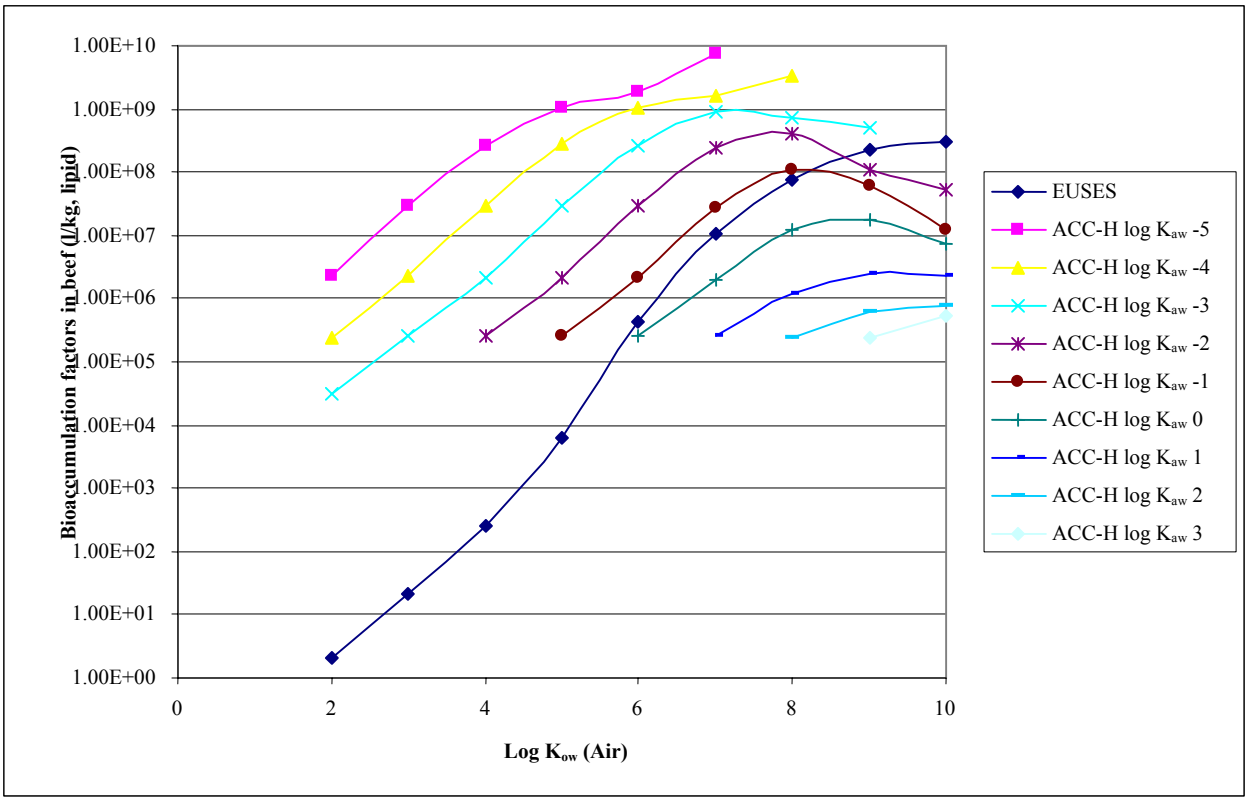

Figure 2.12 Plot of log BAF in beef against log K_{ow} using the TGD approach and the ACC-HUMAN method (air) ($BAF_{meat-air}$)

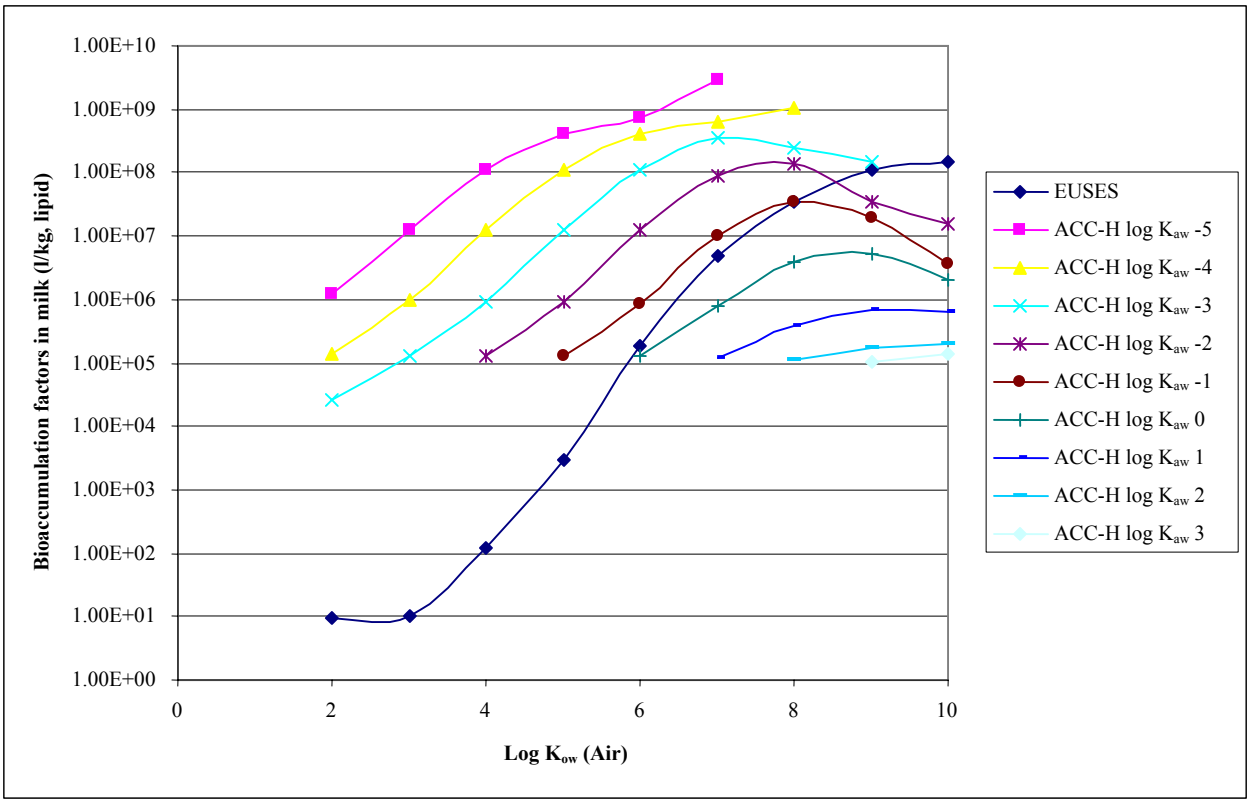

Figure 2.13 Plot of log BAF in milk against log K_{ow} using the TGD approach and the ACC-HUMAN method (air) (BAFmilk-air)

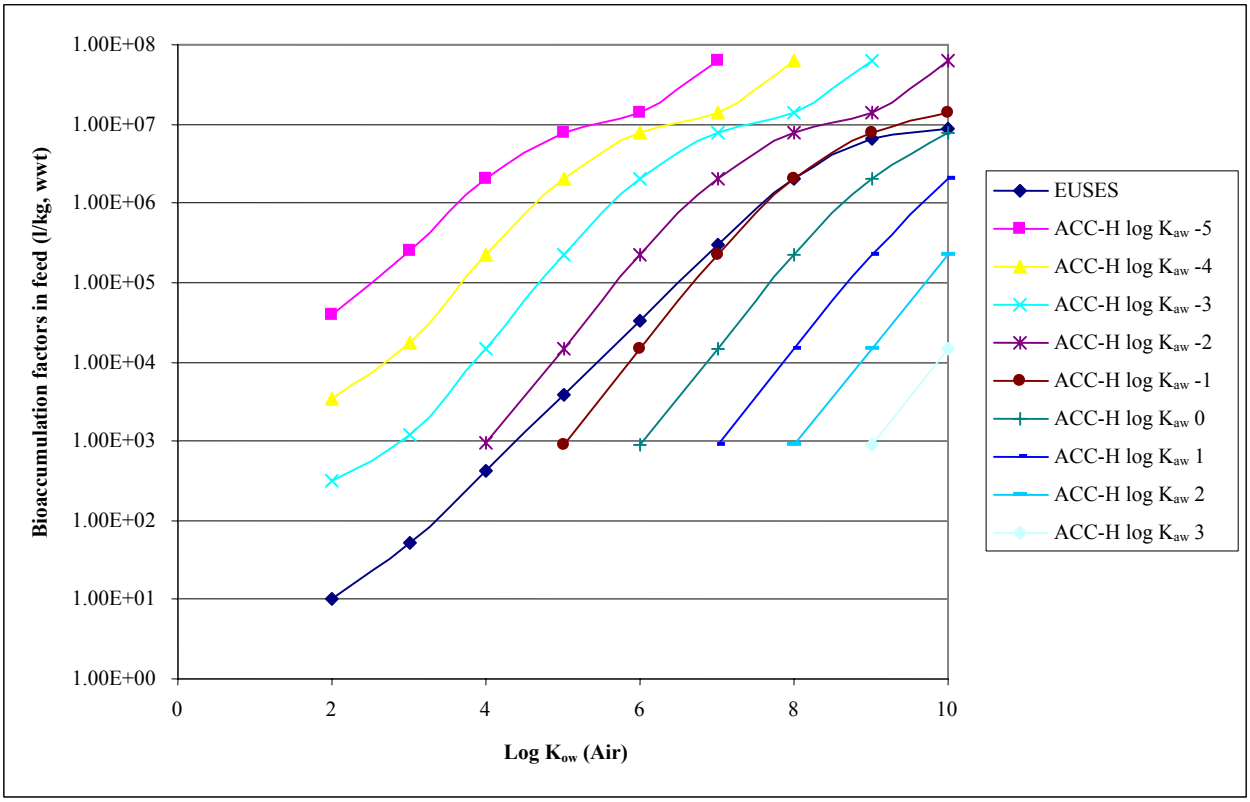

Figure 2.13 Plot of log BAF in grass/feed against log K_{ow} using the TGD approach and the ACC-HUMAN method (air) ($BAF_{feed/grass-air}$)

Figure 2.15 to Figure 2.16 show plots of predicted BAFs in beef, milk and feed/grass in EUSES and ACC-HUMAN for uptake from soil. In EUSES, a local PEC in agricultural soil of 1,000 ng kg^{-1} wet weight was assumed, and a constant concentration of 1×10^{-6} g m^{-3} was assumed in the calculations performed using the ACC-HUMAN model (equivalent to a concentration of 0.59 ng kg^{-1} wet weight using the density of wet soil taken from TGD of 1,700 kg m^{-3}, where this concentration on a mass basis was used to derive the BAFs). As seen from the plots, predictions using the two models are very different. BAFs predicted using ACC-HUMAN decrease with increasing log K_{ow}, and predictions follow the same trend for all values of log K_{aw}. In EUSES, predicted bioaccumulation factors increase slightly with increasing log K_{ow} until seven to eight, when the values remain fairly constant.

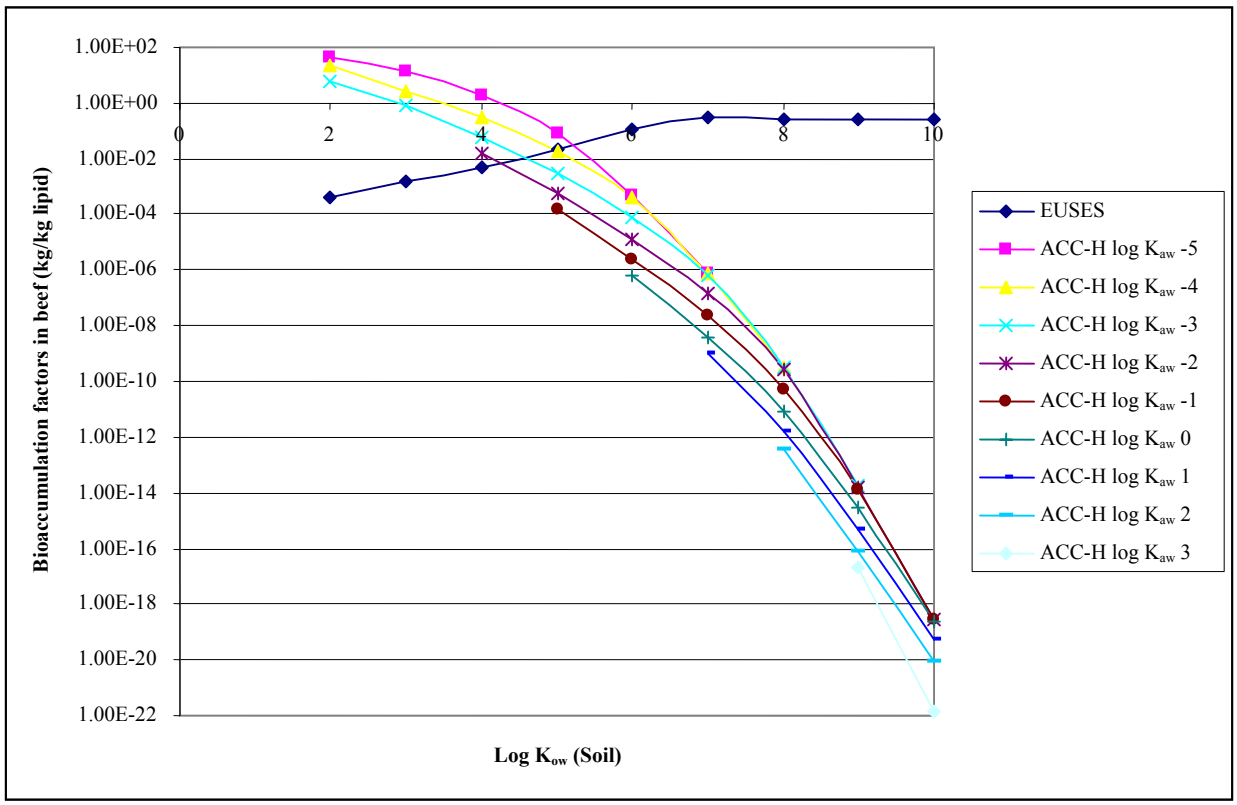

Figure 2.14 Plot of log BAF in beef against log K_{ow} using the TGD approach and the ACC-HUMAN method (soil) ($BAF_{meat\text{-}soil}$)

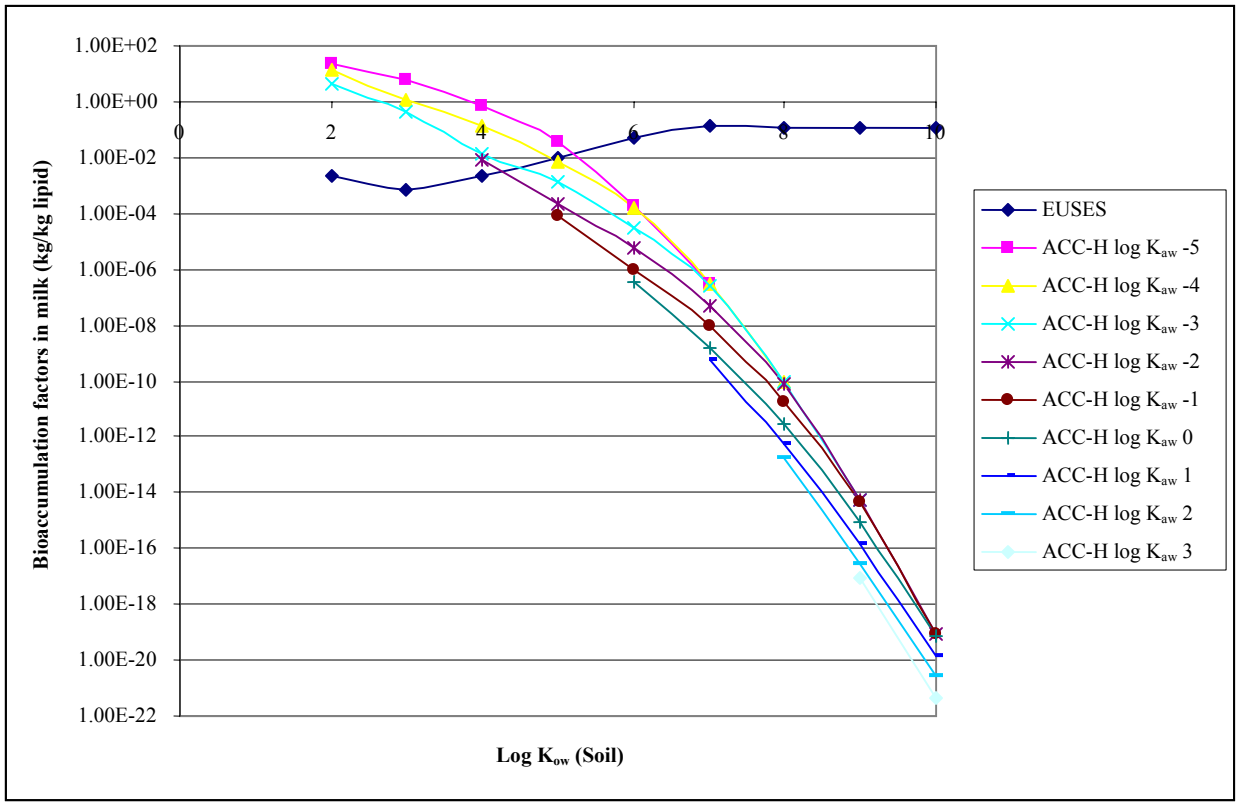

Figure 2.15 Plot of log BAF in milk against log K_{ow} using the TGD approach and the ACC-HUMAN method (soil) ($BAF_{milk-soil}$)

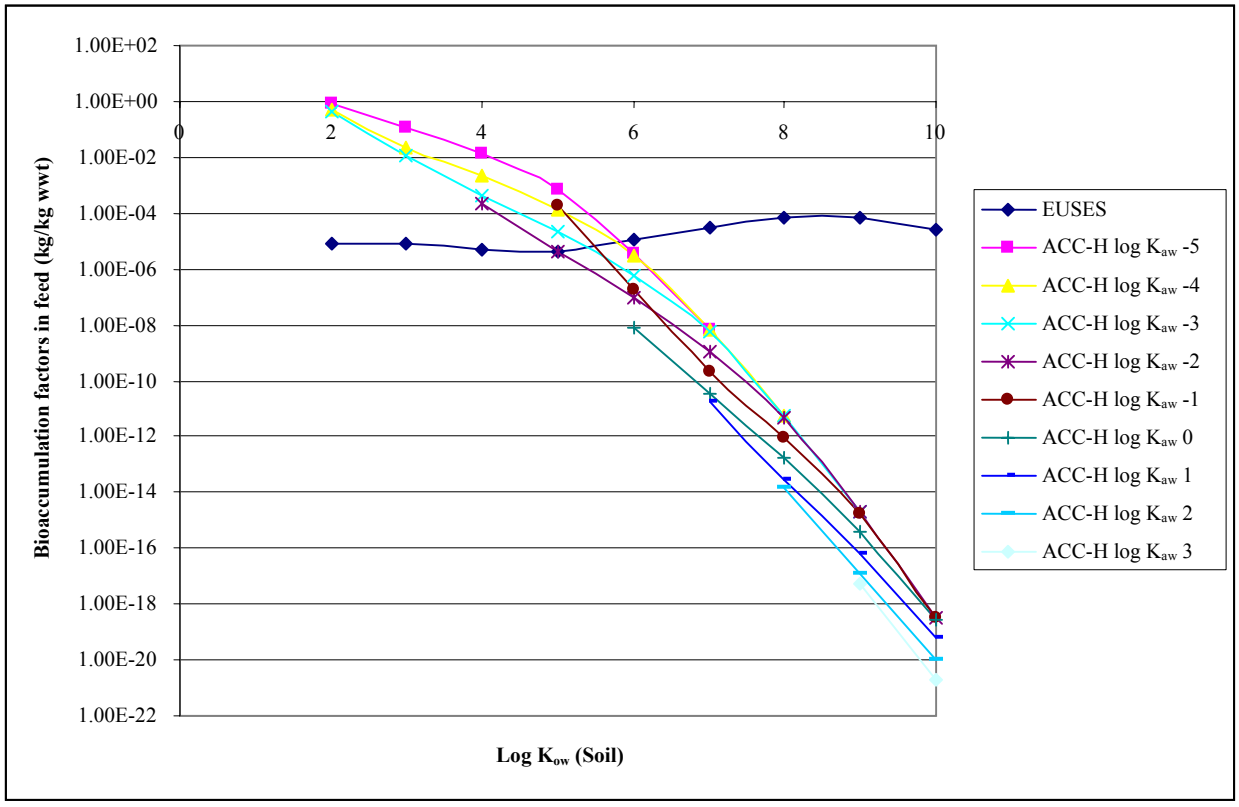

Figure 2.16 Plot of log BAF in grass/feed against log K_{ow} using the TGD approach and the ACC-HUMAN method (soil) ($BAF_{feed/grass-soil}$)

2.5 Summary of findings

Analysis of the two methods using a set of hypothetical chemicals covering a range of log K_{ow} (and log K_{aw} values for ACC-HUMAN) identified a number of similarities and major differences between the patterns of uptake and accumulation predicted by the two methods. In particular, when exposure is assumed to be mainly via soil, ACC-HUMAN predicts a generally decreasing trend in the levels of accumulation in meat and milk with increasing log K_{ow}, whereas the TGD method predicts the opposite. A similar pattern is also evident in the predicted accumulation from soil in grass/feed.

Predictions for exposure via soil also take into account the partitioning behaviour of the substance in soil as well as the actual accumulation in plants, meat and milk. In both approaches, the predicted adsorption to soil is expected to increase with increasing log K_{ow} (or more importantly, the predicted fraction in the soil pore water is predicted to decrease with increasing log K_{ow}). Thus, there is a pattern of reducing bioavailability in the soil phase with increasing log K_{ow} that is superimposed on top of any trends in the uptake from soil pore water into plants, meat and milk in the models. As discussed in Section 3, some of the field/experimental data allow the effects of partitioning in the soil to be separated out from other parts of the accumulation process; for example, data are available on the uptake into cattle/milk from feed, which allow these specific parts of the models to be tested without influence from the soil partitioning properties).

For exposure via air and water, a similar pattern of uptake and accumulation with log K_{ow} is predicted using both the TGD method and ACC-HUMAN. However, a key finding is that concentrations predicted by ACC-HUMAN are strongly dependent on two physico-chemical properties (log K_{ow} and log K_{aw}), whereas the TGD method is mainly dependent on log K_{ow}.

3 Testing against experimental data

3.1 Introduction

The extent of verification that could be carried out for the food chain models was limited to some extent by the availability of suitable data sets. For example, few data were available on the simultaneous exposure of plants via air and soil, and similarly few data were available for the simultaneous exposure of cattle via drinking water, air and food. Therefore, verification of the models was necessarily done in a piece-meal fashion, whereby only certain parts of the model could be validated using any one data set.

Both the TGD and the ACC-HUMAN method can predict the concentration of the chemical in fish. Part A of this report series considers in detail the TGD and two alternative methods for predicting accumulation in fish in relation to wildlife exposure, and so these parts of the methods are not tested further here. Thus, the fish accumulation part of ACC-HUMAN was not tested. However, one of the other methods considered in Part A (the Food Chain Bioaccumulation/ECOFATE/AQUAWEB model) is very similar in principle to the fish accumulation model included in ACC-HUMAN. From a regulatory point of view, it would be desirable to have a similar method for predicting concentrations in fish for both wildlife exposure and human exposure, and so the findings of Part A of this report are also relevant to the human food chain. This aspect is discussed further in Section 4.

The ACC-HUMAN model can also calculate concentrations in humans resulting from exposure via the food chain. This part of the model was not tested here for two reasons. Firstly, there is a lack of usable experimental data relating human body burden of a chemical to concentration in the total diet. Secondly, in terms of setting standards, the effects on humans are normally determined in terms of a dose in intake media rather than an internal body concentration. Therefore, we focused on predicting concentrations in the human intake media, rather than the resulting internal concentration in the human.

The predictive methods rely crucially on certain physico-chemical properties of the chemical. The two most important properties are the log K_{ow} and Henry's law constant. These values are difficult to measure for highly lipophilic substances of low water solubility and vapour pressure (as is the case for many of the chemicals in the test set) and many different values exist in the literature for such properties. For this analysis, log K_{ow} values were generally taken from the original paper outlining the accumulation data. However, for several of the chemicals, different log K_{ow} values were given in different data sets. Therefore, in order to make the predictions as consistent as possible across the different methods and data sets, a single preferred value for log K_{ow} was generally used for the chemical in question. These values are summarised in Part D of this report series for all chemicals considered. No actual validation of log K_{ow} values was undertaken in this analysis, but rather the preferred values reflected the more commonly quoted values in the literature. A similar problem also arose for Henry's law constants. Here, values from the EPIWIN v3.12 program (USEPA, 2000) were mostly used, with preference given to the values in the database within the EPIWIN program rather than predicted values (database values represent in many cases values of the Henry's law constant derived from a measured water solubility and vapour pressure).

The ACC-HUMAN model only works with chemicals with a log K_{ow} value between two and 10. For chemicals with log K_{ow} values outside of this range, the model was run with a log K_{ow} of either two or 10 as appropriate.

3.2 Comparison of predicted and experimental data

3.2.1 Accumulation in plants by exposure via air

Paterson *et al.* (1991) reported a set of leaf-air bioaccumulation factors ($BAF_{leaf\text{-}air}$) based on the experimental work of Bacci *et al.* (1991a and 1991b) using azalea leaves. These $BAF_{leaf\text{-}air}$ values were defined by Paterson *et al.* (1991) as the ratio of the volume concentration (mg m^{-3}) in leaf to the volume concentration (mg m^{-3}) in air. These BAF values are shown in Table 3.1. Paterson *et al.* (1991) gave the density of the wet leaf as 0.89 g cm^{-3} (890 kg m^{-3}) and this allowed BAF values to be converted to a concentration in wet plant (mg kg^{-1})/concentration in air (mg m^{-3}) basis.

Predicted BAFs for plant leaves are shown in Table 3.1 and displayed in Figure 3.1. The predictions were carried out by assuming a nominal exposure concentration (1×10^{-3} mg m^{-3}) in air[4] (the concentrations in water and soil were set to zero) and calculating the resulting concentration (in mg kg^{-1} wet weight) in plant leaves (TGD method) or feed (ACC-HUMAN). The ratio of these predicted concentrations then gave the $BAF_{leaf\text{-}air}$ directly. Calculations were carried out twice, firstly using log K_{ow} values given in the paper by Paterson *et al.* (1991) and secondly, using the preferred log K_{ow} values from Part D of this series.

As can be seen, agreement between predicted and measured log $BAF_{plant/leaf\text{-}air}$ values is variable. Both TGD and ACC-HUMAN appear to give similar predictions of the log BAF in most cases, with the TGD method generally resulting in slightly higher estimates of log BAF than ACC-HUMAN.

It is also worth noting that $BAF_{plant\text{-}air}$ values are predicted to increase with increasing log K_{ow} using both methods (see Section 2.3), and this trend is evident for the experimental data with azalea leaves.

[1] For TGD, as the method does not include a contribution to plant leaves from particulate-bound substances in the air, the air concentration was assumed to represent the concentration in the vapour phase rather than the total concentration. For ACC-HUMAN, the concentration represents the total concentration (this model does include a contribution from aerosol-bound substance).

