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Review of bioaccumulation models for use in environmental standards

Science Report – SC030197/SR1

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Steve Killeen

Head of Science

Executive summary

Bioaccumulative substances have the potential to biomagnify via the food chain and affect organisms at higher trophic levels. When the substance is toxic as well as persistent or continuously released into the environment, bioaccumulation is of particular concern.

Current standards to protect the aquatic environment are based on the potential effects on organisms in direct contact with water. Other routes of exposure and the possibility of effects on higher predators have not generally been considered. Exposure via contaminated food or sediment may also be important.

When setting soil standards, indirect exposure routes for organisms at the top of the terrestrial food chain are an important consideration. The Environment Agency and the Department for Environment, Food and Rural Affairs are developing a tiered terrestrial ecological risk assessment framework into which methods for considering bioaccumulation and persistence when deriving soil standards will be fed.

Bioaccumulation in, or uptake through, the food chain is also of importance when considering human exposure to contaminants. Although there are methods for determining human exposure to chemicals as a result of some types of soil contamination, equivalent methods for determining exposure from other routes, such as the aquatic food chain, are not generally available.

This report reviews available bioaccumulation models and their potential use for setting environmental standards.

The following models are recommended for further consideration, for the purpose of taking into account bioaccumulation when setting environmental standards.

Aquatic food chain:

- Prediction of Bioaccumulation in Aquatic Food Webs model
- Food Chain Bioaccumulation/ECOFATE models
- EU Technical Guidance Document

Terrestrial food chain:

- Arctic Terrestrial Food-chain Bioaccumulation model
- EU Technical Guidance Document

Human food chain:

- EEU Technical Guidance Document
- ACC-Human model

All models (with the exception of the Prediction of Bioaccumulation in Aquatic Food Webs model) need some degree of further development, either to parameterise them in order to better represent the UK situation or to take account of recent developments. In addition, consideration should be given to validating the models against UK datasets. This validation should consider as wide a range of chemical types (and physico-chemical properties) as possible.

A framework is also presented in this report for how the modelled bioaccumulation data could be used in deriving standards.

Contents

1 Introduction

This project forms part of a broader programme of work to support the Environment Agency in developing chemical standards for the protection of the environment and human health (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 role in pollution control. This project will help to provide a sound scientific basis and a transparent and consistent approach to setting standards across different functions within the Environment Agency.

Bioaccumulative substances are of concern to the Environment Agency, as they have the potential to biomagnify through the food chain and affect organisms at higher trophic levels. Bioaccumulation is of particular concern when the substance 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 account for the possibility of 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 which bioaccumulate, direct exposure via water is unlikely to be the only route of exposure, and exposure via contaminated food or sediments may become important in these cases. 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 future EU meetings to agree environmental quality standards for pollutants and priority substances detailed in Annexes VIII to X to the Water Framework Directive (WFD) (Directive 2000/60/EC).

When setting soil standards, the Environment Agency needs to consider indirect exposure routes for organisms at the top of the terrestrial food chain. The method for considering bioaccumulation and persistence when deriving soil standards will feed into the tiered terrestrial ecological risk assessment (ERA) framework 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 IIA of the Environmental Protection Act 1990 to assess the impacts of soil contamination on wildlife top predators; it is also likely to have other uses such as under the Habitats Directive.

Bioaccumulation in, or uptake through, food chain is also of importance when considering human exposure to environmental contaminants. Methods for determining human exposure to chemicals as a result of soil contamination are already available in the Contaminated Land Exposure Assessment (CLEA) approach (Environment Agency and Defra, 2002). However, equivalent methods for determining the exposure to chemicals from other routes, such as the aquatic food chain, are not generally available.

This review was commissioned by the Environment Agency to identify models which can take into account bioaccumulation of organic chemicals when setting environmental standards. The models selected for review in this report are based on the results of an initial evaluation of a large number of possible models. The initial review is given in Appendix D.

Each model is reviewed and scored against a standard set of criteria, which are outlined in Appendix C. The overall score obtained for each model is used to generate

a ranking/grouping in terms of models' predictive ability and overall usefulness for setting standards. The diverse nature of the available models means that, by necessity, the scoring against many of the criteria is subjective and based on expert judgement. Therefore, the overall score should be seen as a guide for selecting the more useful models rather than an absolute ranking of models.

2 Use of bioaccumulation models in standard setting

2.1 Introduction

Until recently, standards for air, water, sediment and soil have generally been based on the potential for effects on organisms directly exposed to the media in question. However, such standards may not necessarily be protective of species that consume the organisms directly exposed, for example top predators such as birds that eat contaminated fish or earthworms. In order to take this into account, it is necessary to consider bioaccumulation through the food chain when setting standards.

A number of frameworks or approaches have been developed for the use of bioaccumulation data in the setting of standards, and the most relevant ones to this project, as identified in the initial review, are discussed in the following sections.

2.2 United States Environmental Protection Agency

The United States Environmental Protection Agency (USEPA) has developed a methodology for deriving ambient water quality criteria (AWQC) for the protection of human health (USEPA, 2000) in relation to Chapter 304(a) of the United States Clean Water Act. A similar approach has also been developed for wildlife criteria for the Great Lakes Water Quality Initiative (USEPA, 1995a; 1995b; Federal Register, 1995).

The methodology for human health considers exposure via the water $\rightarrow$ fish and shell fish $\rightarrow$ humans food chain. The framework is applicable to all types of chemicals, including inorganic and organometallic chemicals. A tiered hierarchy of methods for deriving bioaccumulation factors (BAFs) for the food chain considered is outlined. Some of these methods are applicable to all chemical types, but others (such as the estimation of BAF from biota-sediment accumulation factors (BSAFs)) are only appropriate for non-ionic, moderately to highly hydrophobic chemicals. A flow chart is provided to help select the most appropriate method.

For human health, the AWQC are estimated using the following generalized approach for non-cancer effects (similar equations are also used for cancer effects, assuming either a nonlinear low-dose extrapolation or a linear low-dose extrapolation). The approach considers two main pathways of exposure: the drinking of water obtained from a water body and the consumption of fish/shell fish obtained from that same water body. No treatment of the drinking water is assumed.

$$AWQC = RfD \times RSC \times \left[\frac{BW}{DI + \sum_{i=2}^{4} \left(FI_i \times BAF_i \right)} \right]$$

$$RfD = \frac{NOAEL}{UF \times MF}$$

where *AWQC* = ambient water quality criterion (mg/l) – based on total water concentration.

RfD = reference dose for non-cancer effects (mg/kg bw/day).

RSC = relative source contribution factor to account for non-water sources of exposure. This may be either a percentage or an amount subtracted, depending on whether multiple criteria are relevant to the chemical. A decision tree is provided in USEPA (2000) providing guidance on how this should be done.

BW = body weight (default of 70 kg for adults; other values of 67 kg and 30 kg can be used for pregnant women and children respectively).

DI = drinking water intake (default of two litres per day for adults).

FI_i = fish intake at trophic level i (i = 2, 3 and 4). Defaults for total intake are 0.0175 kg/day for general adult population and sport anglers (broken down as 0.0038 kg/day from trophic level two, 0.0080 kg/day from trophic level three and 0.0057 kg/day from trophic level four), and 0.1424 kg/day for subsistence fishermen. For pregnant women and children, a total fish consumption rate of 0.1655 kg/day and 0.1563 kg/day respectively is recommended.

BAF_i = national bioaccumulation factor at trophic level i (i = 2, 3 and 4).

NOAEL = no observed adverse effect level (mg/kg bw/day). A lowest observed adverse effect level (LOAEL) can also be used, along with an additional uncertainty factor to take account of the LOAEL to NOAEL extrapolation.

UF = uncertainty factor. This includes a factor of one, three or 10 for extrapolation of data from studies using long-term exposure to average healthy humans (to account for intraspecies variation within the human population), an additional factor of one, three or 10 to extrapolate from long-term animal studies to humans (interspecies variation), an addition factor of one, three or 10 when using subchronic studies (to account for the uncertainties involved from subchronic to chronic extrapolation), an additional factor of one, three or 10 when the data represent a LOAEL rather than a NOEAL and an additional factor of three or 10 when an "incomplete" database of tests is available.

MF = modifying factor. This is applied by professional judgment of the uncertainties of the study database not explicitly covered by the uncertainty factors above. The default value is one but values smaller than one and up to 10 can be used.

The national BAF used in the method is estimated for specific water bodies and food chains from a BAF that has been normalized to the lipid content of the organism and the freely dissolved concentration in water (these normalized BAFs are termed baseline BAFs in the methodology), taking into account the percentage of lipid in aquatic organisms commonly consumed by the United States population and the freely dissolved fraction of the chemical that would be expected to occur in ambient waters of interest. Full details of how to carry out these normalizations are given in USEPA (2000). The relationship between the national and baseline BAF is shown below.

National BAF = (baseline BAF $\times$ lipid fraction of organism consumed at trophic level + 1) $\times$ fraction of total chemical that is freely dissolved.

The baseline BAF can be obtained (or predicted) using one or more of the following methods (in decreasing order of priority):

- A measured BAF from a field study.
- A BAF predicted from a field-measured BSAF. This method can be used only for moderately to highly hydrophobic organic chemicals (defined in the procedure as having a log K_{ow} greater than or equal to four). The approach uses reference compounds (for which both a BAF and a BSAF are available) and assumes that the relative BSAFs for two or more chemicals are good indicators of the relative BAFs between the chemicals.
- A BAF predicted from a laboratory-measured bioconcentration factor (BCF). This uses a food chain multiplier (the ratio of a baseline BAF for a particular trophic level to the baseline BCF) to account for uptake via the food chain. These food chain multipliers can either be obtained from field data, or can be estimated from log K_{ow} from the tabulated results of a modelled ecosystem (food chain multipliers are given for trophic levels two, three and four). The model used to develop the food chain multipliers is the food chain accumulation model (Gobas, 1993; see Chapter 8) and considers phytoplankton (trophic level one), zooplankton (trophic level two), forage fish (such as sculpin and smelt; trophic level three) and predatory fish (such as salmonids; trophic level four). The BAF is the resulting product of BCF $\times$ food chain multiplier. Food chain multipliers are typically only used for chemicals with a log K_{ow} greater than or equal to four.
- A BAF predicted from the log K_{ow} value. Again, a food chain multiplier is also used. In this case, the BAF (on a lipid basis) is predicted directly as the product of the K_{ow} $\times$ food chain multiplier. This method is not used when substantial metabolism of the chemical in known to occur. The assessment of the extent of metabolism is made on a case-by-case basis.

The methodology developed for wildlife criteria for the Great Lakes Water Quality Initiative (USEPA, 1995a and 1995b; Federal Register, 1995) is essentially very similar to that outlined above, but this methodology considers also protection of aquatic organisms (based on direct toxicity to aquatic life by exposure via water) and wildlife (assumed to consume aquatic organisms) as well as humans. For wildlife, the following equation is used to estimate a wildlife criteria value.

$$WV = \frac{\dfrac{TD}{UF_A \times UF_S \times UF_L} \times Wt}{W + \sum \left(F_{TLi} \times {}^{WL}BAF_{TLi} \right)}$$

where WV = wildlife criteria value (mg/l)

TD = test dose (mg/kg day) from toxicity test. This value is either a NOAEL or a LOAEL.

UF_A = uncertainty factor for extrapolating toxicity data across all species (value between one and 100).

UF_S= uncertainty factor for extrapolating from subchronic exposure to chronic exposure (value is between one and 10).

UF_L = uncertainty factor for extrapolating from a LOAEL to a NOAEL (value is between one and 10).

Wt = average weight (kg) of wildlife species.

W = average daily volume of water consumed by the wildlife species (l/day).

F_{TLi} = average daily amount of food consumed from trophic level i by the wildlife species (kg/day). Examples are given for mink, otter, kingfishers, herring gull and bald eagle. A general allometric equation is also given for estimating the feeding rate from body weight.

$^{WL}BAF_{TLi}$ = bioaccumulation factor for food in trophic level i (l/kg). This BAF is derived in a similar way as for the national BAFs outlined above. For consumption of piscivorous birds by other birds (such as herring gulls by eagles), the BAF is derived by multiplying the BAF for trophic level three for fish by a biomagnification factor to account for the biomagnification from fish to the consumed bird.

The feasibility of developing AWQCs expressed in terms of concentrations in tissues of aquatic organisms (tissue residue criteria) is currently being evaluated (USEPA, 2000). In addition, the guidance should be developed further in the future to incorporate inhalation and dermal exposure.

2.3 Canadian tissue residue guidelines

Canada has developed a protocol to derive tissue residue guidelines (TRGs) for the protection of wildlife that consumes aquatic biota (Canadian Council of Ministers, 1999). The protocol assumes that for substances that are persistent and bioaccumulative, the main route of exposure for wildlife in aquatic ecosystems is through consumption of contaminated prey species such as fish. Thus, the guidelines are set by defining the level of contaminant in prey fish that would be protective for wildlife consuming food from the aquatic environment (such food could include fish, shellfish, aquatic invertebrates or aquatic plants).

Three assumptions are made in the process:

- dose rates from toxicity studies on mammalian and avian species can be extrapolated to wildlife species using biological data on body weight and food ingestion;
- consideration of ecologically significant endpoints such as reproduction, growth, development and survival of young and adult individuals from toxicity tests in the derivation of the guidelines will also be protective of populations of wildlife species;
- for wildlife, 100 per cent of the exposure to a substance is from aquatic food sources (although adjustment for other routes of exposure may be considered on a site-specific basis).

In order to be protective of all life-stages of species during a lifetime exposure to a substance in aquatic food sources, the dietary TRGs are set to protect the most sensitive life-stage of the most sensitive wildlife species.

A number of steps are involved in the calculation of a TRG, as outlined below.

- Tolerable daily intakes (TDIs), in mg/kg bw/day, are calculated for both mammalian and avian species from the results of oral chronic tests where a sensitive endpoint was measured. The TDI is calculated based on the geometric mean of the LOAEL and NOAEL from the study, using an appropriate uncertainty factor: TDI = $(LOAEL \times NOAEL)^{0.5}$/uncertainty factor.
- The minimum uncertainty factor that can be used is 10, but may be higher depending on the substance and the type, amount and quality of available data. Selection of the uncertainty factor takes into account the type of test data available (if only subchronic studies are available, then an additional uncertainty factor of 10 is applied to allow for subchronic-chronic extrapolation). Similarly, an additional uncertainty factor of 10 or 100 may be used to account for differences in interspecies sensitivity, depending on the quantity and quality of the data available. No uncertainty factor is currently recommended to account for intra-species variability in sensitivity.
- The next step is to calculate reference concentrations for wildlife species using the following equation: Reference concentration = TDI/(food ingestion ÷ body weight), where food ingestion is the rate of food ingestion (kg wet wt/day) and body weight is the body weight of the wildlife species in question. Reference concentrations (units of mg/kg) are estimated for a number of wildlife species (as the lowest TDI will not necessarily result in the lowest acceptable dietary concentration, due to differences in food ingestion and body weight ratios between different species) and the lowest reference concentration is carried forward to the TRG. An extensive collection of body weight and food ingestion data is given in the protocol covering a wide range of wildlife species.
- The final step is to use the lowest reference concentration as the TRG; this is the maximum concentration in aquatic organisms (such as fish) that is protective for wildlife feeding on that aquatic organism. For substances with a high potential to biomagnify within food chains, it is important that the TRG is applied to the highest aquatic trophic level in order to protect wildlife that feeds at that trophic level. This approach is also then protective of wildlife feeding at lower trophic levels.

2.4 The Netherlands

A large amount of work has been carried out in the Netherlands on methods for incorporating bioaccumulation into standard setting. Examples include the work of Everts *et al.* (1993), Jongbloed *et al*. (1994 and 1996) and Traas *et al*. (1996 and 2001). Most of these reports go into the methodology in great detail and so only a brief summary of the main points of the method(s) is given here.

The current methodology used within the Netherlands for deriving environmental risk limits (ERLs), maximum permissible concentrations (MPCs), ecotoxicologically serious risk concentrations (SRC_{eco}s) and negligible concentrations (NCs) for water, groundwater, soil, sediment and air is given in Traas *et al*. (2001). The method involves back-calculating from a “safe” concentration in the food of a predator (bird/mammal) to a concentration in water or soil using an appropriate BCF (for example, fish or mussel for water and earthworm for soil). The methods outlined are similar, in many respects, to those in the EU Technical Guidance Document (See Chapter 3). The basic method is summarised below.

$$NOEC_{water,\ fish\_to\_predator} = \frac{NOEC_{predator}}{BCF_{fish}} \times 0.32$$

$$NOEC_{water,\ mussel\_to\_predator} = \frac{NOEC_{predator}}{BCF_{mussel}} \times 0.20$$

$$NOEC_{soil,\ worm\_to\_predator} = \frac{NOEC_{predator}}{BCF_{worm}} \times 0.23$$

where $NOEC_{water,\ fish\_to\_predator}$ = concentration in water that would lead to the $NOEC_{predator}$ being reached in fish.

$NOEC_{water,\ mussel\_to\_predator}$ = concentration in water that would lead to the $NOEC_{predator}$ being reached in mussels.

$NOEC_{soil,\ worm\_to\_predator}$ = concentration in soil that would lead to the $NOEC_{predator}$ being reached in worms.

$NOEC_{predator}$ = the no effect concentration in diet of predators. These are estimated from laboratory toxicity studies (using appropriate conversion factors to convert by weight concentrations to concentrations in food) using a method very similar to those used in the EU Technical Guidance Document.

BCF_{fish} = fish BCF.

BCF_{mussel} = mussel BCF.

BCF_{worm} = earthworm BCF.

The correction factors of 0.32, 0.20 and 0.23 are based on differences in calorific content between laboratory food and fish, mussels and worms.

The final ERLs can then be estimated using statistical methods (the fifth percentile of the NOECs; also known as the fifth percentile hazardous concentration or HC_5) if sufficient information is available, or by using assessment factors very similar to those used in the EU Technical Guidance Document.

A similar method for water and soil food chains in given in Crommentuijn *et al.* (2000).

Although this method is based on BCF (and so does not account for bioaccumulation through the food chain), a BAF could equally be used in place of the BCF.

Several other methods have been proposed for taking into account bioaccumulation in setting standards. Some of these are summarised below.

Everts *et al.* (1993) described a generic approach that could be used to take into account bioconcentration when setting standards. The method considers a simple food chain of marine water to fish or mussel to bird. Uptake into the fish and mussel is assumed to occur via the water phase (as described by a BCF), and the method takes into account the differences in energy content between laboratory food and field food and in metabolic rates between caged birds and wild birds. The method requires the BCF for mussels and/or fish, the energy content of laboratory food used in toxicity tests with the chemical, the energy content of the prey species (fish or mussels), and the metabolic rate of the wild bird species under normal conditions and conditions of peak activity. The basis of the method is outlined below.

The first step is to define a $NOEC_{prey}$ from a $NOEC_{lab\ food}$ derived from a bird-feeding study using laboratory food.

$$NOEC_{prey} = NOEC_{lab\ food} \times \frac{E_{prey}}{E_{lab\ food}} \times \frac{EMR_{test\ bird}}{FMR_{species\ of\ concern}} \times \frac{FMR_{normal\ conditions}}{FMR_{peak\ activity}}$$

where $NOEC_{prey}$ = no effect concentration in diet for bird eating prey (fish or mussels).

$NOEC_{lab\ food}$ = experimental no effect concentration in diet for bird eating a laboratory diet.

$E_{lab\ food}$ = energy content of laboratory food (kJ/kg) (a value is given for grain fodder).

E_{prey} = energy content of prey (kJ/kg) (values are given for sprat, herring, mackerel, smelt, trout, turbot, cod, shrimp, mussel, amphipods and insect larvae).

$EMR_{test\ bird}$ = existence metabolic rate of laboratory bird used in toxicity test (kJ/day per animal).

$FMR_{species\ of\ concern}$ = field metabolic rate for bird species of concern under normal field conditions (kJ/day per animal).

$FMR_{peak\ activity}$ = field metabolic rate at peak activity (kJ/day per animal) – applied if extrapolating to peak activity.

$FMR_{normal\ conditions}$ = field metabolic rate under normal conditions (kJ/day per animal) – applied if extrapolating to peak activity.

The equivalent concentration in water (MPC) can then be estimated by dividing the $NOEC_{prey}$ by the BCF for the prey species (fish or mussel).

Although this method is based on BCFs, a similar approach could also be constructed based on ecosystem BAFs. Similarly, the approach could also be applied to mammals. For example, Traas *et al*. (1996) extended the approach to consider top predators in more complex food webs, for example soil to food (plants, earthworms, insects) to birds and mammals. This method requires the overall BAF for the food of the species of concern (relating the concentration of chemical in the foodstuff to the concentration of chemical in soil), as well as the energy contents of the various laboratory and field foods and the metabolic rates of the laboratory and mammalian species being considered. The approach presented consists of five steps, as follows.

- The first step is to extrapolate NOECs from laboratory studies to NOECs for species in the wild using correction factors (in a similar way as done above for the aquatic food chain) including metabolic rates, calorific content of food, food assimilation efficiency, pollutant assimilation efficiency and species sensitivity.
- The species NOECs are used to construct uncertainty distributions.
- Different food webs are used to calculate the difference in exposure of top predators with different feeding habitats (BAFs for different food chains) and these are used to construct uncertainty distributions.

- Possible MPCs are calculated (NOEC/BAF) by random sampling of these distributions (the BAF used is calculated by sampling the BAFs for the different prey items in the food web and weighting these BAFs according to the diet composition of the predator). The fifth percentile MPC (MPC_5) is then determined from the MPC distribution. This value is regarded as a "safe" level.
- An uncertainty analysis (Monte-Carlo simulation) is then undertaken to identify the parameters that contribute most to the model uncertainty.

Examples of this model were applied to cadmium (Traas *et al*., 1996; Jongbloed *et al.,* 1996) and DDT (Jongbloed *et al*., 1996).

This method requires BAF data (and metabolic data) to be available for a number of food chains and so would probably only be useful for data-rich substances for which many field BAFs are available. The data are used to define statistical distributions, to allow an MPC_5 to be estimated. However, it would be possible to use a similar scheme with less BAF data, where uncertainties within the MPC in relation to different species were accounted for by uncertainty factors, rather than addressed statistically.

Jongbloed *et al.* (1994) developed a simplified terrestrial food web that could be used for deriving MPCs. The authors performed calculations for six compounds (DDT, dieldrin, lindane, pentachlorophenol, cadmium and methyl mercury). The food web has three trophic levels: plants and invertebrates at level one, small birds and mammals at level two and birds and beasts of prey at level three. The method used is similar in principle to that outlined by Traas *et al*. (1996), in that correction factors (for calorific content and assimilation efficiency of food and metabolic rate of birds/mammals) are applied to NOECs to account for differences between laboratory and field conditions; probability distributions are then generated for MPCs by treating BCFs, BAFs and NOECs as stochastic variables. The method considers the relevant food chains for eight bird of prey species (sparrowhawk, goshawk, buzzard, kestrel, long-eared owl, tawny owl, barn owl and little owl) and two beasts of prey (badger and weasel).

Again, the data requirements of this method make it most useful for data-rich substances. However, the method does include the following regression equations, developed by Garten and Trabalka (1983) for estimating BAFs for uptake from food into the fat of ruminants and birds. These equations may be useful for other methods, although r^2 values are generally low, meaning that correlations are relatively poor.

For food $\rightarrow$ ruminant fat

$$\log BAF = -3.935 + 0.511 \times \log K_{ow} \qquad r^2 = 0.34, \; N = 66$$

For food $\rightarrow$ non-ruminant fat

$$\log BAF = -3.849 + 0.617 \times \log K_{ow} \qquad r^2 = 0.35, \; N = 56$$

For food $\rightarrow$ poultry fat

$$\log BAF = -2.743 + 0.542 \times \log K_{ow} \qquad r^2 = 0.54, \; N = 47$$

Log K_{ow}s of the substances used in this study were in the range -3.05 to 7.05.

2.5 United Kingdom: CLEA

Methods for determining the exposure of humans to chemicals in the United Kingdom as a result of soil contamination are already available in the CLEA approach (Environment Agency and Defra, 2002). The CLEA approach estimates child and adult exposures to soil contaminants for those potentially living, working and/or playing on contaminated sites over extended timeframes; the method is used to set soil guideline values (SGVs) for the protection of these populations within the United Kingdom. The routes of exposure considered in the CLEA model include the ingestion of contaminated soil, inhalation of contaminated dust and vapour, absorption of the contaminant through skin and from ingestion of home/allotment-grown vegetables grown on contaminated land. A detailed review of the CLEA model is beyond the scope of this project. Similarly, other models that primarily cover these routes of exposure, such as CalTOX[1] and CSOIL[2], are not considered here.

2.6 Consideration of internal body concentration

A developing area of assessment is the internal concentration (Escher and Hermens, 2004). So far, such approaches have focused on acute toxicity in aquatic organisms for substances that act by non-polar or polar narcotic mechanisms. For narcotic chemicals, whole-body internal concentrations can be used to express toxicity as, for this type of chemical, all biological membranes within the organism are affected by the chemical (the first symptom is disturbed transmission of nerve cell signals); furthermore, lethal body burdens in a given species have been shown to be relatively constant for a wide variety of compounds (Escher and Hermens, 2004).

The method is essentially an extension of the critical body burden (CBB) method that assumes that effects occur in an organism when the total body burden of a chemical reaches a certain threshold level. Such approaches have so far been applied mainly to narcotic chemicals in aquatic organisms (fish, invertebrates and algae) and are known under a variety of names, such as internal effect concentration (IEC; Traas *et al*., 2004) and the target lipid model (TLM; McGrath *et al.*, 2004, Di Toro *et al.,* 2000). In TLM and IEC, the threshold level is expressed in terms of a concentration in the target lipids rather than a total body burden.

The basis of the method is that the target lipid is the site of toxic action within an organism, and has similar physico-chemical properties in all organisms (similar properties to n-octanol). This implies that the slope of a plot of log $L(E)C_{50}$ against log K_{ow} should be the same for all species, but the intercept will vary from species to species, depending on the body burden of target lipids in each species. Such relationships have been shown to hold for acute toxicities for a range of aquatic species; Di Toro *et al.* (2000) identified 33 species including fish, amphibians, arthropods, molluscs, polychaetes, coelenterates and protozoans, and McGrath *et al.* (2004) found the same for five species of algae. The relationships hold for chemicals up to log K_{ow} of around 5.3; at higher log K_{ow}s, decreasing aqueous solubility means that insufficient chemical can be taken up from water to reach the toxic threshold level.