Table 3.1 Leaf-air bioaccumulation factors from Paterson *et al.* (1991)

Substance	Preferred physico-chemical properties		Physico-chemical properties given in Paterson *et al.* (1991)		Experimental log $BAF_{plant-air}$		Predicted log $BAF_{plant-air}$					
							TGD				ACC-HUMAN	
							Using preferred physico-chemical properties		Using physico-chemical properties given in Paterson *et al.* (1991)		Using preferred physico-chemical properties	Using physico-chemical properties given in Paterson *et al.* (1991)
	log K_{ow}	log K_{aw}	log K_{ow}	log K_{aw}	(mg m^{-3} leaf)/ (mg m^{-3} air)	(mg kg^{-1} leaf)/(mg m^{-3} air)	(mg m^{-3} leaf)/(mg m^{-3} air)	(mg kg^{-1} leaf)/(mg m^{-3} air)	(mg m^{-3} leaf)/(mg m^{-3} air)	(mg kg^{-1} leaf)/(mg m^{-3} air)	(mg kg^{-1} leaf)/(mg m^{-3} air)	(mg kg^{-1} leaf)/(mg m^{-3} air)
Triflurialin	5.33	-2.36	3.00	-2.77	5.02	2.07	5.40	2.56	3.66	0.81	1.98	-0.21
Hexachloro benzene	5.50	-1.14	6.00	-1.26	5.62	2.67	4.36	1.52	4.95	2.10	0.73	1.47
Mirex	5.28	-1.46	6.90	-1.66	7.07	4.12	4.47	1.63	6.11	3.26	0.85	2.93
Thionazin	1.86	-4.43	1.20	-4.44	4.43	1.48	4.52	1.68	4.33	1.49	0.96	0.97
Sulfotep	3.99	-3.99	3.00	-3.91	4.35	1.40	5.74	2.90	4.80	1.95	2.32	1.12
DDT	6.19	-3.45	6.00	-2.60	7.64	4.69	6.68	3.84	6.17	3.33	3.76	2.97
DDE	6.51	-2.75	5.70	-2.47	7.48	4.53	6.56	3.71	5.84	2.99	3.52	2.53
Hexachlorocyclo hexane (alpha-isomer)	3.70	-3.66	3.80	-3.44	6.01	3.06	5.17	2.33	5.04	2.20	1.60	1.46
Hexachlorocyclo hexane (gamma-isomer)	3.70	-3.66	3.80	-4.26	5.88	2.93	5.17	2.33	5.83	2.98	1.60	2.41
PCBs (60% chlorinated)	6.10	-2.52	6.90	-2.14	7.28	4.33	6.19	3.35	6.44	3.59	2.98	3.33
Alachlor	3.52	-6.45	2.80	-5.58	5.45	2.50	6.75	3.91	6.18	3.33	3.87	2.80
Dieldrin	5.40	-3.37	3.70	-3.33	6.03	3.08	6.32	3.48	4.84	2.00	3.11	1.21

Substance	Preferred physico-chemical properties		Physico-chemical properties given in Paterson *et al.* (1991)		Experimental log $BAF_{plant-air}$		Predicted log $BAF_{plant-air}$					
							TGD				ACC-HUMAN	
							Using preferred physico-chemical properties		Using physico-chemical properties given in Paterson *et al.* (1991)		Using preferred physico-chemical properties	Using physico-chemical properties given in Paterson *et al.* (1991)
	log K_{ow}	log K_{aw}	log K_{ow}	log K_{aw}	(mg m^{-3} leaf)/ (mg m^{-3} air)	(mg kg^{-1} leaf)/(mg m^{-3} air)	(mg m^{-3} leaf)/(mg m^{-3} air)	(mg kg^{-1} leaf)/(mg m^{-3} air)	(mg m^{-3} leaf)/(mg m^{-3} air)	(mg kg^{-1} leaf)/(mg m^{-3} air)	(mg kg^{-1} leaf)/(mg m^{-3} air)	(mg kg^{-1} leaf)/(mg m^{-3} air)
3,3',4,4'-Tetrachloro biphenyl (PCB 77)	6.63	-2.33	6.10	-2.39	7.93	4.98	6.40	3.55	6.09	3.25	3.27	2.86
1,2,3,4-TCDD	6.60	-3.07	6.60	-2.80	7.96	5.01	6.68	3.84	6.61	3.76	3.77	3.62

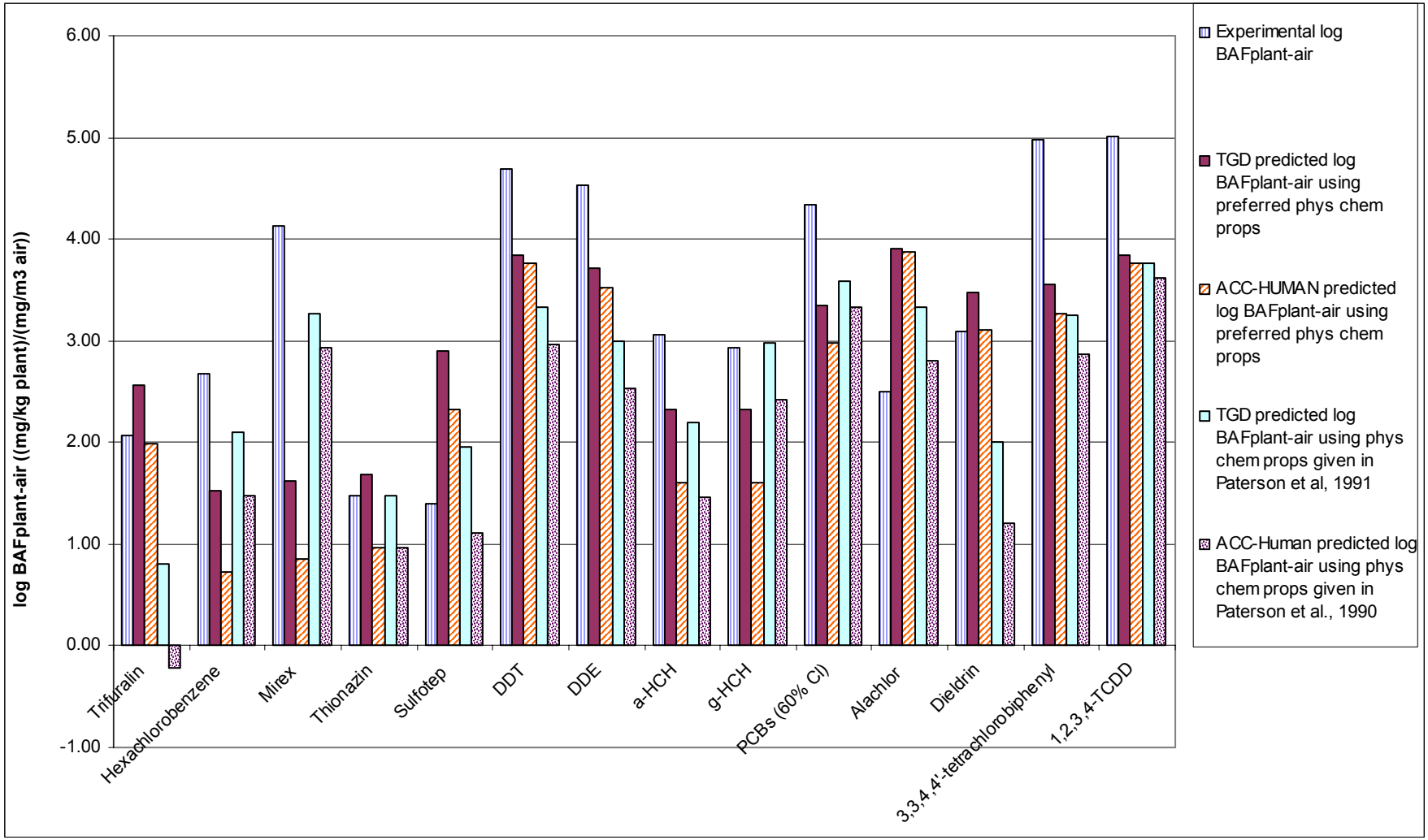

Figure 3.1 Predicted and experimental bioaccumulation factors for uptake by plant leaves from air

Figure 3.2 shows a plot of the residual in the prediction, which is the actual log BAF minus the predicted log BAF; a positive residual indicates that the method is underpredicting the value of BAF and a negative residual indicates that the method is overpredicting the value of BAF. As can be seen from this plot, the residual is generally within around two log units (meaning that the predicted BAF is within a factor of 100 of the actual BAF). In addition, both methods appear to show a trend in increasing underprediction of the actual BAF with increasing log K_{ow}. However, there are likely to be differences between the properties of plant species used to obtain the experimental data (azalea leaves) and the assumptions made over the plant properties used in the model (where the models are designed to predict concentrations in grass and, in the case of the TGD, a "generic" leaf crop). These differences in properties (such as leaf volume or lipid content) may well account for some of the differences seen. However, such differences would be expected to result in a systematic under or overprediction of the actual BAF, rather than the pattern seen here. For the substances in this data set, TGD predictions are in general closer to experimental values than those from ACC-HUMAN.

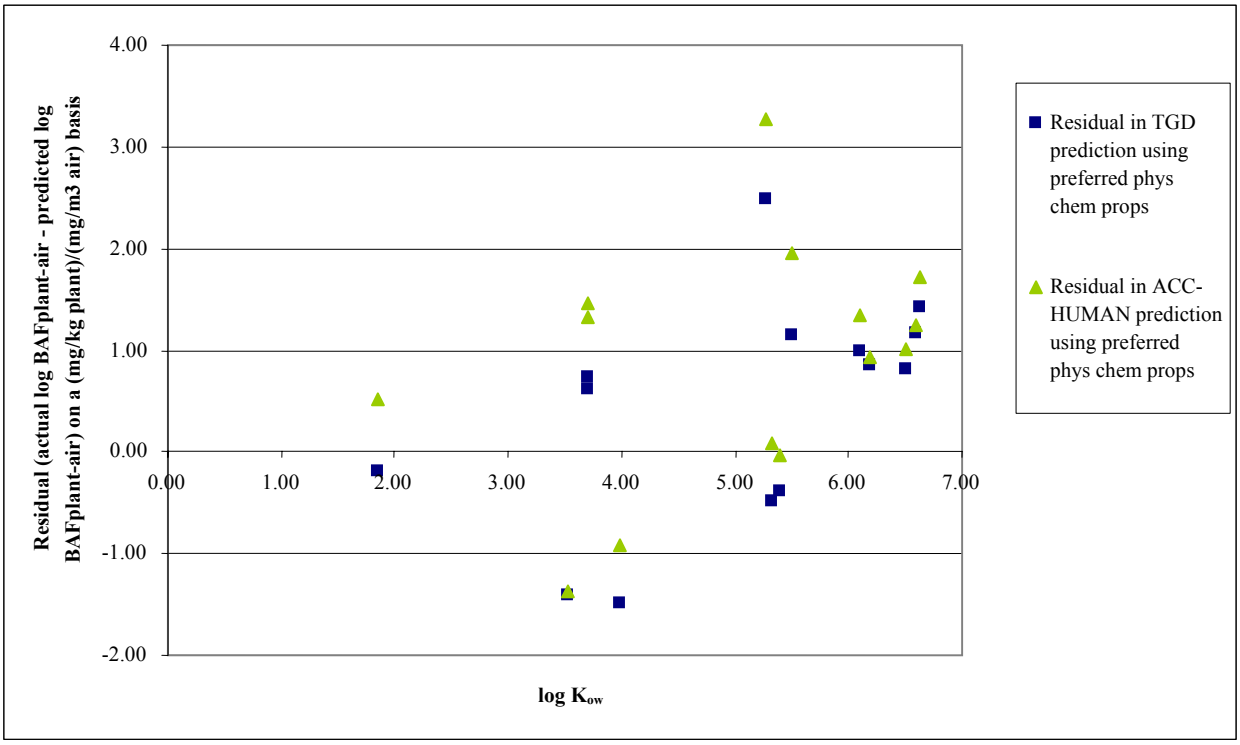

Figure 3.2 Residual in the prediction of log $BAF_{plant-air}$

3.2.2 Accumulation in plants by exposure via soil or soil pore water

A number of data compilations are available which can be used to test part of the TGD method related to uptake by plants from soil or soil pore water.

Uptake into plant roots

Polder *et al.* (1994 and 1995) carried out a validation exercise of the plant uptake model in the forerunner of EUSES. The model was called Uniform System for the Evaluation of Substances (USES) and used a different method for estimating root uptake from soil pore water than is currently used in EUSES, but a similar method for estimating transportation in the transpiration stream. For the evaluation, Polder *et al.* (1995) tabulated literature values for the soil pore water-root partition coefficient. These are summarised in Table 3.2, along with equivalent values predicted using the method in EUSES. The data used by Polder *et al.* (1995) were taken from studies using either whole soil or nutrient solutions carried out by Aguero-Alvarado and Appleby (1991), Businelli *et al.* (1975), Boersma *et al.* (1991), Casterline Jr *et al.* (1985), De la Cruz and Rakanna (1975), Eshel *et al.* (1978), Harris and Sans (1969), Isensee and Jones (1971), McCrady *et al.* (1990), McFarlane *et al.* (1990), O'Connor *et al.* (1990), Shone and Wood (1974), Trapp and Pussemier (1991), Voerman and Besemer (1975), Wild and Jones (1992) and Worobey (1988).

Briggs *et al.* (1982) carried out a series of experiments investigating the uptake of non-ionised O-methylcarbamoyloximes and substituted phenylureas into barley roots from nutrient solution. A regression equation relating the root concentration factor to log K_{ow} was derived from this data and was used to estimate root uptake in an earlier version of the TGD/EUSES (this was the version that was tested in the study of Polder *et al.* (1994 and 1995) discussed above). This data set is also considered here in relation to testing the updated method in the current version of the TGD.

A number of other data were also collected for this project. The complete test data set is summarised in Table 3.2. The same table also outlines the predicted BAF_{root} (calculated here on a mg kg^{-1} wet root/mg kg^{-1} wet soil basis) using the TGD method.

The TGD method relies on estimates of the soil pore water concentration. In order to calculate this, a value for the organic carbon-water partition coefficient (K_{oc}) is needed. TGD provides several methods for estimating K_{oc} values from log K_{ow} values. For this exercise, two of the more commonly used methods from the TGD were used. These were the quantitative structure activity relationship (QSAR) for non-hydrophobics[5] (the default QSAR in the TGD) and the QSAR for predominantly hydrophobics[6].

It was not possible to test the ACC-HUMAN model using this data set as the ACC-HUMAN model does not give concentrations in root crops directly.

[5] $\log K_{oc} = 0.52 \times \log K_{ow} + 1.02$
[6] $\log K_{oc} = 0.81 \times \log K_{ow} + 0.10$

Table 3.2 Comparison of literature and predicted values for the uptake of chemicals into plant roots from soil pore water

Substance	Log K_{ow}	Soil concentration (mg kg^{-1} dry weight)	Nutrient solution concentration (mg l^{-1})[a]	Soil organic carbon content	Plant	Conc^{n} in plant roots (mg kg^{-1} wet wt)	Experimental log BAF root (concentration in wet root / concentration in wet soil)		Predicted log BAF root		Reference
							a	b	a	b	
Acenaphthene/ fluorene	3.92	4.06		1.2%	Carrot peel	2.19	-0.21	-0.21	0.79	0.57	Wild and Jones, 1992 (as quoted in Polder, 1994)
		8.38		1.7%	Carrot peel	3.27	-0.35	-0.35	0.65	0.44	
		17.74		2.3%	Carrot peel	4.08	-0.58	-0.58	0.52	0.31	
		51.00		4.4%	Carrot peel	3.57	-1.10	-1.10	0.23	0.02	
		3.57		1.2%	Peeled carrot (core)	1.25	-0.40	-0.40	0.79	0.57	
		7.09		1.7%	Peeled carrot (core)	2.27	-0.44	-0.44	0.65	0.44	
		16.53		2.3%	Peeled carrot (core)	3.14	-0.67	-0.67	0.52	0.31	
		53.00		4.4%	Peeled carrot (core)	2.12	-1.34	-1.34	0.23	0.02	
Acetone O-methylcarbamoyl oxime	-0.13		1[c]	2.0%	Barley	0.95[c]	0.54	0.85	0.53	0.84	Briggs *et al.,* 1982
Aldicarb	1.15		1[c]	2.0%	Barley	0.94[c]	0.04	0.49	0.11	0.56	Briggs *et al.,* 1982
Aldoxycarb	-0.57		1[c]	2.0%	Barley	0.66[c]	0.50	0.72	0.65	0.87	Briggs *et al.,* 1982

Substance	Log K_{ow}	Soil concentration (mg kg^{-1} dry weight)	Nutrient solution concentration (mg l^{-1})[a]	Soil organic carbon content	Plant	Conc^{n} in plant roots (mg kg^{-1} wet wt)	Experimental log BAF root (concentration in wet root / concentration in wet soil)		Predicted log BAF root		Reference
							a	b	a	b	
Aroclor 1248	6.30	0.50		0.6%	Carrot peel	0.02	-1.34	-1.34	2.09	1.19	O'Connor *et al.,* 1990 (as quoted in Polder, 1994)
		0.75		0.6%	Carrot peel	0.053	-1.10	-1.10	2.09	1.19	
		0.50		0.1%	Carrot peel	1.275	0.46	0.46	2.83	1.93	
		0.75		0.1%	Carrot peel	2.25	0.53	0.53	2.83	1.93	
Aroclor 1254	6.47	100.00		0.3%	Carrot	50	-0.25	-0.25	2.43	1.47	Iwata and Gunther, 1976
Atratone	2.69		0.1	2.0%	Barley	0.128	-0.57	-0.43	0.11	0.24	Shone and Wood, 1974 (as quoted in Polder, 1994)
Atrazine	2.65		0.1	2.0%	Barley	0.185	-0.39	-0.24	0.09	0.24	Shone and Wood, 1974 (as quoted in Polder, 1994)
Benfluralin	5.29	0.46		0.7%	Carrot	0.214	-0.28	-0.28	1.62	1.01	Businelli *et al.,* 1975 (as quoted in Polder, 1994)
		0.76		0.7%	Carrot	0.243	-0.44	-0.44	1.62	1.01	
		0.46		0.7%	Peeled carrot	0.017	-1.38	-1.38	1.62	1.01	

Substance	Log K_{ow}	Soil concentration (mg kg^{-1} dry weight)	Nutrient solution concentration (mg l^{-1})[a]	Soil organic carbon content	Plant	Conc[n] in plant roots (mg kg^{-1} wet wt)	Experimental log BAF root (concentration in wet root / concentration in wet soil)		Predicted log BAF root		Reference
							a	b	a	b	
		0.76		0.7%	Peeled carrot	0.019	-1.55	-1.55	1.62	1.01	
Benzaldehyde O-methylcarbamoyl oxime	1.49		1[c]	2.0%	Barley	1.48[c]	0.08	0.49	0.03	0.44	Briggs *et al.,* 1982
Bromacil	2.11		58	2.0%	Soy bean	345.8	0.39	0.68	-0.01	0.28	Boersma *et al.,* 1991 (as quoted in Polder, 1994)
4-(4-Bromo phenoxy)phenyl urea	3.70		1[c]	2.0%	Barley	34.9[c]	0.35	0.20	0.48	0.33	Briggs *et al.,* 1982
4-Bromo phenylurea	1.98		1[c]	2.0%	Barley	3.17[c]	0.18	0.50	-0.02	0.30	Briggs *et al.,* 1982
Carbofuran	2.32		0.1	2.0%	Garden bean	0.13	-0.38	-0.14	0.02	0.25	Trapp *et al.,* 1991 (as quoted in Polder, 1994)
4-Chloro benzaldehyde O-methylcarbamoyl oxime	2.27		1[c]	2.0%	Barley	2.8[c]	-0.02	0.23	0.01	0.26	Briggs *et al.,* 1982
4-Chloro phenylurea	1.80		1[c]	2.0%	Barley	2[a]	0.07	0.42	-0.01	0.34	Briggs *et al.,* 1982
3,4-Dichloro benzaldehyde O-methylcarbamoyl oxime	2.89		1[c]	2.0%	Barley	5.61[c]	-0.03	0.05	0.17	0.25	Briggs *et al.,* 1982

Substance	Log K_{ow}	Soil concentration (mg kg^{-1} dry weight)	Nutrient solution concentration (mg l^{-1})[a]	Soil organic carbon content	Plant	Conc[n] in plant roots (mg kg^{-1} wet wt)	Experimental log BAF root (concentration in wet root / concentration in wet soil)		Predicted log BAF root		Reference
							a	b	a	b	
2,4-Dichlorophenol	3.06		0.1	2.0%	Soy bean	13.5	1.27	1.30	0.23	0.26	Isensee and Jones, 1971 (as quoted in Polder, 1994)
			0.11	2.0%	Oat	13.5	1.22	1.26	0.23	0.26	
2,4-Dichloro phenoxyacetic acid (2,4-D)	2.81		0.1	2.0%	Barley	1.614	0.17	0.27	0.14	0.25	Shone and Wood, 1974(as quoted in Polder, 1994)
3-(3,4-Dichlorophenoxy) benzaldehyde O-methylcarbamoyl oxime	4.60		1[c]	2.0%	Barley	81.1[c]	0.25	-0.16	0.87	0.45	Briggs *et al.,* 1982
3,4-Dichloro phenylurea	2.64		1[c]	2.0%	Barley	5.86[c]	0.12	0.27	0.09	0.24	Briggs *et al.,* 1982
DDT	6.19	0.57		2.1%	Sugar beet	0.03	-1.22	-1.22	1.53	0.66	Harris and Sans, 1969 (as quoted in Polder, 1994)
		56.50		1.7%	Rye-grass	57.21	0.06	0.06	1.61	0.74	Voerman *et al.,* 1975 (as quoted in Polder, 1994)

Substance	Log K_{ow}	Soil concentration (mg kg^{-1} dry weight)	Nutrient solution concentration (mg l^{-1})[a]	Soil organic carbon content	Plant	Conc^{n} in plant roots (mg kg^{-1} wet wt)	Experimental log BAF root (concentration in wet root / concentration in wet soil)		Predicted log BAF root		Reference
							a	b	a	b	
Dieldrin	5.40	1.12		2.1%	Potato	0.03	-1.52	-1.52	1.19	0.55	Harris and Sans, 1969 (as quoted in Polder, 1994)
		1.12		2.1%	Carrot	0.04	-1.39	-1.39	1.19	0.55	
		1.12		2.1%	Sugar beet	0.07	-1.15	-1.15	1.19	0.55	
		0.57		0.8%	Potato	0.03	-1.22	-1.22	1.60	0.96	
		0.57		0.8%	Carrot	0.05	-1.00	-1.00	1.60	0.96	
		0.12		0.8%	Carrot	0.01	-1.02	-1.02	1.69	0.98	
		7.64		1.7%	Rye-grass	11.3	0.23	0.23	1.27	0.62	Voerman *et al.,* 1975 (as quoted in Polder, 1994)
Diuron	2.68		0.2	2.0%	Barley	0.62	-0.18	-0.04	0.10	0.24	Shone and Wood, 1974 (as quoted in Polder, 1994)
Ethirimol	4.39		0.2	2.0%	Barley	0.1322	-1.73	-2.08	0.78	0.42	Shone and Wood, 1974 (as quoted in Polder, 1994)
Ethofumesate	3.27	1.00		1.7%	Sugar beet	1.34	0.18	0.18	0.38	0.36	Eshel *et al.,* 1978 (as quoted in Polder, 1994)

Substance	Log K_{ow}	Soil concentration (mg kg^{-1} dry weight)	Nutrient solution concentration (mg l^{-1})[a]	Soil organic carbon content	Plant	Conc[n] in plant roots (mg kg^{-1} wet wt)	Experimental log BAF root (concentration in wet root / concentration in wet soil)		Predicted log BAF root		Reference
							a	b	a	b	
Fluoranthene	5.20	47.00		1.2%	Carrot peel	0.47	-1.94	-1.94	1.34	0.75	Wild and Jones, 1992 (as quoted in Polder, 1994)
		42.90		1.7%	Carrot peel	4.29	-0.94	-0.94	1.20	0.61	
		72.00		2.3%	Carrot peel	5.76	-1.04	-1.04	1.07	0.48	
		140.25		4.4%	Carrot peel	5.61	-1.34	-1.34	0.78	0.19	
4-Fluoro phenylurea	1.04		1[c]	2.0%	Barley	1.1[c]	0.16	0.61	0.15	0.59	Briggs *et al.,* 1982
Haloxyfop	4.63		1	2.0%	Soy bean	6.86	-0.84	-1.26	0.88	0.46	Aguero-Alvarado *et al.,* 1991 (as quoted in Polder, 1994)
			1	2.0%	Red fescue	100	0.32	-0.10	0.88	0.46	
			1	2.0%	Tall fescue	43.19	-0.04	-0.46	0.88	0.46	
Lindane	3.70	0.33		1.7%	Ryegrass	0.33	0.06	0.06	0.54	0.39	Voerman *et al.,* 1975 (as quoted in Polder, 1994)
Medium-chain chlorinated paraffins	7.00	4.90		2.0%	Carrot	0.194	-1.35	-1.35	1.90	0.79	ECB, 2006
3-Methyl phenylurea	-0.12		1[c]	2.0%	Barley	0.73[c]	0.42	0.73	0.53	0.84	Briggs *et al.,* 1982
3-(Methylthio) phenylurea	1.57		1[c]	2.0%	Barley	0.94[c]	-0.15	0.25	0.01	0.41	Briggs *et al.,* 1982

Substance	Log K_{ow}	Soil concentration (mg kg^{-1} dry weight)	Nutrient solution concentration (mg l^{-1})[a]	Soil organic carbon content	Plant	Conc^{n} in plant roots (mg kg^{-1} wet wt)	Experimental log BAF root (concentration in wet root / concentration in wet soil)		Predicted log BAF root		Reference
							a	b	a	b	
Mirex	5.28	3.50		0.5%	Garden bean	0.177	-1.24	-1.24	1.75	1.14	De la Cruz *et al.,* 1975 (as quoted in Polder, 1994)
		3.40		0.02%	Garden bean	0.252	-1.07	-1.07	3.05	2.47	
		0.80		0.5%	Garden bean	0.0735	-0.98	-0.98	1.75	1.14	
		0.80		0.02%	Garden bean	0.1035	-0.83	-0.83	3.05	2.47	
		0.30		0.5%	Garden bean	0.0315	-0.92	-0.92	1.75	1.14	
		0.31		0.02%	Garden bean	0.0345	-0.90	-0.90	3.05	2.47	
		3.50		0.5%	Soybean	0.1875	-1.22	-1.22	1.75	1.14	
		3.40		0.02%	Soybean	0.2205	-1.13	-1.13	3.05	2.47	
		0.80		0.5%	Soybean	0.0735	-0.98	-0.98	1.75	1.14	
		0.80		0.02%	Soybean	0.0735	-0.98	-0.98	3.05	2.47	
		0.30		0.5%	Soybean	0.0255	-1.02	-1.02	1.75	1.14	
		0.31		0.02%	Soybean	0.048	-0.75	-0.75	3.05	2.47	
		3.50		0.5%	Sorghum	0.1215	-1.40	-1.40	1.75	1.14	
		3.50		0.02%	Sorghum	0.2565	-1.08	-1.08	3.05	2.47	
		0.80		0.5%	Sorghum	0.066	-1.03	-1.03	1.75	1.14	
		0.80		0.02%	Sorghum	0.1005	-0.85	-0.85	3.05	2.47	
		0.30		0.5%	Sorghum	0.03	-0.94	-0.94	1.75	1.14	
		0.31		0.02%	Sorghum	0.042	-0.81	-0.81	3.05	2.47	
		3.50		0.5%	Wheat	0.1755	-1.24	-1.24	1.75	1.14	
		3.40		0.02%	Wheat	0.1995	-1.18	-1.18	3.05	2.47	
		0.80		0.5%	Wheat	0.0405	-1.24	-1.24	1.75	1.14	
		0.80		0.02%	Wheat	0.0825	-0.93	-0.93	3.05	2.47	
		0.30		0.5%	Wheat	0.0345	-0.88	-0.88	1.75	1.14	
		0.31		0.02%	Wheat	0.054	-0.70	-0.70	3.05	2.47	

Substance	Log K_{ow}	Soil concentration (mg kg^{-1} dry weight)	Nutrient solution concentration (mg l^{-1})[a]	Soil organic carbon content	Plant	Conc^{n} in plant roots (mg kg^{-1} wet wt)	Experimental log BAF root (concentration in wet root / concentration in wet soil)		Predicted log BAF root		Reference
							a	b	a	b	
Naphthalene	3.70	1.88		1.2%	Carrot peel	1.58	-0.02	-0.02	0.70	0.55	Wild and Jones, 1992 (as quoted in Polder, 1994)
		1.59		1.2%	Peeled carrot (core)	0.62	-0.35	-0.35	0.70	0.55	
		1.47		1.7%	Peeled carrot (core)	0.78	-0.22	-0.22	0.56	0.41	
		6.58		2.3%	Peeled carrot (core)	1.25	-0.67	-0.67	0.43	0.28	
		39.40		4.4%	Peeled carrot (core)	1.97	-1.25	-1.25	0.14	-0.01	
Nitrobenzene	1.85		8	2.0%	Soybean	8.8	-0.22	0.13	-0.02	0.33	McFarlane *et al.,* 1990 (as quoted in Polder, 1994)
			8	2.0%	Barley	4.56	-0.50	-0.16	-0.02	0.33	
			8	2.0%	Lettuce	7.36	-0.29	0.05	-0.02	0.33	
			8	2.0%	Russian olive	12	-0.08	0.26	-0.02	0.33	
			8	2.0%	Autumn olive	7.2	-0.30	0.04	-0.02	0.33	
			8	2.0%	Green ash	11.2	-0.11	0.23	-0.02	0.33	
			8	2.0%	Hybrid popular	7.2	-0.30	0.04	-0.02	0.33	
			8	2.0%	Honey-suckle	16	0.04	0.39	-0.02	0.33	

Substance	Log K_{ow}	Soil concentration (mg kg^{-1} dry weight)	Nutrient solution concentration (mg l^{-1})[a]	Soil organic carbon content	Plant	Conc[n] in plant roots (mg kg^{-1} wet wt)	Experimental log BAF root (concentration in wet root / concentration in wet soil)		Predicted log BAF root		Reference
							a	b	a	b	
Oxamyl	-0.47		1[c]	2.0%	Barley	0.91[c]	0.61	0.86	0.62	0.87	Briggs *et al.,* 1982
Pentachloro phenol	5.24	4.00		1.2%	Soybean	40.5	1.06	1.06	1.38	0.78	De la Cruz *et al.,* 1975 (as quoted in Polder, 1994)
		5.40		1.2%	Spinach	20.57	0.64	0.64	1.38	0.78	
Phenanthrene	4.57	16.27		1.2%	Carrot peel	1.79	-0.90	-0.90	1.07	0.66	Wild and Jones, 1992 (as quoted in Polder, 1994)
		48.67		1.7%	Carrot peel	1.46	-1.47	-1.47	0.93	0.52	
		74.25		2.3%	Carrot peel	2.97	-1.34	-1.34	0.80	0.40	
		130.00		4.4%	Carrot peel	2.6	-1.64	-1.64	0.51	0.11	
		15.00		1.2%	Peeled carrot (core)	0.3	-1.64	-1.64	1.07	0.66	
		36.00		1.7%	Peeled carrot (core)	0.72	-1.64	-1.64	0.93	0.52	
		83.00		2.3%	Peeled carrot (core)	0.83	-1.94	-1.94	0.80	0.40	
3-Phenoxy benzaldehyde O-methylcarbamoyl oxime	3.12		1[c]	2.0%	Barley	8.72[c]	0.04	0.06	0.25	0.27	Briggs *et al.,* 1982

Substance	Log K_{ow}	Soil concentration (mg kg^{-1} dry weight)	Nutrient solution concentration (mg l^{-1})[a]	Soil organic carbon content	Plant	Conc[n] in plant roots (mg kg^{-1} wet wt)	Experimental log BAF root (concentration in wet root / concentration in wet soil)		Predicted log BAF root		Reference
							a	b	a	b	
4-Phenoxy phenylurea	2.80		1[c]	2.0%	Barley	7.08[c]	0.12	0.22	0.14	0.25	Briggs *et al.,* 1982
Phenylurea	0.80		1[c]	2.0%	Barley	1.2[c]	0.30	0.74	0.23	0.67	Briggs *et al.,* 1982
Polybrominated diphenyl (mainly hexabromo diphenyl ether)	9.10	10.00		2.0%	Carrot	0.02	-2.64	-2.64	2.80	1.08	Jacobs *et al.*, 1976
		100.00		2.0%	Carrot	0.04	-3.34	-3.34	2.80	1.08	
Pyrene	5.18	41.50		1.2%	Carrot peel	0.83	-1.64	-1.64	1.33	0.75	Wild and Jones, 1992 (as quoted in Polder, 1994)
		63.63		1.7%	Carrot peel	5.09	-1.04	-1.04	1.19	0.61	
		111.83		2.3%	Carrot peel	6.71	-1.17	-1.17	1.06	0.48	
		258.75		4.4%	Carrot peel	10.35	-1.34	-1.34	0.77	0.19	
Simazine	2.18		0.2	2.0%	Barley	0.908	0.24	0.51	0.00	0.27	Shone and Wood, 1974 (as quoted in Polder, 1994)
3,3',4,4'-Tetrachloroazo benzene	6.46	0.02		1.9%	Carrot peel	0.0019	-0.97	-0.97	1.69	0.73	Worobey, 1988 (as quoted in Polder, 1994)
		10.00		1.9%	Carrot peel	0.375	-1.37	-1.37	1.69	0.73	
		0.02		1.9%	Carrot root pulp	0.0011	-1.20	-1.20	1.69	0.73	
		10.00		1.9%	Carrot root pulp	0.01	-2.94	-2.94	1.69	0.73	

Substance	Log K_{ow}	Soil concentration (mg kg^{-1} dry weight)	Nutrient solution concentration (mg l^{-1})[a]	Soil organic carbon content	Plant	Conc[n] in plant roots (mg kg^{-1} wet wt)	Experimental log BAF root (concentration in wet root / concentration in wet soil)		Predicted log BAF root		Reference
							a	b	a	b	
2,3,7,8-TCDD	6.80		1.3×10^{-4}	2.0%	Soybean	0.117	0.15	-0.90	1.81	0.76	McCrady *et al.,* 1990 (as quoted in Polder, 1994)
			1.8×10^{-4}	2.0%	Maize	0.115	0.01	-1.04	1.81	0.76	

a) For these calculations the default QSAR given in the TGD was used to estimate the value of K_{oc} for the soil.

b) For these calculations the QSAR for predominantly hydrophobics given in the TGD was used to estimate the value of K_{oc} for the soil.

c) Concentrations in nutrient solution in the Briggs *et al.* (1982) study were all 1 mmol l^{-1}. The resulting root concentrations were not given. The values given here were estimated using the reported root concentration factor, assuming a nutrient solution concentration for the test substance of 1 mg l^{-1}.

d) Soil organic carbon contents were estimated from soil organic matter contents given in the paper, assuming that soil organic matter is around 58 per cent organic carbon. Where the soil organic matter content was not given, and for calculations from experiments using nutrient solutions, a standard soil organic carbon content of two per cent (the TGD default) was used in the calculations.

The experimental and predicted BAF_{root} are displayed graphically in Figure 3.3 (for experimental values obtained via exposure to nutrient solution, only values derived using the TGD default QSAR are shown). Figure3.4 shows the residual in the prediction (defined here as the experimental log BAF_{root} – predicted log BAF_{root}) against log K_{ow}. A negative residual indicates that the TGD method overpredicts BAF_{root}, whereas a positive residual indicates that the TGD method underpredicts BAF_{root}. The magnitude of the residual indicates the extent of over- or underprediction (on a log_{10} scale). For example, a residual of -1, -2 and -3 indicates that the TGD method overpredicts the actual BAF_{root} by a factor of 10, 100 or 1,000 respectively.

As can be seen from Table 3.2, the data set used for this comparison includes soils of different organic carbon contents; this may account for some of the scatter seen in the plots, and so may hide some of the trends in the data. In order to take this into account, Figure 3.5 shows the same data set normalised to a soil with a standard organic carbon content of two per cent.

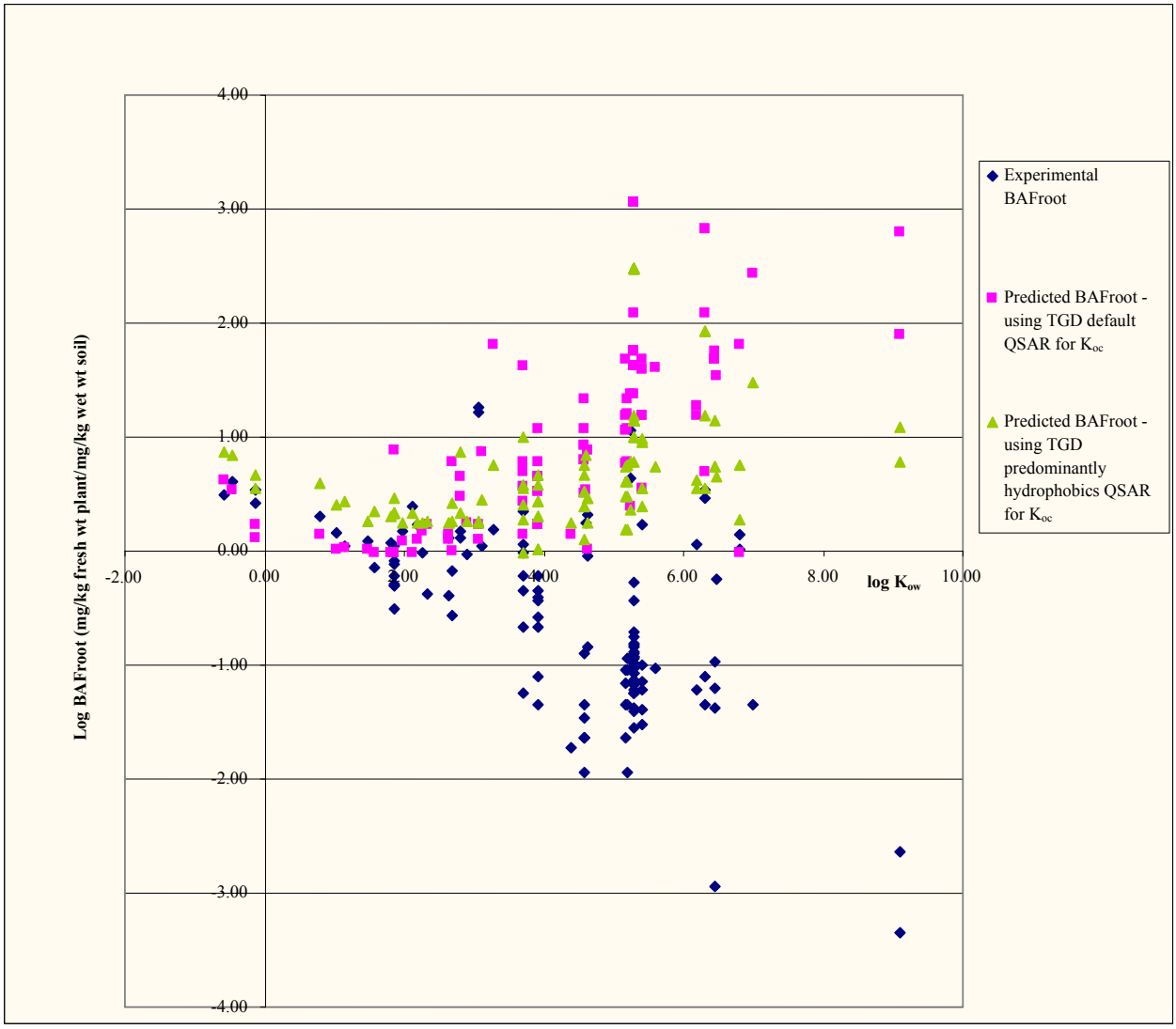

Figure 3.3 Plot of experimental and predicted BAF_{root} against log K_{ow}

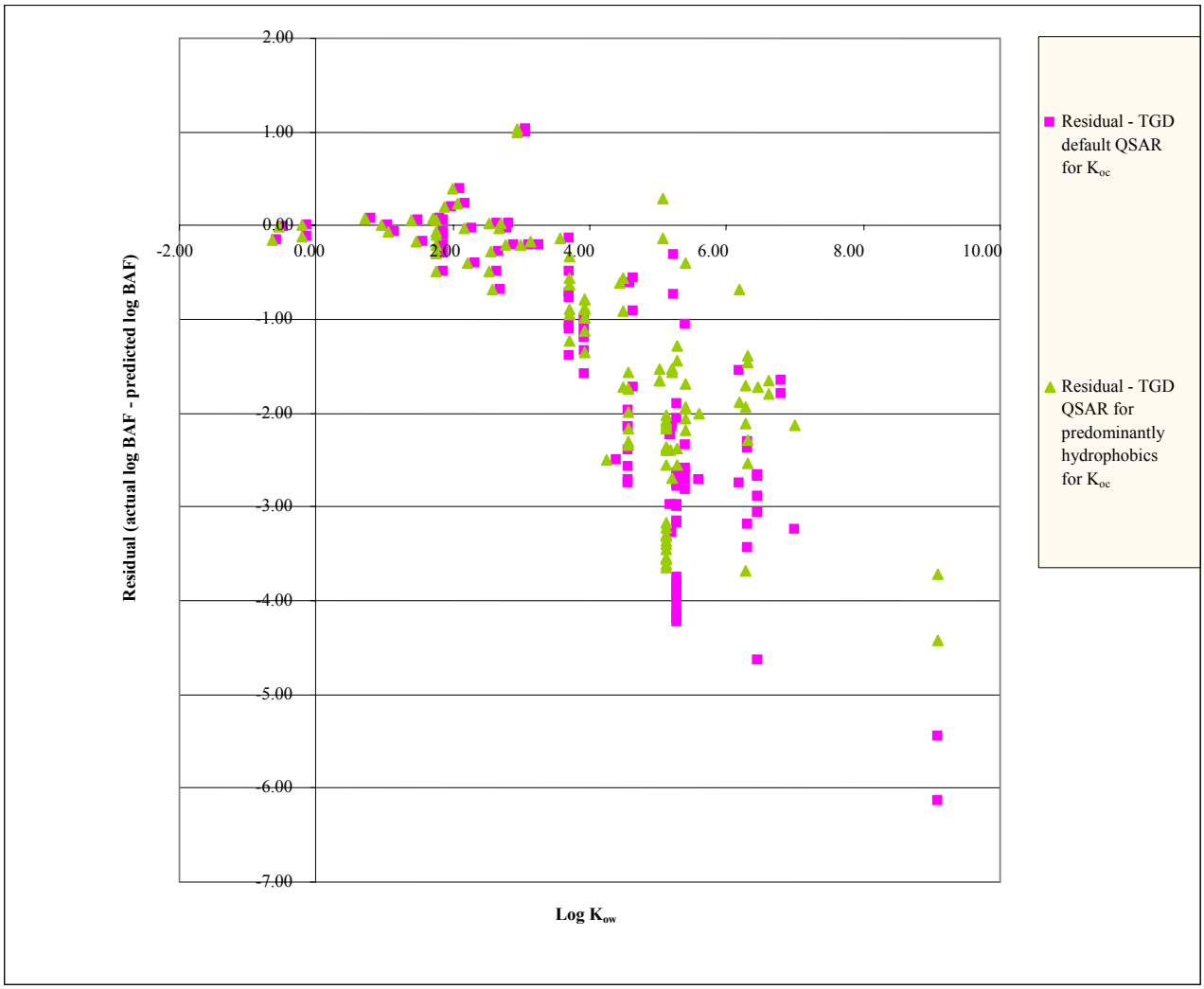

Figure 3.4 Plot of residual in the prediction (experimental log BAF – predicted log BAF)

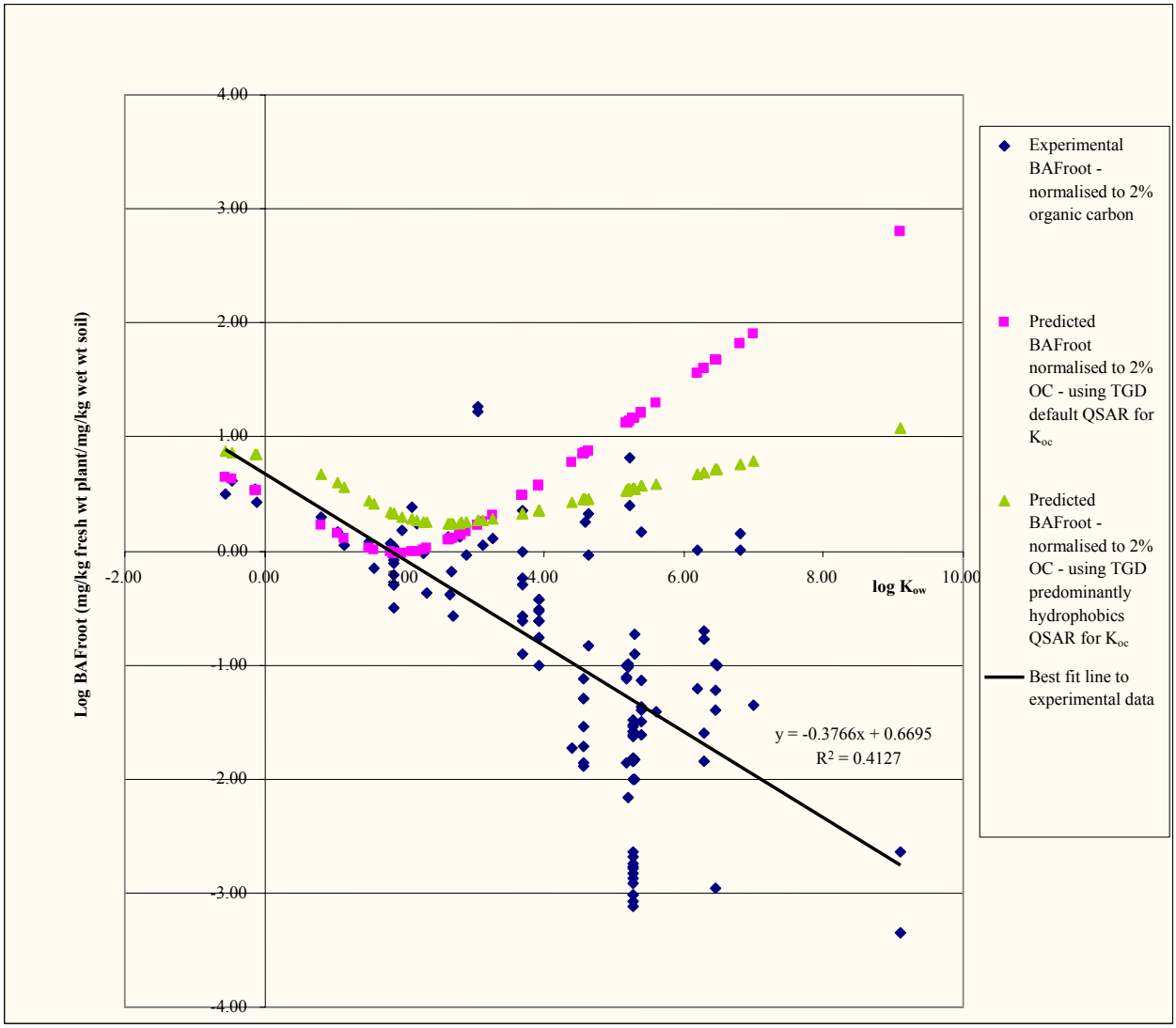

Figure 3.5 Plot of experimental and predicted BAF_{root} against log K_{ow} normalised to a standard soil organic carbon content of two per cent

As can be seen from Figure 3.3 to 3.5, the TGD method predicts well the BAF_{root} for chemicals with log K_{ow} values up to around three. For chemicals with log K_{ow} between three and four, the TGD method tends to overpredict the actual BAF_{root} (as evidenced by a negative residual), but this overprediction is generally less than a factor of 10 (one log unit in the log BAF_{root}). For chemicals with a log K_{ow} above four, overprediction in the BAF_{root} becomes progressively worse with increasing log K_{ow} and, as is evident from Figure 3.5 in particular, this overprediction results from the TGD method predicting an increasing trend in log BAF_{root} with increasing log K_{ow}, whereas the experimental data show a decreasing trend in log BAF_{root} with increasing log K_{ow}.

These results strongly suggest that the underlying assumption in the TGD method - that $K_{plant\text{-}water}$ increases with increasing log K_{ow} - is not valid at high log K_{ow} values.

From Figure 3.5 it can be seen that experimental log BAF_{root} values show an approximately linear decrease with increasing log K_{ow} over the entire data set, when the data are normalised to a standard soil organic carbon content of two per cent (although there is still a large amount of scatter in the data set). The following regression equation can be fitted to the data (for the experimental values obtained via exposure to nutrient solution, only values derived from the TGD default QSAR were used to generate this equation):

$$\log BAF_{root} = -0.38 \times \log K_{ow} + 0.67 \qquad R^2 = 0.41$$

This equation could be used to provide a better estimate of the actual BAF_{root} for substances with log K_{ow} values greater than four. However, the correlation is relatively poor, as seen by the low value of the correlation coefficient (R^2), meaning that there would still be a relatively large uncertainty in the BAF_{root} derived by this method.

Uptake into plant leaves from soil and soil pore water

The second part of the TGD method that could be tested was uptake into the above ground parts of plants (stems and leaves) from soil and soil pore water. Again, a number of data compilations were available for this purpose. The ACC-HUMAN model gives a prediction of the concentration in cattle feed resulting in uptake from soil, and so the same data set could be used to test this part of the ACC-HUMAN model.

Predictive methods for uptake into the above ground parts of plants incorporate uptake into plant roots followed by transport to the leaves; thus, the findings in Section 0 will have some implications for subsequent predictions of concentrations in the above ground parts of plants.

The data sets used for this exercise are discussed briefly below, and the data are summarised in Table 3.3.

Travis and Arms (1988) investigated the uptake of chemicals into the above ground parts of plants from soil. The study defined a bioaccumulation factor[7] for vegetation as the ratio of the concentration in above ground parts of plants (mg chemical/kg dry plant) to the concentration in soil (mg chemical/kg dry soil). The data used to derive these factors were taken from a number of sources including Beall Jr (1976), Beall Jr and Nash (1972), Beynon *et al.* (1972), Bruce *et al.* (1965), Bull and Ivie (1978), Businelli *et al.* (1975), Dejonckheere *et al.* (1975), De La Cruz and Rajanna (1975), Dorough and Pass (1972), Edwards (1983), Eshel *et al.* (1978), Helling *et al.* (1973), Iwata and Gunther (1976), Iwata *et al.* (1977), Jacobs *et al.* (1976), Jalali and Anderson (1976), Lichtenstein (1959 and 1960), Maitlen and Powell (1982), Nash (1974), Popov and Sboeva (1974), Tafuri *et al.* (1977), Viswanathan *et al.* (1978), Voerman and Besemer (1975), and Weisgerber *et al.* (1974), along with a small amount of unpublished data.

A similar exercise was also carried out by Dowdy and McKone (1997). This study used broadly similar data sources as used by Travis and Arms (1988), supplemented by data from Barrentine and Cain (1969), Beynon and Wright (1972), Brass and Ware (1960), Dorough and Randolph (1969), Isensee and Jones (1971), Khan and Marriage (1997), Lichtenstein *et al.* (1973), Reed and Priester (1969), Terriere and Ingalsbe (1953), Trapp *et al.* (1990) and Young (1969).

Predicted values for the log BAF_{plant} using both the TGD method and ACC-HUMAN method are shown in Table 3.3. Both the TGD and ACC-HUMAN method give predicted concentrations in leaves (TGD method) or cattle feed (ACC-HUMAN) on a wet weight plant basis. In order to covert the resulting concentrations to a dry weight plant basis, a water

[7] These were termed bioconcentration factors in the Travis and Arms paper but the term bioaccumulation factor is used here to be consistent with the terminology used throughout the report.

content of 65 per cent by volume (75.6 per cent by weight) was assumed (the TGD default value). For the calculations, a standard soil concentration of 1 mg kg^{-1} wet weight (~1.14 mg kg^{-1} dry weight using the default water content in the TGD) was used for the TGD method and a standard soil concentration of 1×10^{-6} g m^{-3} (~6.7×10^{-7} mg kg^{-1} dry weight) was used for the ACC-HUMAN method. For the TGD method, soil pore water concentrations were estimated using two methods, firstly based on the K_{oc} obtained using the TGD default QSAR and secondly, based on the K_{oc} obtained using the TGD QSAR for predominantly hydrophobic chemicals. A soil organic carbon content of two per cent was assumed by default for the TGD calculations.

Both the TGD and the ACC-HUMAN methods contain the transpiration stream concentration factor (TSCF) as defined by Briggs *et al.* (1982). The TGD method recommends that for substances with a log K_{ow} of greater than 4.5 (or less than -0.5), the TSCF for the substance should be limited to the value estimated for a substance with a log K_{ow} of 4.5 (or a log K_{ow} of -0.5 for substances of very low log K_{ow}), and this correction is automatically applied when using the EUSES program. Therefore, for chemicals with a log K_{ow} greater than 4.5, the TSCF is set to a constant value of 0.0378. Such a limitation on the TSCF is not applied in the ACC-HUMAN method, and this probably accounts to some extent for the differences in the predicted accumulation found using the hypothetical test set in Section 2.3.

In order to test if the TGD recommendation was appropriate, estimates using the TGD method were carried out both with and without this correction.

Table 3.3 Bioaccumulation factors for uptake from soil into above ground parts of plants from Travis and Arms (1988) and Dowdy and McKone (1997).

Chemical	Physico-chemical properties assumed		Experimental log BAF_{plant} (on a dry plant and dry soil weight basis)		Predicted log BAF_{plant} (on a dry plant and dry soil weight basis)				
	log K_{ow}	log K_{aw} (m^3 m^{-3})	Travis and Arms (1988)	Dowdy and McKone (1997)	TGD method – not restricting the TSCF		TGD method – restricting the TSCF to 0.0378 for log K_{ow}>4.5		ACC-HUMAN
					a	b	a	a	
Aldicarb	1.15	-7.21	0.85	0.26	1.59	2.03	1.59	2.03	1.88
Aldrin	6.50	-2.73	-1.67	-0.90	-5.10	-6.07	-2.45	-3.42	-6.84
Aroclor 1254	6.47	-1.92	-1.77		-5.59	-6.54	-2.99	-3.94	-7.43
Atrazine	2.65	-7.00	-2.00	0.11	0.91	1.05	0.91	1.05	1.35
Benfluralin	5.29	-1.91	-3.12		-4.32	-4.93	-3.44	-4.05	-5.42
Benomyl	3.11	-9.68	-0.47	0.25	0.56	0.57	0.56	0.57	0.88
Benzo[a]pyrene	6.13	-4.71	-1.25	-1.28	-4.07	-4.93	-2.02	-2.88	-5.33
Chlordane	6.00	-2.68	-1.81	-1.06	-4.35	-5.17	-2.49	-3.31	-5.98
Cyanazine	2.02	-9.90	-0.06	0.01	1.41	1.72	1.41	1.72	2.25
DDE	6.51	-2.75	-0.98		-5.11	-6.08	-2.44	-3.41	-6.84
DDT	6.19	-3.45	-1.80	-1.22	-4.30	-5.17	-2.15	-3.03	-5.69
Diazinon	3.31	-5.32	-0.59		-0.13	-0.17	-0.13	-0.17	-0.44
3,4-Dichloroaniline	2.69	-3.20	-0.30	0.25	-2.02	-1.89	-2.02	-1.89	-0.96
Dichlobenil	2.74	-3.36		-0.48	-1.86	-1.74	-1.86	-1.74	-1.01
2,6-Dichloro benzamide	0.77	-8.33		0.43	1.80	2.24	1.80	2.24	2.25
2,4-Dichlorophenol	3.06	-4.06		-0.33	-1.19	-1.16	-1.19	-1.16	-1.17
Dieldrin	5.40	-3.37	-1.01	-1.29	-3.12	-3.76	-2.10	-2.75	-4.46
Diflubenzuron	3.82	-6.71	-0.53	-0.40	-0.25	-0.43	-0.25	-0.43	-0.30
Endrin	5.60	-3.37	-1.82	-1.08	-3.37	-4.07	-2.09	-2.79	-4.79
Ethofumesate	3.27	-5.80	-0.32		0.16	0.13	0.16	0.13	-0.05
O-Ethyl O-*p*-nitro phenylphospho thionate	4.78	-4.72		0.45	-1.72	-2.19	-1.43	-1.90	-2.44
Fluchloralin	4.79	-3.33	-1.07		-2.57	-3.04	-2.27	-2.74	-3.59
Heptachlor	6.10	-1.90	-1.48	-1.31	-5.13	-5.98	-3.12	-3.97	-6.78

Chemical	Physico-chemical properties assumed		Experimental log BAF_{plant} (on a dry plant and dry soil weight basis)		Predicted log BAF_{plant} (on a dry plant and dry soil weight basis)				
	log K_{ow}	log K_{aw} (m^3 m^{-3})	Travis and Arms (1988)	Dowdy and McKone (1997)	TGD method – not restricting the TSCF		TGD method – restricting the TSCF to 0.0378 for log K_{ow}>4.5		ACC-HUMAN
					a	b	a	a	
Heptachlor epoxide	5.40	-3.05	-1.62		-3.35	-4.00	-2.34	-2.98	-4.68
Hexachlorobenzene	5.50	-1.14	-0.32	-0.82	-5.26	-5.93	-4.11	-4.79	-6.17
Lindane	3.70	-3.66	-0.41	-0.51 -0.75[d]	-1.71	-1.86	-1.71	-1.86	-2.11
Mirex	5.28	-1.46	-1.14	-1.12	-4.75	-5.36	-3.88	-4.50	-5.62
Pentachloroaniline	4.82	-4.45		-1.08	-1.86	-2.33	-1.53	-2.00	-2.72
Pentachloro benzene	5.18	-1.52		-5.91	-4.61	-5.19	-3.87	-4.45	-5.41
Pentachloronitro benzene	4.18	-2.72	-0.35	-0.78	-2.80	-3.09	-2.80	-3.09	-3.24
Phorate	4.70	-3.73	-1.70	0.23	-2.16	-2.60	-1.96	-2.40	-3.14
Polybrominated biphenyl[c]	9.10	-3.74	-4.00		-11.77	-13.49	-3.55	-5.27	-14.60
Simazine	2.18	-7.39	0.22	-0.004	1.26	1.53	1.26	1.53	1.89
2,7-DiCDD	5.75	-2.60		-0.85	-4.10	-4.85	-2.62	-3.36	-5.59
2,3,7,8-TCDD	6.80	-2.67	-1.87	-0.87	-5.69	-6.74	-2.52	-3.57	-7.46
Tetrachlorobenzene	4.60	-1.49		-0.22	-4.25	-4.66	-4.15	-5.56	-4.35
Trichlorobenzene	4.19	-1.09		-0.45	-4.33	-4.73	-4.33	-4.73	-3.72
Trifluralin	5.33	-2.36	-0.37		-3.91	-4.53	-2.98	-3.61	-5.16

a) Calculation using the TGD default QSAR for estimation of the K_{oc} value.
b) Calculation using the TGD QSAR for predominantly hydrophobics for estimation of the K_{oc} value.
c) Appears to be a mixture of mainly hexabromobiphenyl with smaller amounts of pentabromobiphenyl and heptabromobiphenyl.
d) This is named benzene hexachloride in the paper by Dowdy and McKone (1997).