The general approach adopted in the TLM and IEC methods uses the relationships between log $L(E)C_{50}$ and log K_{ow} to generate a distribution of $L(E)C_{50}$ for each chemical covering a number of species, and to use this distribution to estimate a fifth percentile

[1] CalTOX is a human exposure model for hazardous waste sites in the United States. Details are available at http://www.dtsc.ca.gov/ScienceTechnology/caltox.html.

[2] CSOIL is a generic exposure model for humans in the Netherlands exposed via contaminated soil. It covers similar routes of exposure as the CLEA model. Details are available in van den Berg (1995), Lijzen *et al*. (2001), Rikken *et al.* (2001) and Rikken and Lijzen (2004).

value for the acute L(E)C_{50} for all species – usually called a HC_5 (McGrath *et al*., 2004; Traas *et al*., 2004). An acute to chronic ratio (usually determined from known acute to chronic ratios for similar chemicals) is then applied to this value to estimate a fifth percentile value for the long-term NOEC for all aquatic species. This value is then assumed to be protective of 95 per cent of all aquatic species.

Traas *et al.* (2004) coupled the IEC approach with a food web model in order to determine environmental quality criteria (EQC). The food web model used was based on Thomann (1989) (see Chapter 11) and Campfens and Mackay (1997) (see Chapter 6) and consisted of a sediment compartment, a water compartment and various organisms including tubificids, chironomids, algae, zooplankton, bivalves, roach, bream, whitebream, eel, perch, ruffe and pike. The model was calibrated using field data on PCBs from the Netherlands and verified using field data on PCBs from Denmark. The model was used to estimate food web BAF or BSAF for each species. These were then used with the fifth percentile IECs based on chronic NOEC data to estimate an EQC for each species in the food web, using the following equations:

$$EQS_{water} = \frac{IEC}{BAF}$$

$$EQS_{sed} = \frac{IEC}{BSAF}$$

For substances that act by specific modes of action, the method would require knowledge of, or an estimate of, the internal organ-specific concentration of the substance rather than the whole body concentration (Escher and Hermens, 2004).

From a regulatory standpoint, it is evident that further work would be necessary to develop this concept for a wider range of chemical types and organisms other than aquatic organisms. However, the approach does appear to be useful, in that exposures of an organism from several sources can be taken into account.

3 EU Technical Guidance Document

3.1 Introduction

The Technical Guidance Document (European Commission, 2003) is used for the risk assessment of both new and existing substances (and also biocides) within the EU. The Technical Guidance Document is frequently abbreviated to TGD. The TGD contains a detailed description of methods (including the necessary equations) to carry out an in-depth risk assessment considering exposure of aquatic organisms, wildlife and humans to a chemical through environmental pathways. The methods within the TGD are also implemented in a computer program called EUSES (European Uniform System for Evaluation of Substances). Both the TGD and EUSES are available free of charge via the internet[3].

3.2 Description of model

The TGD method uses the concentrations in air and soil and the dissolved concentration in surface water and marine water as inputs. These can either be estimated using the TGD method/EUSES or can be input as known concentrations. The method allows the calculation of concentrations at two spatial scales: the local scale (which represents concentrations in the vicinity of a point source of release) and a larger, regional scale. The method takes into account degradation in soil, water, sediment and air. The main routes to soil considered are the application of sewage sludge and aerial deposition.

The chemical-specific parameters used in the calculations of air, soil and water concentrations are:

- log K_{oc}, the organic carbon-water partition coefficient, and log K_{ow} , the octanol-water partition coefficient (the method can calculate log K_{oc} from log K_{ow} in the absence of data); these govern the partitioning behaviour between water and solid phases;
- Henry's law constant (which can be estimated from water solubility and vapour pressure); this governs the partitioning behaviour between water and air;
- the degradation rate constant or half-life for water, sediment, soil and air, which can include both biotic and abiotic degradation; default methods are given for estimating rate constants for biotic degradation based on the results of standard biodegradation screening tests.

The method also takes into account loss from soil by volatilization and leaching. A standard environmental temperature of 12°C is assumed (9°C for the marine environment) and properties (such as size, water content, rainfall, organic carbon content) of the environmental compartments used in the model are based on typical European values. A standard set of properties are assumed for the soil and sediment phases; these are an organic carbon content of 10 per cent for suspended sediment,

[3] See http://ecb.jrc.it/existing-chemicals/.

five per cent for bulk sediment and two per cent for soil. These properties are important to the assumed partitioning behaviour of a substance in these phases.

All default properties used in the method could be easily adapted to other situations.

Concentrations in air, surface water, marine water and soil are used as the basis for estimating concentrations in various food chains. These include an aquatic food chain (both freshwater and marine), a terrestrial food chain (earthworms) and the human food chain. The methods used for estimating the uptake of chemicals in these food chains are described below.

3.2.1 Aquatic food chain

Transfer from water to fish is estimated using the fish bioconcentration factor (BCF_{fish}). If available, an experimental value for BCF_{fish} can be used but, in the absence of experimental data, BCF_{fish} can be estimated from the log K_{ow}.

Two equations are given in the TGD for estimating BCF_{fish}. The first was developed by Veith *et al.* (1979) and is applicable for substances with a log K_{ow} in the range of one to 6.89. The equation (relating log BCF_{fish} to log K_{ow}) was derived from experimental data for 55 substances including halogenated compounds, phosphate esters, phenolic compounds, aromatic compounds and amines. The correlation coefficient (r^2 value) of the derived equation is 0.897. According to the TGD, this equation has been validated externally using BCF data for 267 substances. The root mean square error of the prediction was 0.58 for a log K_{ow} below six.

The second is a parabolic equation (again relating log BCF_{fish} to log K_{ow}) recalculated from work published by Connell and Hawker (1988) and is applicable for substances with a log K_{ow} greater than six. The chemicals considered in the Connell and Hawker (1988) paper were mainly chlorinated aromatic hydrocarbons (the total number of chemicals was 42 and included two non-halogenated aromatics and two chlorinated alkanes) with a log K_{ow} in the range 2.6 to 9.05. The r^2 value of the derived equation presented in the TGD is 0.78.

According to the TGD, both equations are applicable to substances with a molecular weight (MW) below 700 g/mole.

In order to take into account possible uptake via food as well as water, the calculation method in the TGD introduces a biomagnification factor (BMF). In this case, BMF is defined as the relative concentration in a predatory animal compared to the concentration in its prey, and the BMF should, wherever possible, be a lipid-normalised value.

In cases where measured BMF data are not available, a default value for the BMF can be assigned based on either the log K_{ow} or the BCF_{fish}. These default values range between one and 10, and reach a maximum at a log K_{ow} of between five and eight and then decrease again with increasing log K_{ow} (see below).

log K_{ow} < 4.5 or BCF_{fish} < 2,000 l/kg	– BMF = 1
log K_{ow} 4.5-5 or BCF_{fish} 2,000-5,000 l/kg	– BMF = 2
log K_{ow} 5-8 or BCF_{fish} > 5,000 l/kg	– BMF = 10
log K_{ow} 8-9 or BCF_{fish} 2,000-5,000 l/kg	– BMF = 3
log K_{ow} > 9 or BCF_{fish} < 2,000 l/kg	– BMF = 1

For the marine environment, a longer food chain is considered. The approach first considers a predator eating fish (as above) and then a top predator eating a predator. Thus, two BMF values (termed BMF_1 and BMF_2) are considered. Again, in the absence of experimental data for the BMF, default values can be assigned based on the log K_{ow} or the BCF_{fish} value. These default values again range between one and 10 (for both BMF_1 and BMF_2) and reach a maximum at a log K_{ow} of between five and eight (see above).

The aquatic food chain model included in the TGD is relatively simplistic (and precautionary in relation to the relatively high BMFs applied by default in some cases). Furthermore, it is difficult to use actual BMF data within the scheme as presented, although this can be done with some relatively simple modifications to the calculation method (Brooke *et al.,* 2003). Thus, the approach is more of a screening approach than a true bioaccumulation model. However, it would be possible to incorporate other aquatic food chain models discussed in this review (or actual BMF or BAF data). This is explored further in Chapter 15

3.2.2 Terrestrial food chain

The terrestrial food chain considered in the TGD is the transfer from soil to earthworms, which are then assumed to be food for the target species (mammals or birds).

The method involves the use of an earthworm bioconcentration factor ($BCF_{earthworm}$). In the absence of experimental data, this is estimated by the method described by Jager (1998) assuming that the bioconcentration process involves equilibrium partitioning between the soil pore water and phases within the earthworm. The model used was supported with experimental data from neutral organic chemicals both in soil (log K_{ow} range three to eight) and water-only experiments (log K_{ow} range one to six), and the recommended range of applicability of the method is given as log K_{ow} between one and eight.

The equation was found to predict well the uptake of chemicals by worms in water phase-only experiments (the equation used had a r^2 value of 0.90 when fitted to data for water phase-only exposure for 11 substances), but the equation was found to systematically overpredict the uptake from soil pore water in experiments with soils.

The overall concentration in the food (earthworm) of a predatory mammal or bird is estimated assuming that, as well as uptake from the soil pore water, the earthworm also contains contaminated soil in the gut.

Other similar, but more recent, earthworm bioaccumulation models are available, for example Jager (2003), Jager *et al.* (2003) and Jager (2004). These models could be incorporated into the existing TGD framework relatively easily.

3.2.3 Human food chain

The TGD assumes that humans are exposed to chemicals via air (inhalation), drinking water and food (fish, root crops, leaf crops, meat and milk).

Drinking water

The TGD assumes that drinking water is obtained from either surface water or groundwater. It assumes that drinking water undergoes treatment in one of two

systems (either storage in open reservoirs or dune recharge). The method assumes complete removal of suspended particulates during treatment and models the removal of dissolved fractions of chemicals by means of purification factors based on Hrubec and Toet (1992). These purification factors take into account the log K_{ow} , Henry's law constant and the aerobic biodegradation rate in a simple way. For groundwater, it is assumed that the purification system used has no effect on the concentration of the chemical.

The highest concentration estimated in either groundwater or drinking water derived from surface water is used for the human exposure estimate.

Fish

Concentrations in fish are estimated using BCF_{fish} as described above. However, calculations only consider uptake by fish from water (the BMF is not considered).

The chemical-specific parameters used in the method are the BCF_{fish} or, in the absence of actual data, the log K_{ow}.

No species-specific data are used.

Plants

The method takes into account uptake into plants from both soil (pore water) and air, and is based on the approach proposed by Trapp and Matthies (1995) which is a simplified version of the four compartment PLANTX model (Trapp, 1995).

The overall model is a one compartment differential mass-balance model that could be used to estimate the concentration in a plant leaf at given time points (root tissue concentrations are estimated using an equilibrium model). The method implemented in the TGD represents the steady-state solution of the model. The key assumptions in the model are as follows:

- the partitioning between water and plant tissue can be described by sorption to plant lipids;
- the concentration in root tissue is governed mainly by physical sorption;
- the transpiration stream concentration factor (TSCF), which is the ratio of the concentration in the transpiration stream to the concentration in pore water, can be estimated using the method of Briggs *et al.* (1982);
- gaseous exchange can be described by leaf-air partitioning;
- the model takes into account growth dilution (it could also take into account removal by metabolism and photolysis if data were available);
- uptake via the leaves only occurs for gaseous-phase substances (particulate/aerosol deposition onto plant surfaces is not accounted for).

The main chemical-specific information required by the method is the log K_{ow}. The method can also incorporate removal processes such as metabolism and photolysis (if no data are available, it is assumed that no removal occurs by these processes).

The plant-specific properties assumed in the method include the volume fractions of water, lipids and air in plant tissue, the bulk density of plant tissue, leaf surface area, conductance, shoot volume, transpiration stream flow, a correction term for differences between plant lipids and octanol, and the growth rate constant for dilution by growth.

The default values used are taken from *Brassica oleracea* (first four parameters; values based on Riederer (1990)) or the suggested values for soybean plants (*Glycine max*) from Trapp and Matthies (1995) (remaining parameters).

The Briggs *et al.* (1982) method was derived from experimental data for two series of non-ionised pesticides: O-methycarbomoyloximes (a total of nine substances) and substituted phenylureas (a total of nine substances) in barley (*Hordeum vulgare*). The chemicals covered the log K_{ow} range of -0.5 to 4.5. The method was derived by fitting a Gaussian curve to the experimental data for 17 out of the 18 chemicals tested.

The overall approach was not tested fully by Trapp and Matthies (1995), although some example calculations were given but, according to the TGD, the original PLANTX model has been validated in short-term experiments. Thus, the reliability of predictions from the TGD method is not clear.

Other, similar plant models could equally be used in this approach. Examples include Calamari *et al.* (1987), Schramm *et al*. (1987), Ryan *et al.* (1988; this is the model currently used in CLEA for uptake from contaminated land into home/allotment-grown vegetables), Patterson *et al*. (1991a, 1991b and 1994), Müller *et al.* (1994), Hung and Mackay (1997), Trapp *et al*. (1990 and 2003), Trapp and Matthies (1998) and Trapp (2000, 2002 and 2004). Similarly, Dowdy and McKone (1997) derived a regression equation for predicting plant uptake of organic chemicals from soil or air using the octanol-water or octanol-air partition coefficient or the molecular connectivity index. In addition, a review of plant uptake models for potential use with CLEA has recently been undertaken by the Environment Agency (Collins *et al.,* 2004). As this report is still in draft, the conclusions are not yet publicly available, but it is likely that the model recommended by this review could be incorporated into the general TGD approach.

Meat and milk

Concentrations in meat and milk are estimated by means of steady-state biotransfer factors (BTF), defined as the concentration in meat or milk divided by the animal's daily intake of the substance in source media (air/grass/soil/drinking water), using the method of Travis and Arms (1988).

Travis and Arms (1988) derived regression equations relating the steady-state log BTF for meat (cattle) and milk to log K_{ow}.

Thirty six chemicals (mainly chlorinated pesticides) were used to generate the regression equation for meat. The log K_{ow} range of the chemicals considered was 1.34 to 6.89. The r^2 value of the regression was 0.81.

Twenty eight chemicals (again mainly chlorinated pesticides but also including naphthalene and naphthol) were used to generate the regression equation for milk. The log K_{ow} range of the chemicals considered was 2.81 to 6.89. The r^2 value of this regression was 0.74.

No further validation of the method was carried out by Travis and Arms (1988).

The main chemical-specific information required by the method in the TGD is the log K_{ow}. In the method, the intake estimated from milk is assumed to represent intake from dairy products in general.

The species-specific information required by the method includes the daily intake (on a wet weight basis) for cattle of grass, soil, air and drinking water. Default values for these parameters are given.

Other methods are available for estimating the BTF from food into cattle (beef) and milk that could be incorporated into the TGD approach. For example, Dowdy *et al*. (1996) presented a regression equation relating the biotransfer factor to the molecular connectivity index of a chemical.

Total daily intake

The total daily intake for humans is estimated as the sum of the doses from the above sources. The key assumptions made include the following (based on data for the EU):

Bioavailability of the chemical through inhalation = 0.75.

Bioavailability of the chemical through oral route = 1.

Body weight of human considered = 70 kg.

Daily intake of drinking water = 2 l/day.

Daily intake of fish = 0.115 kg wet wt/day.

Daily intake of leaf crops = 1.20 kg wet wt/day.

Daily intake of root crops = 0.384 kg wet wt/day.

Daily intake of meat = 0.301 kg wet wt/day.

Daily intake of dairy products = 0.561kg wet wt/day.

Inhalation rate = 20 m^3/day.

3.3 Summary of the TGD method

The main points of the TGD method are summarised in Table 3.1.

Table 3.1 Summary of the TGD method

Criteria	Comment
Structure of the method	The method is outlined in a series of equations given in the TGD, and is also available as an integrated computer program (EUSES).
Scope of the method	The method is intended to be used in the risk assessment of new and existing chemicals and biocides within the EU. The method considers the exposure of predators via a freshwater food chain, a marine food chain and a terrestrial food chain, and the exposure of humans via food (fish, meat, milk, root crops, leaf crops), drinking water and air. The method is intended to be applicable to many types of organic chemicals. However, the validity of some parts of the method have only been established over certain ranges, for example: • estimation of fish BCF – log K_{ow} 2 to > 6, MW < 700 g/mole; • estimation of earthworm BCF – log K_{ow} 1 to 8 (neutral organic chemicals); • estimation of meat BTF – log K_{ow} 1.34 to 6.89 (mainly chlorinated pesticides); • estimation of milk BTF – log K_{ow} 2.81 to 6.89 (mainly chlorinated pesticides); • estimation of TSCF – log K_{ow} -0.5 to 4.5 (O-methycarbomyloximes and substituted phenylureas).
Type of method	Steady-state calculations.
Calculation method	Computer program. Many of the calculations can also be performed by hand if required.
Outputs from the method	Concentration in freshwater fish (mg/kg wet wt). Concentration in marine fish (mg/kg wet wt). Concentration in earthworms (mg/kg wet wt). Concentration in root crops (mg/kg wet wt). Concentration in leaf crops (mg/kg wet wt). Concentration in meat (mg/kg wet wt). Concentration in milk (mg/kg wet wt). Concentration in drinking water (mg/l). Total daily human intake (mg/kg bw/day).
Focus of the method	The method does not focus specifically on sensitive groups (such as children or young animals) but could be adapted to do so.
Chemical-specific input parameters	Physico-chemical properties, in particular log K_{ow} and Henry's law constant (or water solubility and vapour pressure). Fish BCF (can be estimated from log K_{ow}). BMF, preferably lipid-normalised (default value can be estimated from log K_{ow} ; currently difficult to incorporate measured BMF values). Organic carbon-water partition coefficient (can be estimated from log K_{ow}). Biodegradation rate constants or half-lives in surface water, sediment and soil (can be estimated from the results of standard biodegradation tests). Abiotic degradation rate constants or half-lives in surface water, air and so on (optional). Metabolic half-life or rate constant in plants (optional).
Key default parameters used in the method	The key default parameters are the organic carbon content of the soil and sediment phases, and also BMF if no measured value is available. All default parameters can be easily adapted within the method. The default parameters were chosen to be representative of the situation within Europe and so are relevant to the situation within the United Kingdom.
Environment considered	The method considers a "generic European environment" consisting of surface water, sediment, soil, air compartments and a marine compartment.

Criteria	Comment
How is persistence considered?	Persistence is considered in relation to the estimation of concentrations in water, sediment, soil and air. In addition, metabolism can be considered in relation to uptake into plants. The other food chains do not explicitly allow metabolism data to be used (although the methods are derived from experimental data which would have included any metabolism in the results).
Are seasonal variations considered?	No. The method considers an average temperature and an average rainfall. It would be possible to use other values for these.
Strengths	Widely used within Europe for regulatory purposes.
Weaknesses and limitations	Some parts of the model (particularly the uptake from soil by plants and the treatment of biomagnification in the aquatic food chain) are best seen as screening assessments. The food chain considered for the aquatic environment is relatively simple compared with some other methods. The earthworm part of the model may systematically overpredict the concentration in earthworms.
Could the model be adapted to the UK situation?	The method is already in use in the UK for certain regulatory purposes. It would be relatively easy to further adapt the method for specific situations in the UK.
Further work	The aquatic food chain considered in this method is relatively simplistic compared with some other methods; the treatment of biomagnification in particular is relatively crude and can be considered a worst case approach in the absence of actual BMF data. Furthermore, it is difficult to use some types of experimental data within this framework and thus, the approach should be viewed as a screening method. Further development of this area in particular would be needed for setting standards (for example, by incorporating a more realistic bioaccumulation model for the aquatic food chain). The method used for the prediction of concentrations in fish for human consumption only considers uptake of the chemical by fish directly from water (bioconcentration). This method would need to be developed further to incorporate other bioaccumulation processes (for example, uptake from food through the aquatic food chain). The plant uptake approach is different from that used currently within the CLEA method. It would be relatively easy to incorporate other models for uptake of chemicals by plants into the overall approach.

3.4 Evaluation against screening criteria

3.4.1 Data requirements

The model requires relatively simple physico-chemical properties that are usually available (or can be easily estimated). More complex data (such as actual BCFs, BTFs, plant metabolism data) can be used in the scheme if available. A score of three is appropriate. The importance rating for this criterion is five. Therefore,

$SCORE_{DATA} = 3 \times 5 = 15$.

3.4.2 Model calibration

The scoring of this parameter is a little complicated. Although the TGD is intended to be applicable to a wide range of chemical types, it is apparent that some of its underlying assumptions have only been calibrated using data for a defined range of chemical types. In this respect, the estimation of the TSCF is probably the limiting factor for the upper end of the log K_{ow} range (log K_{ow} 4.5) and the BTF for milk is probably the limiting factor for the lower end of the log K_{ow} range (log K_{ow} 2.81). On this basis, the overall TGD method is only strictly applicable to organic substances with a log K_{ow} in the range 2.81 to 4.5. However, many of the estimation methods (when considered in isolation) have a much wider range of applicability, particularly in relation to substances with a log K_{ow} of one and above. Therefore, a score of two is considered appropriate. The importance rating for this criterion is five. Therefore,

$SCORE_{CALIBRATION} = 2 \times 5 = 10$.

3.4.3 Model validation

Similar to model calibration, only parts of the overall method have been validated. For example, the plant model has been validated in short-term experiments whereas the meat and milk parts of the model, although based on experimental datasets, have not been further validated, and the BMF part for aquatic food chains has not been validated. This makes it difficult to give a meaningful score for the model as a whole. Based on the criteria outlined in Appendix C, an overall score of two is considered appropriate. The importance rating for this criterion is five. Therefore,

$SCORE_{VALIDATION} = 2 \times 5 = 10$.

3.4.4 Ease of use

The model is available in a format that requires some experience/knowledge to use and would require some interpretation of the results for use in setting standards. The score for this criterion is therefore two. The importance rating for this criterion is two. Therefore,

$SCORE_{EASE} = 2 \times 2 = 4$.

3.4.5 Transparency

The underlying methods used in the model are clear and so a score of three is appropriate. The importance rating for this criterion is five. Therefore,

$SCORE_{TRANS} = 3 \times 5 = 15$.

3.4.6 Prediction uncertainty

Based on expert judgement, the model has moderate uncertainty and relies to some extent on conservative or precautionary approaches and so a score of two is appropriate. The importance rating for this criterion is five. Therefore,

$SCORE_{UNCERT} = 2 \times 5 = 10$.

3.4.7 Ability to predict the concentration near the top of the food chain

The model allows predictions of concentrations in two or less trophic levels near the top of the food chain and so a score of two is appropriate. The importance rating for this criterion is four. Therefore,

$SCORE_{TOP\ FOOD} = 2 \times 4 = 8$.

3.4.8 Relevance to England and Wales

The model is a generic model for Europe and so is directly relevant to England and Wales. It is also relatively easy to adapt the model for specific situations in England and Wales. A score of three is therefore appropriate. The importance rating for this criterion is four. Therefore,

$SCORE_{RELEVANCE} = 3 \times 4 = 12$.

3.4.9 Overall score

Using the methodology outlined in Appendix C, the overall score can be estimated as follows:

$$\text{TOTAL SCORE} = SCORE_{DATA} + SCORE_{CALIBRATION} + SCORE_{VALIDATION} + SCORE_{EASE} + SCORE_{TRANS} + SCORE_{UNCERT} + SCORE_{TOP\ FOOD} + SCORE_{RELEVANCE}$$

$$= 15 + 10 + 10 + 4 + 15 + 10 + 8 + 12$$

$$= 84.$$

4 ACC-Human model

4.1 Introduction

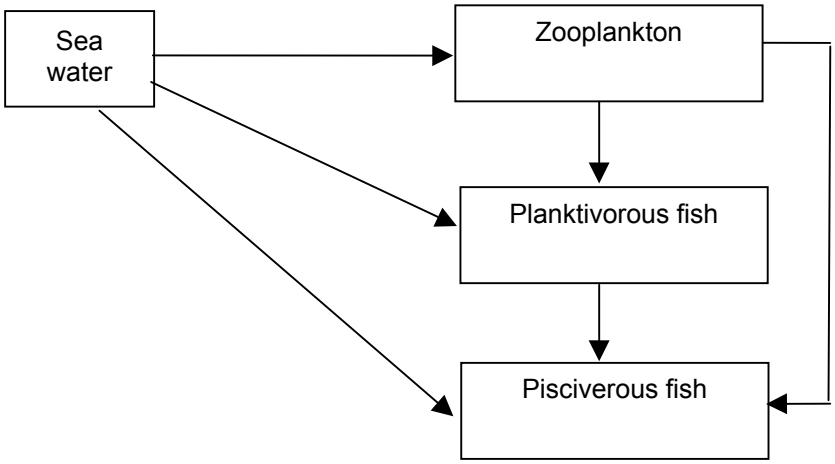
The ACC-Human model is a food chain model for predicting the levels of lipophilic organic chemicals in humans. The model was published in a paper by Czub and McLachlan (2004) and a computerised version is available for download from the Stockholm University website[4]. The model was developed for research purposes and does not appear to have been used as yet in a regulatory context.

4.2 Description of model

The model is a fugacity-based, non-steady state, mechanistic model that considers the bioaccumulation of lipophilic organic chemicals by humans exposed through air, water, soil and food. The model incorporates recent advances in the scientific understanding of bioaccumulation processes in agricultural and aquatic food chains, as well as in humans. The model predicts human tissue levels, as well as levels in various other parts of the food chain, from concentrations of a chemical in air, water and soil.

Within the model a representative food chain is constructed for an agricultural soil system and a marine water system. The top predator in each system is considered to be humans. Each link in the food chain is treated as being composed of one or several homogenous compartments (for example, mammals are assumed to consist of water and lipid phases) that are assumed to be in equilibrium with each other. As the fugacity capacity is generally sensitive to temperature, the calculations are carried out at 37°C for mammals and ambient temperatures for plants and poikilothermal animals. Each link in the food chain is interconnected with the appropriate abiotic environmental compartments (air, water, soil) and the next link below it in the food chain. A mass balance is defined for each compartment and these first-order differential equations are solved in a step-wise fashion based on a set of initial and boundary conditions.

For the marine water system, the model assumes a simple pelagic food chain consisting of zooplankton, planktivorous fish and pisciverous fish as follows. It is assumed that the main fish species harvested for human consumption (such as herring and cod) feed little on benthic organisms.