Figure.6 shows a plot of predicted and experimental log BAF_{plant} values against log K_{ow} when the TSCF in the TGD method is not restricted at high log K_{ow}. As can be seen from the plot, both the TGD and the ACC-HUMAN methods give broadly similar predictions across the range of chemicals considered.

A plot of residuals in the prediction (experimental log BAF_{plant} – predicted log BAF_{plant}) for the ACC-HUMAN and TGD method without a restriction on the TSCF is shown in Figure3.7 for the Dowdy and McKone (1997) data set. This shows that both the TGD and ACC-HUMAN methods tend to overestimate the actual value of BAF_{plant} (as shown by a negative residual) for chemicals with a log K_{ow} up to around three, but underestimate the value of BAF_{plant} for chemicals with a log K_{ow} greater than three. Predictions appear to generally be within a factor of 10 of the actual BAF_{plant} (or one log unit for the log BAF_{plant}) over a relatively narrow log K_{ow} range of approximately 2.5 to four. A similar trend is also seen if the Travis and Arms (1988) data set is considered.

Equivalent plots showing the TGD method with the recommended restriction of the TSCF are shown in Figure3.8 (plot of predicted BAF_{plant} against log K_{ow}), Figure3.9 (residuals for the Dowdy and McKone (1997) data set) and Figure3.10 (residuals for the Travis and Arms (1988) data set). As can be seen from these plots, when the recommended restriction to the TSCF is applied, the TGD method predicts better the experimental data across the entire log K_{ow} range (up to around 9.10 has been tested here), but the predicted BAF_{plant} is generally still lower than the experimental value. The residual in the predicted log BAF is still up to four log units over the log K_{ow} range of approximately four to six (meaning that the actual BAF can be up to 10,000 times lower than predicted over this range) and the residual is only marginally lower (two to three log units) outside of this log K_{ow} range.

For chemicals with very high log K_{ow} values, both methods predict a relatively low level of uptake from soil into the above ground parts of plants. This is also borne out in the experimental data. Therefore, a large error in this prediction is not necessarily important when considering the use of the methods for setting standards, as the exposure route is not likely to be important.

There is likely to be some uncertainty associated with the experimental BAF data, as the uptake seen in any given experiment will depend on the soil properties as well as the plant species and chemical considered. More importantly, it is difficult to carry out experiments that completely rule out other possible routes of exposure. For example, although the chemical may be applied to soil, it is possible that a small amount of the chemical may volatilise from the soil during the experiment and be taken up into the leaves via the air. Thus, the results from experiments may not always represent uptake solely from soil. This is an important consideration in relation to substances with high log K_{ow} values, where the models predict a much lower BAF_{plant} than is found experimentally. As discussed in Sections 2.3 and 3.2.1, chemicals with high log K_{ow} values are predicted to show a high level of uptake into plant leaves via air, and so this may at least partly explain the discrepancy between the experimental data and the predicted uptake from soil into leaves.

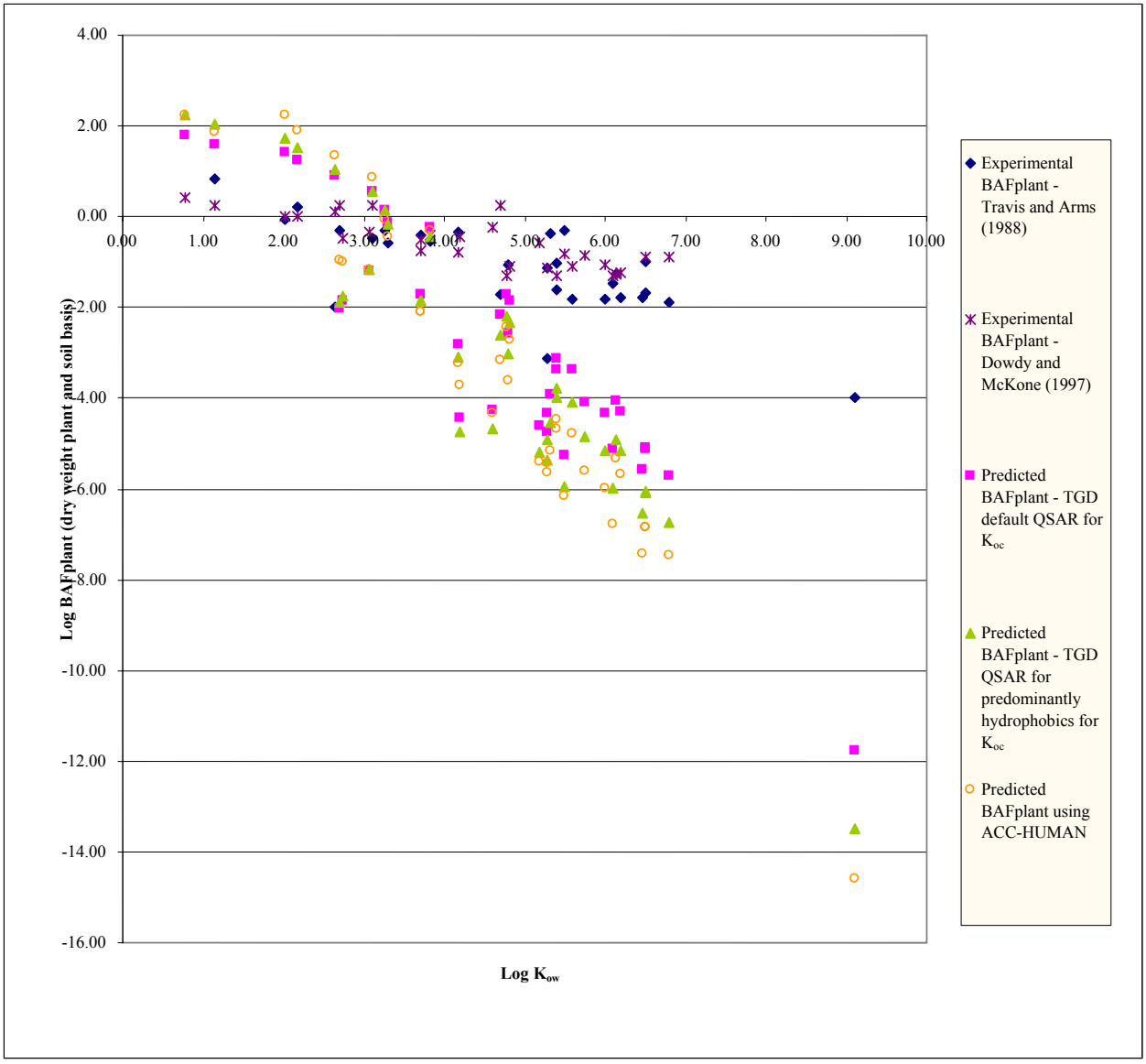

Figure 3.6 Experimental and predicted BAF_{plant} (not restricting the TSCF)

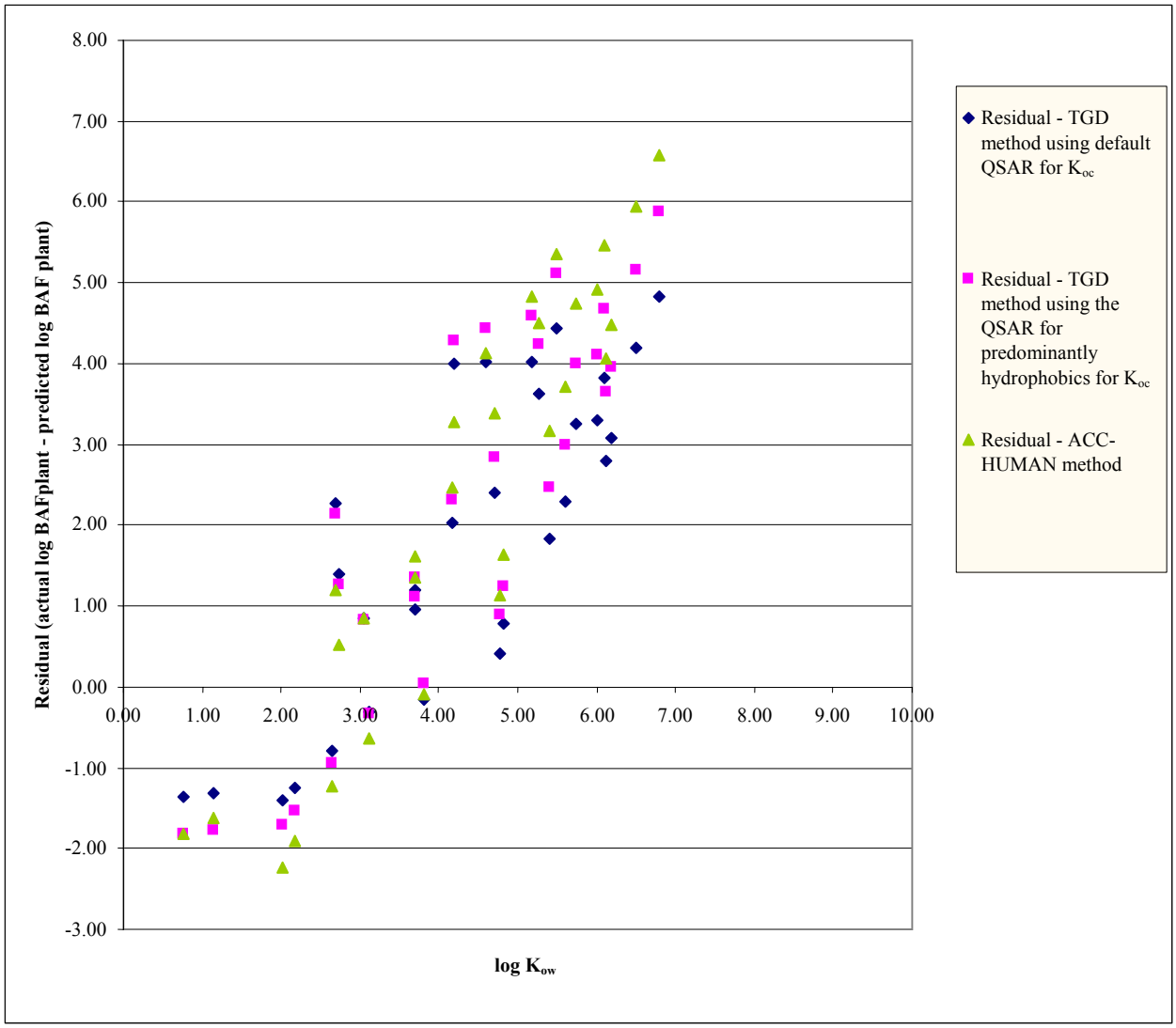

Figure 3.7 Plot of residuals against log K_{ow} for the Dowdy and McKone (1997) data set (not restricting the TSCF)

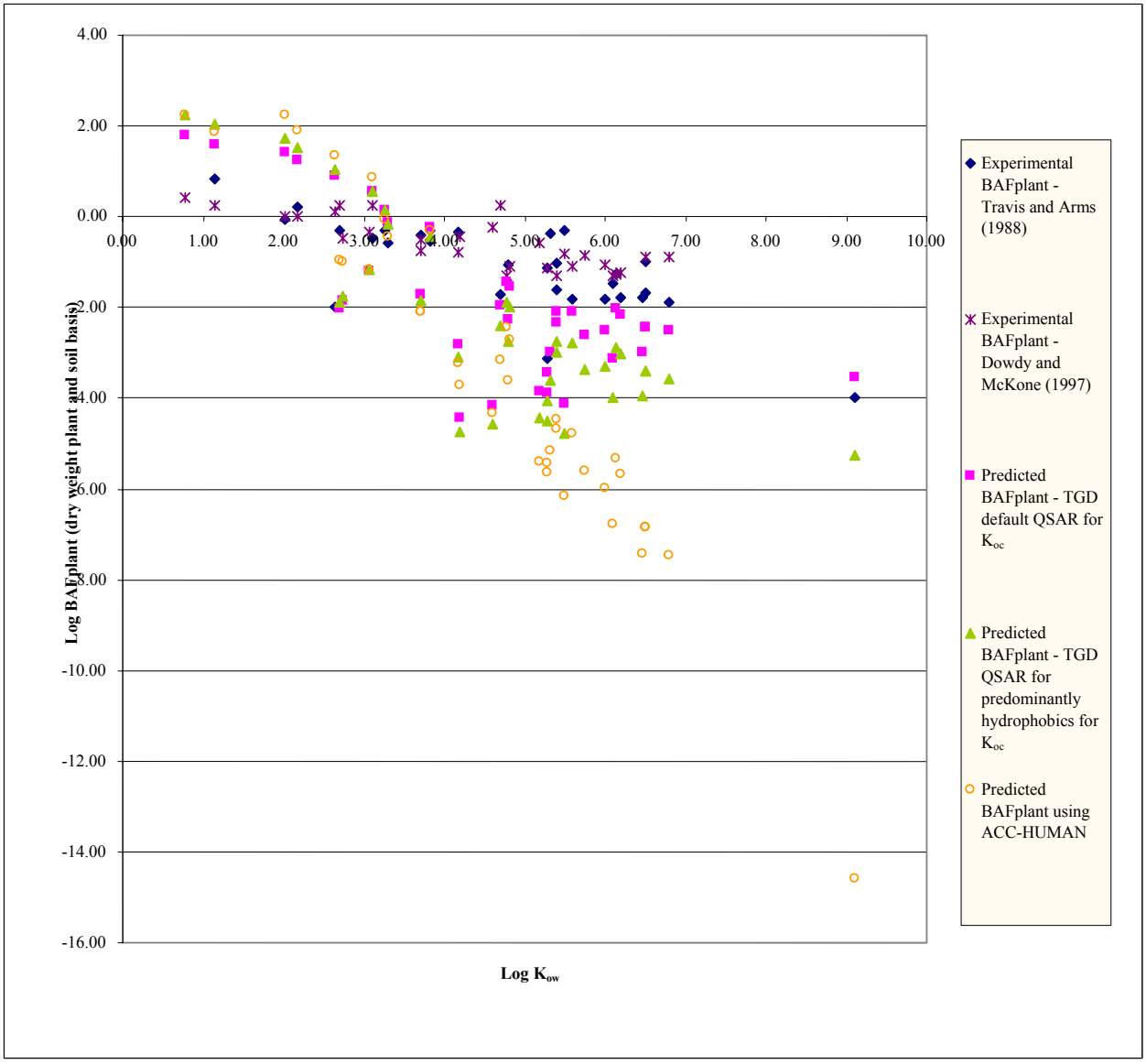

Figure 3.8 Experimental and predicted BAF_{plant} (restricting the TSCF to 0.0378 for log K_{ow} greater than 4.5 for the TGD method)

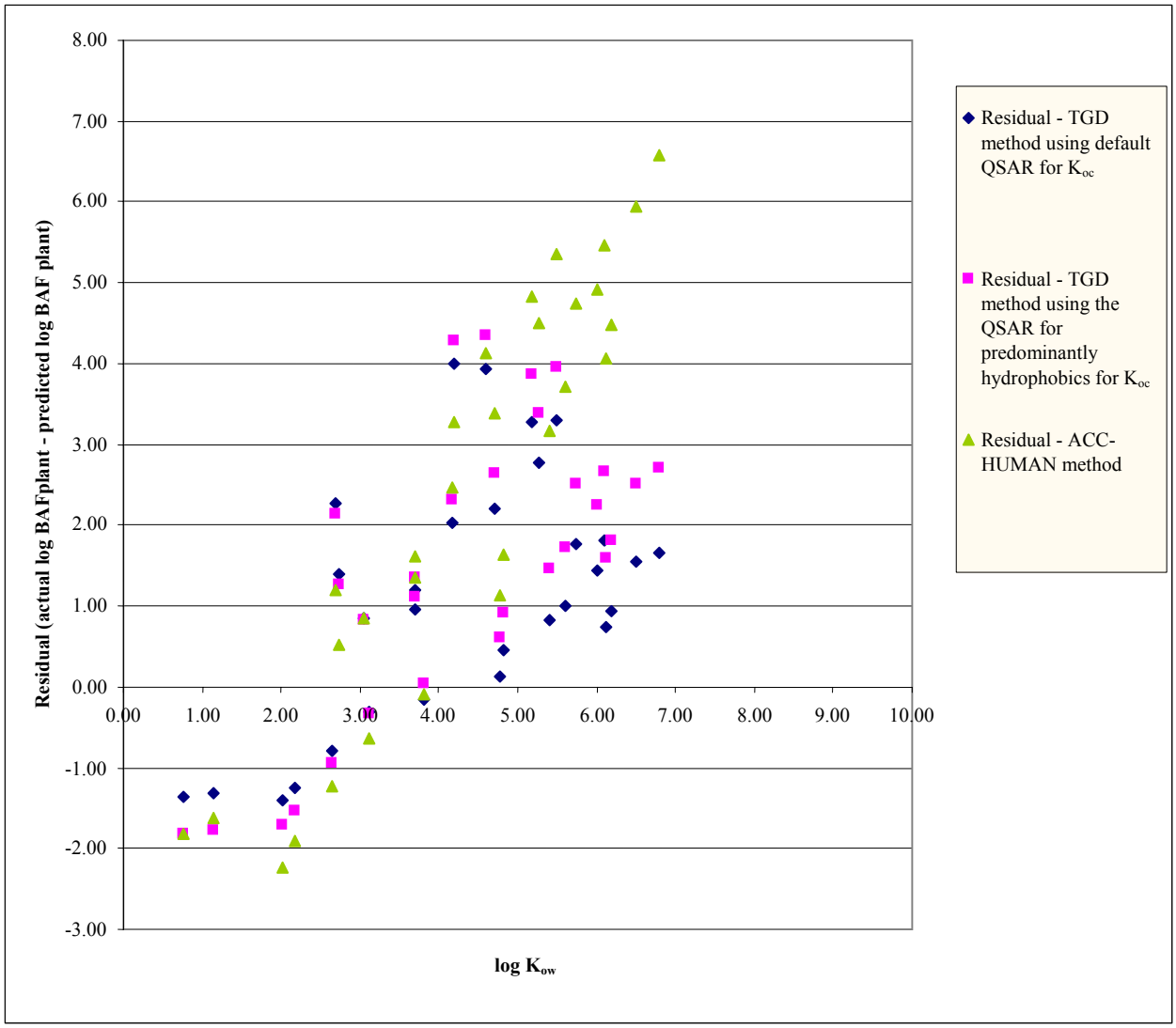

Figure 3.9 Plot of residuals against log K_{ow} for the Dowdy and McKone (1997) data set (restricting the TSCF to 0.0378 for log K_{ow} greater than 4.5 for the TGD method)

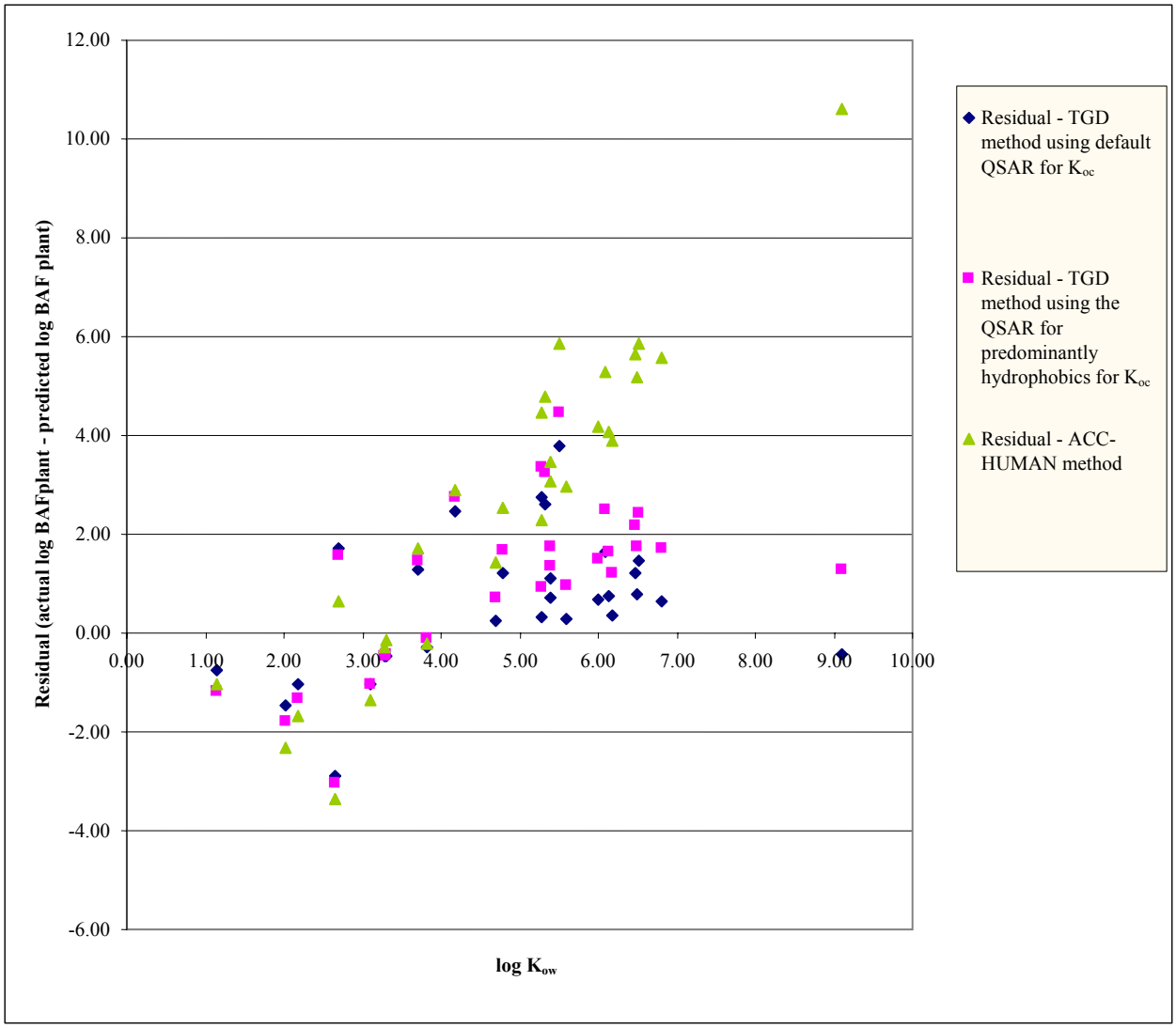

Figure 3.10 Plot of residuals against log K_{ow} for the Travis and Arms (1988) data set (restricting the TSCF to 0.0378 for log K_{ow} greater than 4.5 for the TGD method)

In addition to the data used by Travis and Arms (1988) and Dowdy and McKone (1997), a small number of other data were collected to further test the estimation methods. These data are summarised in Table 3.4. For this analysis, concentrations in soil were used as inputs to the models and concentrations in plants were estimated using the soil properties where available (or TGD default values where these were not available). As can be seen from this analysis, both the TGD and ACC-HUMAN models generate similar predicted concentrations in the plants. However, as found in the analysis of available BAF_{plant} values, the concentrations predicted are much lower than actually found for substances with relatively high log K_{ow} values (five and above in this data set). Only for one substance (alachlor with a log K_{ow} of 3.52) are the predicted concentrations close to measured. Therefore, these data confirm the above findings using the BAF_{plant} data.

Table 3.4 Summary of data used on plants exposed via soil

Substance	Physico-chemical properties		Experimental data		Predicted concentration in plant			Plant	Comment	Reference
	log K_{ow}	log K_{aw} (m^3 m^{-3})	Concentration in soil	Concentration in plant	TGD method – restricting TSCF to 0.0378 for log K_{ow} >4.5		ACC-HUMAN			
					a	b				
Alachlor	3.52	-6.45	0.52 mg kg^{-1} dry wt	0.047 mg kg^{-1} wet wt	0.13 mg kg^{-1} wet wt	0.11 mg kg^{-1} wet wt	0.18 mg kg^{-1} wet wt	Corn (stem)	Data from Pylwpiw *et al.* (1993). Levels refer to the concentration in stems. The soil organic matter content was 3-5%.	Polder *et al.* (1993)
Atrazine	2.65	-7.00	1.50 mg kg^{-1} dry wt	0.032 mg kg^{-1} wet wt	2.6 mg kg^{-1} wet wt	3.6 mg kg^{-1} wet wt	8.1 mg kg^{-1} wet wt	Corn (stem)	Data from Pylwpiw *et al.* (1993). Levels refer to the concentration in stems. The soil organic matter content was 3-5%.	Polder *et al.* (1993)
Dieldrin	5.40	-3.37	0.24 mg kg^{-1} dry wt	0.029 mg kg^{-1} dry wt	1.9×10^{-3} mg kg^{-1} dry wt	4.3×10^{-4} mg kg^{-1} dry wt	8.3×10^{-6} mg kg^{-1} dry wt	Grass (pasture)	Field study by Gilbert and Lewis (1982) determining the levels in soil and pasture following application of a commercial pesticide at the rate of 1.1 kg ha^{-1} in the top 15 cm of soil.	Cullen and Connell (1994)
			0.12 mg kg^{-1} dry wt	0.018 mg kg^{-1} dry wt	9.5×10^{-4} mg kg^{-1} dry wt	5.3×10^{-5} mg kg^{-1} dry wt	4.2×10^{-6} mg kg^{-1} dry wt			
			0.47 mg kg^{-1} dry wt	0.029 mg kg^{-1} dry wt	3.7×10^{-3} mg kg^{-1} dry wt	8.4×10^{-4} mg kg^{-1} dry wt	1.6×10^{-5} mg kg^{-1} dry wt			
			0.24 mg kg^{-1} dry wt	0.011 mg kg^{-1} dry wt	1.9×10^{-3} mg kg^{-1} dry wt	4.3×10^{-4} mg kg^{-1} dry wt	8.4×10^{-6} mg kg^{-1} dry wt			
Heptachlor	6.10	-1.19	0.35 mg kg^{-1} dry wt	0.014 mg kg^{-1} dry wt	2.6×10^{-4} mg kg^{-1} dry	3.7×10^{-5} mg kg^{-1} dry	5.7×10^{-8} mg kg^{-1} dry wt	Grass (past-	Field study by Gilbert and Lewis	Cullen and Connell (1994)

Substance	Physico-chemical properties		Experimental data		Predicted concentration in plant			Plant	Comment	Reference
	log K_{ow}	log K_{aw} (m^3 m^{-3})	Concentration in soil	Concentration in plant	TGD method – restricting TSCF to 0.0378 for log K_{ow} >4.5 a	TGD method – restricting TSCF to 0.0378 for log K_{ow} >4.5 b	ACC-HUMAN			
					wt	wt		ure)	(1982) as above.	
Metolachlor	3.13	-6.41	2.63 mg kg^{-1} dry wt	0.028 mg kg^{-1} wet wt	1.6 mg kg^{-1} wet wt	1.6 mg kg^{-1} wet wt	2.5 mg kg^{-1} wet wt	Corn (stem)	Data from Pylwpiw *et al.* (1993). Levels refer to the concentration in stems. The soil organic matter content was 3-5%.	Polder *et al.* (1994)
Pentachloro phenol	5.24		4.0 mg kg^{-1} dry wt	6.1 mg kg^{-1} wet wt	0.046 mg kg^{-1} wet wt	0.012 mg kg^{-1} wet wt	6.8×10^{-4} mg kg^{-1} wet wt	Soy-bean (shoot)	Data from Casterline *et al.* (1985). The soil organic matter content was 2%.	Polder *et al.* (1994)
			4.0 mg kg^{-1} dry wt	11.8 mg kg^{-1} wet wt	0.046 mg kg^{-1} wet wt	0.012 mg kg^{-1} wet wt	6.8×10^{-4} mg kg^{-1} wet wt	Soy-bean (stem)		
			4.0 mg kg^{-1} dry wt	5.54 mg kg^{-1} wet wt	0.046 mg kg^{-1} wet wt	0.012 mg kg^{-1} wet wt	6.8×10^{-4} mg kg^{-1} wet wt	Soy-bean (leaf)		
			4.0 mg kg^{-1} dry wt	0.75 mg kg^{-1} wet wt	0.046 mg kg^{-1} wet wt	0.012 mg kg^{-1} wet wt	6.8×10^{-4} mg kg^{-1} wet wt	Soy-bean (pod)		
			4.0 mg kg^{-1} dry wt	0.2 mg kg^{-1} wet wt	0.046 mg kg^{-1} wet wt	0.012 mg kg^{-1} wet wt	6.8×10^{-4} mg kg^{-1} wet wt	Soy-bean (seed)		
			5.4 mg kg^{-1} dry wt	9.4 mg kg^{-1} wet wt	0.062 mg kg^{-1} wet wt	0.016 mg kg^{-1} wet wt	9.2×10^{-4} mg kg^{-1} wet wt	Spin-ach (shoot)		
3,3',4,4'-Tetrachloro zobenzene	6.46		0.02 mg kg^{-1} dry wt	5×10^{-5} mg kg^{-1} wet wt	8.2×10^{-6} mg kg^{-1} wet wt	9.1×10^{-7} mg kg^{-1} wet wt	2.6×10^{-10} mg kg^{-1} wet wt	Carrot tops	Data from Worobey, 1988. The soil organic matter content was 3%.	Polder *et al.* (1994)
			10 mg kg^{-1} dry wt	0.03 mg kg^{-1} wet wt	4.3×10^{-3} mg kg^{-1} wet wt	4.5×10^{-4} mg kg^{-1} wet wt	1.3×10^{-7} mg kg^{-1} wet wt			

a) Calculation using the TGD default QSAR for estimation of the K_{oc} value.
b) Calculation using the TGD QSAR for predominantly hydrophobics for estimation of the K_{oc} value.

3.2.3 Accumulation in cattle and milk by exposure via feed

A number of data sets were available to test the methods for predicting the concentration in cattle (beef) resulting from exposure via feed.

As discussed in Section 2.1, the publication by Travis and Arms (1988) documents biotransfer factors for uptake into beef or milk from feed on a mg kg^{-1} meat or milk per mg day^{-1} intake basis. These factors can be converted into a BMF on a mg kg^{-1} meat or milk per mg kg^{-1} feed basis by multiplying by the feeding rate in kg day^{-1} (on either a kg wet weight or kg dry weight basis). This BMF is then the ratio of the concentration in the meat to the concentration in the feed of the cattle, and is in a form that can easily be estimated using both the TGD approach and ACC-HUMAN. For this analysis, the default TGD feeding rate of 67.6 kg wet weight day^{-1} was used.

The Travis and Arms (1988) data was used in the development of the TGD method and so strictly speaking cannot be used as an independent test of the method. However, given the differences in the patterns of accumulation predicted between the TGD method and ACC-HUMAN for the hypothetical test set (see Section 2.3), it is relevant to consider how both models perform against this test set here.

In addition to the Travis and Arms (1988) data set, several other data sets were also available, covering chemicals with log K_{ow} values higher than those in the Travis and Arms (1988) data set, and these are also considered here.

Huwe and Smith (2005) fed cattle a mineral supplement contaminated with chlorinated dibenzo-*p*-dioxins and chlorinated dibenzofurans, mixed into the total maintenance ration (the total maintenance ration consisted of 71 per cent forage and 29 per cent grain concentrate by wet weight) for 40 days. The daily food intake for each cow was estimated to be 39.8 kg day^{-1} on a wet weight basis or 23.7 kg day^{-1} on a dry weight basis (based on these figures, a water content of around 40 per cent can be estimated in the feed). The paper reported the concentrations of several substances in the diet (representing the concentrations in the total maintenance ration) and the steady-state concentrations in milk (the mean concentrations from two cattle, where the values obtained in each cow were similar). The fat content of the milk was around three per cent. Using these data, it was possible to estimate the BMF_{milk} directly as the concentration in milk (mg kg^{-1} either on a whole milk or fat basis)/concentration in feed (mg kg^{-1} either on a wet or dry feed basis).

Schulz *et al.* (2005) determined the levels in milk from cattle grazing on pasture with elevated levels of chlorinated dibenzo-*p*-dioxins and dibenzofurans for 10 weeks. The concentrations of 2,3,7,8-TCDD were given in both the pasture (in mg kg^{-1} dry weight) and in milk (in mg kg^{-1} lipid). The water content of the pasture was given as 12 per cent and this was used to covert the soil concentrations to a mg kg^{-1} wet weight basis. In order to covert the milk concentration to a whole milk basis, a milk fat content of three per cent was assumed as in the above study.

McLachlan *et al.* (1990) carried out a mass balance study on a cow fed for five weeks on a diet consisting of fodder beets (12 kg wet weight day^{-1}), corn silage (12.5 kg wet weight day^{-1}), grass silage (14 kg wet weight day^{-1}), hay (first cut; 1.7 kg wet weight day^{-1}), hay (second cut; 4.3 kg wet weight day^{-1}) and grain feed (8 kg wet weight day^{-1}). The data were reported in terms of the chemical fluxes (expressed as ng day^{-1}) into the cow in feed, water and air, and the chemical fluxes out of the cow (again expressed as ng day^{-1}) in faeces and milk. In order to convert these to concentrations in feed and milk for this analysis, the values for the feeding rate (total ration 52.5 kg wet weight day^{-1}), water consumption (30 l day^{-1}), respiration

rate (150 m^3 day^{-1}) and milk production rate (28 l $day^{-1)}$ found in the study were used. The fat content of the milk was five per cent. The contribution from air and water to the total intake was thought to be negligible in this study.

A further mass balance study in lactating dairy cows was carried out by Thomas *et al.* (1999). In this study, five cows were fed a diet containing the natural background of polychlorinated biphenyls for up to fifteen weeks under typical winter husbandry conditions in the United Kingdom. Measurement of feed intake, milk and milk fat output were made regularly during the study, and true steady-state concentrations were found not to be attained during the study. The feed used in the study consisted of silage (average consumption 12 kg dry weight day^{-1}) and concentrate feed (fed at 6 kg day^{-1}). The mean milk yield was 27 kg day^{-1} and the average milk fat content was four per cent. For the PCB congeners that could be detected in both feed and tissue fat, the report gave the ratio of the concentrations (concentration in fat/concentration in dry feed). These ratios are equivalent to a BMF_{meat} on a mg kg^{-1} lipid/mg kg^{-1} dry feed basis. In order to convert these into a mg kg^{-1} wet weight tissue/mg kg^{-1} wet weight feed basis, it was assumed that beef has a 25 per cent lipid content (as was assumed by Travis and Arms (1988) in their analysis) and that the wet weight feed consumption is four times the dry weight feed consumption (the default assumption in the TGD).

Thomas *et al.* (1999) also gave information on the concentrations in milk relative to feed. The data were presented as a "carry over" rate defined as the daily contaminated flux in milk (ng day^{-1})/daily contaminant flux in feed (ng day^{-1}). In order to convert these data into a BMF_{milk} on a mg kg^{-1} whole milk/mg kg^{-1} wet weight feed basis, a milk production rate of 27 kg day^{-1} was assumed and a wet weight feeding rate as above was used.

The BMFs derived from these data are summarised in Table 3.5 for meat and Table 3.6 for milk, along with the predicted BMFs using both the TGD method and ACC-HUMAN. In order to carry out the predictions, a nominal soil concentration of 1×10^{-6} g m^{-3} was used as the input to the ACC-HUMAN model. No metabolism was assumed in the simulation (a metabolism rate constant of zero was used for all chemicals). The resulting predicted concentrations in meat or milk (the model output was on a lipid weight basis; a lipid content of 25 per cent for meat or 3.7 per cent for milk (from Travis and Arms, 1988) was assumed to covert the concentrations to a whole meat or milk basis) and feed were then used to derive the predicted BMF. BMFs using the TGD method were estimated directly from the equations for the biotransfer factor, using the default feeding rate.

Plots of the experimental and predicted BMFs against log K_{ow} are shown in Figure 3.11 (meat) and Figure3.12 (milk). Plots of the residuals in the predictions are shown in Figure 173.13 and Figure 184.

Table 3.5 Summary of data used on uptake into meat via feed

Substance	Physico-chemical properties assumed		log BMF_{meat} (mg kg^{-1} wet weight meat/mg kg^{-1} wet weight feed) derived from experimental data	Predicted log BMF_{meat} (mg kg^{-1} wet weight meat/mg kg^{-1} wet weight feed)		Residual in the prediction (actual log BMF_{meat} – predicted log BMF_{meat})[b]		Reference
	log K_{ow}	log K_{aw}		TGD method	ACC-HUMAN method	TGD method	ACC-HUMAN method	
Aldrin	6.50	-2.73	0.76	0.73	1.51	0.03	-0.75	Travis and Arms, 1988
Aroclor 1254	6.47	-1.92	0.55	0.70	1.51	-0.15	-0.96	Travis and Arms, 1988
Benzoylprop-ethyl	4.57	-7.31	-2.98	-1.20	1.29	-1.78	-4.27	Travis and Arms, 1988
Chlordane	6.00	-2.68	-0.30	0.23	1.52	-0.53	-1.82	Travis and Arms, 1988
Chlorpyrifos	4.97	-3.90	-1.72	-0.80	1.53	-0.92	-3.25	Travis and Arms, 1988
Clopidol	2.90	-7.36	-2.93	-2.87	1.46	-0.06	-4.39	Travis and Arms, 1988
Coumaphos	4.13	-5.88	-3.37	-1.64	1.59	-1.73	-4.96	Travis and Arms, 1988
Cyhexatin	5.39	-5.25	-2.61	-0.38	1.53	-2.23	-4.14	Travis and Arms, 1988
2,4-Dichloro phenoxyacetic acid	2.81	-5.82	-3.49	-2.96	1.44	-0.53	-4.93	Travis and Arms, 1988
DDD	6.02	-3.55	-0.07	0.25	1.52	-0.32	-1.59	Travis and Arms, 1988
DDE	6.51	-2.75	0.52	0.74	1.50	-0.22	-0.98	Travis and Arms, 1988
DDT	6.19	-3.45	0.28	0.42	1.52	-0.14	-1.24	Travis and Arms, 1988
Dicamba	3.01	-7.03	-2.75	-2.76	1.47	0.01	-4.22	Travis and Arms, 1988
3,6-Dichloropicolinic acid	1.75	-6.89	-3.67	-4.02	1.12	0.35	-4.79	Travis and Arms, 1988
Dieldrin	5.40	-3.37	-0.27	-0.37	1.52	0.10	-1.80	Travis and Arms, 1988
Endosulfan	3.83	-2.56	-1.83	-1.94	1.40	0.11	-3.23	Travis and Arms, 1988
Endrin	5.60	-3.37	-0.09	-0.17	1.52	0.08	-1.61	Travis and Arms, 1988
Famphur	2.28	-6.34	-2.28	-3.49	1.28	1.21	-3.56	Travis and Arms, 1988
Fenoprop	3.86	-5.82	-2.72	-1.91	1.52	-0.81	-4.24	Travis and Arms, 1988
Fenthion	3.16	-4.20	-2.67	-2.61	1.48	-0.06	-4.15	Travis and Arms, 1988
Flamprop-isopropyl	4.41	-5.96	-2.37	-1.36	1.52	-1.01	-3.89	Travis and Arms, 1988
Heptachlor	6.10	-1.90	0.02	0.33	1.52	-0.31	-1.50	Travis and Arms, 1988
Heptachlor epoxide	5.40	-3.05	0.73	-0.37	1.52	1.10	-0.79	Travis and Arms, 1988
Hexachlorobenzene	5.50	-1.14	0.48	-0.27	1.45	0.75	-0.97	Travis and Arms, 1988
Kerb	3.18	-6.38	-2.86	-2.59	1.49	-0.27	-4.35	Travis and Arms, 1988
Lindane	3.70	-3.66	0.05	-2.07	1.50	2.12	-1.45	Travis and Arms, 1988
Malathion	2.89	-6.68	-2.91	-2.88	1.46	-0.03	-4.37	Travis and Arms, 1988
Mirex	5.28	-1.46	0.58	-0.49	1.47	1.07	-0.89	Travis and Arms, 1988

Substance	Physico-chemical properties assumed		log BMF_{meat} (mg kg^{-1} wet weight meat/mg kg^{-1} wet weight feed) derived from experimental data	Predicted log BMF_{meat} (mg kg^{-1} wet weight meat/mg kg^{-1} wet weight feed)		Residual in the prediction (actual log BMF_{meat} – predicted log BMF_{meat})[b]		Reference
	log K_{ow}	log K_{aw}		TGD method	ACC-HUMAN method	TGD method	ACC-HUMAN method	
Oxadiazon	4.09	-5.51	-1.40	-1.68	1.53	0.28	-2.93	Travis and Arms, 1988
PCB 4	4.97	-2.01	0.49	-0.80	1.50	1.29	-1.01	Thomas *et al*., 1999
PCB 18	5.60	-1.97	-0.15	-0.17	1.52	0.02	-1.67	Thomas *et al*., 1999
PCB 28	5.80	-2.07	-0.30	0.03	1.52	-0.33	-1.82	Thomas *et al*., 1999
PCB 31	5.67	-2.09	-0.05	-0.10	1.52	0.05	-1.57	Thomas *et al*., 1999
PCB 33	5.60	-2.16	-0.40	-0.17	1.52	-0.23	-1.92	Thomas *et al*., 1999
PCB 37	5.90	-2.37	-0.10	0.13	1.52	-0.23	-1.62	Thomas *et al*., 1999
PCB 44	6.00	-2.22	-0.40	0.23	1.52	-0.63	-1.92	Thomas *et al*., 1999
PCB 47	5.90	-2.09	0.53	0.13	1.52	0.40	-0.99	Thomas *et al*., 1999
PCB 49	6.10	-2.05	0.00	0.33	1.52	-0.33	-1.52	Thomas *et al*., 1999
PCB 52	6.10	-2.07	-0.40	0.33	1.52	-0.73	-1.91	Thomas *et al*., 1999
PCB 60	5.90	-2.02	-0.15	0.13	1.52	-0.28	-1.67	Thomas *et al*., 1999
PCB 66	5.80	-2.29	0.40	0.03	1.52	0.37	-1.12	Thomas *et al*., 1999
PCB 74	6.20	-2.37	0.76	0.43	1.52	0.33	-0.75	Thomas *et al*., 1999
PCB 82	6.20	-2.09	0.85	0.43	1.51	0.42	-0.66	Thomas *et al*., 1999
PCB 87	6.50	-2.50	-0.22	0.73	1.51	-0.95	-1.73	Thomas *et al*., 1999
PCB 101	6.40	-2.41	-0.22	0.63	1.51	-0.85	-1.73	Thomas *et al*., 1999
PCB 105	6.00	-1.92	0.99	0.23	1.52	0.76	-0.53	Thomas *et al*., 1999
PCB 110	6.50	-2.09	-0.40	0.73	1.50	-1.13	-1.90	Thomas *et al*., 1999
PCB 114	6.95	-2.09	1.18	1.18	1.47	0.00	-0.29	Thomas *et al*., 1999
PCB 118	6.40	-1.91	1.08	0.63	1.51	0.45	-0.43	Thomas *et al*., 1999
PCB 123	6.93	-2.09	0.45	1.16	1.47	-0.71	-1.02	Thomas *et al*., 1999
PCB 128	6.74	-3.25	1.08	0.97	1.49	0.11	-0.41	Thomas *et al*., 1999
PCB 138	6.70	-3.05	1.04	0.93	1.50	0.11	-0.45	Thomas *et al*., 1999
PCB 141	7.33	-3.01	0.80	1.56	1.40	-0.76	-0.60	Thomas *et al*., 1999
PCB 149	7.21	-1.23	-0.30	1.44	1.43	-1.74	-1.73	Thomas *et al*., 1999
PCB 151	7.16	-2.60	-0.10	1.39	1.44	-1.49	-1.54	Thomas *et al*., 1999
PCB 153	6.90	-3.01	1.11	1.13	1.47	-0.02	-0.36	Thomas *et al*., 1999
PCB 156	7.60	-2.21	1.20	1.83	1.32	-0.63	-0.11	Thomas *et al*., 1999
PCB 157	7.44	-2.16	0.90	1.67	1.37	-0.77	-0.47	Thomas *et al*., 1999
PCB 167	7.68	-2.16	1.28	1.91	1.28	-0.63	-0.01	Thomas *et al*., 1999
PCB 170	7.08	-3.41	1.26	1.31	1.45	-0.05	-0.20	Thomas *et al*., 1999

Substance	Physico-chemical properties assumed		log BMF_{meat} (mg kg^{-1} wet weight meat/mg kg^{-1} wet weight feed) derived from experimental data	Predicted log BMF_{meat} (mg kg^{-1} wet weight meat/mg kg^{-1} wet weight feed)		Residual in the prediction (actual log BMF_{meat} – predicted log BMF_{meat})[b]		Reference
	log K_{ow}	log K_{aw}		TGD method	ACC-HUMAN method	TGD method	ACC-HUMAN method	
PCB 180	7.20	-3.37	1.30	1.43	1.43	-0.13	-0.13	Thomas *et al*., 1999
PCB 183	7.00	-2.23	1.28	1.23	1.46	0.05	-0.19	Thomas *et al*., 1999
PCB 187	7.19	-2.23	0.38	1.42	1.43	-1.04	-1.05	Thomas *et al*., 1999
PCB 189	8.00	-2.23	1.04	2.23	1.12	-1.19	-0.08	Thomas *et al*., 1999
PCB 191	7.93	-2.23	0.92	2.16	1.16	-1.24	-0.24	Thomas *et al*., 1999
PCB 193	7.92	-2.23	0.96	2.15	1.17	-1.19	-0.21	Thomas *et al*., 1999
PCB 194	7.40	-3.37	1.23	1.63	1.38	-0.40	-0.15	Thomas *et al*., 1999
PCB 202	7.73	-3.11	0.40	1.96	1.26	-1.56	-0.86	Thomas *et al*., 1999
Phosphamidon	1.34	-6.67	-2.98	-4.43	1.12	1.45	-4.10	Travis and Arms, 1988
Ronnel	4.88	-2.86	-1.33	-0.89	1.52	-0.44	-2.85	Travis and Arms, 1988
2,3,7,8-TCDD[a]	6.80	-2.67	0.57	1.03	1.49	-0.46	-0.92	Travis and Arms, 1988
2,4,5-Trichloro phenoxyacetic acid (2,4,5-T)	3.36	-5.91	-2.99	-2.41	1.50	-0.58	-4.49	Travis and Arms, 1988
Toxaphene	5.50	-3.59	-0.96	-0.27	1.52	-0.69	-2.48	Travis and Arms, 1988
Trichlopyr	2.09	-7.38	-4.02	-3.68	1.18	-0.34	-5.20	Travis and Arms, 1988
3,5,6-Trichloro pyridinol	2.27	-3.85	-2.54	-3.50	1.14	0.96	-3.68	Travis and Arms, 1988

a) In Travis and Arms (1988), this chemical is given as TCDD. The physico-chemical properties for the 2,3,7,8-isomer were assumed here.

b) Some of the calculations were done by spreadsheet using full precision and so the reported residual may not match precisely the individual log BMF values owing to rounding.

Table 3.6 Summary of data used uptake into milk via feed

Substance	Physico-chemical properties assumed		log BMF_{milk} (mg kg^{-1} wet weight milk/mg kg^{-1} wet weight feed) derived from experimental data	Predicted log BMF_{milk} (mg kg^{-1} wet weight milk/mg kg^{-1} wet weight feed)		Residual in the prediction (actual log BMF_{milk} – predicted log BMF_{milk})[b]		Reference
	log K_{ow}	log K_{aw}		TGD method	ACC-HUMAN method	TGD method	ACC-HUMAN method	
Aldrin	6.50	-2.73	0.21	0.23	0.27	-0.02	-0.06	Travis and Arms, 1988
Arochlor 1254	6.47	-1.92	-0.12	0.20	0.28	-0.32	-0.40	Travis and Arms, 1988
Benzoylprop-ethyl	4.57	-7.31	-2.89	-1.70	0.30	-1.19	-3.19	Travis and Arms, 1988
Chlordane	6.00	-2.68	-1.60	-0.27	0.29	-1.33	-1.89	Travis and Arms, 1988
Chloropropylate	4.49	-6.46	-1.82	-1.78	0.30	-0.04	-2.12	Travis and Arms, 1988
Chlorpyrifos	4.97	-3.90	-2.90	-1.30	0.30	-1.60	-3.20	Travis and Arms, 1988
2,4-Dichlorophenoxyacetic acid (2,4-D)	2.81	-5.82	-3.29	-3.46	0.25	0.17	-3.54	Travis and Arms, 1988
DDD	6.02	-3.55	-0.69	-0.25	0.29	-0.44	-0.98	Travis and Arms, 1988
DDE	6.51	-2.75	-0.19	0.24	0.27	-0.43	-0.46	Travis and Arms, 1988
DDT	6.19	-3.45	-0.79	-0.08	0.29	-0.71	-1.08	Travis and Arms, 1988
Dicamba	3.01	-7.03	-2.77	-3.26	0.27	0.49	-3.04	Travis and Arms, 1988
Dieldrin	5.40	-3.37	-0.14	-0.87	0.30	0.73	-0.44	Travis and Arms, 1988
Endrin	5.60	-3.37	-0.93	-0.67	0.30	-0.26	-1.23	Travis and Arms, 1988
Fenthion	3.16	-4.20	-3.77	-3.11	0.28	-0.66	-4.05	Travis and Arms, 1988
Fenvalerate	6.20	-5.83	-1.26	-0.07	0.29	-1.19	-1.55	Travis and Arms, 1988
Flamprop-isopropyl	4.41	-5.96	-2.59	-1.86	0.30	-0.73	-2.89	Travis and Arms, 1988
Heptachlor	6.10	-1.90	-0.66	-0.17	0.29	-0.49	-0.95	Travis and Arms, 1988
Heptachlor epoxide	5.40	-3.05	0.38	-0.87	0.30	1.25	0.08	Travis and Arms, 1988
1,2,3,4,6,7,8-Heptachloro dibenzo-*p*-dioxin	8.20	-2.13	-1.53	1.93	-0.34	-3.46	-1.20	Huwe and Smith, 2005
			-1.27	1.93	-0.34	-3.20	-0.93	McLachlan *et al.*, 1990
1,2,3,4,6,7,9-Heptachloro dibenzo-*p*-dioxin	8.85	-0.86	-1.53	2.58	-0.90	-4.11	-0.63	McLachlan *et al.*, 1990
1,2,3,4,6,7,8-Heptachloro dibenzofuran	7.92	-1.89	-1.56	1.65	-0.14	-3.21	-1.42	Huwe and Smith, 2005
			-1.20	1.65	-0.14	-2.85	-1.06	McLachlan *et al.*, 1990
1,2,3,4,7,8,9-Heptachloro dibenzofuran	7.92	-1.89	-1.46	1.65	-0.14	-3.11	-1.32	Huwe and Smith, 2005
			-0.82	1.65	-0.14	-2.47	-0.68	McLachlan *et al.*, 1990
Hexachlorobenzene	5.50	-1.14	-0.24	-0.77	0.27	0.53	-0.51	Travis and Arms, 1988

Substance	Physico-chemical properties assumed		log BMF_{milk} (mg kg^{-1} wet weight milk/mg kg^{-1} wet weight feed) derived from experimental data	Predicted log BMF_{milk} (mg kg^{-1} wet weight milk/mg kg^{-1} wet weight feed)		Residual in the prediction (actual log BMF_{milk} – predicted log BMF_{milk})[b]		Reference
	log K_{ow}	log K_{aw}		TGD method	ACC-HUMAN method	TGD method	ACC-HUMAN method	
1,2,3,4,7,8-Hexachloro dibenzo-*p*-dioxin	7.80	-3.77	-0.91	1.53	-0.07	-2.44	-0.84	Huwe and Smith, 2005
			-0.52	1.53	-0.07	-2.05	-0.46	McLachlan *et al.*, 1990
1,2,3,6,7,8-Hexachloro dibenzo-*p*-dioxin	7.98	-2.44	-0.79	1.71	-0.18	-2.50	-0.62	Huwe and Smith, 2005
			-0.58	1.71	-0.18	-2.29	-0.40	McLachlan *et al.*, 1990
1,2,3,7,8,9-Hexachloro dibenzo-*p*-dioxin	8.21	-2.44	-1.00	1.94	-0.35	-2.94	-0.66	Huwe and Smith, 2005
			-0.47	1.94	-0.35	-2.41	-0.12	McLachlan *et al.*, 1990
1,2,3,4,7,8-Hexachloro dibenzofuran	7.92	-1.40	-0.89	1.65	-0.14	-2.54	-0.75	Huwe and Smith, 2005
			-0.46	1.65	-0.14	-2.11	-0.32	McLachlan *et al.*, 1990
1,2,3,6,7,8-Hexachloro dibenzofuran	7.92	-1.40	-0.90	1.65	-0.14	-2.55	-0.76	Huwe and Smith, 2005
			-0.50	1.65	-0.14	-2.15	-0.36	McLachlan *et al.*, 1990
2,3,4,6,7,8-Hexachloro dibenzofuran	7.92	-1.40	-0.98	1.65	-0.14	-2.63	-0.84	Huwe and Smith, 2005
			-0.56	1.65	-0.14	-2.21	-0.42	McLachlan *et al.*, 1990
Lindane	3.70	-3.66	-0.77	-2.57	0.29	1.80	-1.06	Travis and Arms, 1988
Methoxychlor	4.40	-5.06	-2.00	-1.87	0.30	-0.13	-2.30	Travis and Arms, 1988
Mirex	5.28	-1.46	-0.19	-0.99	0.28	0.80	-0.47	Travis and Arms, 1988
Naphthalene	3.70	-1.73	-1.87	-2.57	-0.05	0.70	-1.82	Travis and Arms, 1988
Naphthol	2.84	-5.61	-2.09	-3.43	0.25	1.34	-2.34	Travis and Arms, 1988
Octachlorodibenzo-*p*-dioxin	8.20	-3.54	-2.41	1.93	-0.34	-4.34	-2.07	Huwe and Smith, 2005
			-1.10	1.93	-0.34	-3.03	-0.77	McLachlan *et al.*, 1990
Octachlorodibenzofuran	8.60	-2.41	-2.55	2.33	-0.67	-4.88	-1.87	Huwe and Smith, 2005
			-1.53	2.33	-0.67	-3.86	-0.85	McLachlan *et al.*, 1990
Oxadiazon	4.09	-5.51	-1.89	-2.18	0.31	0.29	-2.20	Travis and Arms, 1988
PCB 18	5.60	-1.97	-1.12	-0.67	0.30	-0.45	-1.42	Thomas et al, 1999
PCB 28	5.80	-2.07	-1.00	-0.47	0.30	-0.53	-1.30	Thomas et al, 1999
PCB 31	5.67	-2.09	-0.90	-0.60	0.30	-0.30	-1.20	Thomas et al, 1999
PCB 33	5.60	-2.16	-1.12	-0.67	0.30	-0.45	-1.42	Thomas et al, 1999
PCB 37	5.90	-2.37	-0.82	-0.37	0.30	-0.45	-1.12	Thomas et al, 1999
PCB 47	5.90	-2.09	-0.20	-0.37	0.29	0.17	-0.50	Thomas et al, 1999
PCB 66	5.80	-2.29	-0.35	-0.47	0.30	0.12	-0.64	Thomas et al, 1999
PCB 74	6.20	-2.37	0.05	-0.07	0.29	0.12	-0.24	Thomas et al, 1999
PCB 101	6.40	-2.41	-0.90	0.13	0.28	-1.03	-1.18	Thomas et al, 1999
PCB 110	6.50	-2.09	-1.30	0.23	0.27	-1.53	-1.57	Thomas et al, 1999

Substance	Physico-chemical properties assumed		log BMF_{milk} (mg kg^{-1} wet weight milk/mg kg^{-1} wet weight feed) derived from experimental data	Predicted log BMF_{milk} (mg kg^{-1} wet weight milk/mg kg^{-1} wet weight feed)		Residual in the prediction (actual log BMF_{milk} – predicted log BMF_{milk})[b]		Reference
	log K_{ow}	log K_{aw}		TGD method	ACC-HUMAN method	TGD method	ACC-HUMAN method	
PCB 118	6.40	-1.91	0.44	0.13	0.28	0.31	0.16	Thomas et al, 1999
PCB 126	6.95	-2.36	-0.83	0.68	0.23	-1.51	-1.06	Huwe and Smith, 2005
PCB 128	6.74	-3.25	0.21	0.47	0.26	-0.26	-0.04	Thomas et al, 1999
PCB 138	6.70	-3.05	0.27	0.43	0.26	-0.16	0.01	Thomas et al, 1999
PCB 141	7.33	-3.01	-0.82	1.06	0.14	-1.88	-0.96	Thomas et al, 1999
PCB 149	7.21	-1.23	-0.90	0.94	0.17	-1.84	-1.08	Thomas et al, 1999
PCB 153	6.90	-3.01	0.32	0.63	0.23	-0.31	0.09	Thomas et al, 1999
PCB 156	7.60	-2.21	0.28	1.33	0.04	-1.05	0.24	Thomas et al, 1999
PCB 167	7.68	-2.16	0.36	1.41	0.00	-1.05	0.36	Thomas et al, 1999
PCB 169	7.50	-2.33	-0.65	1.23	0.08	-1.88	-0.73	Huwe and Smith, 2005
PCB 170	7.08	-3.41	0.21	0.81	0.20	-0.60	0.01	Thomas et al, 1999
PCB 180	7.20	-3.37	0.22	0.93	0.18	-0.71	0.05	Thomas et al, 1999
PCB 183	7.00	-2.23	0.21	0.73	0.22	-0.52	-0.01	Thomas et al, 1999
PCB 187	7.19	-2.23	-0.65	0.92	0.18	-1.57	-0.83	Thomas et al, 1999
1,2,3,7,8-Pentachloro dibenzo-*p*-dioxin	6.64	-3.02	-0.83	0.37	0.26	-1.20	-1.09	Huwe and Smith, 2005
			-0.47	0.37	0.26	-0.84	-0.73	McLachlan *et al.*, 1990
1,2,3,7,8-Pentachloro dibenzofuran	6.92	-2.12	-1.87	0.65	0.23	-2.52	-2.10	Huwe and Smith, 2005
			-0.95	0.65	0.23	-1.60	-1.18	McLachlan *et al.*, 1990
2,3,4,7,8-Pentachloro dibenzofuran	6.92	-2.12	-0.85	0.65	0.23	-1.50	-1.08	Huwe and Smith, 2005
			-0.33	0.65	0.23	-0.98	-0.57	McLachlan *et al.*, 1990
2,3,7,8-Tetrachloro dibenzo-*p*-dioxin[a]	6.80	-2.67	-1.34	0.53	0.25	-1.87	-1.58	Schulz *et al.*, 2005
			-0.19	0.53	0.25	-0.72	-0.44	McLachlan *et al.*, 1990
			-0.16	0.53	0.25	-0.69	-0.41	Travis and Arms, 1988
2,3,7,8-Tetrachloro dibenzofuran	6.53	-1.95	-0.85	0.26	0.27	-1.11	-1.12	McLachlan *et al.*, 1990
2,4,5-Trichlorophenoxy acetic acid (2,4,5-T)	3.36	-5.91	-2.72	-2.91	0.29	0.19	-3.01	Travis and Arms, 1988
Toxaphene	5.50	-3.59	-1.37	-0.77	0.30	-0.60	-1.67	Travis and Arms, 1988

a) In Travis and Arms (1988), this chemical is given as TCDD. The physico-chemical properties for the 2,3,7,8-isomer were assumed here.
b) Some of the calculations were done by spreadsheet using full precision and so the reported residual may not match precisely the individual log BMF values owing to rounding.