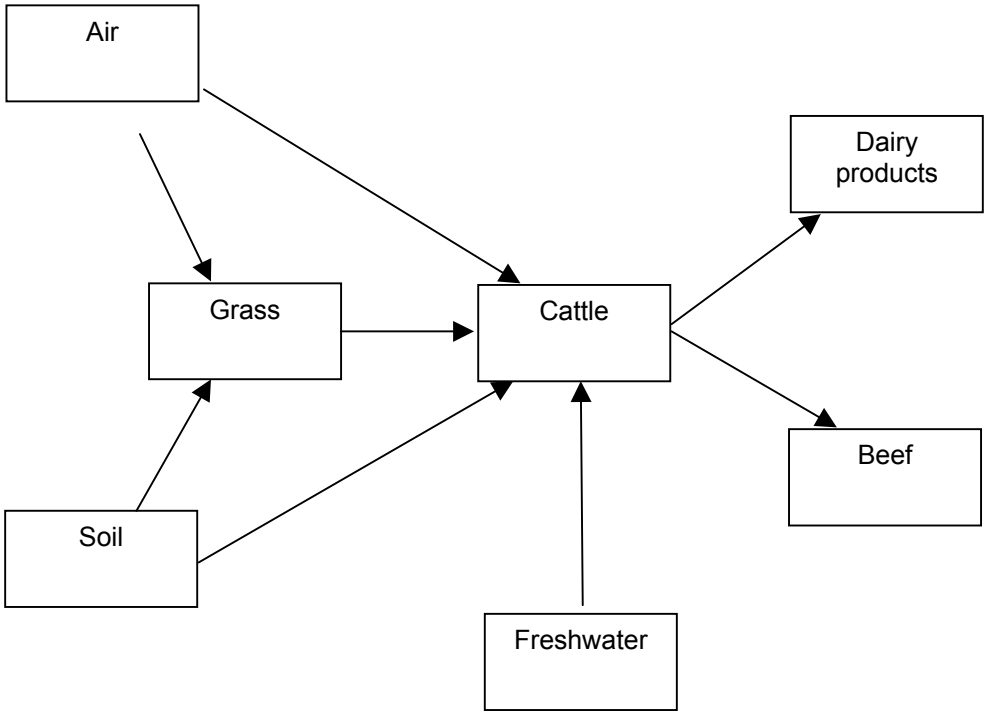


[4] http://www.itm.su.se/research/model.php

The concentration of chemical in zooplankton is assumed to be in equilibrium with the concentration in marine water. For fish, the bioaccumulation is described using a non-steady state model based on the model developed by Gobas *et al*. (1988) and is similar in principle to the Foodweb model (see Chapter 6, although the Foodweb model is solved at steady state). The fish model considers uptake both from water and food, and metabolism of the chemical by the fish. For both piscivorous fish and planktivorous fish, ten different age classes are represented within the model. Thus the model assumes that on the 1st March each year, the fish enters the next age class and a new generation is created, initially as eggs. The initial fugacity of the fish/eggs is assumed to be equal to the fugacity of the mother fish; for model initiation (when there are no mother fish), the initial fugacity of the eggs is assumed to be equal to the fugacity of the water. Uptake of the chemical by fish from food is dependent, amongst other things, on the food consumption rate. Within the model, the food consumption rate is defined for each fish species, age and season. Thus, the model can be used to investigate accumulation of chemicals over successive generations of fish, and can take into account seasonal differences in food consumption behaviour.

The model is intended to represent the main pathways for human exposure in northern Europe, where consumption of shellfish is a minor source of human exposure compared to fish.

The agricultural system considers beef and dairy products in the following food chain.



Grass is the main pathway used in the model to represent exposure of cattle to the chemical. The model assumes that transfer of the chemical to grass can occur from the atmosphere and from soil. The grass model uses a mass balance approach to describe uptake in a one m^2 plot of pasture land. Atmospheric deposition of both gaseous and particle-bound contaminants are considered. The gaseous uptake is modelled using a two-resistance model as developed by Riederer (1990). The deposition of aerosol-associated chemical is calculated using an average net deposition velocity. Root uptake into the plants is treated as an inflow of soil pore water equal to the grass transpiration rate, which is corrected for by the transpiration

stream concentration factor based on the work of Briggs *et al*. (1982); a similar approach is used in other plant models such as the TGD (see Chapter 3).

The model assumes that grass can be harvested up to five times per year during the growing season (the length of the growing season, the time points of harvest, and the yield of each harvest can be user-specified). The model then calculates the yield-weighted mean contaminant concentration in the harvested grass after the last harvest and this is used as the concentration in cattle feed for the following 12-month period. The soil content of the feed is also taken into account.

The milk cow model is based on McLachlan (1994). The milk-cow is treated as two compartments, the digestive tract and the cow itself. The original model considered dietary ingestion, dietary egestion, transformation and lactation, and the version in the ACC-Human model has been extended to also consider inhalation, exhalation and urination. The model assumes that the cow is at steady state (this was thought to be a reasonable assumption owing to the comparatively large rate of lipid excretion via lactation compared to the total quantity of lipid in the cow). Transfer of chemical across the wall of the intestinal tract is described using a two-film model. Air-lung exchange is modelled based on work by Hickie *et al*. (1999). Seventy percent of the inhaled air is assumed to come into intimate contact with the aveoli and equilibrates with the cow. Urination and lactation are treated as advection processes. The dietary uptake includes contributions from feed (a factor of 25 per cent is added to the intake from grass in order to account for the contribution from other feeds), soil and water.

The beef-cattle model is similar to the milk-cattle model except that steady-state behaviour is not assumed. In the model, a steer is born on the day of the last grass harvest of each year with an initial fugacity equal to the fugacity of cow's milk. The steer is then fed for twenty eight months until slaughter (the volume of the steer is assumed to increase linearly with time).

The final step in the food chain is the human exposure resulting from inhalation, consumption of drinking water (freshwater), and consumption of food (planktivorous fish, piscivorous fish, dairy products and beef).

As the aim of this work is to predict concentrations in the food chain and not necessarily the resulting concentrations in humans, the human uptake model used in ACC-Human is not directly relevant. However, brief details of the model are given below for completeness. The model is a two-compartment equilibrium model similar to that of the milk cow. The human tissue compartment is modelled as a mixture of water and lipids (the model does not consider binding of contaminants to proteins). It considers uptake via diet and inhalation, and elimination via metabolism, percutaneous excretion, digestive tract excretion, exhalation and, in the case of women, childbirth and nursing. The basis is a digestive tract absorption model (Moser and McLachlan, 2002) that has been extended to include the elimination processes. The consumption rate for each food group − fish (as a fresh volume), dairy products and beef (both as a lipid volume) − can be specified by the user. In the model, a human is born every 10 years on December 31st. The baby is breast fed for the first six months (the baby's initial fugacity and the fugacity of mother's milk are assumed to be equal to the fugacity of a twenty-year old woman or the fugacity of cow's milk during the first two decades of the simulation). The intervals between childbirth of a given woman can be specified within the model. The concentrations in each person within the model are simulated for up to eighty years.

The actual ACC-Human model is available as a computer program and accompanying manual. The user-entered inputs to the model are summarised in Table 4.1.

Table 4.1 Inputs required for ACC-Human model

Parameter	Comment
Chemical-specific data	
Log K_{ow}	
Log K_{aw} (air-water partition coefficient) and/or log K_{oa} (octanol-air partition coefficient)	The log K_{aw} can be estimated from log K_{oa} and *vice versa* if required.
Heat of phase transfer – octanol-water	Units of J $mole^{-1}$.
Heat of phase transfer – air-water and/or octanol-air	Units of J $mole^{-1}$. The value of air-water can be estimated from the value for octanol-air and *vice versa*.
Concentration in air	Can be entered as a constant concentration (g/m^3) or a fugacity (Pa). A file with varying concentrations with time can also be used.
Concentration in seawater	
Concentration in freshwater	
Concentration in soil	
Metabolism rate constant in humans	Units of $hour^{-1}$.
Metabolism rate constant in milk cows	Units of $hour^{-1}$.
Metabolism rate constant in beef cattle	Units of $hour^{-1}$.
Metabolism rate constant in grass	Units of $hour^{-1}$.
Metabolism rate constant in fish	Units of $hour^{-1}$.
Faeces-blood partition coefficient in humans	Default = 2×10^{-8}. Value can be varied.
Model parameters	
Temperature in seawater	Default values relevant to the Baltic area are used (initial default 7°C – varies with season). A constant temperature can be user-defined.
Temperature in air, soil and freshwater	Default values relevant to the Baltic area are used (initial default 17°C – varies with season). A constant temperature can be user-defined.
Grass parameters	The date of start of growing period (1st March), the dates of harvest (15th May, 1st July, 1st October), the fraction of each harvest in cattle diet (0.45, 0.40 and 0.15), the transpiration rate (1×10^{-5} m^3/m^2/hour), the specific surface area of grass (5,000 m^2/m^3), and crop (6×10^{-3} m^3/m^2/year) can all be varied.
Mass transfer coefficients for grass	For gaseous deposition, the values for atmosphere-plant surface (8 m/h) and plant surface-contaminant reservoir (2.80×10^{-8} m/h) can be varied. For wet and dry particle-bound deposition, the value for the deposition velocity (3 m/h) can be varied.
Milk cattle	
Water volume of the cow	Default = 0.36 m^3. Value can be varied.
Lipid volume of the cow	Default = 0.1 m^3. Value can be varied.
Water content in milk	Default = 0.87 g/g. Value can be varied.
Fat content in milk	Default = 0.044 g/g. Value can be varied.
Lactation rate	Default = 6,100 l/year. Value can be varied.

Parameter	Comment
Grass consumption rate	Default = 13 kg dry weight/day or 49 kg fresh weight/day. Value can be varied.
Fraction of contamination due to grass consumption	Default = 0.80. Value can be varied.
Beef cattle	
Water content in steer	Default = 0.70 g/g. Value can be varied.
Lipid content in steer	Defaults = 0.01 m^3 at birth, 0.15 m^3 at slaughter. Values can be varied.
Grass consumption rate	Defaults = 3.5 kg dry weight/day or 13 kg fresh weight/day after birth, 13 kg dry weight/day or 49 kg fresh weight/day at slaughter. Values can be varied.
Soil content in feed	Default = 0.023 g/g dry weight. Value can be varied.
Fish food chain (values are specified for both winter and summer)	
Lipid content of zooplankton	Default = 0.04. Value can be varied.
Lipid content of fish	Defaults = 0.035 for herring and 0.044 for cod (total fish) or 0.035 and 0.005 (fillets). Values can be varied.
Food composition for cod	Values are given for the fraction of cod (for ages one to 10) diet composed of zooplankton, herring (ages one to 10) and cod (ages one to 10).
Humans	
Body lipid excretion rate	Default = 0.80 g lipid/day or 8.89×10^{-7} m^3/day. Values can be varied.
Age at start of model	Default = 0 years. Value can be varied.
Air and water balance of a 25-year old man	Defaults = 15 m^3/day (air) and 0.003 m^3/day (water) for uptake and elimination. Values can be varied.
Food consumption rate of a 25-year old man	Defaults = 21.08 g lipid/day of dairy products, 9.7 g lipid/day of beef and 79.1 g wet weight/day of fish. Values can be varied.
Fraction of fish items in diet	Defaults = 0.75 herring, 0.25 cod. Values can be varied.
Age pattern of fish in human's diet	Default values are given for the age profile of the fish (between one and 10 years of age) in the diet.
Mother's age at birth of first child	Default = 29. Value can be varied.
Nursing period	Default = 182 days. Value can be varied.

The model can be run over a user-defined period of years using either constant concentrations in air, water, soil and sediment or time-varying concentrations. The time step for the simulation can be set to one, three, six, 12 or 24 hours and the results can be stored representing 24-hour, 120-hour (five day), 1,752-hour (73 day) or 8,760-hour (365 day) periods. The outputs from the model are (for each time period) as follows.

Marine system

Concentration in seawater (g/m^3)

Concentration in zooplankton (ng/g lipid)

Concentration in herring (ng/g lipid) – values are calculated for ten one-year age groups.

Concentration in cod (ng/g lipid) – values are calculated for ten one-year age groups.

Terrestrial system

Concentration in air (g/m^3)

Concentration in freshwater (g/m^3)

Concentration in soil (g/m^3)

Concentration in grass (pg/g lipid)

Concentration in cattle feed (pg/g lipid)

Concentration of soil in grass (pg/g lipid)

Concentration in milk (pg/g lipid)

Concentration in milk cow (pg/g lipid)

Concentration in beef cattle (pg/g lipid) – values are given for cattle of age zero to one years, one to two years and two years-slaughter

Concentration in beef (pg/g lipid)

Humans

Concentrations in males and females (pg/g lipid) – values are given for 10-year ranges from ages 0-10 to 70-80.

The predictability of the model was evaluated using PCBs (PCB 52, 101, 118, 138, 153 and 180) in the Swedish environment as a case study. For the marine model, the results predicted for PCB 153 in four-year old herring and cod were generally in good agreement with measured (lipid-normalised) values in fish from the Baltic (the comparison for herring was confounded by high variability in the available monitoring data). Other data from 1999 for a range of PCB congeners showed that the model tended to underpredict the actual concentrations found in this dataset by a factor of up to two (with the exception of PCB 138 which was overpredicted by a factor of 1.5 to two). It was thought that this could be related to the log K_{ow} values used in the model, as the fish model was reported to be very sensitive to the log $_{Kow}$ value. The results for other years were found to be similar, with the exception of a tendency to overpredict concentrations in three- to four-year old herring, which was thought to be related to differences in lipid levels in the fish. Overall, reasonably good agreement was obtained between the modelled and measured levels in fish. It was concluded that a more

detailed knowledge of herring lipid dynamics would be useful to improve the model, and would help to explain the large variability in monitoring data.

The agricultural food chain was evaluated based on reported levels of PCBs in beef cattle and dairy products from southern Sweden or Denmark. Good agreement was obtained between model predictions and measured levels (lipid-normalised) of PCBs in milk and beef. The highest deviation (a factor of two) was seen for PCB 52, which is a labile substance; given the simplistic system used for selecting metabolism rate constants, the agreement was nevertheless thought to be good. PCB 138 was underpredicted by a factor of two, likely as a result of uncertainties in the log K_{ow} (dietary adsorption in the cow is roughly inversely proportional to the log K_{ow} in the range studied).

Predicted human tissue levels for PCBs were compared with actual data from Swedish mothers' milk collected between 1972 and 1997. Predicted concentrations agreed well with measured (lipid-normalised) concentrations in milk from samples taken six weeks after birth. In addition, the model was able to predict the temporal trend in measured levels correctly. Again, comparatively poor agreement was obtained for PCB 138.

The input screen for the model indicates that the accepted range of physico-chemical properties is two to 10 for log K_{ow} and -10 to +10 for log K_{aw}. However, the Briggs *et al*. (1982) method was derived from experimental data for chemicals with log K_{ow} in the range -0.45 to 4.5 (see Chapter 3), and so the validity outside of this range is unknown.

In summary, the model is flexible and could be easily modified to other food chains, provided the lipid contents and diet constituents are available. However, in its current computerised form, it is not possible to add extra steps to the food chain. In addition, the soil organic carbon content used in the simulation is unclear (and does not appear to be a variable within the model).

4.3 Summary of the ACC-Human model

An overview of the method is given in Table 4.2.

Table 4.2 Summary of the ACC-Human model

Criteria	Comment
Structure of the method	The model is available as a computer program. Details of the methods used in the model are given as a series of equations in the published literature.
Scope of the method	The model is intended for research purposes. The method considers the exposure of marine fish via a seawater food chain; cattle via air, grass, soil and water; and humans via food (beef, milk and fish). The method is intended to be applicable to lipophilic organic chemicals with a log K_{ow} in the range two to 10 and a log K_{aw} in the range -10 to +10.
Type of method	Non-steady state, fugacity-based, mechanistic model.
Calculation method	Computer program.
Outputs from the method	Concentration in zooplankton (ng/g lipid). Concentration in herring (ng/g lipid). Concentration in cod (ng/g lipid). Concentration in grass (pg/g lipid). Concentration in cattle feed (pg/g lipid). Concentration of soil in grass (pg/g lipid). Concentration in milk (pg/g lipid).

Criteria	Comment
	Concentration in milk cow (pg/g lipid). Concentration in beef cattle (pg/g lipid). Concentration in beef (pg/g lipid). Concentrations in humans (males and females) (pg/g lipid).
Focus of the method	The method considers fish, cattle and humans of various age ranges and so does consider sensitive groups (such as children and young animals).
Chemical-specific input parameters	The main chemical-specific input parameters required by the model are summarised in Table 4.1. These include log K_{ow} , log K_{aw}, heats of phase transfers, and metabolism rate constants.
Key default parameters used in the method	The key default parameters used in the model are summarised in Table 4.1. All default parameters (with the possible exception of the soil organic carbon content) can be easily adapted within the program. Default parameters are representative of a Northern European country and so may not be appropriate for the general situation in the United Kingdom.
Environment considered in the method	The method considers a generic Northern European environment consisting of marine water, freshwater (drinking water), soil and air compartments.
How is persistence considered?	Metabolism in humans, milk cows, beef cattle, grass and fish can be included in the model provided sufficient chemical-specific data are available. (Bio)degradation of the chemical in the environment is not considered directly, although one of the model inputs is the concentration in various environmental media, so this could be accounted for indirectly by suitable input concentrations.
Are seasonal variations considered?	Yes. The model can consider seasonal variations in temperatures.
Strengths	The model is easy to use and uses a relatively small amount of chemical-specific data.
Weaknesses and limitations	It is not clear what value for the soil organic carbon content (or other soil-related parameters) is used in the model. This potentially makes the model difficult to adapt for different soil types. The aquatic food chain in the model does not appear to consider uptake from sediment into the food chain.
Overall assessment of whether the model could be adapted to the UK situation	The model could be adapted to the situation in the UK. In particular, UK-specific consumption rates for the food items included could easily be incorporated. The one exception is that the soil-type included is unclear and it is currently not possible to adapt the model for different soil types. The model could also be adapted to include other fish species, although the availability of data for other species could limit the number of fish age classes that could be incorporated.
Further work	If the soil organic carbon content could be included as an input variable, this would then allow the model to be adapted to different soil types.

4.4 Evaluation against screening criteria

4.4.1 Data requirements

The model requires some simple physico-chemical properties that are usually readily available (or can be easily estimated). However, more complex data (such as metabolism data for plants, fish, humans and cattle) would be needed for accurate

predictions; the model can be run assuming no metabolism, but this would have implications for the accumulation predicted. In addition, the heats of phase transfer for octanol-water and air-water and/or octanol-air are required. These data may be of limited availability for a wide range of chemicals. A score of one is appropriate. The importance rating for this criterion is five. Therefore,

$SCORE_{DATA} = 1 \times 5 = 5$.

4.4.2 Model calibration

The model is generally based on theoretical considerations and so is not calibrated as such. Overall, a score of two is considered appropriate. The importance rating for this criterion is five. Therefore,

$SCORE_{CALIBRATION} = 2 \times 5 = 10$.

4.4.3 Model validation

The model has been validated using data for PCBs in the Swedish Environment. Agreement between the predicted and field data was found to be generally satisfactory (less than a factor of two in difference was generally found). Based on the criteria outlined in Appendix C, an overall score of three is considered appropriate. The importance rating for this criterion is five. Therefore,

$SCORE_{VALIDATION} = 3 \times 5 = 15$.

4.4.4 Ease of use

The model is available in a format that requires some experience/knowledge to use and would require some interpretation of the results for use in setting standards. The score for this criterion is therefore two. The importance rating for this criterion is two. Therefore,

$SCORE_{EASE} = 2 \times 2 = 4$.

4.4.5 Transparency

The underlying methods used in the model are mostly clear, the one exception being how soil partitioning is taken into account, and so a score of two is appropriate. The importance rating for this criterion is five. Therefore,

$SCORE_{TRANS} = 2 \times 5 = 10$.

4.4.6 Prediction uncertainty

Based on expert judgement, the model has low uncertainty and does not rely on conservative or precautionary approaches and so a score of three is appropriate. However, this score relies on the availability of all the necessary chemical-specific input data. Uncertainty in the prediction would increase if, for example, assumptions had to be made over the metabolism rate in the various organisms (the data requirements are scored separately; see Chapter 4.4.1). The importance rating for this criterion is five. Therefore,

$SCORE_{UNCERT} = 3 \times 5 = 15.$

4.4.7 Ability to predict the concentration near the top of the food chain

The model allows predictions of concentrations in more than two trophic levels near the top of the food chain. Howeve,r the aquatic food chain does not consider some important routes of exposure (from sediment) and so a score of two is judged appropriate. The importance rating for this criterion is four. Therefore,

$SCORE_{TOP\ FOOD} = 2 \times 4 = 8.$

4.4.8 Relevance to England and Wales

The model is a generic model for Northern Europe and so is not directly relevant to England and Wales. It is relatively easy to adapt the model for specific situations in England and Wales. A score of two is therefore appropriate. The importance rating for this criterion is four. Therefore,

$SCORE_{RELEVANCE} = 2 \times 4 = 8.$

4.4.9 Overall score

Using the methodology outlined in Appendix C, the overall score can be estimated as follows.

TOTAL SCORE $= SCORE_{DATA} + SCORE_{CALIBRATION} + SCORE_{VALIDATION} + SCORE_{EASE} + SCORE_{TRANS} + SCORE_{UNCERT} + SCORE_{TOP\ FOOD} + SCORE_{RELEVANCE}$

$= 5 + 10 + 15 + 4 + 10 + 15 + 8 + 8$

$= 75.$

5 System dynamic model

5.1 Introduction

The concept of the system dynamic model was outlined in a paper by Carbonell *et al.* (2000). The model was developed to further the debate on how ecological risk assessment protocols (such as the EU TGD discussed in Chapter 3) could be improved to take more account of the potential for bioaccumulation/biomagnification through the food chain, including exposure from direct ingestion of sediment-bound substances and food, thus leading to more scientifically-supported conclusions. A version of this model has been incorporated in the guidance document for risk assessments for birds and mammals under Council Directive 91/414/EEC[5] in relation to plant protection products (European Commission, 2002).

Further information on this model has been requested from the original authors as part of this work, however no further details have been provided. Therefore, this review is based on the published outlines of the model.

5.2 Description of model

The model is a generic model for food chain biomagnification. The paper by Carbonell *et al.* (2000) discusses an aquatic food chain model, but similar principles could be applied to other food chains. The model outline is flexible and there are effectively no limits (other than availability of data) to the number of steps or organisms that could be incorporated into the scheme. Two versions of the model are presented, called the "simplified" and "complete" versions here.

The simplified version is intended to represent a worst-case calculation and assumes an instantaneous equilibrium between water, sediment and all organisms considered in the food chain. This version requires information on bioconcentration factors (BCFs), and biota-food (BFAF) and biota-sediment (BSAF) accumulation factors. The concentration in any one organism in this food chain is estimated as follows:

$$PEC_{organism} = [PEC_{water} \times BCF] + [PEC_{food} \times BFAF] + [PEC_{sediment} \times BSAF]$$

where: $PEC_{organism}$ = predicted concentration in organism (mg/kg).

PEC_{water} = predicted concentration in water (mg/l).

PEC_{food} = predicted concentration in food (mg/kg).

$PEC_{sediment}$ = predicted concentration in sediment (mg/kg).

Where exposure via water (and hence sediment) is not continuous, the dissipation of the chemical can be modelled (using the dissipation half-life) and the time-weighted

[5] Council Directive 91/414/EEC of 15 July 1991 concerning the placing of plant protection products on the market. Official Journal L230, 19/08/1991, p1-32.

average concentration in the organisms or food can be estimated from the time-weighted average concentration in water and sediment.

The complete version of the model takes into account the chemical uptake and depuration rates in the organisms in the food chain. In this version of the model, the concentration of the chemical in the organism is calculated as follows, using kinetic data on accumulation and depuration:

$$C_{organism,\ water} = (k_1/k_2)\times PEC_{water}\times(1\text{-}e)^{-k_2 t}$$

$$C_{organism,\ sediment} = (k_1/k_2)\times PEC_{sediment}\times(1\text{-}e)^{-k_2 t}$$

$$C_{organism,\ food} = (\alpha\times F/k_2)\times PEC_{food}\times(1\text{-}e)^{-k_2 t}$$

$$PEC_{organism} = C_{organism,\ water} + C_{organism,\ sediment} + C_{organism,\ food}$$

where: $C_{organism,\ water}$ = concentration in organism from water exposure (mg/kg).

$C_{organism,\ sediment}$ = concentration in organism from sediment ingestion (mg/kg).

$C_{organism,\ food}$ = concentration in organism from food ingestion (mg/kg).

k_1 = uptake rate constant (for water and sediment) (day^{-1}).

k_2 = depuration rate constant (day^{-1}).

α = assimilation efficiency from food[6].

F = feeding rate (fraction of body weight/day).

t = time (days).

These equations allow time-dependent concentrations in each step of the food chain to be estimated.

Carbonell *et al.* (2000) considered the following food chain in a pond consisting of water and sediment:

- Unicellular algae. This is the primary producer in the system. Algae were assumed to have a cell diameter of 3.57 µm and a wet and dry weight of 1.2×10^{-7} mg and 1.14×10^{-8} mg respectively. Exposure was via water.
- Primary consumer. This was assumed to be a cladoceran which fed on the algae. The feeding rate was assumed to be 50 per cent of its body weight per day.
- Secondary consumer. This was assumed to be a fish feeding on the cladoceran. The feeding rate was assumed to be 20 per cent of its body weight per day.

[6] Similar to several other models, this model assumes that the assimilation efficiency of the chemical from food is constant with increasing body concentration. However, according to Barber (2005a) such an assumption may be incorrect, and assimilation efficiency would be expected to decrease with increasing body concentration.

- Tertiary consumer. This was assumed to be a fish feeding on the secondary consumer. The feeding rate was assumed to be 15 per cent of its body weight.

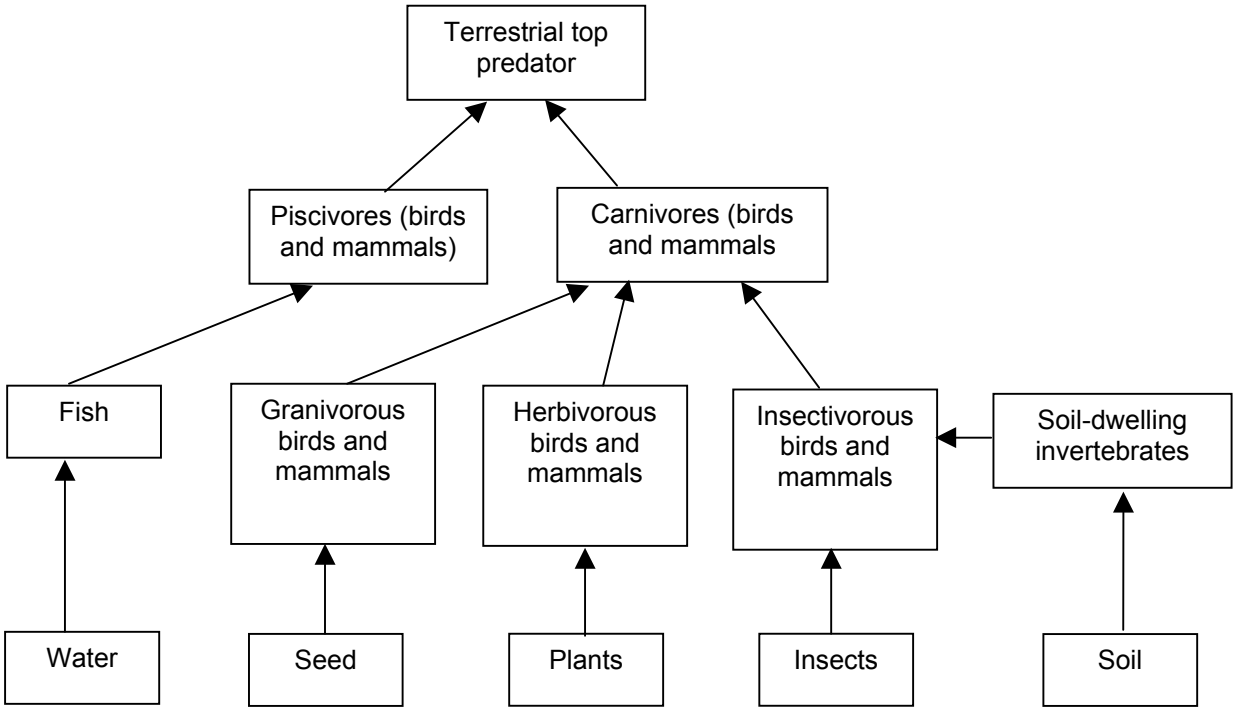
The model was run for four hypothetical lipophilic pollutants outlined below, assuming a single pollutant event with an initial concentration of one mg/l.

- Chemical 1. Of medium persistence in water (dissipation half-life 20 days). The BCF was assumed to be 5,000, 3,000, 4,000 and 5,000 l/kg for algae, first, second and third consumer respectively. The assimilation efficiency in all organisms was assumed to be 30 per cent. The substance was assumed to be easily metabolised, particularly in fish; the depuration rate constant was assumed to be 0.5, 0.1, 0.3 and 0.3 (units were not given but are probably day^{-1}) respectively for algae, first, second and third consumers respectively.
- Chemical 2. This was the same as chemical 1 with the exception that it was slowly metabolised by fish; the depuration rate constant was 0.01 for second and third consumers respectively.
- Chemical 3. This was highly persistent in water (dissipation half-life was 100 days) and only slowly metabolised in invertebrates and fish; the depuration rate constant was assumed to be 0.5, 0.05, 0.01 and 0.01 l/kg for algae, first, second and third consumers respectively. The BCF was 5,000, 3,000, 40,000 and 50,000 l/kg for algae, first, second and third consumer respectively and the assimilation efficiency was assumed to be 30 per cent for all organisms.
- Chemical 4. This was similar to chemical 1 with the exception that it was highly persistent in water (dissipation half-life 1×10^7 days). The BCF was assumed to be 5,000, 5,000, 5,000 and 6,000 l/kg for algae, first, second and third consumers respectively. The assimilation efficiency was assumed to be 0.6, 0.3 and 0.3 for first, second and third consumers respectively. The depuration rate constant was assumed to be 0.3, 0.1, 0.3 and 0.3 day^{-1} for algae, first, second and third consumers respectively.

The results of this analysis showed that the simplified approach led to the worst-case concentrations in various parts of the food chain. The time-dependent complete version of the model would lead to similar results if a constant exposure and extended time periods were considered (at steady state).

Although exposure via sediment was not specifically included in the model given in Carbonell *et al*. (2000), it could easily be incorporated into the framework provided BSAFs or uptake rate constants were available.

A version of the system dynamic model is incorporated in the guidance document for risk assessments of birds and mammals under Council Directive 91/414/EEC (European Commission, 2002). This model is based on aquatic and terrestrial food chains and is summarised below.



Within this framework, it is proposed that the diets of various levels of the food chain consist of the following:

- Insectivores: 100 per cent contaminated insects (for small mammals); and 100 per cent contaminated insects or 100 per cent contaminated soil-dwelling invertebrates (for small and medium-sized birds).
- Herbivores: 100 per cent contaminated plants (for small and medium-sized mammals and small and medium-sized birds).
- Omnivores: 33 per cent contaminated invertebrates, 33 per cent contaminated seeds and 33 per cent contaminated plants (for medium-sized mammals and small birds).
- Carnivores: 100 per cent contaminated mammals (for medium-sized mammals and medium-sized birds).
- Piscivore: 100 per cent contaminated fish (for medium-sized mammals and medium and large-sized birds).
- Carnivore/piscivore: 50 per cent contaminated birds and mammals and 50 per cent contaminated fish (for medium and large-sized birds).
- Aquatic herbivore/insectivore: 50 per cent contaminated aquatic invertebrates and 50 per cent aquatic plants (for medium-sized birds).
- Top predators: either 100 per cent carnivores or 100 per cent piscivores.

The calculations involved are similar to those outlined above for the aquatic food chain. In particular, for each consumer in the food chain the steady-state concentration is calculated using the assimilation efficiency, feeding rate, depuration rate constant and estimated concentration (or dose) in the food item from the preceding trophic level. For episodic or intermittent exposures, a kinetic version of the model can also be derived (similar to that outlined for the aquatic compartment) which incorporates the dissipation rate constants.

No validation of the model appears to have been carried out.

Overall, the model provides a reasonable framework for incorporating the known accumulation properties of a substance into an assessment of a given food chain or ecosystem. However, the model is not able to predict the bioaccumulation potential of a chemical without knowing a significant amount about its behaviour in the various trophic levels.

5.3 Summary of the system dynamic model

An overview of the method is given in Table 5.1.

Table 5.1 Summary of the system dynamic model

Criteria	Comment
Structure of the method	The model is presented as a series of equations. A spreadsheet version of the model was used by Carbonell *et al.* (2000) but this does not appear to be generally available.
Scope of the method	An adaptation of the method is proposed for the assessment of risks to mammals and birds from plant protection products under Council Directive 91/414/EEC
Type of method	The method can either be used to derive steady-state concentrations in the food chain or to estimate time-dependent concentrations.
Calculation method	Hand calculations (for simplified version). The method could be readily implemented in a spread sheet program.
Outputs from the method	Concentrations in organisms within each trophic level within the food chain. For the example model in Carbonell *et al.* (2000), these would include: • Concentration in algae (mg/kg). • Concentration in invertebrates (mg/kg). • Concentration in fish feeding on invertebrates (mg/kg). • Concentration in predatory fish (mg/kg). For the proposal in European Commission (2002), these would include: • Concentration in granivorous birds and mammals (mg/kg). • Concentration in herbivorous birds and mammals (mg/kg). • Concentration in insectivorous birds and mammals (mg/kg). • Concentration in piscivorous birds and mammals (mg/kg). • Concentration in carnivorous birds and mammals (mg/kg). • Concentration in terrestrial top predators (mg/kg).
Focus of the method	The method does not focus specifically on sensitive groups (such as children or young animals).

Criteria	Comment
Chemical-specific input parameters	The key chemical-specific input data are the BCF, BFAF or BSAF for each organism considered in the food chain (for the steady-state solution). In addition, for the time-dependent calculations knowledge is also needed of the dissipation rate constant for the media considered, the depuration rate constant from each of the organisms in the food chain, assimilation efficiency from food or the uptake rate constant from water, sediment and so on,
Key default parameters used in the method	The key default parameters used in the model are the feeding rates and composition of diet for each organism in the food chain.
Environment considered in the method	The model considers a generic (European) environment. The method could be adapted to site-specific food chains, provided the necessary accumulation factors and kinetic data were available for the organisms in question.
How is persistence considered?	The steady-state calculation is based on a constant or time-weighted average concentration. Metabolism in the organism is implicitly included in these calculations if measured BCFs, BFAFs and BSAFs are used. The time-dependent calculation can incorporate the rate of dissipation (such as degradation) in various environmental media and the uptake and depuration kinetics. As the model is formulated in terms of a depuration rate constant, the processes that are taken into account (for example, fish depuration could occur via the gills, faeces, metabolism and growth dilution[7]) will depend on how this value is chosen/determined.
Are seasonal variations considered?	No.
Strengths	The model is flexible, simple to use, and could be adapted to many food chains.
Weaknesses and limitations	The reliability of the model depends on the availability of data on BCFs, BFAFs, BSAFs, assimilation efficiencies, and/or uptake and depuration rate constants for each organism considered in the food chain. Such data are not likely to be routinely available for chemicals in general. Although it is possible to estimate some of these values (such as fish BCFs), the uncertainty in these values would then translate into uncertainties in the modelled results.
Overall assessment of whether the model could be adapted to the UK situation	The model is a generic model based on the EU. It could be adapted to specific situations in the UK provided information on the necessary accumulation factors, kinetic data and feeding data was available for the organisms in question.
Further work	The model would need to be implemented in a spread sheet if it was to be routinely used.

[7] Although growth dilution is not strictly related to the persistence or loss of the chemical, it is frequently grouped with other depuration processes (such as metabolism, excretion) within bioaccumulation models, as the effect of growth dilution is to lower the overall concentration of a chemical in an organism.

5.4 Evaluation against screening criteria

5.4.1 Data requirements

The model requires a BCF, BFAF and/or BSAF for each organism considered (for the steady-state solution) and details of the dissipation rate constants for the media considered (such as water, sediment, soil), the assimilation efficiency from food, the uptake rate constant from water, sediment and so on, and the depuration rate constant for each organism considered (for the time-dependent calculations). Many of these data may be of limited availability for a wide range of chemicals. A score of one is appropriate. The importance rating for this criterion is five. Therefore,

$SCORE_{DATA} = 1 \times 5 = 5$.

5.4.2 Model calibration

The model is generally based on theoretical considerations and so is not calibrated as such. Therefore, a score of two is considered appropriate. The importance rating for this criterion is five. Therefore,

$SCORE_{CALIBRATION} = 2 \times 5 = 10$.

5.4.3 Model validation

No validation has been carried out, so a score of two is considered appropriate. The importance rating for this criterion is five. Therefore,

$SCORE_{VALIDATION} = 2 \times 5 = 10$.

5.4.4 Ease of use

The model is available as a series of equations that would require some experience or knowledge to use. The score for this criterion is therefore two. The ease of use of the model could be simplified by use of a spreadsheet. The importance rating for this criterion is two. Therefore,

$SCORE_{EASE} = 2 \times 2 = 4$.

5.4.5 Transparency

The underlying methods used in the model are clear and so a score of three is appropriate. The importance rating for this criterion is five. Therefore,

$SCORE_{TRANS} = 3 \times 5 = 15$.

5.4.6 Prediction uncertainty

The uncertainty in the model's predictions will depend crucially on the availability and quality of accumulation factors, depuration rate constants and so on. If these data are available, the prediction uncertainty will be low. However, for most chemicals such data are unlikely to be available for all organisms in the food chain and so conservative/precautionary approaches would be needed. Therefore, based on expert judgement, a score of one is considered appropriate (although this score may be higher for certain data rich substances).

$SCORE_{UNCERT} = 1 \times 5 = 5$.

5.4.7 Ability to predict the concentration near the top of the food chain

The model allows predictions of concentrations in more than two trophic levels near the top of the food chain (data permitting), and so a score of three is judged appropriate. The importance rating for this criterion is four. Therefore,

$SCORE_{TOP\ FOOD} = 3 \times 4 = 12$.

5.4.8 Relevance to England and Wales

The model is a generic model for Europe and so is likely to be directly relevant to England and Wales. It is relatively easy to adapt the model for specific situations in England and Wales. A score of three is therefore appropriate. The importance rating for this criterion is four. Therefore,

$SCORE_{RELEVANCE} = 3 \times 4 = 12$.

5.4.9 Overall score

Using the methodology outlined in Appendix C, the overall score can be estimated as follows.

$$\text{TOTAL SCORE} = SCORE_{DATA} + SCORE_{CALIBRATION} + SCORE_{VALIDATION} + SCORE_{EASE} + SCORE_{TRANS} + SCORE_{UNCERT} + SCORE_{TOP\ FOOD} + SCORE_{RELEVANCE}$$

$$= 5 + 10 + 10 + 4 + 15 + 5 + 12 + 12$$

$$= 73.$$

6 Foodweb model

6.1 Introduction

The Foodweb model has been developed by the Canadian Environmental Modelling Centre at Trent University. The model is available free of charge from their modelling website[8]. Details of the theory behind the model are given in Campfens and Mackay (1997). The model is supplied with an example output file and a brief description file.

6.2 Description of model

The model is a fugacity-based mass balance model of the contaminant flux through an aquatic food web. Uptake by organisms in the food web is assumed to occur by diffusion from water (water column or sediment pore water) and via diet (both benthic and pelagic food organisms are considered). Clearance of the chemical from the organisms is modelled as a result of respiration, egestion and metabolism. The model also takes into account growth dilution. The food web can consist of any number of organisms, and each organism can be specified to feed on any others within the food web (including their own species).

The model presented by Campfens and Mackay (1997) is an extension of an earlier model for fish developed by Clark *et al*. (1990). The model is based on the fugacity approach, where at steady state the concentration or fugacity of a chemical in an organism exposed via both contaminated water and food can be expressed using the following equation:

$$f_W D_W + f_A D_A = f_F (D_W + D_E + D_M + D_G)$$

where: f_W = fugacity[9] in water.

f_A = fugacity in food.

f_F = fugacity in fish.

D_W = D-value[10] for exchange with water.

D_A = D-value for food uptake.

D_E = D-value for egestion.

D_M = D-value for metabolism.

D_G = D-value for growth dilution.

[8] http://www.trentu.ca/cemc/models/Foodweb.html.

[9] Fugacity is related to concentration (in units of mol/m^3) by the equation concentration = Z × fugacity, where Z is the fugacity capacity (units of mol/m^3.Pa) and fugacity has units of Pa.

[10] Within the fugacity approach, D-values are transport parameters with units of mol/Pa.h. The rates of transport (or loss) are obtained by multiplying the D-value by the fugacity.

The model assumes that the concentration of chemical in organisms at the bottom of the food chain (such as algae) is in, or is close to, equilibrium with the concentration in water. For feeding organisms, uptake from water and food is assumed. Both uptake from the water column and sediment (via pore water) are included in the model.

The water (gill) uptake and elimination rate constants used within the model are estimated based on the following correlation equation (Gobas and Mackay, 1987 and Gobas, 1993):

$$\frac{1}{k_1} = (V_F / Q_w) + \frac{(V_F / Q_L)}{Kow} = \frac{1}{(L \times Kow \times k_2)}$$

where: k_1 = water (gill) uptake rate constant.

k_2 = elimination rate constant.

V_F = the fish volume.

L = fish lipid content.

K_{ow} = octanol-water partition coefficient.

Q_W = transport parameter that expresses water phase conductivity ($Q_W = 88.3 \times V_F^{0.6}$).

Q_L = transport parameter that expresses lipid phase conductivity ($Q_L = 0.001 \times Q_W$).

The equation is derived from theoretical considerations (assuming the gill uptake rate is dependent on the gill ventilation rate and the diffusion rate of the chemical across the gills) and experimental data investigating the relationship between gill uptake efficiencies and K_{ow} over the log K_{ow} range <4.5 to >7.

The food uptake rate is estimated using the gut absorption efficiency (estimated from log K_{ow} , see Table 6.1) and the feeding rate.

Within the model it is assumed that all transport and removal processes are first order in the chemical concentration, and that the growth rate of organisms is linear. The model also assumes a constant exposure concentration via the water and sediment phases.

Adsorption of the chemical onto suspended matter in the water column is taken into account (the K_{oc} is assumed to be $0.41 \times K_{ow}$).

The chemical, lake and species-related parameters required to run the model are summarised in Table 6.2.

Table 6.1 Inputs required for Foodweb model

Parameter	Comment
Chemical-specific data	
Molecular mass	
Henry's law constant	Units of Pa m^3/mole.
Log K_{ow}	
Concentration in water column	
Concentration in sediment	
Metabolic half life	This is entered under the properties for each fish.
Lake properties	
Suspended particulate matter concentration	Units of g/m^3. The default value of 1.25 g/m^3 is used for Lake Ontario.
Volume fraction of sediment solids	Dimensionless. The default value of 0.1 is used for Lake Ontario.
Organic carbon content of suspended matter	Dimensionless. The default value of 0.2 is used for Lake Ontario.
Organic carbon content of sediment particulates	Dimensionless. The default value of 0.02 is used for Lake Ontario.
Organism properties	
Number of species	Any number of species can be simulated in the food web. The model contains an example eight-species food web for Lake Ontario consisting of plankton, mysids, pontoporeia, oligochaete, sculpin, alewife, smelt and salmonids.
Volume	Defined for each species. Values are given for plankton (0.0005 cm^3), mysids (0.1 cm^3), pontoporeia (0.002 cm^3), oligocheate (0.1 cm^3), sculpin (5.4 cm^3), alewife (32 cm^3), smelt (16 cm^3) and salmonids (385.6 cm^3).
Lipid volume fraction	Dimensionless. Defined for each species. Values are given for plankton (0.015), mysids (0.04), pontoporeia (0.03), oligochaete (0.01), sculpin (0.08), alewife (0.07), smelt (0.04) and salmonids (0.16).
Metabolic half-life.	Defined for each species (see above). For non-metabolisable substances a relatively long half-life (such as 5,000 days) should be used.
Digestion factor	This is essentially the maximum or limiting biomagnification factor and relates to the ratio of the rate of intake from food and the rate of egestion. A value of three is suggested as a default.
Growth rate	Units of g/g/day. Values are given for plankton (0.025), mysids (0.02), pontoporeia (0.02), oligochaete (0.015), sculpin (0.005), alewife (0.004), smelt (0.005) and salmonids (0.002).
Feeding rate	Units of g/g/day. Values are given for plankton (0), mysids (0.2), pontoporeia (0.224), oligochaete (0.17), sculpin (0.04), alewife (0.035), smelt (0.04) and salmonid (0.02).
Fractional water respiration rates	These are used to distinguish between benthic organisms (given a value of zero) and pelagic organisms (given a value of one). The fraction represents the fraction of time the organism spends in the water column (a value between zero and one can be used for organisms that spend time both in the benthos and water column). Values are given for plankton (1), mysids (1), pontoporeia (0), oligochaete (0), sculpin (1), alewife (1), smelt (1) and salmonids (1).

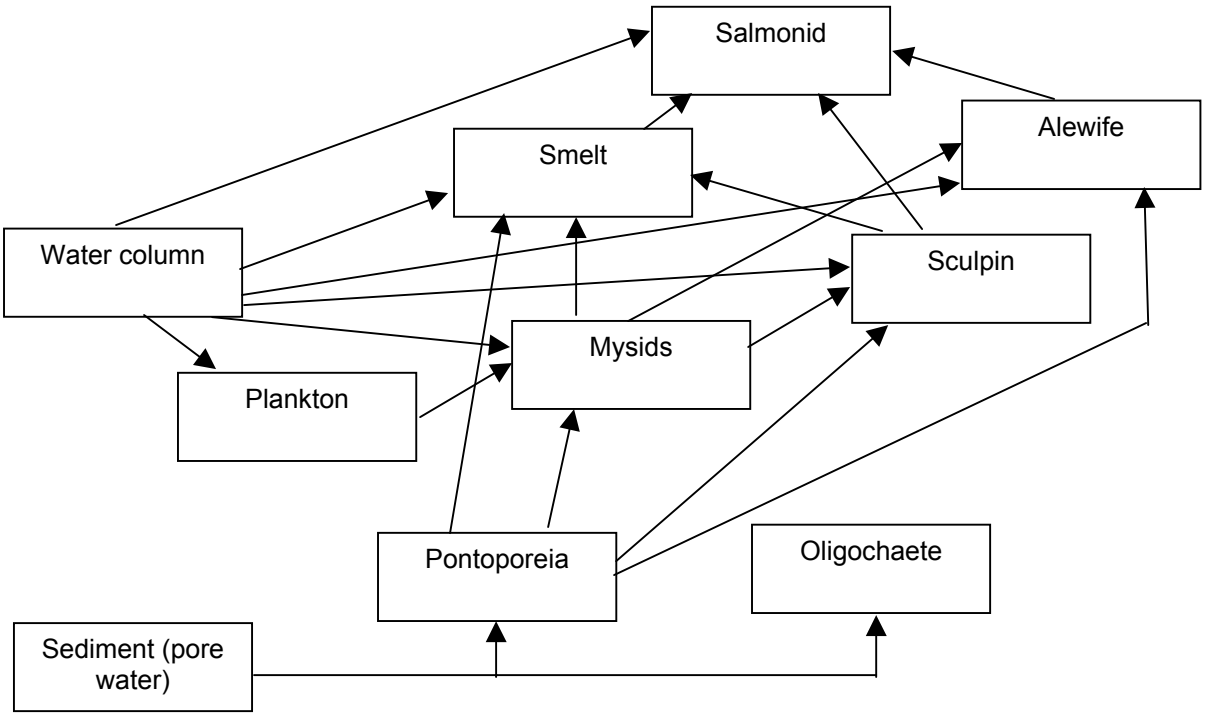
Parameter	Comment
Gut absorption efficiency parameter (E)[11]	These can be entered directly, or can be estimated using the following equation (from Gobas *et al*., 1988): $1/E = 5.3\times10^{-8} \times K_{ow} + 2.3$ This equation was derived from data on chlorinated organic chemicals (PCBs, chlorobenzenes, chlorinated dibenzo-*p*-dioxins and chlorinated pesticides) with six species of fish (*Poecilia reticulata, Carassius auratus, Salmo salar, Oncorhynchus mykiss, Pimephales promelas and Moxostoma macrolepidotum*). The regression equation was based on 36 data points, covering a log K_{ow} range of 5.0 to 8.3. The slope and intercept (95 per cent confidence limits given in brackets) of the plot of 1/E against K_{ow} were 5.3×10^{-8} ($\pm1.5\times10^{-8}$) and 2.3 (±0.3) respectively.
Diet	The diet of each species can be specified. The values used for the Lake Ontario food chain were as follows. Plankton – assumed to photosynthesize or consume organic carbon and detritus. Mysids – 80% plankton, 20% pontoporeia. Pontoporeia – not relevant – assumed to photosynthesize or consume organic carbon and detritus. Oligochaete – assumed to consume organic carbon and detritus. Sculpin – 18% mysids, 82% pontoporeia. Alewife - 60% mysids, 40% pontoporeia. Smelt – 54% mysids, 21% pontoporeia, 25% alewife. Salmonids – 10% sculpin, 50% alewife, and 40% smelt.

The outputs from the model include the following:

- Z-values (fugacity capacities);
- net contaminant flux from prey to consumer;
- steady-state environmental concentrations and fugacities;
- concentrations and fugacities in each species.

The model, as supplied, is set up for an eight-species food web in Lake Ontario but, as the required lake properties and organism properties are relatively modest, it could be easily modified to address other lakes/water bodies and fish species. The Lake Ontario food web is shown schematically below.

[11] Similar to several other models, this model assumes that the assimilation efficiency of the chemical from food is constant with increasing body concentration. However, according to Barber (2005a) such an assumption may be incorrect, and assimilation efficiency would be expected to decrease with increasing body concentration.



The model was validated by Campfens and Mackay (1997) by comparing model predictions for several PCB congeners (log K_{ow} values ranging from 5.6 to 7.4, and Henry's law constants between 12.2 and 58.1 Pa m^3/mole) with measured values from Lake Ontario. Predicted results were generally found to be within a factor of three of measured data. The agreement found was within a factor of two for mysids, two to three (overprediction) for pontoporeia, three for fish and a factor of four for benthos. For plankton, predictions were generally found to be close to measured data, but the predictions tended to exceed the measured data at high log K_{ow} values. Predictions for oligochaetes were generally lower than measured for test substances with lower log K_{ow} values (5.6 to 6.4), but higher than measured for substances with higher log K_{ow} values (6.7 to 7.4). The overall agreement (based on the standard deviation on a log scale plot of predicted versus measured concentration for all organisms) was a factor of 2.2. These comparisons were made using measured concentrations on a wet weight basis. The agreement on a lipid weight basis was not given (normalisation of the measured concentrations to the lipid content may remove some of the variability inherent in the measured data).

Campfens and Mackay (1997) warned that comprehensive validation of the model would require reliable measured data for a wide variety of food webs, organisms and chemicals. Their validation covered chemicals with only a relatively small range of chemical properties.

The authors concluded that this approach could be readily extended to include air-breathing organisms such as birds and marine mammals, whose diet was obtained primarily from aquatic (freshwater or marine) environments, and also possibly to include vegetation. Such extensions of the model would also need to include the air compartment.

An example of such an extension was a model for biomagnification and metabolism of contaminants for harp seals (*Phoca groenlandica*) in the Barents Sea (Fraser *et al*., 2002). The seals fed primarily on polar cod (*Boreagadus saida*) and a pelagic

crustacean (*Themisto libellula*). The model was used to estimate the biomagnification factors, rates of contaminant uptake and loss and metabolic half-lives in seals for 15 PCB congeners and 27 pesticides, using measured data for the concentrations of these substances in the food items.

6.3 Summary of the Foodweb model

An overview of the method is given in Table 6.2. This model is very similar in principle to the Food Chain Bioaccumulation model developed by Simon Fraser University based on the work of Gobas (1993) that forms part of the ECOFATE model (see Chapter 8).