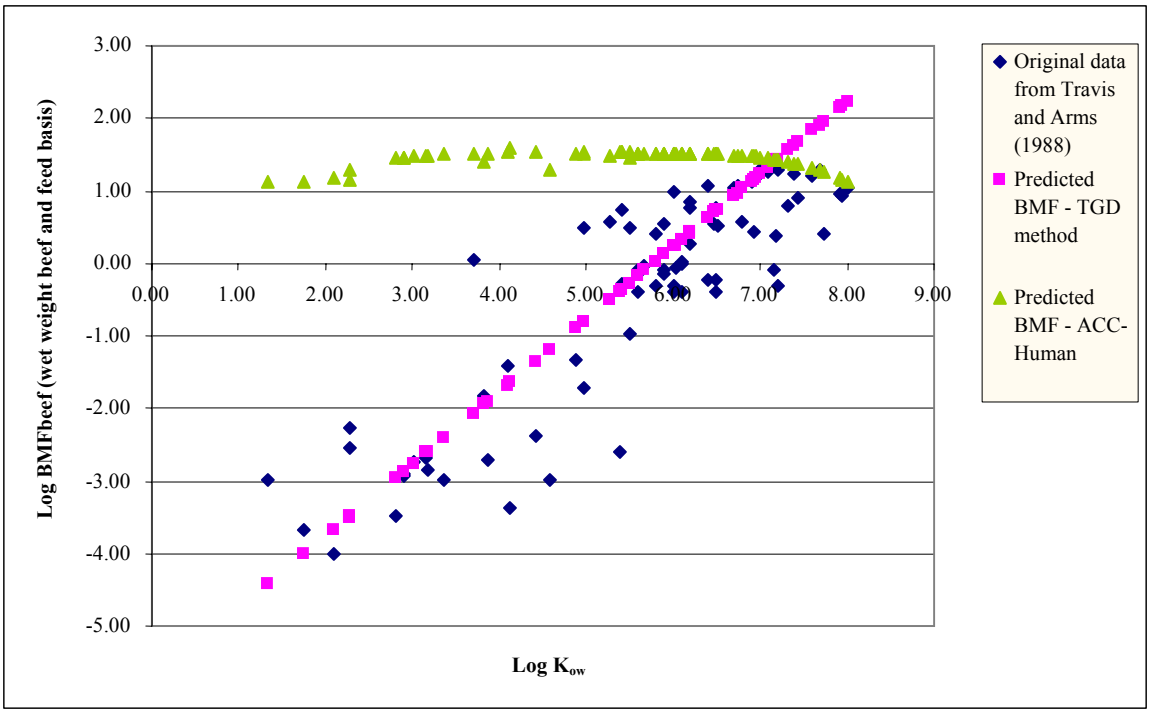

Figure 3.11 Experimental and predicted BMF_{meat}

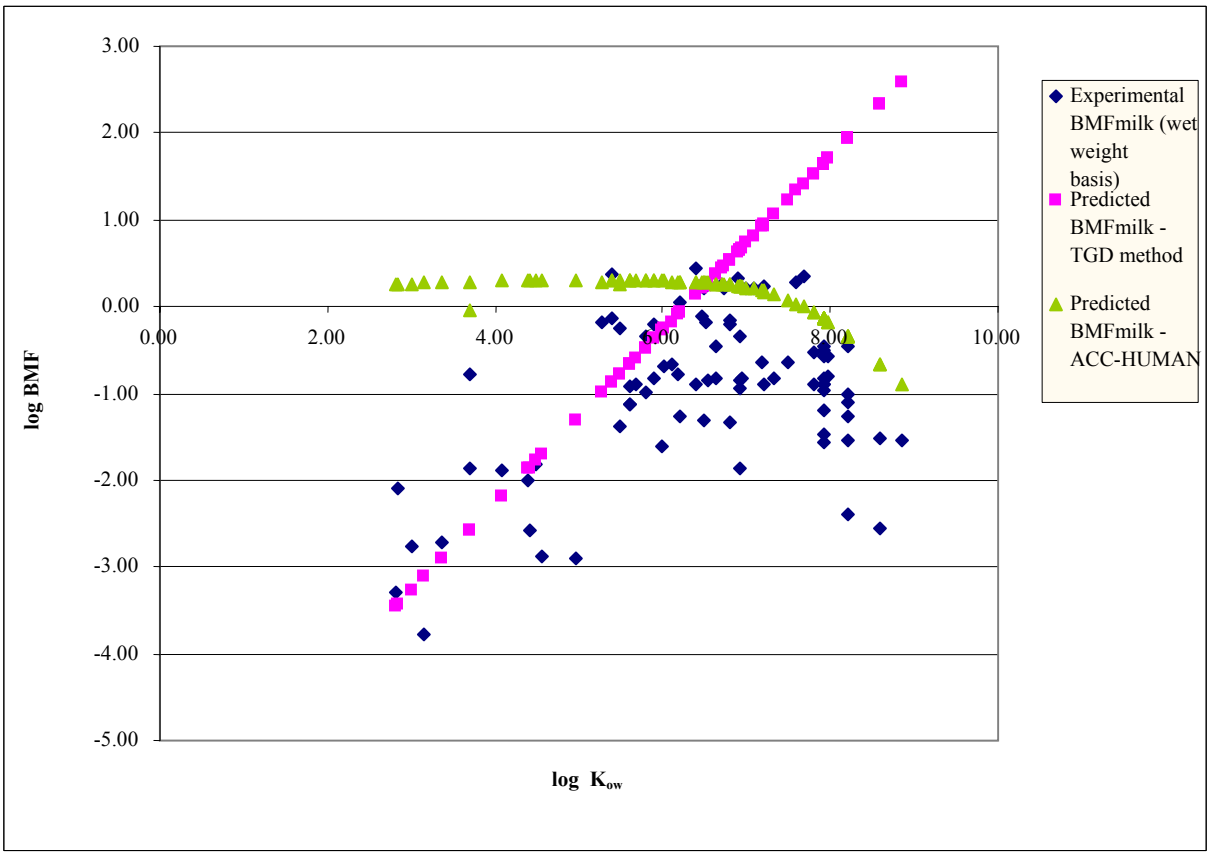

Figure 3.12 Experimental and predicted BMF_{milk}

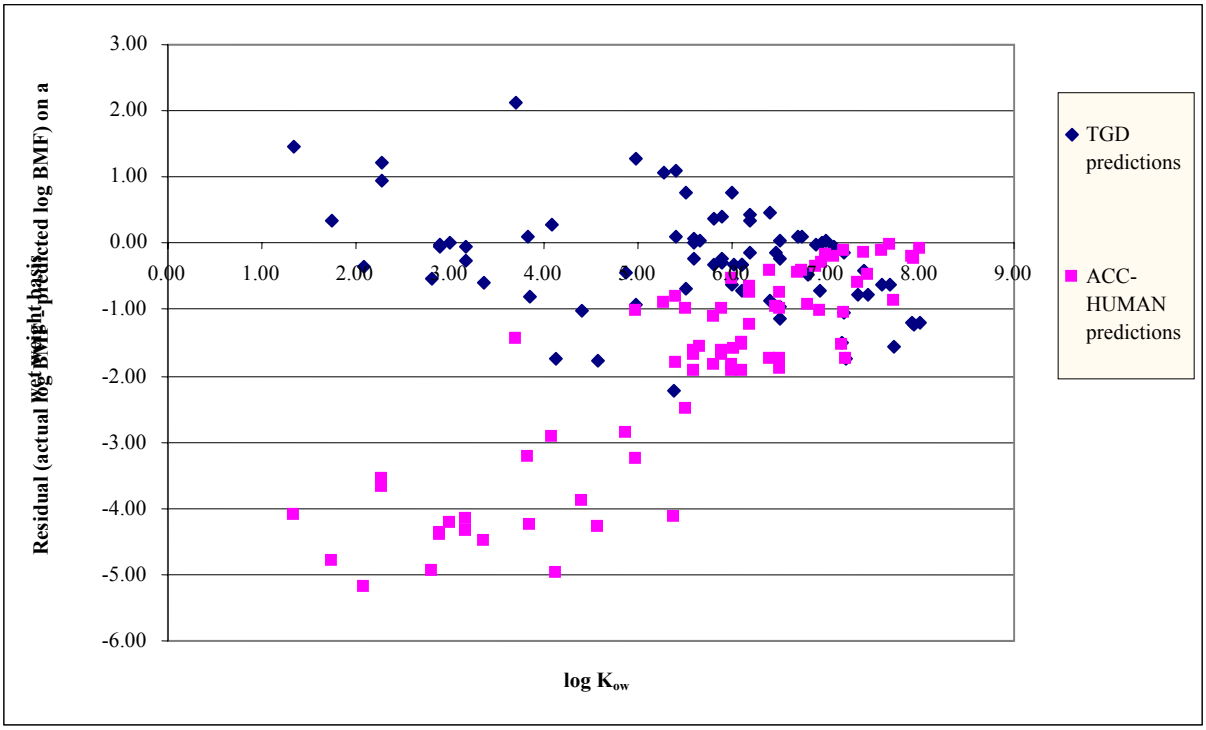

Figure 17.13 Residuals in the predicted BMF_{meat}

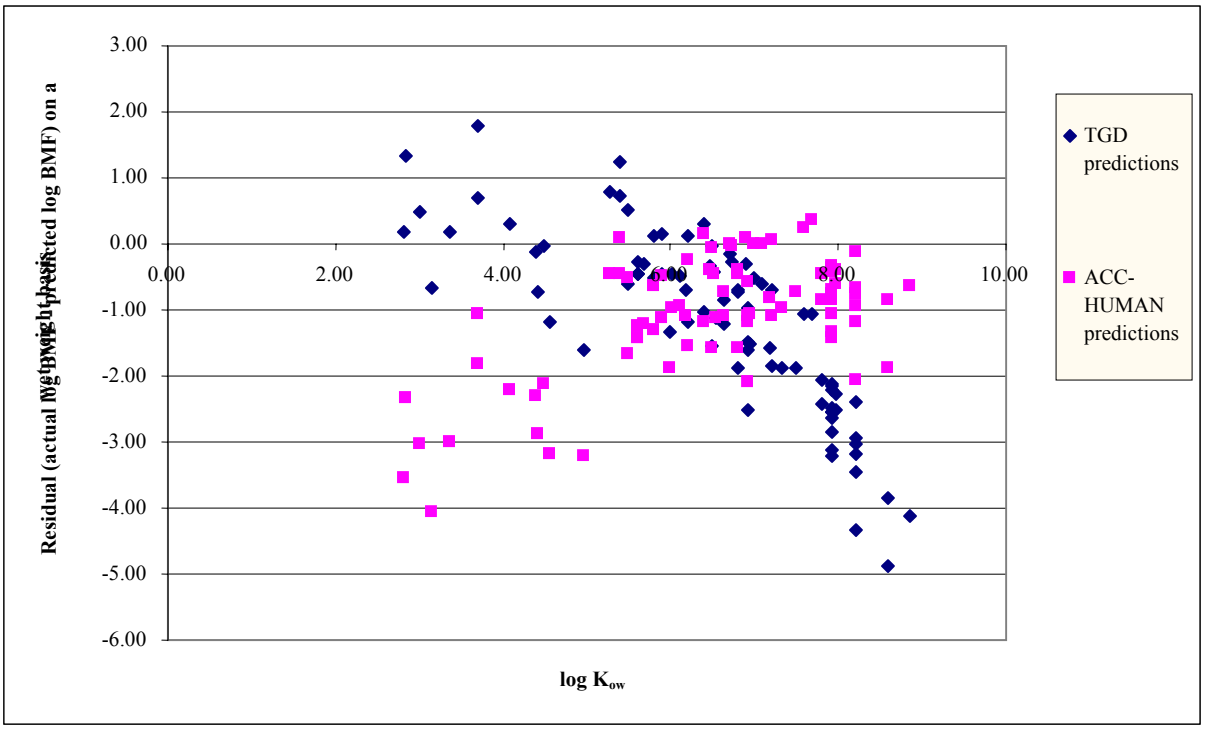

Figure 184 Residuals in the predicted BMF_{milk}

Predictions using the TGD method reflect the linear relationship of the degree of accumulation with log K_{ow} as found originally by Travis and Arms (1988). The mass balance study of McLachlan *et al.* (1990) found transfer of chlorinated dibenzo-*p*-dioxins and dibenzofurans from food to milk showed a decreasing trend with increasing log K_{ow}. This is in direct contrast to the method of Travis and Arms (1988), and hence the TGD method. As can be seen from the plots, when the data set is extended to log K_{ow} values above those originally used in the Travis and Arms (1988) analysis, a decrease in BMF with increasing log K_{ow} is evident for both the meat and milk data. The ACC-HUMAN model predicts this decrease well, but does not appear to predict the linear increase with increasing log K_{ow} at lower log K_{ow} values. One possible reason for this is that the simulations carried out using ACC-HUMAN did not include a rate constant for metabolism.

As indicated above, the comparison of predicted and measured BMFs using ACC-HUMAN was carried out assuming no metabolism of the chemical. This will clearly lead to an overestimate of the BMF for chemicals that are readily metabolised, but it is doubtful whether this factor alone will account for the relatively poor performance of the ACC-HUMAN model at low log K_{ow} values, even though these chemicals are most likely to be susceptible to rapid metabolism. In order to test this, metabolic or elimination half-lives were obtained where available from the studies underlying the Travis and Arms (1988) data set, and these were used to obtained improved predictions of the BMF for both beef and milk using the ACC-HUMAN model. The results of this analysis are summarised in Table 3.7.

Inclusion of a rate constant for metabolism leads to a marked improvement in the prediction of the BMF for both meat and milk, including substances with relatively low log K_{ow} values. This implies that for substances likely to be metabolised reasonably quickly in cattle, data on the actual rate of metabolism in cattle may be needed for reliable predictions of the BMF to be made using ACC-HUMAN. Although the metabolism rate is a chemical-specific property, in general terms it is often the case that the rate of metabolism is higher for substances of relatively low log K_{ow} than for substances of very high log K_{ow} (although exceptions exist), and this may at least partly explain why, when ACC-HUMAN was run assuming a zero metabolism rate, predicted BMFs agreed more closely with the experimental data at high log K_{ow} values than at lower log K_{ow} values.

The Travis and Arms (1988) method that is included in the TGD approach is based on a data set which includes substances that are both metabolised readily in cattle and more recalcitrant in cattle. Therefore, this method already takes account of metabolism to some extent, but the method may not be appropriate for substances that are metabolised much more or much less rapidly than substances of similar log K_{ow} used to generate the Travis and Arms (1988) equation.

The need for metabolism data for the ACC-HUMAN model is considered further in Section 4.

Table 3.7 Refined ACC-HUMAN predictions incorporating metabolism/ elimination data

Substance (log K_{ow})	Measured log BMF[a]		Estimated log BMF[a] assuming no metabolism		Elimination data		Estimated log BMF[a] assuming metabolism		Reference of metabolic rate constant
	Beef	Milk	Beef	Milk	Half-life (days)	Assumed rate constant ($hour^{-1}$)	Beef	Milk	
Aroclor 1254 (6.47)	0.56	-0.12	1.51	0.28	~70	4.2×10^{-4}	0.88	-0.01	Fries *et al.*, 1973
Chlordane (6.00)	-0.28	-1.60	1.52	0.29	<7	4.2×10^{-3}	-0.03	-0.72	Dorough and Hemken, 1973
Dicamba (3.01)	-2.68	-2.77	1.47	0.27	<0.25	0.12	-1.48	-2.14	Oehler and Ivie, 1980
Dieldrin (5.40)	-0.19	-0.14	1.52	0.30	≥42	7.1×10^{-4}	0.71	-0.11	Wilson and Cook, 1972
DDT (6.19)	0.35	-0.79	1.52	0.29	120-220	1.3×10^{-4}	1.24	0.18	Whiting *et al.*, 1973
Fenthion (3.16)	-2.56	-3.77	1.48	0.28	<<7	0.029	-0.85	-1.51	Johnson Jr and Bowman, 1972
Hexachloro benzene (5.50)	0.61	-0.24	1.45	0.27	35-69	4.2×10^{-4}	0.88	-0.01	Fries and Marrow, 1976
DDE (6.51)	0.58	-0.19	1.50	0.27	43-69	4.2×10^{-4}	0.87	-0.02	Fries and Marrow, 1976

a) BMFs on a mg kg^{-1} wet wt. beef or milk per mg kg^{-1} wet wt. feed basis.

3.2.4 Accumulation in cattle and milk by exposure via air

No data was found with which to test this part of the model.

3.2.5 Data sets testing several parts of the model

Douben *et al.* (1997) used a data set of 'typical' levels of polychlorinated dibenzo-*p*-dioxins and dibenzofurans in the UK in the early to mid-1990s to test a series of models. This data set is summarised in Table3.8. The air levels (representing total concentrations) were taken from Davis (1993), with some values derived from König *et al.* (1994). Levels in grass were taken from Kjeller *et al.* (1996) and levels in milk were taken from MAFF (1992 and 1995). Levels in rural soil were taken to be the average levels from a survey by HMIP (1995).

Predicted concentrations obtained with both the TGD and ACC-HUMAN methods (using the measured concentrations in air and soil as inputs) are summarised in Table3.8, and displayed in Figure 19.15 (grass/feed) and Figure 19.15 Measured and predicted concentrations in grass/feed using the Douben *et al.* (1997) data set

There is relatively good agreement between measured and predicted levels in grass (with most predictions being within a factor of 10 of the measured values using either method). For chemicals with very high log K_{ow} values (such as octachlorodibenzo-*p*-dioxin and octachlorodibenzofuran), agreement with the grass/feed data is much better using the ACC-HUMAN model than the TGD method. The probable reason for this is that ACC-HUMAN includes deposition of aerosol/ particulate-bound substance onto plant leaves, whereas this is not covered in the TGD method. This route of exposure of grass/leaves is likely to become increasingly important as the log K_{ow} increases.

For levels in milk, both the ACC-HUMAN and TGD methods overpredict the actual concentrations found, particularly for some substances with four to six chlorine atoms per molecule. One possible reason for this is that no metabolism was assumed in the calculations. For substances with higher degrees of chlorination, agreement between the actual and predicted concentration in milk is somewhat better, possibly reflecting the fact that these substances may not be metabolised as quickly as some congeners of lower chlorine contents (and so the assumption of no metabolism may be more applicable to these substances). Overall, ACC-HUMAN appears to give slightly better predictions of the actual concentration in milk than the TGD method (in line with earlier findings for chemicals with log K_{ow} values greater than six), but this data set did not include chemicals of low to moderate log K_{ow} (where the TGD method may be expected to perform better than the ACC-HUMAN in the absence of metabolism rate data).

Table 3.8 Measured and predicted levels of polychlorinated dibenzo-*p*-dioxins and dibenzofurans in air, soil, grass and milk in the UK (Douben *et al.*, 1997)

Substance	Input data				Output data							
	log K_{ow}	log K_{aw}	Level in air (pg/m^3)	Level in soil (ng/kg dry weight)	Grass[a] (ng/kg)				Milk (ng/kg)			
					Measured	Predicted			Measured	Predicted		
						TGD		ACC-HUMAN		TGD		ACC-HUMAN
						b	c			b	c	
2,3,7,8-Tetrachloro dibenzo-*p*-dioxin	6.80	-2.67	0.002	0.05	0.12	0.008	0.008	0.009	<0.01	0.015	0.015	0.013
1,2,3,7,8-Pentachloro dibenzo-*p*-dioxin	6.64	-3.02	0.009	0.04	0.07	0.007	0.007	0.052	<0.02-0.03	0.013	0.013	0.079
1,2,3,4,7,8-Hexachlorodibenzo-*p*-dioxin	7.80	-3.77	0.013	2.1	0.10	0.004	0.003	0.364	0.03	0.029	0.027	0.254
1,2,3,6,7,8-Hexachlorodibenzo-*p*-dioxin	7.98	-2.44	0.047	7	0.17	0.014	0.012	0.433	<0.01-0.04	0.099	0.093	0.234
1,2,3,7,8,9-Hexachlorodibenzo-*p*-dioxin	8.21	-2.44	0.035	7	0.08	0.011	0.009	0.364	0.03	0.093	0.088	0.134
1,2,3,4,6,7,8-Heptachlordi benzo-*p*-dioxin	8.20	-2.13	0.53	38	2.8	1.020	1.010	4.688	<0.05-0.26	2.140	2.110	1.761
Octachlorodi benzo-*p*-dioxin	8.20	-3.54	2.31	150	15.6	0.074	0.045	86.500	0.29-2.1	1.730	1.630	32.430
2,3,7,8-Tetrachloro dibenzofuran	6.53	-1.95	0.024	4.1	1.28	0.040	0.039	0.017	<0.01	0.121	0.109	0.026
1,2,3,7,8-Pentachloro dibenzofuran	6.92	-2.12	0.031	37.4	0.29	0.129	0.115	0.067	<0.01	0.667	0.586	0.093
2,3,4,7,8-Pentachloro dibenzofuran	6.92	-2.12	0.032	0.26	0.28	0.118	0.118	0.069	0.03-0.06	0.203	0.202	0.096
1,2,3,4,7,8-Hexachloro dibenzofuran	7.92	-1.40	0.029	4.1	0.21	0.128	0.127	0.106	0.02-0.03	0.261	0.258	0.063
1,2,3,6,7,8-Hexachloro dibenzofuran	7.92	-1.40	0.016	3.3	0.09	0.071	0.070	0.058	0.01-0.03	0.156	0.153	0.035

Substance	Input data				Output data							
	log K_{ow}	log K_{aw}	Level in air (pg/m^3)	Level in soil (ng/kg dry weight)	Grass[a] (ng/kg)				Milk (ng/kg)			
					Measured	Predicted			Measured	Predicted		
						TGD		ACC-HUMAN		TGD		ACC-HUMAN
						b	c			b	c	
1,2,3,7,8,9-Hexachloro dibenzofuran	7.58	-1.85	0.005	0.20	0.017	0.024	0.023	0.022	<0.01	0.042	0.042	0.020
2,3,4,6,7,8-Hexachloro dibenzofuran	7.92	-1.40	0.024	1.4	0.09	0.106	0.106	0.088	0.01-0.03	0.195	0.194	0.052
1,2,3,4,6,7,8-Heptachloro dibenzofuran	7.92	-1.89	0.073	24	1.02	0.326	0.321	0.486	<0.02-0.28	0.813	0.793	0.288
1,2,3,4,7,8,9-Heptachloro dibenzofuran	7.92	-1.89	0.011	10	0.13	0.051	0.048	0.073	<0.01-<0.02	0.194	0.185	0.043
Octachloro dibenzofuran	8.60	-2.41	0.08	10	0.98	0.001	2.910E-04	1.088	<0.04-0.94	0.108	0.104	0.189

a) ACC-HUMAN currently only gives the concentration in cattle feed. This concentration is taken within the model to be the same as the concentration predicted in grass.

b) Calculations carried out using the TGD default QSAR to estimate the K_{oc}.

c) Calculations carried out using the TGD QSAR for predominantly hydrophobics for K_{oc}.

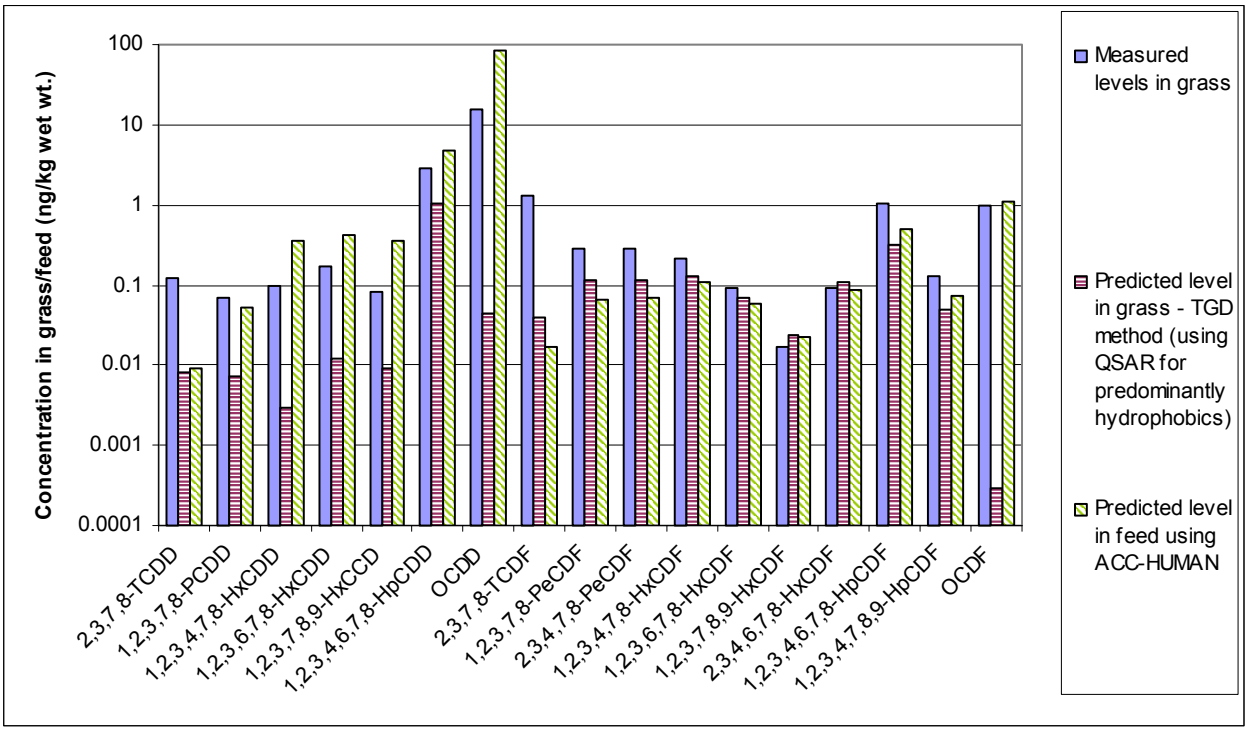

Figure 19.15 Measured and predicted concentrations in grass/feed using the Douben *et al.* (1997) data set

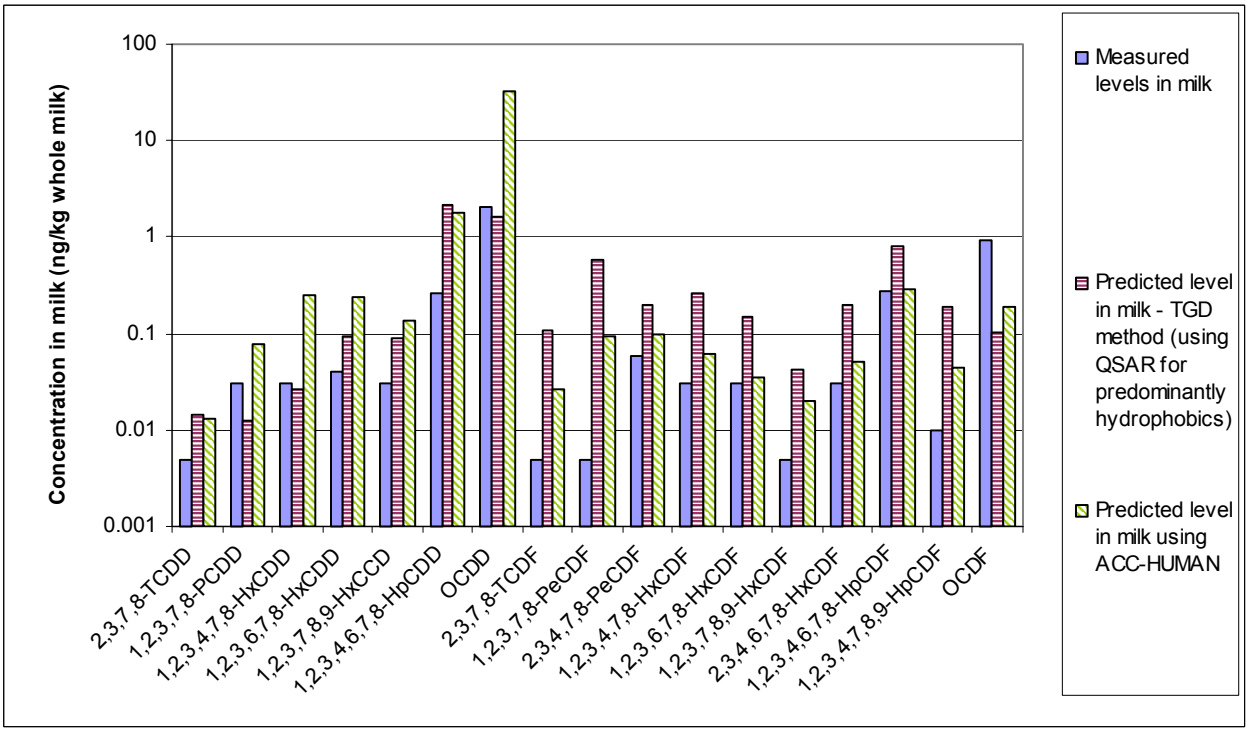

Figure 20.16 Measured and predicted concentrations in milk using the Douben *et al.* (1997) data set

3.3 Summary of findings

The available experimental and field data allowed various parts of both the TGD method and the ACC-HUMAN model to be tested.

For uptake into plants by air, both methods appeared to perform similarly against a test set of experimental data obtained using azalea leaves, with agreement between the predicted BAF and the experimental data being somewhat variable. In general, both models appeared to predict the measured BAF to within a factor of 100. An important difference between the two approaches is that the ACC-HUMAN method takes account of deposition of aerosol-bound substances onto plant surfaces, whereas this possible route to plant leaves is not included in the TGD method. This route of exposure may be most important for substances with very high log K_{ow} values which are expected to be present in the atmosphere and mainly adsorbed to particulates/aerosols.

For uptake into plant roots from soil, only the TGD method could be tested (the ACC-HUMAN method does not predict concentrations in plant roots). Here, it was found that the TGD method predicts well the BAF_{root} for chemicals with log K_{ow} values up to three. For chemicals with log K_{ow} values between three and four, the method tends to overpredict the actual BAF slightly (generally by less than a factor of 10). For chemicals with a log K_{ow} of four and above, the overprediction becomes progressively worse with increasing log K_{ow}; in particular, the TGD method predicts an increasing trend in BAF with increasing log K_{ow} in this region, whereas the experimental data show the opposite trend. This suggests that underlying assumptions in the TGD method may not be valid at high log K_{ow} values. An analysis of the available data suggests that the actual BAF_{root} can be related to log K_{ow} by the following relationship (when using the TGD default QSAR to estimate the K_{ow} value used for soil partitioning):

$$\log BAF_{root} = -0.38 \times \log K_{ow} + 0.67$$

For uptake into plant leaves from soil, both the TGD and ACC-HUMAN methods use similar principles, and result in generally similar predictions. Both methods tend to overestimate the actual BAF_{plant} for substances with log K_{ow} values up to three, and underestimate the actual BAF_{plant} for substances with log K_{ow} values above three. Predictions using both methods are generally within a factor of 10 of the measured BAF_{plant} within the log K_{ow} range of approximately 2.5 to four. However, one important difference (relevant to chemicals with log K_{ow} values lower than -0.5 or greater than 4.5) is that the TGD method applies a limit to the TSCF, whereas this is not applied in the ACC-HUMAN method. The result of this is that the TGD method tends to give much better predictions than ACC-HUMAN at higher log K_{ow} values, but even so the TGD method still appears to underestimate the actual BAF by up to a factor of 10,000 over a log K_{ow} range of four to six, though it gives slightly better predictions (within a factor of 100-1,000) outside of this range. There are also considerable uncertainties and variation associated with the experimental and field data, most notably that it is difficult to carry out soil uptake experiments that totally eliminate exposure via air. This could at least partly explain why the uptake seen in the experiments appears to be higher than predicted in some cases.

For predictions in cattle (meat) and milk exposed via diet, different overall trends in uptake are predicted using the TGD method compared with the ACC-HUMAN one. In the absence of information on the rate of metabolism of the chemical, the TGD method appears to make more reliable predictions than ACC-HUMAN over the log K_{ow} range one to around five or six, but the ACC-HUMAN method appears to provide more reliable predictions at a log K_{ow} above five to six. At lower log K_{ow}, ACC-HUMAN only appears to give reliable predictions of the actual accumulation if information on the rate of metabolism in cattle is available.

The original Travis and Arms (1988) method (that is incorporated into the TGD method for meat and milk) was also reviewed by Birak *et al.* (2001). In this study, a validation exercise was carried out on the original equations for uptake into meat and milk from feed given by Travis and Arms (1988), to check that they could be reproduced. In addition, the study also undertook a review of the more recent literature data to see if there were any further data that could be used to update the equation. This analysis similarly found that the Travis and Arms (1988), and hence TGD method, does not correctly predict actual accumulation for substances with very high log K_{ow} values (or at log K_{ow} values below 2.5); the authors recommended that the equation should be used mainly for substances with log K_{ow} values in the approximate range 2.5 to 6.5.

Although predictions obtained from both methods agree generally with experimental and field data, at least over certain ranges of physico-chemical properties, their predictions are often only within a factor of around 100 at best of the actual data. Some of this variability probably reflects the natural variability in the experimental data, and indeed the difficulties in determining accumulation factors experimentally; some of this variability probably results from the simplifications and assumptions made in the models and predictive methods used.

4 Conclusions and recommendations

When considering the results of this modelling exercise, it should be borne in mind that there are numerous sources of variability and uncertainty in the data. These include uncertainties in the physico-chemical properties of the chemicals used in the models, uncertainties in the actual measured accumulation factors, and uncertainties resulting from assumptions and simplifications made in the models. For example, the log K_{ow} value measured 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 increasing difficult with increasing log K_{ow}. Similar problems also exist for the measurement or prediction of other key physico-chemical properties such as Henry's law constants. Therefore, it should not be expected that the model results agree completely with the available experimental data, but rather the model should be expected to provide a general agreement (to within an order of magnitude) with the measured data.

For both methods, validation of the calculations for uptake into fish was not considered in this report, as the TGD method and a method similar to that included in ACC-HUMAN are reviewed in detail in report Part A in relation to exposure of fish-eating wildlife and these conclusions are equally valid here. Of particular importance for human food chain calculations, the current TGD method for predicting the accumulation of a chemical in fish does not include a BMF value. This therefore may underestimate the extent of accumulation in fish for some chemicals.

The analysis of the TGD method and the ACC-HUMAN model has highlighted some similarities between the two approaches, and equally importantly, some differences. No one method provides the best estimates across all endpoints considered, and so it is recommended that both models are used selectively, with different models being used for different endpoints. The recommendations for each endpoint are summarised below.

For accumulation in plants exposed via air, both methods appear to given similar predictions. However, the ACC-HUMAN model includes deposition onto plant leaves from aerosol-bound substances, whereas this is not included in the TGD method. Therefore, for substances where binding to atmospheric particulates/aerosols is important, the ACC-HUMAN model would be preferred in order to give more reliable predictions for animal feed. The ACC-HUMAN model currently does not give predictions for plants for human consumption, but predictions for grass/feed could equally well be used for leaf crops in general (and indeed, grass and leaf crop models in the TGD method are essentially the same). However, it should be considered whether aerosol deposition onto leaves is relevant for human exposure, as most leaf crops will be washed prior to ingestion.

For uptake into plant roots from soil, only the TGD method is available. This method gives reliable predictions of uptake for chemicals with log K_{ow} values up to around three. For chemicals with log K_{ow} values between three and four, the method tends to over-predict the actual BAF slightly (generally by less than a factor of 10). For chemicals with a log K_{ow} of four and above, the overprediction becomes progressively worse with increasing log K_{ow}; in particular, the TGD method predicts an increasing trend in the BAF with increasing log K_{ow} in this region, whereas the experimental data show the opposite trend. This suggests that underlying assumptions in the TGD method may not be valid at high log K_{ow} values. An analysis of the available data suggests that the actual BAF_{root} can be related to log K_{ow} by the following relationship (when using the TGD default QSAR to estimate the K_{oc} value used for soil partitioning):

$$\log BAF_{root} = -0.38 \times \log K_{ow} + 0.67$$

For uptake into plant leaves from soil, both methods are based on similar principles and give similar predictions over the log K_{ow} range -0.4 to 4.5. However, outside of this range the TGD method limits the value of an important partition coefficient used in the method (the transpiration stream concentration factor or TSCF) and the TGD method gives better predictions of the actual uptake than the ACC-HUMAN model outside of this log K_{ow} range. Therefore, it is recommended that the TGD approach is used for uptake into plant leaves from soil. However, the TGD method still provides predictions that may significantly underestimate actual uptake over the log K_{ow} range four to six in particular. There are also considerable uncertainties and variation associated with the experimental and field data (most notably, that it is difficult to carry out soil uptake experiments that totally eliminate exposure via air), and this could at least partly explain why the uptake seen in the experiments appears to be higher than predicted in some cases.

For predictions in cattle (meat) and milk for exposed via diet, different overall trends in uptake are predicted using the TGD method compared with the ACC-HUMAN one. It was found that, in the absence of information on the rate of metabolism of the chemical, the TGD method appears to give more reliable predictions than the ACC-HUMAN method over the log K_{ow} range one to five or six, but the ACC-HUMAN method appears to provide more reliable predictions at a log K_{ow} above five to six. At lower log K_{ow}, ACC-HUMAN only appears to give reliable predictions of actual accumulation if information on the rate of metabolism in cattle is available. Therefore, in the absence of metabolism data, it is recommended that the TGD method is used for chemicals up to a log K_{ow} of around six, and the ACC-HUMAN model is used for chemicals with a log K_{ow} greater than six. If metabolism data are available, then the ACC-HUMAN model should be used.

It was not possible to test the models for uptake into cattle and milk for exposure via drinking water and air, owing to the lack of suitable test data. However, the above conclusions for exposure via feed would be expected to apply in this case.

One important finding from this work relates to the prediction of accumulation in cattle and milk. Although the ACC-HUMAN model is much more sophisticated than the approach taken in the TGD, this does not necessarily lead to better predictions of the accumulation in meat and milk for chemicals with a log K_{ow} less than six. The probable reason for this is that the ACC-HUMAN model requires an estimate of the metabolism rate constant to give reliable predictions for these types of chemicals, and predictions using the method for substances with log K_{ow} values higher than this are also improved with the inclusion of metabolism rate constant data. The TGD method is based on a data set that includes chemicals metabolised in cattle, and so already takes account of metabolism to some extent. This raises the question of the availability of suitable metabolism rate constant data for use in the ACC-HUMAN model. Ideally, this should be generated with experiments on cattle. However, such experiments are costly and difficult to carry out, and the data generated are generally part of feeding studies in any case. Thus, for chemicals where metabolism data are available, it is likely that a BAF would also be available from the same study, meaning that an actual prediction would not be needed. The second potential problem is that most studies looking at metabolism actually 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 the various loss processes). As other loss processes (such as faecal egestion) are already built into the ACC-HUMAN model, rate constants derived from total depuration half-lives in cattle may overestimate the rate of metabolism. This then raises the question of whether such a

predictive method that relies on the availability of metabolism data is actually useful in practice. One possible approach to address this would be to investigate if it is possible to extrapolate or predict rates of metabolism in cattle from species that are more commonly studied (such as laboratory rodents).

In terms of using the models to set standards, it is relevant to consider an approach whereby BAFs for different parts of the food chain are estimated separately. This allows the most reliable model to be selected for different parts of the food chain, and also allows the recommendations for the prediction of accumulation in fish in Part A to be taken into account. Both the TGD and ACC-HUMAN methods can be used, with limitations, to calculate the concentration in plants, meat and milk resulting from exposure via one of water, soil or air. If the concentration predicted in the food item is divided by the concentration in the exposure medium, this then provides a BAF of suitable form for use in setting standards; such a BAF can be used to readily back-calculate from a 'no observed effect concentration' (NOEC) in food (or some similar endpoint derived from mammalian toxicity data) to the associated concentration in either air, water or soil. This type of approach is recommended by the Environment Agency (2007) and further details of how it could be applied are given in that report.

This approach may not, however, be precautionary if the exposure of an individual occurs by several routes, as the NOEC or 'safe concentration' could be exceeded through the combined exposure. An alternative approach would be to use the estimated fraction that each food chain makes to the total diet of the target species. This fraction could be used to adjust the standard for each medium, so that if an individual is exposed simultaneously via all food chains at the standard concentrations, the total exposure would equal the NOEC or 'safe concentration'. An approach like this has been developed in the Netherlands (Bontje *et al*., 2005). This uses the EUSES program with a fixed emission of a substance to generate regional PEC values for each compartment. The TGD human exposure routes considered above are augmented with others relevant for contaminated sites, and the total exposure is calculated. This is compared with the tolerable daily intake (TDI) or other measure of 'safe' exposure. If the calculated exposure exceeds the TDI, then the PEC values are reduced (by reducing the emission) until the exposure is the same as the TDI. The PEC values giving this exposure can then be used as the standards. As well as considering the combined exposure, this approach also provides concentrations in the environmental compartments which are consistent with each other. One aspect which might need to be considered is that the route of release (to air, water or soil) can affect the relative concentrations, and so knowledge of the emission pattern would be useful. This approach is intended for exposure to concentrations resulting from dispersed emissions and not for specific local exposures.

An important point to consider for human food chain models is that agreement of the predicted data with experimental data is generally within a factor of 100 at best when the whole data set is considered. This raises the question of whether this uncertainty in the estimation methods is reasonable in the context of standard setting. For example, an overly precautionary approach may lead to a too conservative standard being set, possibly leading to problems (and costs) associated with monitoring (where, for example, the standard is set at a concentration below one that can actually be measured analytically) and enforcement.

An alternative approach that could be considered would be to set the standard based on the concentration in the food item itself (such as fish, milk, meat, leaf crops, root crops). This would have the advantage that there would be less uncertainty in the standard, and it would probably be easier to monitor analytically. In this respect, predictive methods would be useful for targeting the most relevant food items for the standard, where they could be used to determine in which food items a given chemical is most likely to accumulate.

During this work, the ACC-HUMAN model gave predicted concentrations of zero for the concentration in grass and the concentration of soil in feed for all of the simulations. As far as could be seen, the underlying calculations appeared to be carried out correctly by the model and the error appeared to be related only to how the results were displayed in the final output file. This would need to be checked and corrected if the model were to be routinely used.

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Glossary of terms

Adapted from USEPA (2000).

Allometric	Relative growth of a part of an organism in relation to the growth of the whole.
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 wt.)/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. The 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 wt.)/concentration in organism at trophic level y (mg/kg wet wt.); 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 wt.)/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 non-polar 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.
Uptake	The acquisition by an organism of a substance from the environment as a result of any active or passive process.

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
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
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)
Kp_{soil}	Solids-water partition coefficient for soil (units of l kg^{-1})
$K_{soil\text{-}water}$	Bulk soil-water partition coefficient
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

QSAR	Quantitative structure-activity relationship
R^2	Correlation coefficient
TGD	Technical Guidance Document
TSCF	Transpiration stream concentration factor
USEPA	United States Environmental Protection Agency
wet wt.	Wet weight basis.

Appendix - Variation in predicted concentrations in biota using ACC-HUMAN across allowed ranges of property values

This appendix presents a greater number of plots than are included in Section 2.3.2, and some further comments on the results obtained. Some of the text here is the same as that in Section 2.3.2, and is repeated here for clarity.

Using the ACC-HUMAN method, predicted concentrations for a set of hypothetical chemicals were calculated for grass/feed, soil in feed, milk, milk cattle, beef (0-1 year old and 1-2 year old) and humans (female 0-10, 30 to 40 and 70-80 year old and male 0-10, 30-40 and 70-80 year old)[8]. For this simulation, the log K_{ow} value was increased from two to 10 in intervals of one log unit and log K_{aw} was increased from -5 to +5 in steps of one log unit. The partition coefficient log K_{oa} (log K_{oa} = log K_{ow} – log K_{aw}) [9] is calculated by the program and simulations were performed for the combinations of log K_{ow} and log K_{aw} where log K_{oa} was greater than or equal to four.

For the first series of calculations, the concentration in fresh water was assumed to be constant at 1×10^{-6} g m^{-3}. Concentrations in air, soil and sea water were set to zero.

Figure A1 shows a plot of concentration (pg g^{-1} lipid or ng g^{-1} in humans) against log K_{ow} with a constant log K_{aw} of -4. As seen from this plot, concentration increases between a log K_{ow} of two and four, remains constant between a log K_{ow} of around four to seven and then starts to decrease at higher log K_{ow} values. Predicted concentrations are higher in milk cows, beef cattle (0-1 and 1-2 year old) and beef (upper series of curves) than in humans (the lower series of curves). The results obtained for the simulation with log K_{aw} of -5 were very similar, hence this plot is not shown. As exposure was via water only, the concentration in grass/feed was zero.

A similar pattern is seen in Figure A2 (log K_{aw} of -3) where concentration in milk cows, beef cattle (0-1 and 1-2 year old) and beef increases with increasing log K_{ow} between a log K_{ow} of two and four, remains constant between a log K_{ow} of four and seven and starts to decrease at higher log K_{ow} values. The concentration curves for humans (the lower series of curves), however, appears to be slightly shifted with respect to the cattle/beef/milk curves (the upper series of curves), and predicted concentrations for humans increase with increasing log K_{ow} until a log K_{ow} value of around five, after which it remains relatively constant until a log K_{ow} of seven, before starting to decrease with increasing log K_{ow}.

[8] The program will also generate data for other age ranges of humans if required.

[9] The allowable range of values that can be used by the program are a log K_{ow} value between two and 10, a log K_{aw} value between -10 to +10 and a log K_{oa} value between zero and 12. The program will not work if values outside of this range are input and so this limits the combinations of log K_{ow} and log K_{aw} that can be tested.

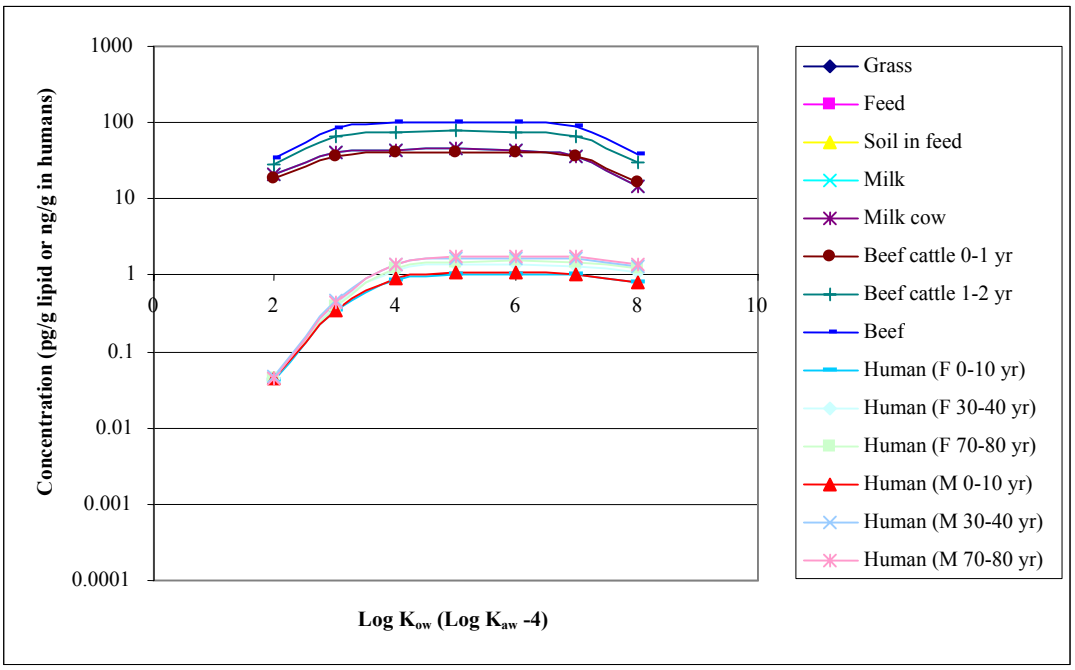

Figure A1 Plot of predicted concentration against log K_{ow} (log K_{aw} of -4) for ACC-HUMAN method (fresh water)

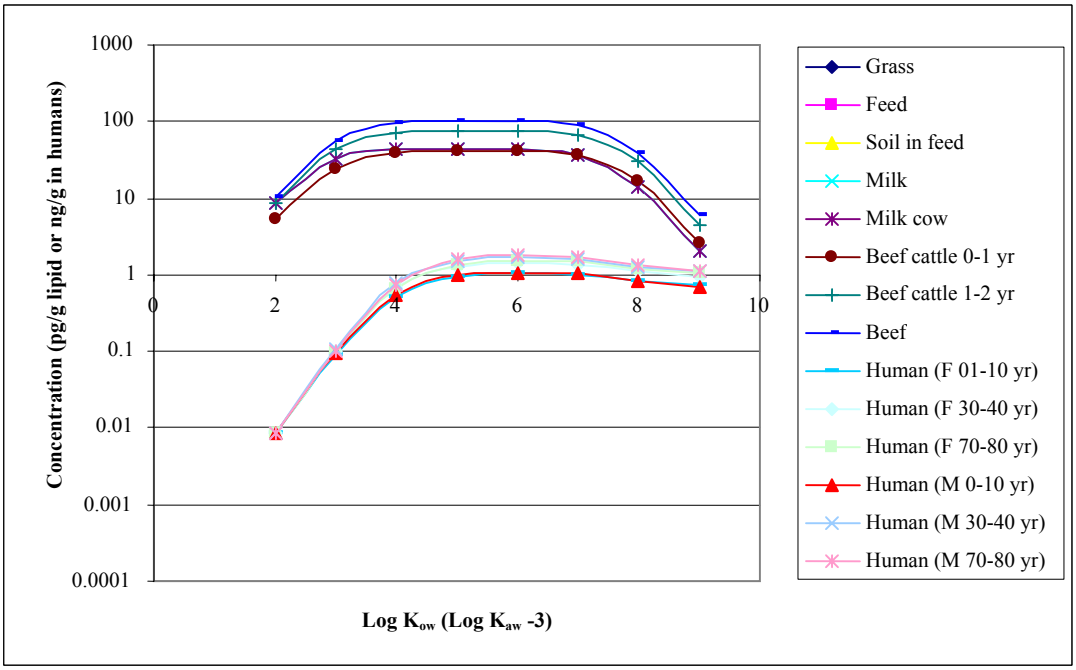

Figure A2 Plot of predicted concentration against log K_{ow} (log K_{aw} of -3) for ACC-HUMAN method (fresh water)

This pattern is more pronounced in Figure A3 (for a higher value of log K_{aw} of -2) where the concentration curves for humans (lower series of curves) are again shifted with respect to the curves for cattle/beef/milk (upper series of curves), increasing to a maximum at a log K_{ow} of around six before decreasing at log K_{ow} values above seven. The concentration curve for milk cows, beef cattle and beef is also shifted as log K_{aw} increases to -2, becoming more pronounced with respect to the plots for lower log K_{aw} values. In this case, predicted concentrations increase with increasing log K_{ow} until a log K_{ow} of around five, remain constant at a log K_{ow} between five and seven and then decrease with further increases in log K_{ow}.

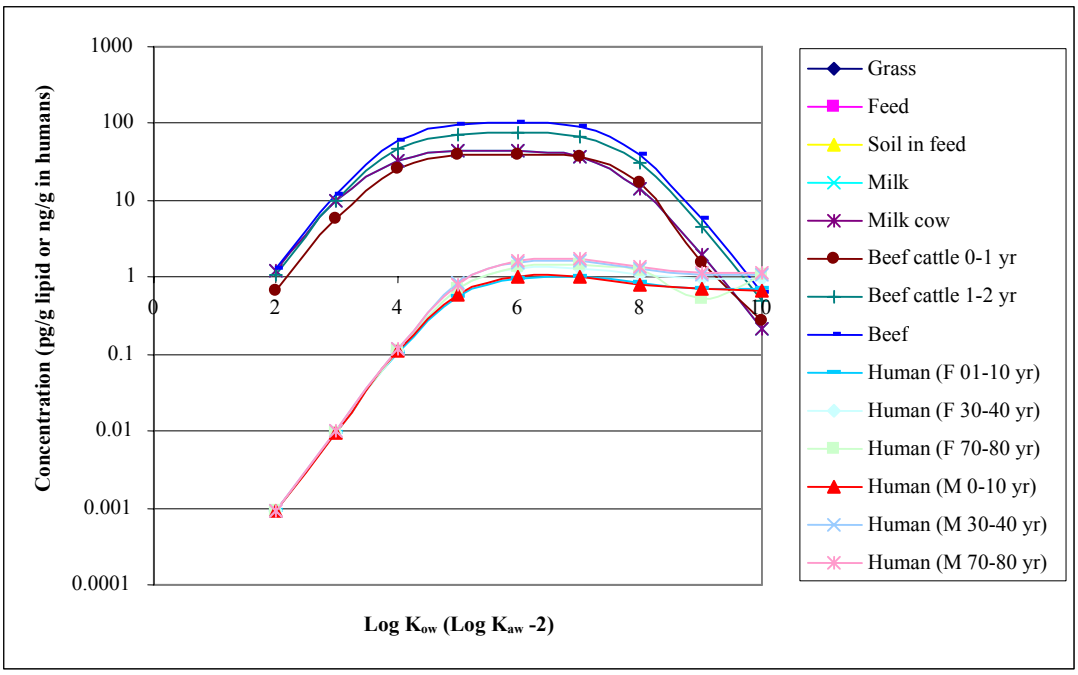

Figure A3 Plot of predicted concentration against log K_{ow} (log K_{aw} of -2) for ACC-HUMAN method (fresh water)

As seen from Figure A3 to Figure A7, the value of log K_{ow} at which the maximum predicted concentration occurs increases with increasing log K_{aw}. As seen from the concentration curves for humans (the lower series of curves on the plots), the maximum occurs at log K_{oa} of 8 (log K_{oa} = log K_{ow} – log K_{aw}). For example, in Figure A3 where log K_{aw} is -2, the concentration curve reaches a maximum at log K_{ow} of six, and in Figure A4 (log K_{aw} of -1), the maximum is at a log K_{ow} of seven. This trend is also observed in Figure A5, Figure A6 and Figure A7. A similar trend is observed for the concentration curves for milk cows, beef cattle and beef (the upper series of curves in the plots), where the value of log K_{ow} at which the maximum concentration is predicted increases as log K_{aw} increases.

Predicted concentrations for grass, feed and soil in feed are zero for all values of log K_{ow} and log K_{aw} in these simulations (exposure via surface water/drinking water only).