Table 6.2 Summary of the Foodweb model

Criteria	Comment
Structure of the method	The model is available as a computer program. Full details of the methods used in the model are given as a series of equations in the published literature.
Scope of the method	The model is intended for research purposes. The food web in the model can theoretically consist of any number of aquatic organisms exposed via water, sediment pore water and food. The method is applicable to lipophilic organic chemicals. Some of the methods used within the model have been calibrated for substances with a log K_{ow} below 4.5 or above seven (gill uptake efficiencies) and 5.0 to 8.3 (gut absorption efficiencies).
Type of method	Steady-state, fugacity-based, mass balance model.
Calculation method	Computer program.
Outputs from the method	Z-values (fugacity capacities). Net contaminant flux from prey to consumers. Steady-state environmental concentrations and fugacities. Concentrations and fugacities in each species (such as oligocahetes, plankton, mysids, fish).
Focus of the method	The method does not consider specific sensitive groups (such as the young).
Chemical-specific input parameters	The main chemical-specific input parameters required by the model are summarised in Table 6.1. These include Henry's law constant, log K_{ow} and metabolic half-life in each fish species.
Key default parameters used in the method	The key default parameters used in the model are summarised in Table 6.1. These include parameters related to lake properties (such as suspended particulate matter concentration, organic carbon content) and organism properties (including volume, lipid fraction, digestion factor, feeding rates, fractional water respiration rates and diet).
Environment considered in the method	The method as presented considers a specific food chain from Lake Ontario consisting of eight species (pontoporeia, oligochaetes, plankton, mysids, sculpin, smelt, alewife and salmonids).
How is persistence considered?	Metabolism in fish can be included in the model if data are available. Other depuration processes (such as gill elimination, faecal egestion and growth dilution) are accounted for in the method.
Are seasonal variations considered?	No.
Strengths	The model is easy to use and uses a relatively small amount of chemical-

Criteria	Comment
	specific data. The method considers several modes of elimination from the organisms and can also take into account metabolism if data are available.
Weaknesses and limitations	It is not possible to use any measured bioaccumulation data (such as a measured BCF value) within the scheme. The model as set up is for a specific food chain in Lake Ontario and so the model may need to be modified to make it more generally applicable.
Overall assessment of whether the model could be adapted to the UK situation	The model is for a specific food chain in Lake Ontario and would need to be adapted to a more representative food chain for the UK. The species-related properties used by the model are relatively modest and it would be easy to adapt this model to other situations.
Further work	The model would need to be adapted to a more representative food chain for the UK. The model is easy to use but the user interface is a little basic. We did encounter problems running the program as supplied (an error message kept appearing). The original program was written in 1997 and it may be that the program is not very compatible with more modern computer systems. Therefore, a new computer program (or spreadsheet model) may need to be written to implement this model if it is to be routinely used on a range of computer systems.

6.4 Evaluation against screening criteria

6.4.1 Data requirements

The model requires mostly readily available chemical-specific information to run. More complex data (such as metabolism half-lives) can be used in the method if available. A score of three is appropriate. The importance rating for this criterion is five. Therefore,

$SCORE_{DATA} = 3 \times 5 = 15$.

6.4.2 Model calibration

The model is based on a combination of theoretical considerations and experimentally-derived correlations. The correlation for gut absorption efficiency was derived directly from experimental data on chlorinated organic compounds with six species of fish, but covers only a relatively small log K_{ow} range of 5.0 to 8.3. The correlation for gill uptake efficiency was based on theoretical considerations, but also experimental data for substances with a log K_{ow} range below 4.5 or above seven (chemical type not clear). On balance, a score of two is considered appropriate as some parts of the model have been calibrated over a relatively small log K_{ow} range. The importance rating for this criterion is five. Therefore,

$SCORE_{CALIBRATION} = 2 \times 5 = 10$.

6.4.3 Model validation

The model has been validated using data for several PCB congeners (log K_{ow} range 5.6 to 7.4) using data from Lake Ontario. The agreement of predictions with the field data was generally satisfactory. A score of three is considered appropriate. The importance rating for this criterion is five. Therefore,

$SCORE_{VALIDATION} = 3 \times 5 = 15$.

6.4.4 Ease of use

The model is easy to use but the user interface is a little basic. However, we did encounter problems running the program as supplied (an error message kept appearing). The original program was written in 1997 and it may be that the program is not very compatible with more modern computer systems. Therefore, a new computer program (or spreadsheet model) may need to be written to implement this model if it is to be routinely used on a range of computer systems. On balance, the score for this criterion is two. The importance rating for this criterion is two. Therefore,

$SCORE_{EASE} = 2 \times 2 = 4$.

6.4.5 Transparency

The underlying methods used in the model are clear and so a score of three is appropriate. The importance rating for this criterion is five. Therefore,

$SCORE_{TRANS} = 3 \times 5 = 15$.

6.4.6 Prediction uncertainty

The uncertainty in the model's predictions will depend to some extent on the availability of metabolism data. In the absence of such data, a zero metabolism rate can be assumed, resulting in a precautionary assessment. If metabolism data are available (or are estimated), this precautionary aspect will be reduced. Overall, a score of three is considered appropriate. The importance rating for this criterion is five. Therefore,

$SCORE_{UNCERT} = 3 \times 5 = 15$.

6.4.7 Ability to predict the concentration near the top of the food chain

The model allows predictions of concentrations in more than two trophic levels, including those near the bottom and top of the food chain (data permitting), and so a score of three is judged appropriate. The importance rating for this criterion is four. Therefore,

$SCORE_{TOP\ FOOD} = 3 \times 4 = 12$.

6.4.8 Relevance to England and Wales

The model is based on a Lake Ontario food chain and so is not directly relevant to the UK as it stands. However, the food chain in the model can be user-specified and it would be relatively easy to adapt the model to an aquatic food chain relevant to the UK. Further, the basic principles behind the model could be used to extend the method to include air-breathing organisms (such as fish-eating birds and mammals). A score of two is therefore appropriate. The importance rating for this criterion is four. Therefore,

$SCORE_{RELEVANCE} = 2 \times 4 = 8$.

6.4.9 Overall score

Using the methodology outlined in Appendix C, the overall score can be estimated as follows.

TOTAL SCORE $= SCORE_{DATA} + SCORE_{CALIBRATION} + SCORE_{VALIDATION} + SCORE_{EASE} + SCORE_{TRANS} + SCORE_{UNCERT} + SCORE_{TOP\ FOOD} + SCORE_{RELEVANCE}$

$= 15 + 10 + 15 + 4 + 15 + 15 + 12 + 8$

$= 94$.

7 BASS/FGETS

7.1 Introduction

The BASS (Bioaccumulation and Aquatic System Simulator) model is currently available as a test version (version 2.2 beta 2). The model is being developed by the United States Environmental Protection Agency (USEPA). The BASS model incorporates an earlier bioaccumulation model developed by the USEPA called FGETS (Food and Gill Exchange of Toxic Substances). The FGETS model (version 3.0.18, September 1994) can still be downloaded from the USEPA website[12] free of charge.

The test version of the BASS model has been used in this evaluation. A user guide is available (Barber, 2005a) outlining full details of the model. Details of the FGETS model have also been published (for example, Barber *et al*., 1988 and 1991).

7.2 Description of model

The BASS model can be used to predict both the population and bioaccumulation dynamics of age-structured fish populations. It consists of a bioaccumulation model coupled to a growth model and a model for population dynamics. The model can be used for hydrophobic organic chemicals and some types of metals.

The overall model is based on the following three mass balance differential equations.

$$\frac{dB}{dt} = J_g + J_i - J_m$$ - for bioaccumulation in fish

where: B denotes the chemical body burden in fish (µg/fish).

J_g denotes the net exchange of chemical across the gills (µg/day).

J_i denotes the net chemical exchange across the intestine from food (µg/day).

J_m denotes the metabolism or biotransformation of the chemical (µg/day).

$$\frac{dW_d}{dt} = F - E - R - EX - SDA$$ - for fish growth

where: W_d denotes the dry body weight of an individual fish (g dry weight/day).

F denotes the fish's feeding (g dry weight/day).

E denotes the fish's egestion (g dry weight/day).

[12] http://www.epa.gov/ceampubl/fchain/fgets/index.htm.

R denotes the fish's routine respiration (g dry weight/day) – relates to the weight loss resulting from respiration of CO_2.

EX denotes the fish's excretion (g dry weight/day).

SDA denotes the fish's specific dynamic action (the respiratory expenditure in excess of R required to assimilate food) (g dry weight/day).

Although many physiologically based models are formulated in terms of energy content (such as units of J/fish or J/day), the above model is stated to be fundamentally the same as these models as the energy densities of fish depend on their dry weight.

$\frac{dN}{dt} = -EM - NM - PM$ - for population dynamics.

where: *N* denotes the population density (number of fish/hectare).

EM denotes the emigration from the food web (number of fish/hectare).

NM denotes the non-predatory mortality (number of fish/hectare).

PM denotes the predatory mortality (number of fish/hectare).

In the model, organism recruitment (such as birth rate) is considered as a boundary condition and so no term is required for recruitment of new organisms in this equation.

The bioaccumulation model in the BASS model is essentially the same as that used in the FGETS model, and is based on diffusion kinetics coupled to a fish-growth model. The model considers the diffusive exchange of chemicals across gill membranes and intestinal mucosa and takes into account both the biological characteristics of fish and the chemical properties that affect this diffusive exchange. The fish is assumed to consist of three phases, a water phase, a lipid phase and a non-lipid organic carbon phase. The exchange from water across the gills is modelled by Fick's first law of diffusion.

Uptake from food is modelled using a thermodynamically based description of dietary uptake. Barber (2005a) notes that the more usual method of modelling uptake from food (based on a feeding rate and an assimilation factor) assumes that the assimilation efficiency (assimilation factor) is constant for a given fish; however, as chemical exchange across the intestine is driven by diffusive gradients, such assimilation efficiencies would be expected to decrease with increasing body concentration. Thus, the method used in the BASS/FGETS model takes this into account. The method assumes that, as the transit time through the gastrointestinal tract is relatively slow, the concentration of chemical in the fish's aqueous blood, intestinal fluids and dry faecal matter are in equilibrium with each other, and that the ratio of the chemical concentration in dry and aqueous phases of faeces can be adequately described by an organic carbon-water partition coefficient. Biotransformation/metabolism in the model is assumed to be described by a first-order reaction of the chemical's concentration in the aqueous phase.

The growth of the fish is simulated using a mass balance bioenergetic model (as outlined above) and takes into account the availability of prey. The effects of temperature on the fish's feeding, assimilation, respiration and egestion are taken into account. In addition to this growth/feeding model, three other growth models are also included in the program. These are the Rashevsky-Holling model (Rashevsky, 1959 and Holling, 1966), a clearance volume model for planktivores, and a model that back-

calculates a fish's feeding rate based on knowledge of the fish's expected growth rate and routine respiratory demands (Thomann and Connolly, 1984).

The food web structure can be user-defined in the model. A number of age classes for individual fish species and predator-prey interactions within these age classes can be set up within the model. Fish within each age class can therefore be assumed to feed upon other fish species, benthos, incidental terrestrial insects, periphyton/attached algae, phytoplankton and zooplankton. The model takes into account both the feeding preference of the fish, and the availability of the food. A number of assumptions are used in order to rank the competitive abilities of different age classes and species. These are as follows:

- The competitive abilities and efficiencies of benthivores and piscivores are positively correlated with their body sizes.
- The competitive abilities of planktivores are inversely related to their body size.
- When forage fish become limiting within the model, piscivores switch to benthic macroinvertebrates or incidental terrestrial insects as alternative prey. However, such piscivores are assumed to be less efficient benthivores than are obligate benthivores. If feeding on benthic organisms is still insufficient to satisfy the metabolic demands of piscivores, then it is assumed that they start feeding on plankton.
- If benthos becomes limiting for benthivores, the model assumes that benthivores can switch their diet to include plankton and terrestrial insects.
- If plankton becomes limiting for planktivores, the model assumes that planktivores can switch their diets to include benthos and terrestrial insects.

Dispersal and non-predatory mortality is modelled based on general empirical observations using a power function relationship. Species recruitment (new born fish) is included in the model by assuming that each fish species turns over a fixed percentage of its potential spawning mass into new young; this percentage is referred to as the reproductive biomass investment. The spawning biomass is determined as the total mass of fish with a body length above a minimum value, where the body length chosen represents the size at sexual maturation. The model can also (indirectly) take into account habitat effects using a series of multipliers between zero and one (the default values for these multipliers are taken as one). These multipliers can be applied to the feeding rate of fish, to take into account a reduced ability to intercept prey resulting, for example, from a habitat with refuges for prey, or a habitat where visibility is reduced in turbid waters. Similar multipliers can also be applied to species recruitment, for example to take into account a reduced number of spawning sites, and dispersal/non-predatory mortality.

As well as the fish compartments, four other compartments are considered within the BASS model. These are benthos, periphyton/attached algae, phytoplankton and zooplankton. The compartments are simulated using a simple mass balance model, and the individual body size of organisms in these compartments can be varied as a function of time if required.

The BASS model can also take into account toxicological effects of chemical exposure on fish populations. The model simulates acute and chronic mortality, assuming that the chemical (or chemicals if more than one is modelled) exhibits a narcotic mode of action. Toxic concentrations can either be estimated within the model, using an approach analogous to the toxic unit (see for example Peterson, 1994), critical body

residue (see for example McCarty and Mackay, 1993) and total molar body residue (see for example van Loon *et al*., 1997) approaches, or they can be based on a user-specified LC_{50}.

Biological characteristics in the model include information on the gill morphology, feeding rate, growth rate and composition (in terms of the fractions of water, lipid and structural organic carbon in the fish). Chemical properties include the octanol-water partition coefficient.

The model is formulated such that its parameterisation relies on relatively simple physical and chemical properties (many of which can be estimated if no experimental data are available) and on ecological, morphological and physiological parameters that can generally be obtained from the published literature or databases.

The model can be run without simulating the population dynamics (in this case, the model essentially becomes the FGETS model). The model considers a one hectare area.

The model itself uses a number of input files. The construction of these files is complex and, in our judgement, expert knowledge of the model is required in order to edit and amend some of the files. Files are grouped into four main areas, as shown in Table 7.1.

Table 7.1 Inputs required for BASS model

Parameter	Comment
Simulation control input file	
Annual_outputs	This specifies the time interval in years between the annual tabulated and plotted outputs (the default is zero – no annual outputs).
Annual_plots	This specifies the variables whose annual dynamics will be plotted for each time interval specified by annual_outputs. Such variables include (for each species as a function of time and species age, length or weight class): • fish aqueous phase activity; • bioaccumulation factor (the concentration in fish/concentration in water); • biomagnification factor (the concentration in predator/concentration in prey); • whole body fish concentration (in mg/kg); • species population density (no of fish/hectare); • total body length of fish (cm/fish); • body weight of fish (g fresh weight/fish).
Biota string$_1$	This specifies the non-fish standing stocks that are to be considered as forcing functions (rather than simulated variables) in the model. These can include benthic organisms, insects, periphyton, phytoplankton and zooplankton. These populations are generated in the model according to a number of functions (either a constant compartment standing stock or a sinusoidal time-varying standing stock) or can be generated from a file.
FGETS	This allows BASS to be run using the FGETS module only.
Header	This allows a header to be printed on each page of the output file (optional).

Parameter	Comment
Length_of_simulation	Specifies the length of the simulation (in days).
Nonfish_QSAR	This specifies the Quantified Structure Acirivity Relationships (QSARs) to be used for the bioconcentration/bioaccumulation properties of the non-fish compartments. The QSAR has to be user-entered as a function of log K_{ow}. This estimated value is not used if an actual BCF is entered (see Nonfish_BCF).
Month_T0	This specifies the starting month of the simulation (optional).
Summary_plots	This specifies the variables whose temporal dynamics will be plotted at the end of the simulation. Options are the same as listed under annual_plots.
Temperature	This specifies the ambient temperature of the food web. Options include a constant temperature, a user-defined sinusoidal time-varying temperature, or input from a file. Stratified waters can also be modelled (values for the epilimnion and hypolimnion can be entered).
Water_level	This allows the depth of water to be set. It can be set to a constant depth, a user-defined sinusoidal time-varying depth or the depth information can be read from a file. For stratified waters, the depth of the epilimnion and hypolimnion can be entered.
Chemical input file	
Exposure	This allows the temporal dynamics of chemical exposure to fish via water or contaminated sediments, or via ingestion of benthic invertebrates, incidental terrestrial insects or plankton, to be defined. The concentrations can be entered directly or can be derived as user-defined functions of other concentrations (for example, the aqueous concentration can be set as a concentration in equilibrium with the benthic sediment concentration). For water, the freely-dissolved concentration, rather than the total concentration is needed.
Lethality	This allows the fish LC_{50} to be entered directly or estimated from the log K_{ow}.
Log_AC	This refers to the $\log_{10}$ of the chemical's aqueous activity coefficient. If this value is not available, the program will estimate the value from the melting point and octanol-water partition coefficient.
Log_KB1 and Log_KB2	These are relevant to metals only and refer to the $\log_{10}$ of the metal's binding constant to non-lipid and refractory organic matter.
Log_P	The log K_{ow} value is needed.
Melting_point	The melting point. This is used along with log K_{ow} to estimate the chemical's aqueous activity coefficient.
Metabolism	This allows the biotransformation/metabolism rate constant to be entered. The value can be entered directly or can be entered as a user-specific function of the log K_{ow}. The transformation/metabolic products can also be modelled.
Molar_volume	The molar volume is needed as it is used within the model to estimate the substance's aqueous diffusivity. The value should be entered in units of cm^3/mole.
Molar_weight	The molecular weight of the chemical.
Nonfish_BCF	The bioconcentration/bioaccumulation factors for the non-fish compartments (benthos, periphyton, phytoplankton and zooplankton). The values can either be entered directly or as a user-defined function of the octanol-water partition coefficient.

Parameter	Comment
Fish input file	
Age_class_duration	Allows the duration of each age class to be defined.
Common_name	The identity of the fish species.
Compositional-parameters	This allows the aqueous and lipid fractions of the fish to be defined. Two options are available: the first specifies the aqueous fraction as a linear function of the lipid fraction, while the second specifies the lipid fraction as an allometric function of the body weight.
Ecological_parameters	This allows trophic interactions, non-predatory mortality, and recruitment of each fish species to be defined. Parameters that are considered include the following: • Dietary consumption – for each age class, the prey items, and their contribution to the total diet, can be defined. This can include other simulated fish species, benthos, insects, periphyton, phytoplankton and zooplankton. The contribution can either be expressed as a constant percentage or as "prey electivity". • Average length of prey – this allows the average length of prey consumed by a fish to be defined, based on the length of the predatory fish. • Maximum length of prey – this allows the maximum length of prey consumed by a fish to be defined, based on the length of the predatory fish. • The maximum lifespan for each species of fish. • The rate of dispersal and non-predatory mortality for each species of fish. • The reproductive biomass investment – this is the grams gametes per gram spawning fish. • Refuge population – this defines the fraction of the species population that is not available to predation (in fish/hectare). The default is set to zero (all fish are available for predation). • The length of fish at which each species is assumed to reach sexual maturity. • Species live weight (this is estimated as an allometric function of its total length). • The live weight of fish recruited into the population as young.
Feeding_options	This allows the various feeding model options within BASS to be selected. The options are an allometric model, a clearance model, the Rashevsky-Holling model and a linear model (see above). Different models can be assigned to different species.
Fishery_parameters	This specifies the stocking and harvest rates for sports fish.
Habitat_parameters	This allows the habitat preferences, tolerances and suitability indices for each species to be specified. Options include temperature preferences and habitat suitability multipliers (see text above).
Initial_conditions	This allows initial ages, whole body chemical concentrations, live body weights and population sizes for each species in the model to be defined.
Morphometric_parameters	These parameters are used to describe the exchange of chemical across the gills. The information required includes the following, where each parameter is entered as a user-defined

Parameter	Comment
	allometric power function of the fish body weight: • Total gill surface area. • Interlamellar distance between adjacent lamellae. • Density of secondary lamellae on the primary gill filaments. • Lamellar length.
Physiological_parameters	These parameters are used for simulating growth of each species within the model. Each parameter is entered either as a constant value or as a temperature-dependent power function of the fish body weight. The information required includes the following: • Assimilation efficiency for periphyton and phytoplankton. • Assimilation efficiency for benthos, insects and zooplankton. • Assimilation efficiency for fish. • Gastric evacuation (only required if the Rashevsky-Holling feeding model is used). • Minimum conditioning factors for a fish's continuing existence (these are estimated based on the live body weight and total length). • Maximum filtering rate (only required if the clearance feeding model is used). • Maximum ingestion (only required if the allometric feeding model is used). • Respiratory quotient (the ratio of CO_2 expired to O_2 consumed). • The ratio of routine respiration to standard respiration (default is set to two). • The ratio of specific dynamic action to ingestion (default is set to 0.17). • Specific growth rate (only required if the linear feeding model is used). • Standard oxygen consumption. • Size of satiation meal consumed and the time to satiation when feeding with an initially empty stomach (only needed if the Rashevsky-Holling model is used).
Prey-switching_off	This allows the prey-switching algorithms within BASS (see text above) to be switched off.
Spawning_period	This allows the months during which spawning occurs to be specified.
Species	This allows the scientific names of the species in the model to be entered. BASS includes default values for several fish species (see main text).
Non-fish input file	
Biomass	This is used when benthos, periphyton, incidental terrestrial insects, phytoplankton or zooplankton are treated as community forcing functions in the model. The options include a constant non-fish standing stock, a user-defined sinusoidal time-varying non-fish standing stock, or the details of the non-fish standing stock can be entered from a file.
Initial_biomass	Allows the initial compartmental standing stock to be defined. Used when benthos, periphyton, phytoplankton or zooplankton

Parameter	Comment
	are to be treated as community variables in the model.
Mean-weight	Allows the average body weight of individuals within each non-fish compartment to be defined. The options include a constant body weight, a user-defined sinusoidal time-varying body weight, or the data can be entered from a file. Used when benthos, periphyton, phytoplankton or zooplankton are to be treated as community variables in the model.
Ingestion	This allows the ingestion rate of individuals within each non-fish compartment to be entered as a user-defined function of body weight and temperature. Used when benthos, periphyton, phytoplankton or zooplankton are to be treated as community variables in the model.
Photosynthesis	This allows the photosynthesis rate of individuals within the non-fish compartment (periphyton and/or phytoplankton) to be entered as a user-defined function of average body weight and temperature. Used when benthos, periphyton, phytoplankton or zooplankton are to be treated as community variables in the model.
Respiration	This allows the specific rate of dry organic matter respiration within each non-fish compartment to be entered as a user-defined function of body weight and temperature. Used when benthos, periphyton, phytoplankton or zooplankton are to be treated as community variables in the model.

The outputs from the model can, to some extent, be user-specified (see Table 7.1) and can include the following.

- A file summarising the user-input parameters.
- A file tabulating selected results of the simulation, which can include the annual bioenergetic fluxes and growth statistics (such as mean body weight, mean growth rate) of individual fish by species and age class, the annual bioaccumulation fluxes and statistics (such as mean whole body concentrations, BAF and BMF) of individual fish by species and age class, and the annual community fluxes and statistics (such as mean population densities and biomasses) for each species and age class.
- A post-script file that contains the plots specified by the user.
- An XML file that contains daily values of community state variables, as well as integrated annual flow summaries and annual mean values for selected variables. A separate program (BASS Output Analyzer) is available which allows users to generate their own customised plots and tables.

The principles behind the FGETS (bioaccumulation) part of the model have been validated by comparing predicted uptake and elimination rates to experimental data published in the literature (see Barber *et al*., 1988; Barber, 2003). In addition, the FGETS model has been validated using simulations of mixtures of PCBs in Lake Ontario salmonids and largemouth bass-bluegill-catfish communities of Lake Hartwell/Twelvemile Creek, South Carolina (Barber *et al.,* 1991, and an unpublished study by Brockway *et al.*, 1996).

In the Barber *et al.* (1991) study, the FGETS model was used to describe the bioaccumulation properties of PCBs in various fish (alewife, coho salmon, rainbow trout, brown trout and lake trout). These results were compared with laboratory BCF results for rainbow trout and field BAFs. The model was found to simulate the

bioconcentration in rainbow trout well when compared to laboratory results. The results from the comparison with field data were more scattered but again, the model appeared to produce results consistent with the field data.

Although the model requires a relatively large amount of fish-specific data, many of these data are available in a compilation (Barber, 2005b) which has been used to parameterise the model for different fish species. Thus, the BASS model contains species-specific information for the following fish (information for other fish species is given in Barber, 2005b).

- alewife (*Alosa pseudoharengus*)
- bluegill sunfish (*Lepomis macrochirus*)
- yellow bullhead (*Ameiurus natalis*)
- mosquito fish (*Gambusia affinis*)
- gar (*Lepisosteus platyrhncus*)
- largemouth bass (*Micropterus saloides*)
- redear sunfish (*Lepomis microlophus*)
- salmonids.

Several example community files are also included in the model, but these relate mainly to food chains in the everglades and Lake Ontario.

Despite the complexity of the model, it is relatively easy to create a new chemical input file. However, many of the fish included in the model are warm-water species and a considerable effort would be required to parameterise the model for species more appropriate to the United Kingdom.

7.3 Summary of the BASS/FGETS model

An overview of the method is given in Table 7.2.

Table 7.2 Summary of the BASS/FGETS model

Criteria	Comment
Structure of the method	The model is available as a computer program. A comprehensive manual is available outlining the main assumptions in the model.
Scope of the method	The model is being developed by the United States Environmental Protection Agency. The intended users include research fisheries ecologists, bioaccumulation researchers and Environmental Protection Agency scientists and ecologists who must routinely estimate bioaccumulation of chemicals in fish for ecological or human health exposure assessments. The method is applicable to hydrophobic organic chemicals and some metals (those that complex with sulfhydryl groups such as cadmium, copper, lead, mercury, nickel, silver and zinc).
Type of method	The fish bioaccumulation model is a kinetic model (based on diffusion kinetics). As well as fish, the model considers benthos, periphyton/attached algae, phytoplankton and zooplankton using a simple mass balance model. The bioaccumulation model is coupled to a fish-growth model and a model for population dynamics. The bioaccumulation model can be run on its own or in

Criteria	Comment
	conjunction with the other sub-models.
Calculation method	Computer program.
Outputs from the method	The outputs from the model are numerous (and can be user-specified). The outputs can include the following: • annual bioenergetic fluxes and growth statistics (such as mean body weight, mean growth rate) of fish; • annual bioaccumulation fluxes and statistics (such as mean whole body concentrations, BAFs, BMFs).
Focus of the method	The method can consider different age classes within individual species and so can target sensitive groups (such as young fish).
Chemical-specific input parameters	The main chemical-specific input parameters required by the model are summarised in Table 7.1. These include the melting point, log K_{ow} , the log aqueous activity coefficient (can be estimated from melting point and log K_{ow} if data are not available), the molar volume, metabolism rate for each fish species, and the BCF for non-fish species (such as benthos, periphyton, phytoplankton and zooplankton).
Key default parameters used in the method.	The model uses many fish-related parameters, outlined in Table 7.1. Values are defined for several (mainly warm water) species. Also, the model uses some environment-related parameters such as depth of water, initial biomass loadings, and habitat preferences, tolerances and suitability indices.
Environment considered in the method.	The model considers a generic one-hectare area of a water body. The actual food chain structure can be user-defined. Example files are provided with the model for food chains in the Everglades and Lake Ontario.
How is persistence considered?	A metabolism rate in fish (which can be varied for different species and age ranges) can be included in the model if data are available. The bioaccumulation model takes account of other depuration processes such as faecal egestion, growth dilution and respiration. Metabolism in non-fish species is not taken into account directly (but would be included if the BCF used for the species already takes account of metabolism). Degradation in the environment is not specifically included, but input concentrations could be adjusted to take this into account if required.
Are seasonal variations considered?	Yes. Many of the input parameters can be entered as sinusoidal time-varying functions.
Strengths	The model is comprehensive and can consider the effects of the substance on the community structure. The food chain within the model can be user-defined. Metabolic/degradation products can also be modelled.
Weaknesses and limitations.	The model is quite complicated and would require a degree of expert knowledge to run. The species-related data requirements are quite extensive and, although appropriate values are given within the model for a number of species, such data may not be available for other species (a data compilation is provided with the model that would be a useful start in this respect). Coupling of the bioaccumulation model with the population dynamics model would complicate the interpretation of the results, as the feeding pattern of the fish may change with changing populations (although it is possible to run the bioaccumulation model independently of the population model).
Could the model be adapted to the UK situation?	The model could be adapted to the UK situation, but this would not be straight forward and would require considerable effort.
Further work	No further development of the model itself would be required. However, if it were to be used for the UK, one or more UK-specific food chains would need to be constructed.