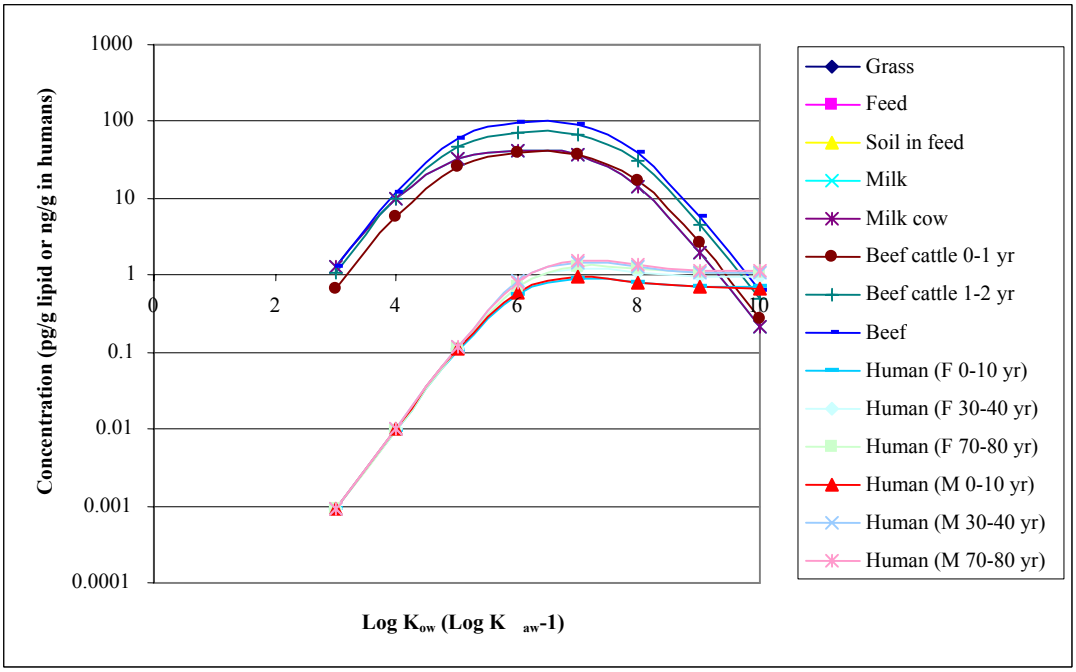

Figure A4 Plot of predicted concentration against log K_{ow} (log K_{aw} of -1) for ACC-HUMAN method (fresh water)

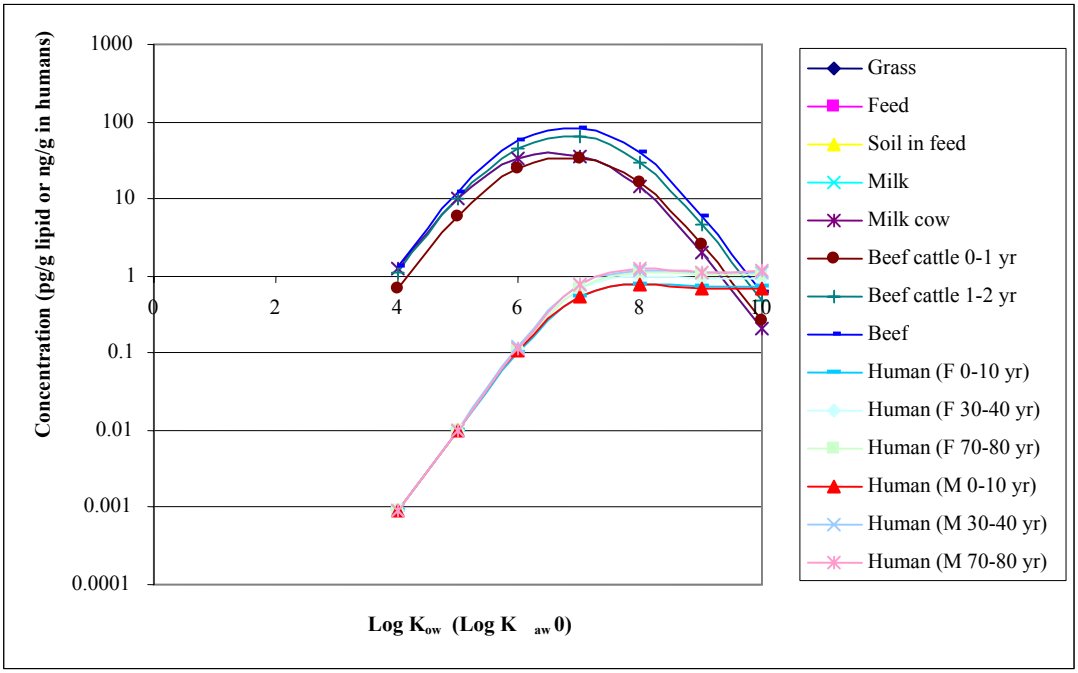

Figure A5 Plot of predicted concentration against log K_{ow} (log K_{aw} of zero) for ACC-HUMAN method (fresh water)

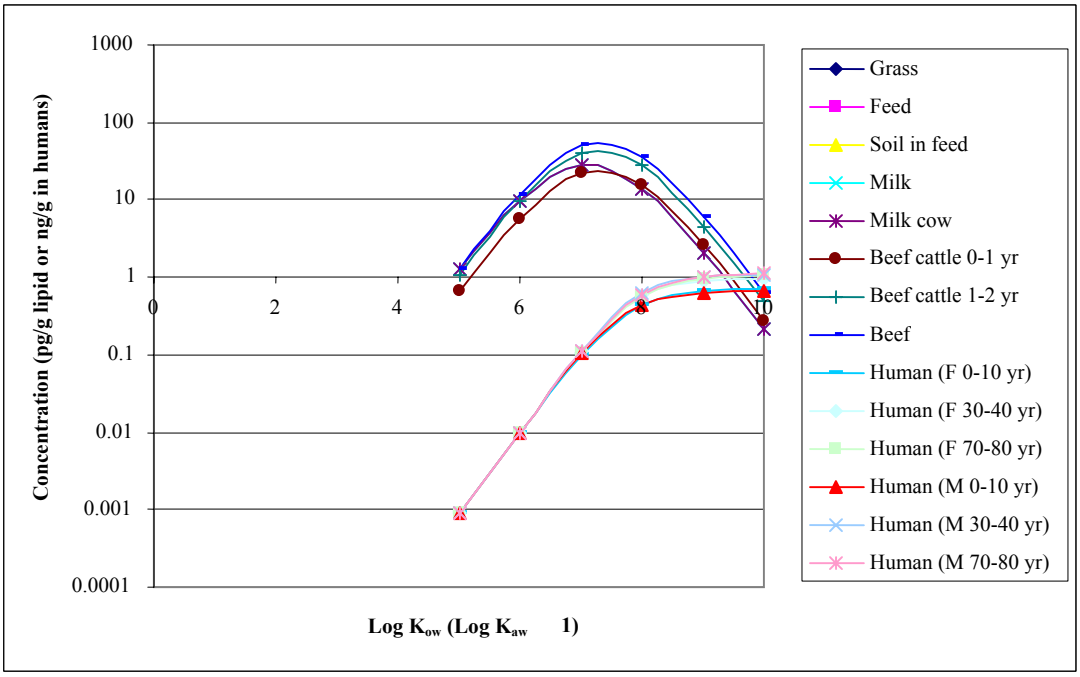

Figure A6 Plot of predicted concentration against log K_{ow} (log K_{aw} of one) for ACC-HUMAN method (fresh water)

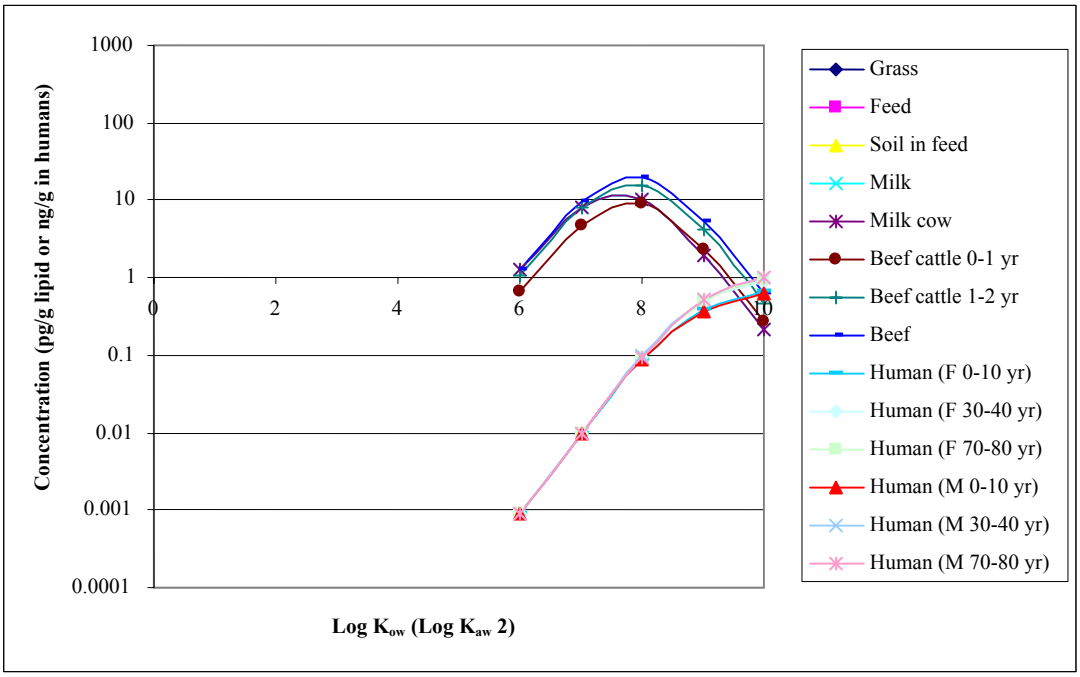

Figure A7 Plot of predicted concentration against log K_{ow} (log K_{aw} of two) for ACC-HUMAN method (fresh water)

For the next series of simulations, the concentration in soil was assumed to be constant at 1×10^{-6} g m^{-3}, and concentrations in air, fresh water and sea water were set to zero. As seen from the plots shown in Figure A8 to Figure A11, predicted concentrations for feed, milk, milk cattle, beef cattle 0-1 year old, beef cattle 1-2 year old, beef (the upper series of curves) and humans (the lower series of curves) decrease with increasing log K_{ow}. Predicted concentrations also decrease with increasing log K_{aw}. Although simulations were performed for log K_{aw} values ranging from -5 to +5, only selected plots are shown since the same trend was observed for the range of log K_{aw} values.

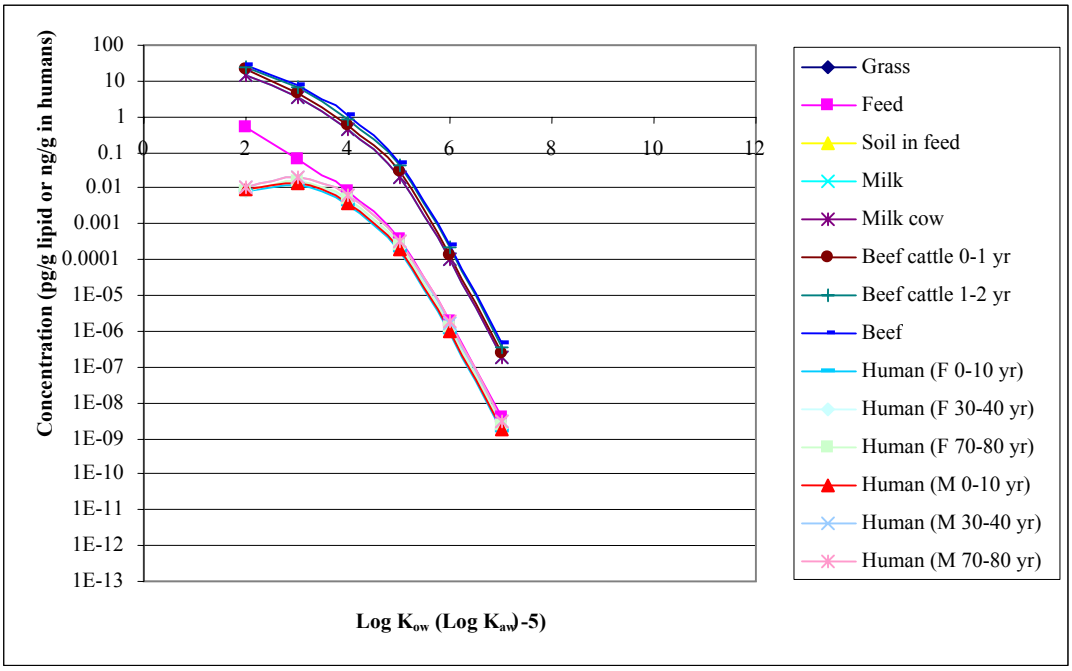

Figure A8 Plot of predicted concentration against log K_{ow} (log K_{aw} of -5) for ACC-HUMAN method (soil)

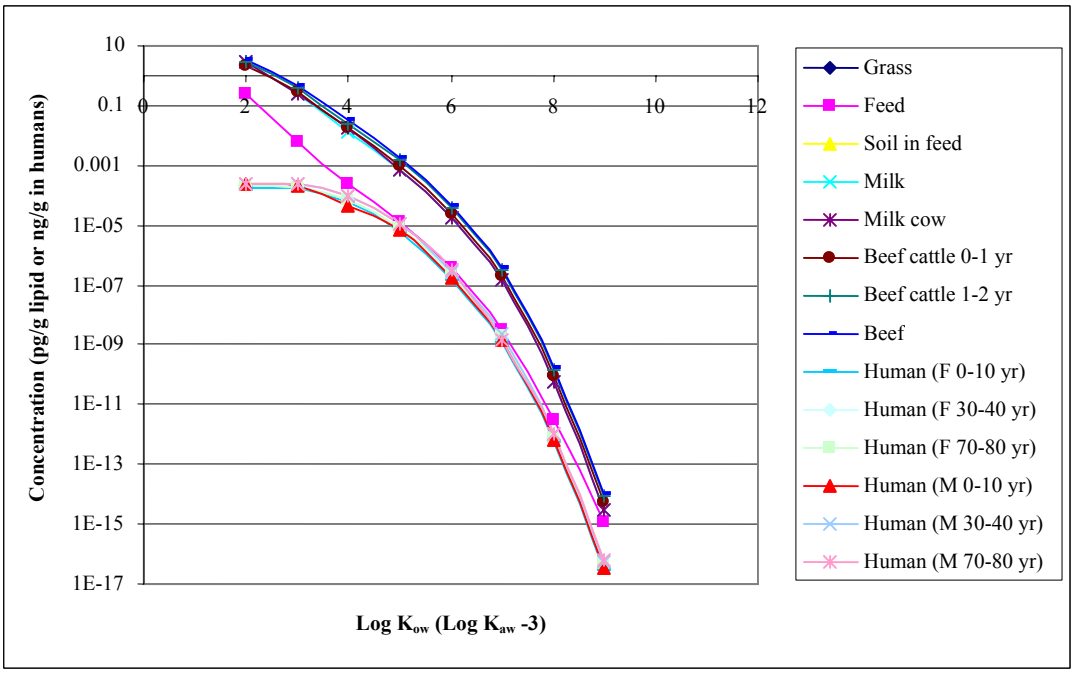

Figure A9 Plot of predicted concentration against log K_{ow} (log K_{aw} of -3) for ACC-HUMAN method (soil)

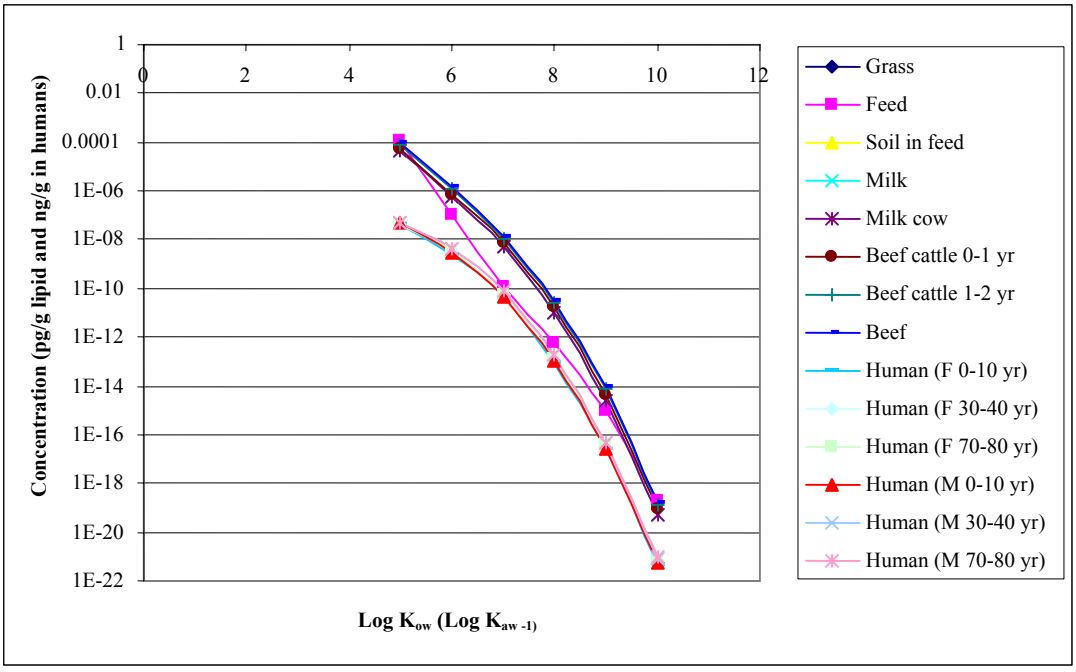

Figure A10 Plot of predicted concentration against log K_{ow} (log K_{aw} of -1) for ACC-HUMAN method (soil)

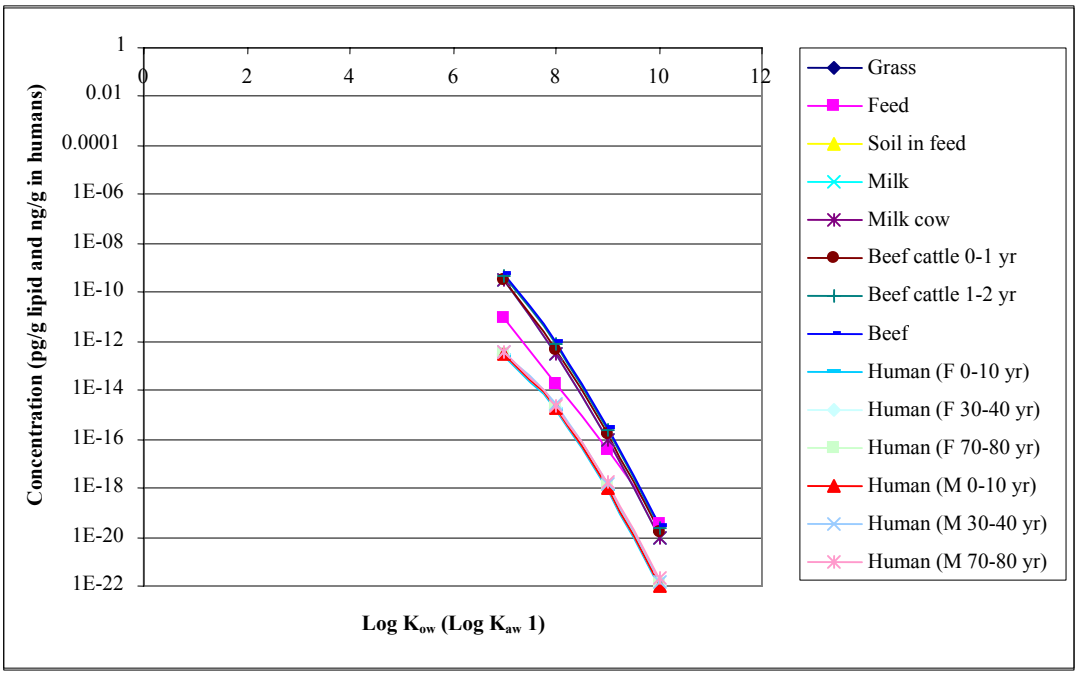

Figure A11 Plot of predicted concentration against log K_{ow} (log K_{aw} of one) for ACC-HUMAN method (soil)

For the final set of simulations, the concentration in air was set to 1×10^{-6} g m^{-3} and concentrations in fresh water, soil and sea water were set to zero. As seen from the plots shown in Figure A12 and Figure A13 (log K_{aw} of -5 and -4), the predicted concentrations for grass/ feed, milk/cattle/beef (upper series of curves) and in humans (the lower series of curves) increase with increasing log K_{ow}.

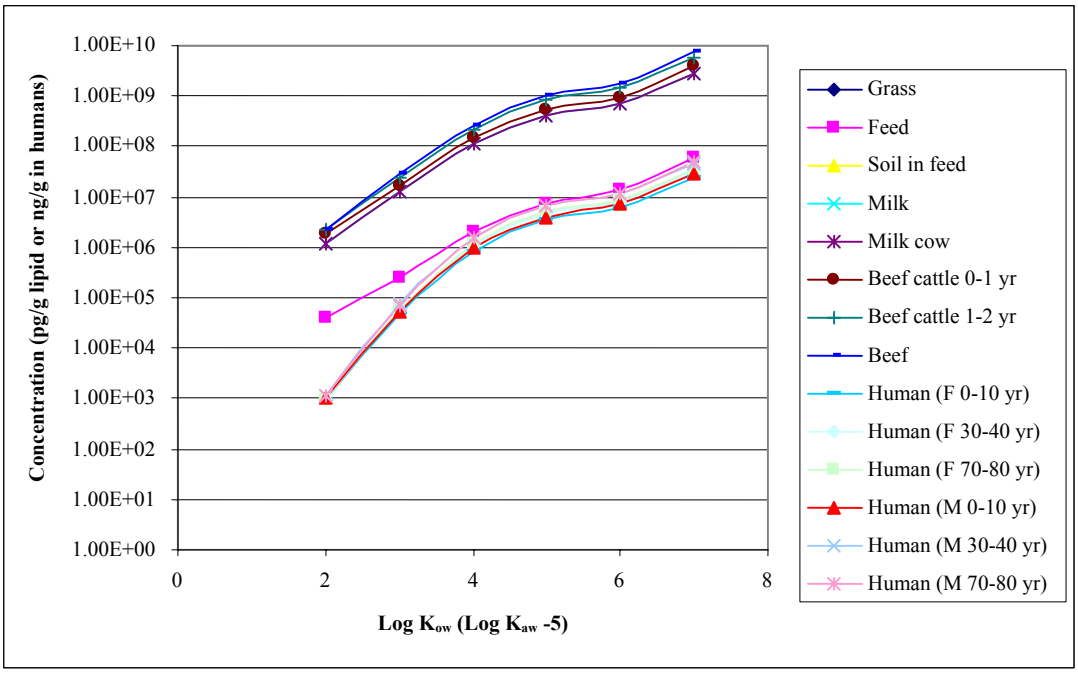

Figure A12 Plot of predicted concentration against log K_{ow} (log K_{aw} of -5) for ACC-HUMAN method (air)

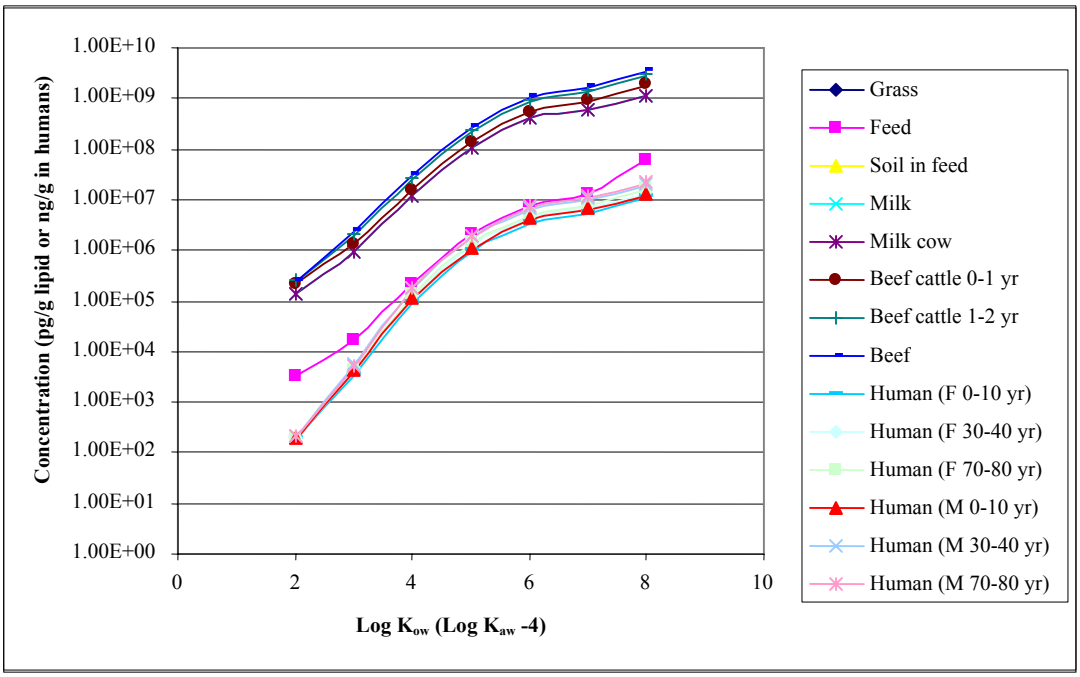

Figure A13 Plot of predicted concentration against log K_{ow} (log K_{aw} of -4) for ACC-HUMAN method (air)

However as seen from Figure A14 (for log K_{aw} of -3), predicted concentrations increase with increasing log K_{ow} to a maximum at log K_{ow} of around seven, before decreasing. The exception is the predicted concentration in feed which continues to increase as log K_{ow} increases. A similar trend is observed for the plots where log K_{aw} is between -2 and +3 (see Figure A15, log K_{aw} of zero as an example). Predicted concentrations increase with increasing log K_{ow} to a maximum, before decreasing. However, the value of log K_{ow} at which the maximum predicted concentration occurs also increases with increasing log K_{aw} (as seen by comparison of Figure A14 and Figure A15). Predicted concentrations also decrease with increasing log K_{aw}.

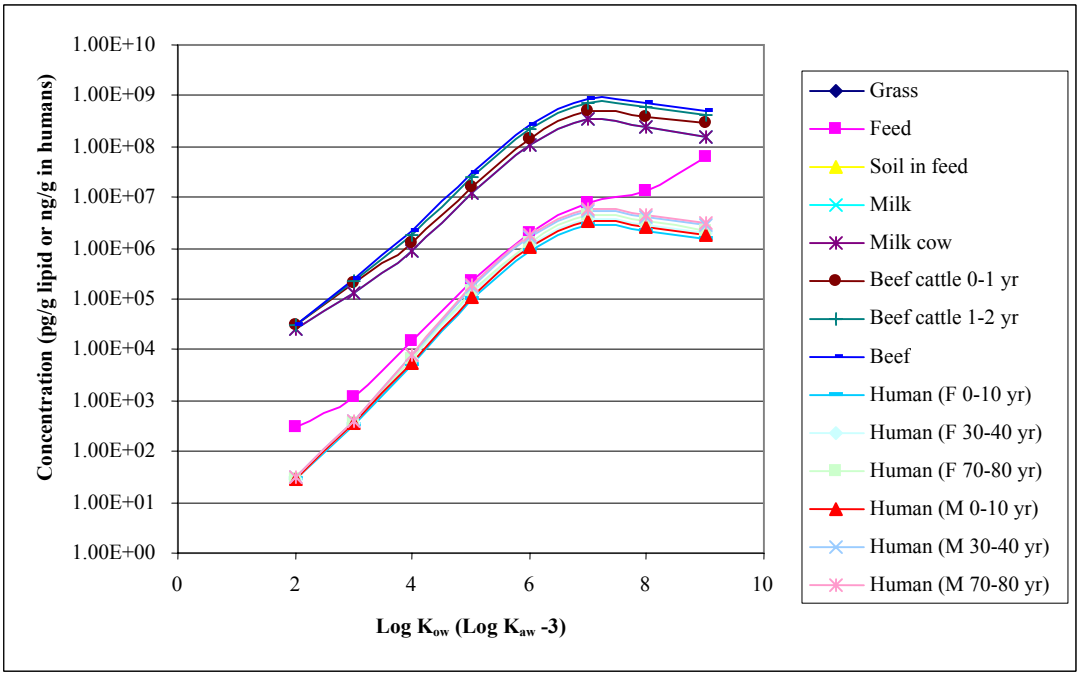

Figure A14 Plot of predicted concentration against log K_{ow} (log K_{aw} of -3) for ACC-HUMAN method (air)

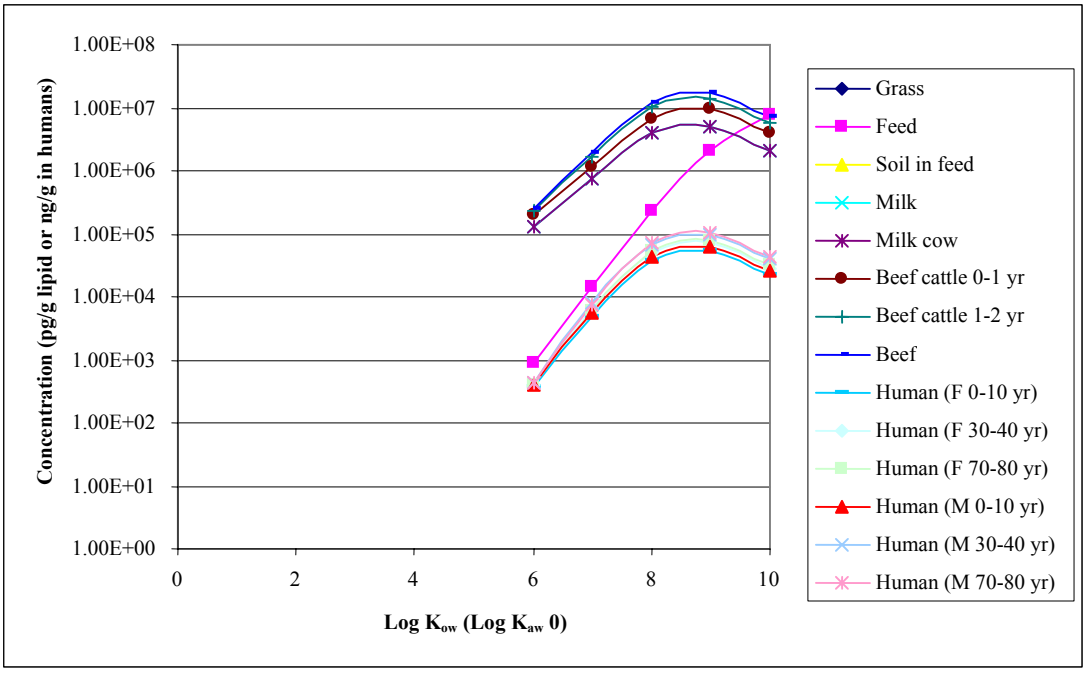

Figure A15 Plot of predicted concentration against log K_{ow} (log K_{aw} of zero) for ACC-HUMAN method (air)

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