7.4 Evaluation against screening criteria

7.4.1 Data requirements

The chemical-related data required to run the model are relatively modest or could be estimated. The more problematic data are probably the BCFs for the non-fish species included in the model, and possibly the molar volume. More complex data (such as metabolism half-lives) can be used if available. There are sufficient species-related data within the model to run it for certain fish species. Overall, a score of two is appropriate. The importance rating for this criterion is five. Therefore,

$SCORE_{DATA} = 2 \times 5 = 10$.

7.4.2 Model calibration

The model is based mainly on theoretical considerations and no calibration appears to have been carried out. The model is applicable to hydrophobic chemicals but the range of applicability (in terms of log K_{ow} , for example) is unclear. A score of two is considered appropriate. The importance rating for this criterion is five. Therefore,

$SCORE_{CALIBRATION} = 2 \times 5 = 10$.

7.4.3 Model validation

The bioaccumulation model has been validated against laboratory BCFs and field BAFs for PCBs. Agreement between experimental and field data was found to be consistent. Other parts of the model do not appear to have been validated. A score of two is appropriate. The importance rating for this criterion is five. Therefore,

$SCORE_{VALIDATION} = 2 \times 5 = 10$.

7.4.4 Ease of use

The model is quite complex and would require considerable experience to use, particularly if user-defined simulations were to be run. A score of one is considered appropriate. The importance rating for this criterion is two. Therefore,

$SCORE_{EASE} = 1 \times 2 = 2$.

7.4.5 Transparency

The main underlying principles of the methods used in the model are clear, but the exact calculations used are not always clear. A score of two is appropriate. The importance rating for this criterion is five. Therefore,

$SCORE_{TRANS} = 2 \times 5 = 10$.

7.4.6 Prediction uncertainty

Uncertainty in the method's predictions will depend to some extent on the availability of metabolism data. In the absence of such data, a zero metabolism rate can be assumed, resulting in a precautionary assessment. If such metabolism data are available (or are estimated), this precautionary aspect will be reduced. Overall, a score of three is appropriate. The importance rating for this criterion is five. Therefore,

$SCORE_{UNCERT} = 3 \times 5 = 15$.

7.4.7 Ability to predict the concentration near the top of the food chain

The model allows predictions of concentrations in more than two trophic levels near the top of the food chain (data permitting) and so a score of three is judged appropriate. The importance rating for this criterion is four. Therefore,

$SCORE_{TOP\ FOOD} = 3 \times 4 = 12$.

7.4.8 Relevance to England and Wales

The fish species within the model are generally not relevant to the UK (several of the fish are warm-water species). It is possible for the user to add other fish species to the model and so it would be possible to construct example food chain(s) relevant to the UK. However, the data requirements for fish species are extensive and so this adaptation may not be straightforward, and would require expert knowledge of the model. A score of one is therefore considered appropriate. The importance rating for this criterion is four. Therefore,

$SCORE_{RELEVANCE} = 1 \times 4 = 4$.

7.4.9 Overall score

Using the methodology outlined in Appendix C, the overall score can be estimated as:

$$\text{TOTAL SCORE} = SCORE_{DATA} + SCORE_{CALIBRATION} + SCORE_{VALIDATION} + SCORE_{EASE} + SCORE_{TRANS} + SCORE_{UNCERT} + SCORE_{TOP\ FOOD} + SCORE_{RELEVANCE}$$

$$= 10 + 10 + 10 + 2 + 10 + 15 + 12 + 4$$

$$= 73.$$

8 ECOFATE and Food Chain Bioaccumulation models

8.1 Introduction

The Food Chain Bioaccumulation model and the ECOFATE model have been produced by workers at Simon Fraser University in Canada. The following three models (all working on very similar principles) are available for download[13] free of charge.

- Food Chain Bioaccumulation model version 1.0
- Food Chain Bioaccumulation model version 1.1
- ECOFATE model version 1.0ß1

The models were originally developed for the Lake Ontario ecosystem but can be adapted to other ecosystems. The ECOFATE model is a ß test version.

The model is used within the USEPA methodology for deriving ambient water quality criteria for the protection of human health (USEPA, 2000), where it is used to define the food chain multipliers used to estimate BAFs by some methods (see Chapter 2.2).

8.2 Description of model

The Food Chain Bioaccumulation model (version 1.0) is based on work published by Gobas (1993). The model is a non-steady state mass balance model for hydrophobic organic chemicals based on a Lake Ontario food chain. The main assumptions used in the model are as follows:

- the bioconcentration factor for a chemical in aquatic macrophytes, phytoplankton and zooplankton can be estimated directly from the K_{ow} value and the lipid content of the macrophytes/phytoplankton/zooplankton;
- the bioaccumulation in benthic invertebrates results from an equilibrium partitioning of the chemical between the lipids of the organism, the organic carbon fraction of the sediment and the interstitial pore water;
- uptake into fish can occur directly from water via the gills and from the consumption of food via the gastrointestinal tract;
- loss of chemical from the fish can occur via the gills to water, via egestion to faecal matter and as a result of metabolic transformation.

The model's basis is that the change in concentration of a chemical with time in an organism is a result of the rate of uptake and loss of the chemical. The effect of growth of the organism is also taken into account. Thus, for fish the following equation is

[13] http://www.rem.sfu.ca/toxicology/models/models.htm.

applicable (at steady state this equation is analogous to the one based on fugacity used as the basis of the Foodweb model, as outlined in Chapter 6).

$$\frac{dC_F}{dt} = k_1 \times C_{WD} + k_D \times C_D - (k_2 + k_E + k_M + k_G) \times C_F$$

where: C_F = chemical concentration in fish (µg/kg).

C_{WD} = dissolved chemical concentration in water (µg/l).

C_D = chemical concentration in food (µg/kg).

k_1 = rate constant for uptake of chemical from water via gills (day^{-1}).

k_D = rate constant for chemical uptake from food (kg food/kg fish/day)

k_2 = rate constant for elimination of chemical via gills (day^{-1}).

k_E = rate constant for elimination via faecal egestion (day^{-1}).

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

k_G = rate constant for growth.

The rate constants for uptake of chemical from water via gills (k_1), for elimination of chemical via gills (k_2) and for uptake from food (k_D) are estimated from the feeding rate and the gut absorption efficiency[14] (or assimilation efficiency; estimated from K_{ow} and the fish size (weight) in a similar way to the Foodweb model (see Chapter 6)). However, the model also takes into account the effects of temperature on the feeding rate, using a simple bioenergetics-based model relating the feeding rate to temperature and the fish's body weight.

The faecal egestion rate constant is set as four times lower than the rate constant for uptake of the chemical via food. This is based on experimental observations that the faecal egestion rate is generally around three to five times lower than the ingestion rate.

Growth of the fish (rate constant k_G) is modelled based on the following generalised growth equations developed by Thomann *et al.* (1992b).

$k_G = 0.00251 \times V_F^{-0.2}$ for temperatures around 25°C.

$k_G = 0.000502 \times V_F^{-0.2}$ for temperatures around 10°C

where: V_F = weight of fish.

Adsorption of the chemical onto suspended particulate matter in the water column is taken into account, as the model assumes that only the chemical in the dissolved phase is bioavailable.

Version 1.1 of the model is essentially the same as above, except that the benthic invertebrate sub-model published by Morrison *et al.* (1996) is also included. This is a steady-state model for the bioaccumulation of organic chemicals for filter feeding and

[14] Similar to other models, this model assumes that the assimilation efficiency of the chemical from food is constant with increasing body concentration. However, according to Barber (2005a) such an assumption may be incorrect, and assimilation efficiency would be expected to decrease with increasing body concentration.

detritivorous organisms. The basis of the model is the same as for fish, where at steady state, the sum of chemical intake from water and food equals the sum of chemical elimination from the respiratory surface, faeces and metabolism). This model was developed for a food web consisting of plankton and benthic/filter feeding invertebrates including *Gammarus fasciatus*, cray fish (*Orconectes propinquus*), zebra mussel (*Dreissena polymorpha*) and caddisfly larvae (*Hydropychidae alterans*), and takes into account uptake from feeding on sediments/suspended sediments as well as from food and water.

Both versions of the Food Chain Bioaccumulation model can carry out Monte-Carlo simulations in order to investigate confidence limits in the modelling results. This simulation is based on the standard deviations (user-entered) of many of the input values. Input parameters of the Food Chain Bioaccumulation model are summarised in Table 8.1.

Table 8.1 Inputs required for Food Chain Bioaccumulation model

Parameter	Comment
Chemical – physico-chemical data	
Molecular weight	
Log K_{ow}	The standard deviation can be entered if running a Monte-Carlo simulation.
Henry's law constant	Units of Pa m^3/mole. The standard deviation can be entered if running a Monte-Carlo simulation.
Dissociation constant	A value of zero is entered if the substance does not dissociate. The standard deviation can be entered if running a Monte-Carlo simulation.
Chemical – environmental data	
Concentration of chemical in water	Units of g/l. A constant exposure concentration is assumed in the model. The standard deviation can be entered if running a Monte-Carlo simulation.
Concentration of suspended solids in water	Units of kg/l. The model takes account of adsorption of the chemical onto suspended solids. The standard deviation can be entered if running a Monte-Carlo simulation.
Organic carbon content of suspended solids	Units of g/g. The standard deviation can be entered if running a Monte-Carlo simulation.
Concentration of chemical in bottom sediments	Units of g/kg. The standard deviation can be entered if running a Monte-Carlo simulation.
Organic carbon content of bottom sediments	Units of g/g. The standard deviation can be entered if running a Monte-Carlo simulation.
pH of water	The standard deviation can be entered if running a Monte-Carlo simulation.
Water temperature	In °C. The standard deviation can be entered if running a Monte-Carlo simulation.
Food chain information – version 1	
Lipid content of plankton	As a weight fraction. Values for two species can be entered. The standard deviation can be entered if running a Monte-Carlo simulation.
Number of benthic species	Any number of benthic species can be added.
Lipid content of benthos	As a weight fraction for each species. The standard deviation can be entered if running a Monte-Carlo simulation.
Number of fish	Any number of fish species, or fish sizes, can be added.
Weight of fish	In kg. This can be defined for each species or can be used to

Parameter	Comment
	define size groups within a species. The standard deviation can be entered if running a Monte-Carlo simulation.
Lipid content of fish	As a weight fraction for each species/size. The standard deviation can be entered if running a Monte-Carlo simulation.
Metabolism rate constant in fish	The rate constant for metabolism of the chemical in each fish species or size can be entered (units day^{-1}). The standard deviation can be entered if running a Monte-Carlo simulation.
Feeding preference	The fraction of the diet that each prey item makes to each predator can be defined using a matrix.
Food chain information – version 1.1	
Lipid content of planktons	As a weight fraction. The standard deviation can be entered if running a Monte-Carlo simulation. A default value of 0.05 is used.
Lipid content of zooplankton	As a weight fraction. The standard deviation can be entered if running a Monte-Carlo simulation. A default value of 0.03 ± 0.01 is used for mysids.
Lipid content of filter feeders	As a weight fraction. The standard deviation can be entered if running a Monte-Carlo simulation.
Lipid content of benthic detrivores	As a weight fraction. The standard deviation can be entered if running a Monte-Carlo simulation. Default values are given for pontoporeia (0.03 ± 0.01) and oligochaetes (0.01 ± 0.005).
Weight of fish	In kg. This can be defined for each species or can be used to define size groups within a species. The standard deviation can be entered if running a Monte-Carlo simulation. Default values are given for sculpins (0.0054 kg), alewife (0.032 kg), smelt (0.2 kg), laketrout (2.41 ± 0.77 kg) and rainbow trout (3.38 ± 0.78 kg) for a Great Lakes food chain.
Lipid content of fish	As a weight fraction for each species/size. The standard deviation can be entered if running a Monte-Carlo simulation. Default values are given for sculpins (0.08), alewife (0.07), smelt (0.08), laketrout (0.174) and rainbow trout (0.13) for a Great Lakes food chain.
Metabolism rate constant in fish	The rate constant for metabolism of the chemical in each fish species or size can be entered (units day^{-1}). The standard deviation can be entered if running a Monte-Carlo simulation. A value of zero (non-metabolised) can be assumed as a default.
Feeding preference	The proportion of the diet that each prey item makes up for each predator can be defined using a matrix. The following values are included as default (based on a Great Lakes food chain): Sculpin – 0.18 mysids, 0.82 pontoporeia. Alewife – 0.60 mysids, 0.40 pontoporeia. Smelt – 0.54 mysids, 0.21 pontoporeia and 0.25 sculpins. Lake trout – 0.10 sculpin, 0.50 alewife and 0.4 smelt. Rainbow trout – 0.1 sculpin, 0.50 alewife and 0.4 smelt.

The ECOFATE model consists of four integrated modules: an environmental fate model, a food web bioaccumulation model, a toxicological hazard assessment model and a human health risk assessment model. The model can be applied to a range of freshwater and marine aquatic systems. The food web bioaccumulation model can be run on its own or in combination with any of the other models. The ECOFATE model can be run as a time-dependent or steady-state model.

The food web bioaccumulation model in ECOFATE is very similar in principle to the Food Chain Bioaccumulation model described above. The principles behind the other models are less clear. The environmental fate model takes into account degradation in sediment and surface water. The toxicological hazard model carries out a comparison of predicted concentrations in water with the known ecotoxicity of the chemical. The human health risk assessment model uses derived concentrations in fish and other aquatic organisms, combined with user-entered consumption rates, to derive a total daily human intake figure and compares this with mammalian toxicity data for the substance.

Input parameters required by the ECOFATE model are summarised in Table 8.2. Similar to the Food Chain Bioaccumulation model, the standard deviation can be entered for many of the parameters when running a Monte-Carlo simulation.

Table 8.2 Inputs required for ECOFATE model

Parameter	Comment
System definition	
Number of compartments in the aquatic ecosystem	This allows the properties of different parts of the water body to be specified; the water body being modelled can be split into a number of connected parts and the appropriate hydrological properties for each part of the water body can then be entered.
Number of layers in aquatic compartment	This allows the properties of different depths (layers) within each compartment to be specified.
Models to be run	One or more of the following sub-models can be specified. Each model can be run as a steady-state and/or time-dependent model. • environmental fate • food web bioaccumulation • human health risk • toxicological hazard.
Food web	
Lipid content of plankton	As a weight fraction. A default of 0.005 is assumed. More than one species can be added.
Lipid content of zooplankton	As a weight fraction. More than one species can be added.
Lipid content of filter feeders	As a weight fraction. More than one species can be added.
Maximum age of fish	Only required for time-dependent model.
Spawning month	Only required for time-dependent model.
Weight of fish	In kg. More than one species, or size for a single species, can be added. For time-dependent calculations, a value for each age of fish is needed.
Lipid content of fish	As a weight fraction for each species or size/age.
Metabolism rate constant in fish	The rate constant for metabolism of the chemical in each fish species or size/age can be entered (units day^{-1}).
Fraction of fish diet	The fraction each species/organism makes to the diet of each fish considered can be specified.
Hydrodynamic data	
Flow rate	The flow rate of water (in l/day) into and out of the model, to and from each aquatic compartment (and layer) considered in the model, can be specified.
Ecosystem parameters	
Length, width and depth	The length, width and depth (in metres) of each compartment

Parameter	Comment
	(and layer) within the aquatic ecosystem can be specified.
Temperature and air temperature	The water temperature and air temperature (in °C) of each compartment (and layer) within the aquatic ecosystem can be specified.
Active sediment layer	The depth of the sediment layer within each compartment (and layer) within the aquatic ecosystem can be specified.
Fraction organic carbon in sediment	The fraction of organic carbon in sediment can be specified within each compartment (and layer).
Fraction organic carbon in suspended sediment	The fraction of organic carbon in suspended sediment can be specified within each compartment.
Chemical loading	
Loading rate	The chemical loading rate (in g/day) can be specified for each compartment (and layer) within the aquatic ecosystem. Different values can be entered for each month of the simulation or a constant input can be assumed.
Chemical properties	
Molecular weight	
Log K_{ow}	
Henry's law constant	Units of Pa m^3/mole.
Dissociation constant	Zero is entered if the substance is non-dissociating.
Transformation half-life in water	The degradation half-life in water (in days).
Transformation half-life in sediment	The degradation half-life in sediment (in days).
Carcinogen – cancer potency factor	Units of kg.day/mg. This value is optional and is only required if the human health risk assessment module is being run for a carcinogen.
Non-carcinogen reference dose	Units of mg/kg/day. Value derived from available mammalian toxicity data. Only required if the human health risk assessment module is being run.
Map	
Map	A simplistic map of the aquatic ecosystem can be generated. The map shows the interconnection of the various water bodies specified under the "compartments" parameter. Predicted concentrations from the model can be displayed on this map.
Human health model	
Body weight	The typical human body weight (in kg). Can be specified for males and females.
Food consumption rate	The consumption rate (in g/day or g/year) of the various fish (and other organisms) included in the model can be specified for both males and females.
Concentration in other food items	These allow the intake of the chemical from other food items (not included in the model) to be taken into account.
Consumption of other food items	
Consumption of water	The consumption of water can be optionally included (in l/day)
Toxicological hazard	
Effect concentration	The toxic effect concentration can be specified (in ng/l) for each species of fish (or age/size class).
Other ecosystem parameters	
Water phase air to water mass transfer coefficient	Units of m/day.
Air phase air to water mass	Units of m/day.

Parameter	Comment
transfer coefficient	
Water to sediment diffusion mass transfer coefficient	Units of m/day.
Suspended solids deposition rate	Units of m/day.
Resuspension rate	A default value of zero is recommended if unknown.
Sediment burial rate	Units of m/day.
pH of water	

The food chain considered in the Food Chain Bioaccumulation model and ECOFATE model can be readily modified to consider different combinations of invertebrates and fish exposed via both the water column and sediment. The default food chain incorporated into the Food Chain Bioaccumulation model version 1.1 is very similar to that considered in the Foodweb model developed by Campfens and Mackay (1997) (see Chapter 6).

The outputs from the Food Chain Bioaccumulation model and ECOFATE model are available graphically and as a spreadsheet. Graphical outputs include log BCF (for uptake from water, on both a fresh weight and lipid weight basis) for each species, the BMF (for uptake from food, on both a fresh weight and lipid weight basis) and the log BAF (the overall bioaccumulation factor, again on a fresh weight and lipid weight basis). Concentration plots for each species (units g/kg on a fresh weight and lipid weight basis) and fugacities (units of Pa) are also presented. Outputs include diagrams showing the relative contributions of food and water to uptake of the chemical and the relative contributions of metabolism, gill exchange, faecal elimination and growth to elimination of the chemical from each species. If a Monte-Carlo simulation is run, the 95 per cent confidence limits of, for example, the BCF, BMF and BAF can be displayed.

The Food Chain Bioaccumulation model (version 1) was tested using measured data for 63 substances (including PCBs, DDT, DDE, chlorobenzenes, mirex, octachlorostyrene, hexachlorobutadiene and lindane amongst others) in a Lake Ontario food web. The model considered zooplankton (such as *Mysis relicta*), two benthic invertebrates (oligochaetes such as *Tubifex tubifex*, and *Pontoporeia affinis*) and four fish species: sculpin (*Cottus cognatus*), alewifes (*Alosa pseudoharengus*), smelt (*Osmeris mordax*) and a composite group of large salmonid species including lake trout (*Salvelinus namaycush*), rainbow trout (*Oncorhynchus mykiss*) and coho salmon (*Oncorhynchus velinus namaycush*). No statistically significant differences ($p = 0.05$) were found between predicted and observed concentrations for total PCBs in fish and benthic invertebrates. Observed concentrations in phytoplankton and zooplankton were generally higher than predicted. No explanation was apparent for this discrepancy, but the comparison may have been affected by sampling difficulties and small samples sizes (two samples for zooplankton and three for phytoplankton). A sensitivity analysis indicated that predicted concentrations in all fish species were more sensitive to changes in sediment concentration than changes in water concentration.

Modelled results from the benthic invertebrate model of Morrison *et al.* (1996) that was incorporated into the Food Chain Bioaccumulation model (version 1.1) and ECOFATE were compared to field measurements of 38 PCBs (covering a log K_{ow} range of 5.6 to 7.5). The following species were modelled: caddisfly larvae (*Hydropsyche alterans;* one composite sample), zebra mussels (*Dreissena polymorpha*; 20 samples), amphipods (*Gammarus fasciatus*; four composite samples) and crayfish (*Orconectes propinquus;* five samples) from Lake Erie. Measured concentrations of PCBs in sediment, water

and plankton from the same area were used as inputs into the model. A comparison was made between predicted and measured steady-state organism-to-sediment fugacity ratios using a goodness-of-fit test comparing the sum of relative squared errors (a similar comparison was also made assuming an equilibrium partitioning model). The steady-state model presented by Morrison *et al*. (1996) was shown to be a much better predictor of bioaccumulation in benthic invertebrates than the equilibrium partitioning model. For example, the sum of relative squared errors for the steady-state model was 33.4 for caddisfly larvae, 48.0 for zebra mussel, 3.3 for *Gammarus* and 16.4 for crayfish compared with 143.1 for caddisfly larvae, 117.5 for zebra mussel, 113.2 for *Gammarus* and 56.2 for crayfish using the equilibrium partitioning model. With the exception of crayfish, the 95 per cent confidence limits of model predictions[15] for the steady-state model were less than a factor of 3.2 (95 per cent confidence limits of predictions for crayfish were a factor of seven). A sensitivity analysis indicated that the diet-related parameters (such as digestibility and absorption of food) and the fugacity ratio between diet and sediment were the most sensitive input parameters for benthic invertebrates.

The model has also been applied to a benthic/pelagic food web for PCBs in Western Lake Erie (Morrison *et al.,* 1997). Measured data of 31 PCBs in fourteen fish species and five benthic invertebrate species was used to verify the model. The results indicated that 95 per cent of observed concentrations in filter-feeding benthic invertebrates, detritus-feeding benthic invertebrates and fish were within a factor of 1.8, 1.9 and 2.0 of the model predictions, respectively.

Using similar principles as those laid out in the Food Chain Bioaccumulation model and the ECOFATE model, Arnot and Gobas (2003) derived a generic QSAR for predicting a BAF for accumulation in aquatic food webs. The model was derived for a fish in the upper trophic level of a Canadian food chain and was represented by the following equation:

$$BAF = \frac{C_B}{C_W} = (1 - L_B) + \left(\frac{k_1 \times \phi + (k_D \times \beta \times \tau \times \phi \times L_D \times K_{OW})}{k_2 + k_E + k_G + k_M} \right)$$

where: BAF = bioaccumulation factor in fish.

C_B = concentration in biota (fish)

C_W = total concentration in water.

ϕ = fraction of total chemical concentration in water that is freely dissolved = $1/(1 + \chi_{POC} \times 0.35 \times K_{ow} + \chi_{DOC} \times 0.1 \times 0.35 \times K_{ow})$, where χ_{POC} = concentration of particulate organic carbon in water (assumed to be 5×10^{-7} g/ml) and χ_{DOC} = concentration of dissolved organic carbon (assumed to be 5×10^{-7} g/ml).

k_1 = rate constant for chemical uptake via gills (l/kg/day) = $1/((0.01 + 1/K_{ow}) \times W^{0.4})$, where W = weight of fish (assumed to be one kilogram).

k_D = rate constant for chemical uptake via diet (kg/kg/day) = $0.02 \times W^{-0.15} \times e^{(0.06\times T)}/(5.1\times10^{-8} \times K_{ow} + 2)$, where T = mean water temperature (assumed to be 10°C).

[15] The 95 per cent confidence limit reflects the factor that should be applied to model predictions in order to account for 95 per cent of the observed data.

k_2 = rate constant for elimination of chemical via respiratory surfaces (day^{-1}) = $k_1/(L_B \times K_{ow})$.

k_E = rate constant for elimination of chemical via faecal egestion (day^{-1}) = $0.125 \times K_D$.

k_G = rate constant for growth dilution (day^{-1}) = $0.0005 \times W^{-0.2}$.

k_M = rate constant for elimination of chemical via metabolism (day^{-1}) – default is zero day^{-1}.

K_{ow} = octanol-water partition coefficient.

L_B = fraction lipid content of fish (assumed to be 0.2).

L_D = fraction lipid content of diet (lowest trophic level organism) (assumed to be one per cent).

The term β is an empirical value derived from calibrating the model to measured data. It represents the degree of food web accumulation and is highly dependent on the species of interest, food web structure and ecosystem characteristics. A value of 130 was used for the example food web (based on a dataset of 936 good quality BAF measurements) but the value would need to be determined on a case-by-case basis for other food webs by calibration of the QSAR to appropriate datasets.

The term τ is a factor that represents the degree of trophic dilution for substances that are metabolised at a significant rate in organisms in a food web = $(0.0065/(k_M + 0.0065))^{n-1}$, where n = number of trophic interactions (levels) in the food web (n was assumed to be three in the Canadian food web).

This approach allows the BAF for fish in higher trophic levels to be estimated using relatively little chemical-related (mainly K_{ow} and metabolism rate constant), species-related (mainly lipid contents of organisms at the top and bottom of the food chain, the weight of individual fish at the top trophic level and number of trophic levels), and environment-related (mainly particulate and dissolved organic carbon contents in the water and the ambient temperature) information. However, the method needs to be calibrated to specific food chains (the β-parameter), and so the applicability of the method as it stands (based on a Canadian food web) will be limited for the UK.

An update to the original model presented by Gobas (1993) has recently been published (Arnot and Gobas, 2004). This model incorporates several new elements and revisions including a new model for the partitioning of chemicals into organisms, new kinetic models for predicting concentrations in algae, phytoplankton and zooplankton, new allometric relationships for predicting gill ventilation rates in a wide range of aquatic species, and a new mechanistic model for predicting gastrointestinal magnification of organic chemicals in a range of species. These developments are based on insights obtained from recent laboratory experiments, analysis of field data and improvements in the availability of data for model parameterization.

The performance of the new model was compared to the Gobas (1993) model using field data (1,019 datapoints for 35 species and 64 chemicals) from three freshwater ecosystems (Lake Ontario, Lake Erie and Lake St. Clair). The food web consisted of algae, phytoplankton and macrophytes, zooplankton and small pelagic invertebrates, benthic invertebrates, water-column filter feeders, small juvenile fish, medium-sized fish and larger (upper-trophic level) fish. The performance of the models was assessed by comparing the geometric means of predicted and observed BAFs for all chemicals in all species for which empirical data were available and defined as the model. Bias represented systematic overprediction (model bias greater than one) or underprediction (model bias less than one); thus, a model bias of two indicated that the model, in general, overpredicted the field data by a factor of two, whereas a model bias of 0.5

indicated that the model generally underpredicted the field data by a factor of two. The overall model bias for the updated model was found to be 1.04 (95 per cent confidence interval 0.13 to 8.08), 1.05 (95 per cent confidence interval 0.24 to 4.64) and 0.78 (95 per cent confidence interval 0.08 to 7.89) for the data from Lake Ontario, Lake Erie and Lake St. Clair, compared with a model bias of 0.86, 0.16 and 0.17 for the three lakes respectively (the 95 per cent confidence intervals were not given in this case) using the original Gobas (1993) model. Overall, it was concluded that the revised model had improved accuracy over the original 1993 model. The model was stated to be applicable to non-ionizing organic chemicals with a log K_{ow} from one to around nine.

The inputs required for the updated model are largely unchanged from the original model. The updated model is, however, not yet implemented in a computer program (although it would be relatively straightforward to implement the calculations in a spreadsheet).

8.3 Summary of the Food Chain Bioaccumulation and ECOFATE models

An overview of the method is given in Table 8.3.

Table 8.3 Summary of the Food Chain Bioaccumulation and ECOFATE model

Criteria	Comment
Structure of the method	The models are available as computer programs. Papers outlining the calculation methods involved have been published.
Scope of the method	The model was developed for research purposes but is also used within the USEPA methodology for deriving ambient water quality criteria for human health (see Chapter 2.2). The method is reported to be applicable to non-ionizing organic chemicals with a log K_{ow} in the range one to nine.
Type of method	The model is a non-steady state mass balance model. The model also contains a steady-state mass balance model for filter feeding and detritivorous organisms.
Calculation method	Computer program. Details of the calculation methods involved have been published and could be implemented in a spreadsheet if desired.
Outputs from the method	Outputs are available as a spreadsheet or graphically and include the following: • Log BCF for each species (both on a wet weight and lipid weight basis). • Log BMF for each species (both on a wet weight and lipid weight basis). • Log BAF for each species (the overall bioaccumulation factor, both on a wet weight and a lipid weight basis). • Concentration in each species (g/kg on both a fresh weight and lipid weight basis). • Fugacities in each species (Pa). • Relative contributions of food and water to the uptake in each organism. • Relative contributions of metabolism, gill exchange, faecal elimination and growth to the elimination of the chemical from each species. • 95 per cent confidence limits for BCF, BMF or BAF if a Monte-Carlo simulation is run.
Focus of the method	The method does not focus specifically on sensitive groups, but specific size/age groups can be defined within the model.
Chemical-specific input	The main chemical-specific input parameters required by the model are summarised in Table 8.1 and Table 8.2. These include the molecular weight,

Criteria	Comment
parameters	log K_{ow} , Henry's law constant, dissociation constant (if applicable), transformation half-life in water, transformation half-life in sediment, metabolism rate constant for each species of fish.
Key default parameters used in the method	The key default parameters required by the model are summarised in Table 8.1 and Table 8.2 and can be divided into two groups. The first relates to the environment and includes parameters such as concentration of suspended solids in water, organic carbon content of suspended and bottom sediments, pH and temperature of water. The second group relates to the organisms in the food chain and includes the lipid contents of plankton, zooplankton, filter feeders and fish, and weight and feeding preferences of fish.
Environment considered in the method	The model considers a generic environment. The default parameters used relate mainly to a Great Lakes food chain, but all key parameters within the model can be easily adapted for other environments and food chains.
How is persistence considered?	A metabolism rate in fish (which can be varied for different species and age groups) can be included if data are available. The bioaccumulation model takes account of other depuration processes such as faecal egestion, growth dilution and respiration. Degradation in water and sediment can also be taken into account in the ECOFATE model.
Are seasonal variations considered?	No. However, several parameters within the model are temperature-dependent (such as feeding rates and growth rates for fish) and so it would be relatively easy to investigate the effects of this by simply changing the temperature used in the simulation.
Strengths	The model is simple to use and can be easily adapted to different food chains and environments. Data requirements (both chemical-related and food chain-related) are modest. Ingestion of sediments/suspended sediments by benthic/filter feeding organisms is included. The method considers several modes of elimination from organisms and can also take into account metabolism if data are available. The model directly calculates the appropriate BAFs that can be used in setting standards (see Chapter 15).
Weaknesses and limitations	It is not possible to use actual BCF data within this method.
Overall assessment of whether the model could be adapted to the UK situation	The model provides a generic framework that could easily be adapted to the UK situation. Default/example values within the model are generally taken from a Great Lakes food chain that may not be appropriate for the UK. but all the relevant parameters can easily be changed. In particular, species-related parameters used by the model are modest (essentially lipid contents and weight of organism) and so a UK food chain could easily be constructed.
Further work	An appropriate food chain for the UK should be constructed (the default food web already considered in the model could be used as a basis for this). Updates presented in the paper by Arnot and Gobas (1993) could also be implemented in the model.

8.4 Evaluation against screening criteria

8.4.1 Data requirements

The model requires mainly readily available chemical-specific information to run. More complex data (such as metabolism half-lives) can be used in the method if available. A score of three is appropriate. The importance rating for this criterion is five. Therefore,

$SCORE_{DATA} = 3 \times 5 = 15$.

8.4.2 Model calibration

Similar to the Foodweb model (see Chapter 6), this method is based on theoretical considerations and experimentally-derived correlations. For example, the correlation for gut absorption efficiency used in the Foodweb model is used here (derived directly from experimental data on chlorinated organic compounds with six species of fish, but covering only a relatively small log K_{ow} range of 5.0 to 8.3). On balance, a score of two (similar to the Foodweb model) is appropriate, as some parts of the model have been calibrated over a small log K_{ow} range. The importance rating is five. Therefore,

$SCORE_{CALIBRATION} = 2 \times 5 = 10$.

8.4.3 Model validation

The model has been validated for a large number of compounds (log K_{ow} ranging from 5.6 to 7.4) using data from different locations and species. Agreement of predictions with field data was generally satisfactory. A score of three is appropriate. The importance rating for this criterion is five. Therefore,

$SCORE_{VALIDATION} = 3 \times 5 = 15$.

8.4.4 Ease of use

The model is easy to use. All three computer programs contain user-friendly interfaces, allowing important variables to be easily changed. Model outputs are in a form that could be used directly for setting standards (see Chapter 15).The score for this criterion is therefore three. The importance rating for this criterion is two. Therefore,

$SCORE_{EASE} = 3 \times 2 = 6$.

8.4.5 Transparency

Underlying methods used in the model are clear and outlined in the literature and so a score of three is appropriate. The importance rating for this criterion is five. Therefore,

$SCORE_{TRANS} = 3 \times 5 = 15$.

8.4.6 Prediction uncertainty

Uncertainty in the method's predictions will depend to some extent on the availability of metabolism data. In the absence of such data, a zero metabolism rate can be assumed, resulting in a precautionary assessment. If such metabolism data are

available (or are estimated), this precautionary aspect will be reduced. Overall, a score of three is appropriate. The importance rating for this criterion is five. Therefore,

$SCORE_{UNCERT} = 3 \times 5 = 15$.

8.4.7 Ability to predict the concentration near the top of the food chain

The model allows predictions of concentrations in more than two trophic levels near the top of the food chain (date permitting) and so a score of three is judged appropriate. The importance rating for this criterion is four. Therefore,

$SCORE_{TOP\ FOOD} = 3 \times 4 = 12$.

8.4.8 Relevance to England and Wales

The model is based on a Great Lakes food chain and so is not directly relevant to the UK. However, the food chain in the model can be user-specified and it would be easy to adapt the model to an aquatic food chain relevant to the UK. A score of two is therefore appropriate. The importance rating for this criterion is four. Therefore,

$SCORE_{RELEVANCE} = 2 \times 4 = 8$.

8.4.9 Overall score

Using the methodology outlined in Appendix C, the overall score can be estimated as:

$$\begin{aligned} \text{TOTAL SCORE} &= SCORE_{DATA} + SCORE_{CALIBRATION} + SCORE_{VALIDATION} + SCORE_{EASE} + SCORE_{TRANS} + SCORE_{UNCERT} + SCORE_{TOP\ FOOD} + SCORE_{RELEVANCE} \\ &= 15 + 10 + 15 + 6 + 15 + 15 + 12 + 8 \\ &= 96. \end{aligned}$$

9 Arctic Terrestrial Food-chain Bioaccumulation model

9.1 Introduction

The Arctic Terrestrial Food-chain Bioaccumulation model was presented in a paper by Kelly and Gobas (2003). Although the model is based on an arctic food chain, it is included in this review as one of the few models that considers terrestrial predators. It is thus of interest to investigate whether this model could be adapted to the situation in the United Kingdom (for example, Kelly and Gobas (2003) indicate some similarities between this food chain and the pasture-cow-human food chain in temperate regions).

9.2 Description of model

The model is designed to predict the bioaccumulation of persistent organic pollutants (POPS) in an arctic terrestrial food chain consisting of lichen, willows, caribou and wolf. The predominant route of exposure to the food chain is considered to be from aerial deposition.

The model consists of a series of mechanistic, mass balance equations relating ambient concentrations in the environment (air and snow concentrations) to the resulting concentration in vegetation, herbivores and carnivores.

Uptake by vegetation is modelled using a homogeneous one-compartment model. The three most important processes for uptake of chemicals in arctic vegetation are considered to be: a) air-to-vegetation partitioning of the chemical from the gas phase; b) direct deposition (both wet and dry) and erosion of the chemical associated with particulate matter in the atmosphere; and c) precipitation and subsequent accumulation of the chemical from overlying snowpacks via water-to-vegetation partitioning during snow melt events.

The bioaccumulation model for terrestrial mammals (caribou and wolves) is a two-compartment model consisting of a gastrointestinal tract and organism compartment (which represents the overall contaminant storage in the animal) for each mammal. Each compartment consists of a lipid phase, a non-lipid organic matter phase and a water phase. It is assumed that the sorption affinity of the lipid phase is similar to octanol, whereas the sorption affinity of the non-lipid organic matter phase is 3.5 per cent of that of octanol.

The basic assumption behind the model is that gastrointestinal magnification is the primary mechanism driving uptake and biomagnification of organic chemicals from the diet. The degree of chemical accumulation in the mammal is modelled on competing rates of uptake (through inhalation and absorption through the gastrointestinal tract) and elimination (through exhalation, urine excretion, faecal egestion, milk excretion, and metabolic transformation). The model also assumes that for continuously exposed animals (at steady state), concentrations in different tissues are homogeneously distributed within the animal when expressed on a lipid-normalised basis. This simplification is backed by experimental data. The mammalian model also considers the concentration in mother's milk (concentrations in milk are assumed to be equal to those in adult females' tissues when expressed on a lipid basis), the fetus

(concentrations in the fetus are assumed to be in equilibrium with the mother) and ingestion of the milk by a calf or pup.

As well as predicting concentrations in the food chain, the equations given in the paper allow bioaccumulation factors (related to the concentration in air) to be estimated directly for lichens, caribou and wolves.

A summary of the chemical-specific and species-specific data required by the model is given in Table 9.1.

Table 9.1 Information required by the Arctic Terrestrial Food Chain Bioaccumulation model

Information	Comment
Chemical-specific information	
Molecular weight	
Log K_{ow}	The value at 20°C is required. Values at other temperatures (ambient temperature for plants, 37°C for mammals) are estimated within the model (the temperature correction for log K_{ow} may be small).
Henry's law constant	Value at 20°C is required. Values at other temperatures are estimated within the model. Units Pa m^3/mole. The temperature correction applied may be chemical-specific.
Log K_{oa} (octanol-air partition coefficient)	Value at 20°C. Values at other temperatures are estimated within the model (the temperature correction applied may be chemical-specific). Can be estimated from the log K_{ow} and Henry's law constant.
Tissue half-life in mammals	Units of days.
Air concentration	These are the starting concentrations for the simulation.
Dissolved concentration in snowpack melt water	
Ambient air parameters	
Aerosol surface area	Values are given for the arctic for May-September (1×10^{-7} cm^2/cm^3) and October to April (1×10^{-6} cm^2/cm^3).
Particulate deposition velocity	Value assumed is three metres per hour.
Vegetation parameters	
Mass transfer coefficient for air-vegetation diffusion	Value assumed was three metres per hour (reduced to 0.5 m/hour during winter owing to snow cover).
Mass transfer coefficient for meltwater-vegetation diffusion	Value assumed was 1×10^{-4} m/hour based on surface water run-off data.
Rate constant for erosion of particle-bound chemical associated with vegetation surface	Value assumed was 0.002 per hour.
Surface area	Values assumed are 1×10^{6} m^2/m^3 for lichens and 1×10^{4} m^2/m^3 for willows.
Non-lipid organic matter	Values assumed are 40 per cent for lichens and 30 per cent for willows.
Lipid content	Values assumed are 0.5 per cent for lichens and one per cent for willows.
Water content	Values assumed are 59.5 per cent for lichens

Information	Comment
	and 69 per cent for willows.
Ecological-physiological parameters	
Diet composition	For caribou, assumed to be 100 per cent snow-covered lichens in winter, 100 per cent lichens in spring and 80 per cent willows/20 per cent lichens in summer and autumn. For wolves, assumed to be 100 per cent caribou all year round.
Feeding rate	Assumed to be 3.0 kg/day for caribou and 2.5 kg/day for wolves.
Faecal excretion rate	Assumed to be 1.3 kg/day for caribou and 0.2 kg/day for wolves.
Lipid absorption efficiency from diet	Assumed to be 65 per cent for caribou and 99 per cent for wolves.
Non-lipid organic matter absorption efficiency from diet	Assumed to be 50 per cent for caribou and 75 per cent for wolves.
Water absorption efficiency	Assumed to be 95 per cent for both caribou and wolves.
Water content in gastrointestinal tract	Assumed to be 50 per cent for both caribou and wolves.
Urinary excretion rate	Assumed to be 0.45 l/day for caribou and 0.25 l/day for wolves.
Dietary uptake efficiency	Assumed to be 25-80 per cent for caribou and 75-98 per cent for wolves. These values are based on data from cows and humans for chemicals with a log K_{ow} in the range 5.0-8.0.
Air uptake efficiency	Assumed to be 70 per cent for both caribou and wolves.
Lactation rate	Assumed to be 1.5 l/day per calf or pup for both caribou and wolves.
Suckling rate	Assumed to be 1.5 l/day per calf or pup for both caribou and wolves.
Lipid content in milk	Assumed to be 12 per cent for caribou and 10 per cent for wolves.
Non-lipid organic carbon content of milk	Assumed to be 20 per cent for both caribou and wolves.
Number of offspring per female	Assumed to be one calf for caribou and three pups for wolves.
Birth weight	Assumed to be 5 kg for caribou and 0.5 kg for wolves.
Time to weaning	Assumed to be 130 days after birth for caribou and 68 days after birth for wolves.
Mean annual lipid content of caribou or wolves	Assumed to be 8 per cent for caribou (range 4-25 per cent) and 12 per cent for wolves (range 7-21 per cent).
Non-lipid organic matter content of caribou or wolves	Assumed to be 20 per cent for both caribou and wolves.
Lung ventilation rates	Assumed to be 18 m^3/day for caribou and 13 m^3/day for wolves. Values estimated from an allometric relationship with body size.
Other information	
Ambient temperature for plants	Assumed to be -20°C during November (no snow cover) and -2°C from December-April.

The model was tested using a group of twenty-five organochlorine chemicals including five pesticides (α- and β-hexachlorocyclohexane, dieldrin, mirex, β-endosulphan), three trichlorbenzenes, sixteen PCBs and octachlorostyrene. Measured concentrations in arctic air and snowpack meltwater were used as input parameters to estimate concentrations in lichen, willows, caribou and wolves at hourly intervals over a 14-year period. A Monte-Carlo simulation was also run in order to determine the 95 per cent confidence intervals in predicted concentrations (based on the mean and standard deviations for several input parameters). In addition, predicted concentrations in caribou and wolf tissues were compared to actual concentrations in lichens, and animals sampled from Cambridge Bay, Bathurst Inlet and Inuvik (Kelly and Gobas, 2001).

Model predictions for lichens were in general agreement with observed concentrations in the environment. The model was also found to predict reasonably closely seasonal fluctuations in the levels of PCB 153 found in male caribou tissues (observed concentrations consistently fell within the model uncertainty determined by the Monte-Carlo simulation). General agreement between modelled and actual concentrations in the environment were also found with hexachlorobenzene and hexachlorocyclohexane in caribou and wolves.

One interesting finding from this model was that the bioaccumulation factors for caribou and wolves increased with increasing log K_{oa}, and were not always related to the chemical's log K_{ow} (as is often the case with aquatic food chains, for example). Thus, substances with relatively low log K_{ow} (two or more), but a high log K_{oa}, were predicted to biomagnify. This was thought to result from the fact that elimination from mammals by respiration was predicted to become increasingly less significant for substances with log K_{oa} greater than six. According to this model, log K_{oa} rather than log K_{ow} is the indicator for the potential to biomagnify in terrestrial food chains. The paper concluded that substances with a log K_{oa} below five should not biomagnify in this food chain regardless of the log K_{ow} value, but substances with a log K_{ow} two or more and a log K_{oa} greater than five have the potential to biomagnify.

Kelly *et al.* (2004) reviewed methods for predicting intestinal absorption and biomagnification of organic contaminants in fish, wildlife and humans. They concluded that emerging evidence indicated that currently-used K_{ow} -based classification methods (based on a log K_{ow} value above a certain cut-off – typically in the range three to five) for identifying potentially bioaccumulative substances were not adequate when considering mammals, birds and humans. The log K_{oa} value was deemed important for assessing bioaccumulation potential in such species, whereas the log K_{ow} alone gave a good indicator of bioaccumulation potential in aquatic organisms. It was argued that for air-breathing organisms, respiratory elimination occurs via lipid-air exchange, and that such exchange declines with increasing octanol-air partition coefficient, with biomagnification predicted to occur in many mammals at a log K_{oa} above five. This biomagnification potential can be mediated only if the substance is rapidly eliminated in urine (having a log K_{ow} of around two or less) or is rapidly metabolised. Thus, the bioaccumulation potential on air-breathing organisms is a function of both log K_{ow} and log K_{oa}. In contrast, for fish, respiratory elimination occurs to water via gill ventilation, and this process is known to be inversely related to the log K_{ow} (hence an increase in log K_{ow} results in a decrease in the rate of elimination and increase in the accumulation potential). Similar conclusions were also reached by Gobas *et al*. (2003).

Based on these findings, Kelly *et al.* (2004) proposed that chemicals can be classified into four groups based on their potential to bioaccumulate in air-breathing organisms. These groups are summarised below.

- Polar volatiles (low log K_{ow} and low log K_{oa}). These substances have low potential for bioaccumulation in air-breathing organisms or aquatic organisms. Examples include chemicals such as styrene and vinyl chloride.
- Non-polar non-volatiles (high log K_{ow} and high log K_{oa}). This group represents the majority of POPs such as PCBs and some organochlorine pesticides. These substances have a high bioaccumulation potential in both air-breathing organisms and aquatic organisms.
- Polar non-volatiles (low log K_{ow} and high log K_{oa}). This group of substances has a low bioaccumulation potential in aquatic organisms, but a high bioaccumulation potential in air-breathing organisms (unless they are rapidly metabolized).
- Non-polar volatiles (high log K_{ow} and low log K_{oa}). This group of substances is predicted to have a high accumulation potential in aquatic organisms, but a low accumulation potential in air-breathing mammals.

These findings are of potential interest for chemicals whose bioaccumulation potential in aquatic systems appears to be limited, but which have been found to occur in terrestrial birds and mammals (such as decabromodiphenyl ether).

9.3 Summary of the Arctic Terrestrial Food Chain Bioaccumulation model

An overview of the method is given in Table 9.2.

Table 9.2 Summary of the Arctic Terrestrial Food-Chain Bioaccumulation model

Criteria	Comment
Structure of the method	The model is currently available only as a series of equations in the published literature.
Scope of the method	The model is intended for research purposes. The method considers an arctic terrestrial food chain consisting of lichen, willows, caribou and wolf. Exposure routes in the model include air, snowmelt water and the food chain. The method is applicable to persistent organic pollutants.
Type of method	Non-steady state, kinetic mass balance model.
Calculation method	Detailed hand calculations. The method would need to be implemented into a computer program/spreadsheet for routine use.
Outputs from the method	The method can be used to estimate concentrations in lichens, caribou and wolves. In addition, methods are also given for estimating bioaccumulation factors (related to the concentrations in air) for lichens, caribou and wolves.
Focus of the method	The method considers the concentration in the fetus, mother's milk and in pups from ingestion of mother's milk. Therefore, some sensitive life stages are considered in the model.
Chemical-specific input	The chemical-specific information required by the model is summarised in Table 9.1. This includes the molecular weight, Henry's law constant, log

Criteria	Comment
parameters	octanol-air partition coefficient (which can be estimated from log K_{ow} and Henry's law constant) and the tissue half-life in mammals.
Key default parameters used in the method	The key default parameters used in the model are outlined in Table 9.1. They include ambient air parameters, vegetation parameters and several physiological/ecological parameters for the mammals in the model. Default values are given for the Arctic food chain considered.
Environment considered in the method	The model considers an Arctic food chain consisting of plants (lichens/willows), caribou and wolves.
How is persistence considered?	Metabolism in mammals can be included in the model if data are available.
Are seasonal variations considered?	Yes. Seasonal variations in caribou diet, temperature, mass transfer coefficient for air-vegetation exchange, and aerosol surface area are taken into account for the Arctic environment.
Strengths	The model is one of the few available that considers terrestrial predators. The data requirements (both chemical- and ecosystem-related) are modest and so the method could be adapted relatively easily for other food chains.
Weaknesses and limitations	The model as formulated considers an Arctic food chain that is of little relevance to the UK. The plant uptake part of the model does not consider uptake via the roots from soil. The model is not yet available in a computerized form.
Overall assessment of whether the model could be adapted to the UK situation	The method as it stands is not applicable to the UK situation. However, the basic frame work could be modified to represent a UK food chain if desired. This would take a considerable amount of effort, but this is one of the few models available that considers terrestrial predators.
Further work	The model would need substantial modification for the UK situation, but the framework could provide the basis of a terrestrial food web model for the UK. In addition to the routes of exposure already included, the model could also consider uptake by plants from soil (using, for example, a modification of the method in CLEA or the EU TGD outlined in Chapter 3). In addition, the model could be extended to include small (worm-eating) mammals by the inclusion of an earthworm uptake model (for examples, see Chapter 3).

9.4 Evaluation against screening criteria

9.4.1 Data requirements

The model requires mainly simple physico-chemical properties of the chemical. The model can also use more complex data such as metabolic half-lives in mammals if such data are available. Ecosystem-related data used by the model are also relatively modest and should be easily adaptable to other situations/species. A score of three is appropriate. The importance rating for this criterion is five. Therefore,

$SCORE_{DATA} = 3 \times 5 = 15$.

9.4.2 Model calibration

The model is generally based on theoretical considerations and so is not calibrated as such. The model is designed for use with persistent organic chemicals. A score of two is considered appropriate. The importance rating for this criterion is five. Therefore,

$SCORE_{CALIBRATION} = 2 \times 5 = 10$.

9.4.3 Model validation

The model has been validated using data for twenty-five organochlorine chemicals. The agreement between predicted concentrations and those found in lichen, willows, caribou and wolves was found to be acceptable. A score of three is considered appropriate. The importance rating for this criterion is five. Therefore,

$SCORE_{VALIDATION} = 3 \times 5 = 15$.

9.4.4 Ease of use

The model is available as a series of equations that would require considerable experience/knowledge to use. The model would need to be implemented as a computer program/spread sheet to be routinely used. The score for this criterion is therefore 1. The importance rating for this criterion is 2. Therefore,

$SCORE_{EASE} = 1 \times 2 = 2$.

9.4.5 Transparency

The underlying methods used in the model are clear and so a score of three is appropriate. The importance rating for this criterion is five. Therefore,

$SCORE_{TRANS} = 3 \times 5 = 15$.

9.4.6 Prediction uncertainty

Uncertainty in the method's predictions will depend to some extent on the availability of metabolism data. In the absence of such data, a zero metabolism rate can be assumed, resulting in a precautionary assessment. If such metabolism data are available (or are estimated), this precautionary aspect will be reduced. Overall, a score of three is considered appropriate. The importance rating for this criterion is five. Therefore,

$SCORE_{UNCERT} = 3 \times 5 = 15$.

9.4.7 Ability to predict the concentration near the top of the food chain

The model allows predictions of concentrations in more than two trophic levels, including those near the bottom and top of the food chain (data permitting), and so a score of three is judged appropriate. The importance rating for this criterion is four. Therefore,

$SCORE_{TOP\ FOOD} = 3 \times 4 = 12.$

9.4.8 Relevance to England and Wales

The model is for an Arctic terrestrial food chain and so is not relevant to the UK. However, the basic framework could be adapted to represent a UK food chain if desired. This would take a considerable amount of effort, but this is one of the few models available that considers terrestrial predators. A score of one is therefore appropriate. The importance rating for this criterion is four. Therefore,

$SCORE_{RELEVANCE} = 1 \times 4 = 4.$

9.4.9 Overall score

Using the methodology outlined in Appendix C, the overall score can be estimated as follows:

$$\begin{aligned} \text{TOTAL SCORE} &= SCORE_{DATA} + SCORE_{CALIBRATION} + SCORE_{VALIDATION} + SCORE_{EASE} + SCORE_{TRANS} + SCORE_{UNCERT} + SCORE_{TOP\ FOOD} + SCORE_{RELEVANCE} \\ &= 15 + 10 + 15 + 2 + 15 + 15 + 12 + 4 \\ &= 88. \end{aligned}$$

10 Prediction of Bioaccumulation in Aquatic Food Webs

10.1 Introduction

This method was published as a research paper (Voutsas *et al.*, 2002) and does not appear to have been used as yet in a regulatory context.

10.2 Description of model

The model consists of a series of regression equations relating field bioaccumulation factors to log K_{ow} for four trophic levels.

The raw data used in the analysis were taken from studies by Oliver and Niimi (1998), Pereira *et al.* (1988), Morrison *et al.* (1996), Burkhard *et al.* (1997), Metcalfe and Metcalfe (1997), Kid *et al.* (1998) and van Hattum *et al.* (1998). The data used covered a wide variety of persistent, non-metabolized organic chemicals including polychlorinated biphenyls, other chlorinated hydrocarbons and polyaromatic hydrocarbons. Many of the data referred to field studies in the Great Lakes area but also included some data from the Canadian Arctic, an estuarine system in Louisiana and various water systems in the Netherlands.

The data used consisted of measurements of concentrations in water and concentrations in various aquatic organisms from the same location. In order to facilitate the analysis, organisms were assigned to one of four generalised trophic levels. These were:

- plankton, including both phytoplankton and zooplankton;
- benthic invertebrates;
- planktivorous fish;
- piscivorous fish.

Concentrations of chemicals in water from the field studies were converted to freely dissolved concentrations using the following equation:

$$\frac{Conc_{Dissolved}}{Conc_{Total}} = \frac{1}{1 + K_{DOC} \times DOC + K_{POC} \times POC}$$

where: $Conc_{Dissolved}$ = freely dissolved concentration in water.

$Conc_{Total}$ = total concentration in water (as measured in the field study).

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

DOC = concentration of dissolved organic carbon in the water (kg/l).

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

POC = concentration of particulate organic carbon in the water (kg/l).

Values for DOC and POC were taken from the respective field studies. The value of K_{POC} was set to be equal to the K_{ow} value and the K_{DOC} value was set as the K_{ow} /10.

The log K_{ow} values used for the chemicals were taken from the compilations of Sangster (1997) and Devillers (1998).

Field BAFs were then determined for each chemical and organism based on the measured concentration in the organism (on a wet weight basis) divided by the concentration in water; BAFs were estimated using both the total concentration in water (termed BAF^t) and the estimated freely dissolved concentration (BAF^{fd}). Correlation equations relating the BAF to log K_{ow} were then constructed for each of the four trophic levels considered. Better correlations were obtained using BAF^{fd} based on the freely dissolved concentration. The correlations are summarised below, along with the relevant statistics (number of data points (N), correlation coefficient (r^2), the static test (F) value and the probability attached to the confidence interval (*p*)).

Trophic level 1: $\log BAF^{fd} = -0.1301 \times (\log K_{ow})^2 + 2.5301 \times \log K_{ow} - 3.52$

N = 94 $r^2 = 0.620$ F = 71.8 $p < 0.001$

Trophic level 2: $\log BAF^{fd} = -0.0995 \times (\log K_{ow})^2 + 2.2855 \times \log K_{ow} - 3.1516$

N = 352 $r^2 = 0.713$ F = 433.7 $p < 0.001$

Trophic level 3: $\log BAF^{fd} = -0.0977 \times (\log K_{ow})^2 + 2.3852 \times \log K_{ow} - 3.693$

N = 325 $r^2 = 0.912$ F = 1661.9 $p < 0.001$

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

N = 103 $r^2 = 0.929$ F = 653.8 $p < 0.001$

The N value given above refers to the number of data points included in the regressions and not the number of individual chemicals (multiple data points were available for some chemicals). The approximate number of individual chemicals included in the analyses, the types of chemicals, and the log K_{ow} range of the chemicals, are shown below.

Trophic level 1: Approx. number of chemicals = 59 (mainly PCBs).

Log K_{ow} range = 5.24 to 8.18.

Trophic level 2: Approx. number of chemicals = 82 (mainly chlorinated benzenes, PCBs and PAHs, but also hexachlorobutadiene, p,p'-DDE and nonachlor).

Log K_{ow} range = 4.02 to 8.18.

Trophic level 3: Approx. number of chemicals = 61 (mainly chlorinated benzenes and PCBs, but also p,p'-DDE, nonachlor, chlorinated butadienes and hexachloroethane).

Log K_{ow} range = 4.02 to 8.18.

Trophic level 4: Approx. number of chemicals = 64 (mainly chlorinated benzenes and PCBs, but also chlorinated butadienes and hexachloroethane).

Log K_{ow} range = 4.02 to 8.45.

The derived regression equations were validated against independent datasets. The results of the validation are summarised below.

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

Log K_{ow} range = 3.72 to 7.14.

Average absolute deviation in log BAF = 0.48.

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

Log K_{ow} range = 3.43 to 7.14.

Average absolute deviation in log BAF = 0.64.

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

Log K_{ow} range = 3.43 to 7.14.

Average absolute deviation in log BAF = 0.52.

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

Log K_{ow} range = 3.72 to 7.14.

Average absolute deviation in log BAF = 0.60.

10.3 Summary of the Voutsas *et al.* (2002) method

An overview of the method is given in Table 10.1.

Table 10.1 Summary of the Voutsas *et al.* (2002) method

Criteria	Comment
Structure of the method	The method is a series of regression equations relating the BAF to log K_{ow} for four trophic levels within a freshwater ecosystem.
Scope of the method	The method is applicable to persistent (or slowly metabolized) chemicals. The method is intended to be generally applicable to many types of organic chemicals that are a) not readily metabolized and b) have a high log K_{ow}. Regression equations are given for four trophic levels and cover chemicals with log K_{ow} values in the general range four to eight.
Type of method	Steady-state calculations.
Calculation method	Hand calculations. Would be easy to implement the calculations in a spread sheet.
Outputs from the method	Bioaccumulation factor for trophic level 1 (plankton). Bioaccumulation factor for trophic level 2 (benthic invertebrates). Bioaccumulation factor for trophic level 3 (planktivorous fish). Bioaccumulation factor for trophic level 4 (piscivorous fish). The bioaccumulation factors are based on a wet weight concentration in the organism/freely dissolved concentration in water basis.
Focus of the method	The method does not focus specifically on sensitive groups (such as children or young animals).
Chemical-specific input parameters	The log K_{ow} value is the only chemical-specific input parameter required.
Key default parameters used in the method	Bioaccumulation factors are based on the estimated dissolved concentration in water.
Environment considered in the method	The method is based on field data from various locations in North America and Europe.
How is persistence considered?	The method is designed for persistent chemicals and so may overestimate the bioaccumulation of non-persistent, easily metabolized, substances.
Are seasonal variations considered?	No.
Strengths	Very simple to use.
Weaknesses and limitations	Only applicable to persistent (or slowly metabolized) substances with relatively high log K_{ow} values.
Overall assessment of whether the model could be adapted to the UK situation	Although some of the data used in the correlations was from North America, data from Europe (such as the Netherlands) were also used in the construction of the correlations. Therefore, the correlations may be directly applicable to the UK, although it is not possible to be conclusive on this at this stage.
Further work	The applicability of the correlations to the UK should be checked by validation against UK datasets.

10.4 Evaluation against screening criteria

10.4.1 Data requirements

The model requires only the log K_{ow} of the chemical. This should be available (or could be estimated) for most non-ionisable organic chemicals. A score of three is appropriate. The importance rating for this criterion is five. Therefore,

$SCORE_{DATA} = 3 \times 5 = 15$.

10.4.2 Model calibration

The model is generally based on regression equations of defined datasets for between 94 and 352 persistent organic chemicals with log K_{ow}s in the approximate range four to eight. The regression equations (particularly for trophic level 3 and 4) showed a good correlation (as shown by the r^2 value). A score of three is considered appropriate. The importance rating for this criterion is five. Therefore,

$SCORE_{CALIBRATION} = 3 \times 5 = 15$.

10.4.3 Model validation

The model has been validated using independent datasets for between 12 and 70 chemicals. The average absolute deviation in the log BAF was between 0.48 and 0.64. A score of three is considered appropriate. The importance rating for this criterion is five. Therefore,

$SCORE_{VALIDATION} = 3 \times 5 = 15$.

10.4.4 Ease of use

The model is easy to use and gives a BAF that could be used directly for setting standards (see Chapter 15). The score for this criterion is therefore three. The importance rating for this criterion is two. Therefore,

$SCORE_{EASE} = 3 \times 2 = 6$.

10.4.5 Transparency

The underlying methods used in the model are simple and clear and so a score of three is appropriate. The importance rating for this criterion is five. Therefore,

$SCORE_{TRANS} = 3 \times 5 = 15$.

10.4.6 Prediction uncertainty

The prediction uncertainty of this method depends to a large extent on the quality of the regression equations. The quality (as measured by the r^2 value) is poorer for trophic levels 1 and 2 than for trophic levels 3 and 4. In addition, regression equations are derived for substances considered to be persistent/non-metabolised in the organisms considered. Thus, the regression equations will overpredict the BAF for substances that are metabolized. Overall, a score of two is considered appropriate. The importance rating for this criterion is five. Therefore,

$SCORE_{UNCERT} = 2 \times 5 = 10.$

10.4.7 Ability to predict the concentration near the top of the food chain

The model allows predictions of concentrations in more than two trophic levels, including those near the bottom and top of the food chain (data permitting), and so a score of three is judged appropriate. The importance rating for this criterion is four. Therefore,

$SCORE_{TOP\ FOOD} = 3 \times 4 = 12.$

10.4.8 Relevance to England and Wales

The appropriateness of the method for the UK is not apparent. The method has been derived using data from the Netherlands amongst others, and so it is likely that it will be relevant to the UK (although this would need to be checked). On this basis, a score of two is proposed. The importance rating for this criterion is four. Therefore,

$SCORE_{RELEVANCE} = 2 \times 4 = 8.$

10.4.9 Overall score

Using the methodology outlined in Appendix C, the overall score can be estimated as follows.

TOTAL SCORE $= SCORE_{DATA} + SCORE_{CALIBRATION} + SCORE_{VALIDATION} + SCORE_{EASE} + SCORE_{TRANS} + SCORE_{UNCERT} + SCORE_{TOP\ FOOD} + SCORE_{RELEVANCE}$

$= 15 + 15 + 15 + 6 + 15 + 10 + 12 + 8$

$= 96.$

11 QEAFDCHN

11.1 Introduction

The QEAFDCHN model was developed by Quantitative Environmental Analysis. It is available as a computer program, and a printed manual for the model is also available (QEA, 2001a). The model is based on work by Connolly, Thomann and co-workers and has been presented, adapted and used in several studies including Thomann (1981), Thoman (1989), Thomann and Connolly (1984), Thomann *et al*. (1992a), Connolly (1991), Connolly *et al.* (2000), Connolly and Glaser (2002), Glaser and Connolly (2002) and QEA (1999 and 2001b). These studies have generally investigated the behaviour of persistent organochlorine compounds (such as PCBs and DDE) in food chains in the United States such as an upper Hudson River food chain, a Lake Michigan trout food chain, a marine bird food chain from the Southern California Bight, a sea lion food chain in the California Channel Islands, and a lobster and winter flounder food chain in New Bedford Harbour.

11.2 Description of model

The computer program (QEAFDCHN version 1.0) is used here as the basis for the description of the model. The necessary inputs are taken from QEA (2001a) and the model program itself. However, the model is flexible and can be used for many different food chains. A brief discussion of the food chains that have been considered using this model is included later, in relation to the validation of the model.

The model is written in FORTRAN and consists of a number of subroutines. In order to run the model, an input file has to be created by the user. The input file should be structured as a text file and have the name “fdchain.inp”. The input file effectively defines the food chain to be modelled. The computer program as supplied does not contain a default food chain and so a suitable input file would need to be constructed before the model could be used.

The data required by the input file are divided into nine groups (labelled Group A to Group I). Each group of information describes a separate component of the food web. Depending on the composition of the food web, data for entire groups or portions of groups may be omitted.

The model can consider both steady-state species and age-dependent species. Within the model, each species is identified by a species number and a step number, whereby the same species is given the same species number throughout but different age groups within a species are assigned different step numbers.

Information required for the groups listed in the input file is summarised in Table 11.1.

Table 11.1 Information required by the QEAFDCHN model

Information	Comment
Group A – Number of species and chemicals being modelled	
Number of species for which age-specific concentrations are calculated	
Number of species for which steady-state concentrations are calculated	

Information	Comment
Number of chemicals being modelled	
Name of chemicals being modelled	
Group B – Chemical-specific parameters	
Flag indicating whether the BCF value is used in calculating the rate at which each chemical is eliminated	Used to indicate whether the chemical elimination rate should be calculated from the BCF value or whether the BCF value should not be used (see also below).
Ratio of the energy efficiency of contaminant transfer across the gill to the efficiency of oxygen transfer across the gill for each chemical	
The resistance factor for transfer of each chemical from lipid to blood	
Group C – Phytoplankton and sediment parameters	
Energy density of water column particulate matter	Required units are kJ/g C.
Energy density of sediment	
Group D – Steady-state species parameters	
Flag to indicate the source of water with which each organism is in contact	The options are: a) in contact with water column; or b) in contact with benthic pore water.
Flag to indicate the method by which the chemical elimination rate for each species will be calculated	The options are: a) elimination rate equals uptake rate from water/BCF; b) elimination rate equals uptake rate from water × fraction aqueous × multiplier (C_R); or c) elimination rate is equal to the BCF value.
Name for each steady-state species	
Respiration rate coefficient for each species	Units of kJ/g wet weight/day.
Growth rate for each species	Units day^{-1}.
Food assimilation efficiency for each species	
Fraction of protein in each species	Units g protein/g wet weight.
Exponential coefficient for temperature dependence of respiration for each species	Units $°C^{-1}$.
Lipid content for each species	Units g lipid/g wet weight.
Toxicant assimilation efficiency for each species	
BCF for each species	This is defined as a factor used to calculate the elimination rate. It is not altogether clear if this is the same as a bioconcentration factor in the classical sense, although it appears to be used as such (see discussion in main text).
Partition coefficient in each species	The units are given as l/kg. Again, it is not altogether clear what this parameter is, but it appears to be the octanol-water partition coefficient.
Group E – Age-dependent species parameters	
Flag to indicate the source of water with which each organism is in contact	The options are: a) in contact with water column; or b) in contact with benthic pore water.
Flag to indicate the method by which the chemical elimination rate for each species will be calculated	The options are: a) elimination rate equals uptake rate from water/BCF; b) elimination rate equals uptake rate from water × fraction aqueous × multiplier (C_R); or c) elimination rate is equal to the BCF value.
Name for each age-dependent species	

Information	Comment
Number of age classes for each species	See main text for discussion of age classes.
Age class size for each species	Units of days.
Respiration rate coefficient for each species	Units of kJ/g wet weight/day.
Respiration weight exponent for each species	
Food assimilation efficiency for each species	
Fraction of protein in each species	Units g protein/g wet weight.
Specific dynamic action of each species	
Exponential coefficient for temperature dependence of respiration for each species	Units $°C^{-1}$.
Swimming speed coefficient for each species	Units cm/s.
Swimming speed weight exponent for each species	
Exponential coefficient for temperature dependence of swimming speed for each species	Units $°C^{-1}$.
Exponential coefficient for swimming speed	Units s/cm.
Flag to separate/identify non-migrating juveniles from migrating adults	
Number of Julian days after start of calculation to the species birth date	
Chemical assimilation efficiency from food for each species	
Number of breaks describing the annual growth pattern for each species	
Time of break in annual growth pattern for each age class	Units days.
Weight of each species at each time break	Units g.
Lipid content of each species at each time break	Units g lipid/g wet weight.
BCF for each species	This is defined as a factor used to calculate the elimination rate. It is not altogether clear if this is the same as a bioconcentration factor in the classical sense, although it appears to be used as such (see discussion in main text).
Partition coefficient in each species	The units are given as l/kg. Again, it is not altogether clear what this parameter is.
Group F – Migrating species parameters	
Number of migrating species in model	
Identification number for each migrating species	
Number of breaks describing the migratory pattern of each species	
Time of each break in the migratory pattern for each species	Units days.
Spatial compartment occupied by each migratory species at each time break	
Group G – Number of compartments	
Number of spatial compartments in the model	
Number of breaks describing the annual temperature (and salinity) cycles in each spatial compartment	
Time of each break in temperature cycle for each compartment	Units days.
Temperature at each time break in each compartment	Units °C.

Information	Comment
Number of species above the plankton level in each compartment	
Species identification number	
Number of prey of each species or age class in each compartment	
Identity of each prey/food item for each species or age class in each compartment	An identification number system is used. This can include any of the species included in the model, sediment or water column particulates.
Number of time breaks describing the feeding preference structure of each age class	This allows the food for the various species to be altered as the age of the species increases.
Time of each break in the feeding preference structure for each species	Units of days.
Fraction of total consumption constituted by each prey species at each time break	This allows the contribution from each prey/food item to the total diet of a predator to be assigned.
Initial concentration of the chemical in each steady-state species or age class in each compartment at the start of the calculation	Units µg/g wet weight.
Group H – Printing and integration control	
Time step for calculation	Units days.
Total run time	Units days.
Print interval for outputting concentrations	Units days.
Julian date at beginning of run	Typically zero days.
Time after start of simulation to start outputting concentrations	Units days.
Option to print diagnostic files	
Group I – Exposure concentrations	
Number of concentration values to be inputted	
Scale factor for water column dissolved concentrations for each chemical in each compartment	The exact meaning of these parameters is not clear, but they appear to be related to the equilibrium partitioning of the chemical between water, sediment and suspended sediment.
Scale factor for water column particulate concentrations for each chemical in each compartment	
Scale factor for pore water dissolved concentrations for each chemical in each sediment compartment	
Scale factor for particulate sediment concentrations for each chemical in each sediment compartment	
Time break for each chemical concentration in each compartment	Unit days.
Dissolved chemical concentration in the water column of each compartment at each time break	Units µg/l.
Adsorbed chemical concentration of each chemical in the water column at each time break	Units µg/g carbon. This represents the suspended sediment concentration.
Dissolved chemical concentration in the sediment in each compartment at each time break	Units µg/l. This represents the sediment pore water concentration.
Adsorbed chemical concentration in sediment in each compartment at each time break	Units µg/g carbon. This represents the bulk sediment concentration.

Details of the calculations and assumptions used in the model are not clear from the user manual (QEA, 2001b). However, several papers have been published on this model and these are discussed below in relation to the calculation methods used.

The model is a dynamic model based on the principles of conservation of mass and energy (QEA, 1999). Chemicals are assumed to be taken up during respiration and ingestion of food/sediment and are lost by diffusion across respiratory surfaces and other elimination processes (such as metabolism, excretion, growth dilution). Rates of uptake are estimated using rates of feeding and respiration, using assimilation[16] or transfer efficiencies. The basic principle behind the model is that the change in concentration in an (aquatic) organism with time can be expressed in terms of the following equation for the *i*th trophic level (Thomann, 1989):

$$\frac{dv_i}{dt} = k'_{ui} \times \omega_i \times c + \alpha_{i,i-1} \times C'_{i,i-1} \times \omega_i \times \frac{v_{m,i-1}}{\omega_{i-1}} - K_i \times v_{mi}$$

where: v_{mi} = chemical whole body burden of the predator (*i*) (µg/organism).

$v_{m,\,i-1}$ = chemical whole body burden for the prey (*i-1*) (µg/organism).

k'_{ui} = uptake rate of chemical from water (l day^{-1} kg wet wt^{-1}) for predator.

ω_i = wet weight of predator (kg).

ω_{i-1} = wet weight of prey (kg).

$\alpha_{i,i-1}$ = chemical assimilation efficiency (µg of chemical absorbed/µg chemical ingested).

$C'_{i,i-1}$ = specific consumption rate (kg wet wt of prey/kg wet wt of predator per day).

K_i = chemical excretion rate constant (day^{-1}).

From the data input file (see Table 11.1), it appears that several methods can be used within the model to estimate the rate of metabolism/depuration of the chemical in each species. These include:

- back-calculating from a BCF value and uptake rate (at steady state, the BCF in a given species equals the rate of uptake/rate of elimination);
- estimating the rate of elimination from the rate of uptake, the aqueous fraction of the substance and a multiplier (no further details of this method appear to be available, but it is possible that the value is estimated from the log K_{ow} value);
- setting the rate of elimination equal to the BCF (no further details of this method appear to be available, but it is possible that this effectively sets a zero rate of elimination or uses the BCF value directly).

Outputs from the model are presented in a series of text files as follows:

- **FDCHAIN.OUT**. This file contains details of all the input data used in the simulation, along with the predicted concentrations for each species.

[16] Similar to other models, this model assumes that the assimilation efficiency of the chemical from food is constant with increasing body concentration. However, according to Barber (2005a) such an assumption may be incorrect, and assimilation efficiency would be expected to decrease with increasing body concentration.

- **FDCHAINA.OUT**. This file contains contaminant concentrations and lipid contents for each time step and each steady-state species and age class.
- **BIOENG1.OUT**. This file contains the weight and lipid content information for the age-dependent species for each time step.
- **BIOENG2.OUT**. This file contains the kinetic and bioenergetic information for the age-dependent species for each time step.
- **DOSE.OUT**. This file contains a summary of the contaminated uptake and total loss rates for all steady-state and age-dependent species for each time step.
- **LOSS.OUT**. This file contains information on the loss rates from individual processes for age-dependent species for each time step.
- **PREY.OUT**. This file contains the food web structure and the dietary preference information for all steady-state and age-dependent species for each time step.

As can be seen from Table 11.1, the QEAFDCHN model is flexible in terms of the design of the food chain. In theory, any number of species could be included in the food chain, and the model can take into account exposure via water, sediment and food. In practice, the usefulness of the model will be limited to a large extent by the requirements for species-specific bioenergetic parameters (see Group D and E of Table 11.1). However, several papers have been published using this model, and these contain values for many of the parameters. Therefore, it would be possible to construct other food chains using these parameters. Some of the published studies are summarised below.

Thomann (1989) outlines a model for a simple generic aquatic food chain consisting of phytoplankton, zooplankton, small fish and top predatory fish exposed to dissolved chemicals in water. The model was calibrated and validated by comparing predictions against laboratory and field data for the BCF for phytoplankton and field data on BAFs for top predators. The main finding of the calibration exercise was that for a log K_{ow} range of 5 to 6.5, the model results were generally found to be within an order of magnitude of the field data, and did not depend significantly on assumptions in the model on the behaviour of chemical assimilation efficiency with log K_{ow} or the behaviour of the phytoplankton BCF with log K_{ow}. In this range, predictions indicated that food chain accumulation was significant. Above a log K_{ow} of 6.5, model results were found to be particularly sensitive to assumptions made on the chemical assimilation efficiency, phytoplankton BCF and top predator growth rate, but food chain accumulation was still calculated to be significant up to a log K_{ow} of around eight.

The Connolly (1991) model was a used as a part of a remedial investigation and feasibility study for a site in New Bedford Harbour that was contaminated with PCBs. The model was constructed for winter flounder (consisting of sediment detrital organic material, polychaetes and phytoplankton) and lobster (consisting of sediment detrital organic material, polychaetes, phytoplankton, mussels, crabs and lobsters) food chains. The model was found to successfully predict the actual concentrations of tri-, tetra-, penta- and hexachlorobiphenyls at all levels of the food chain and across a two order of magnitude concentration gradient in the system.

Thomann *et al*. (1992a) used a five-compartment steady-state food web model that included a benthic invertebrate compartment, a phytoplankton/detritus compartment, a zooplankton compartment, a forage fish compartment and a piscivorous fish compartment. Four routes of exposure were considered for benthic invertebrates: ingestion of particulate contaminants associated with sediment organic carbon, ingestion of overlying phytoplankton, ventilation of freely dissolved contaminant in

interstitial water and ventilation of freely dissolved contaminant in overlying water. The model was calibrated and validated using data for PCBs from an amphipod-sculpin food web for Lake Ontario. The model was found to satisfactorily represent the field data up to a log K_{ow} of around 7.5 (above this, the amphipod BSAF tended to be overestimated by the model)

QEA (1999) and Connolly *et al*. (2000) took part in a detailed study of the fate and behaviour of PCBs in the upper Hudson River. Their bioaccumulation model considered the uptake of water-borne and sediment-borne PCBs by invertebrates and sequential transfer through the food chain via predation. Four trophic levels were considered: particulate matter (including sediment and suspended sediment), invertebrates (including benthic macroinvertebrates in contact with sediment and periphyton in contact with the water column), forage fish (pumpkinseed and brown bullhead) and predatory fish (largemouth bass). The model was parameterised and calibrated/validated with laboratory and field data for the upper Hudson River. Around 90 per cent of the estimated data were found to lie within a factor of two of the available field measurements on a wet weight basis (or 92 per cent on a lipid weight basis). Some of this uncertainty was thought to result from uncertainties in field measurements and so it was concluded that uncertainty in the model was less than a factor of two.

QEA (2001b) considered the fate and behaviour of PCBs in an aquatic food chain in the Lower Fox River and Green Bay. The food chain consisted of benthic macroinvertebrates, phytoplankton/zooplankton, gizzard shad, rainbow smelt, alewife and walleye and brown trout and represented three trophic levels (invertebrates, forage fish and predatory fish). The model was calibrated with data for PCBs using simulations for a ten-year period. The model was calibrated to provide the best overall match between predictions and actual data for all species, both on a wet weight and lipid-normalised basis. Overall, more than 90 per cent of the average simulated wet weight and lipid weight PCB concentrations were found to lie within a factor of two of the calibration dataset, and all of the average simulated concentrations were within a factor of three of observed average values in the dataset. The calibrated model was then used to evaluate the efficacy of different remedial options for reducing the PCB levels in fish in the catchment for 100-year projections.

Connolly and Glaser (2002) presented a model for the distribution of *p, p'*-DDE in female sea lions in the California Channel Islands exposed via their diet. The model was a time-variable, age-dependent, physiologically-based toxicokinetic model, whereby the uptake and loss of chemicals was described by mass and energy balance equations. The model considered the distribution of the chemicals into milk and the fetus. The model was validated/calibrated using field data for the levels of *p ,p'*-DDE in the diet of sea lions. Predicted and observed concentrations were generally within a factor of two of the measured levels from the area.

Glaser and Connolly (2002) considered a food chain consisting of fish and invertebrates, sea lions and birds, with the peregrine falcon, bald eagle and double-crested cormorant being representative of top predators. Exposure was assumed to be via water, terrestrial sources and the food chain. Transfer to birds' eggs was also considered. The model was validated using data on PCBs and DDE levels from the Southern California Bight. Measured (field) levels of these substances in various parts of the food chain were used as input into the model, and the resulting modelled concentrations in peregrine falcon and bald eagle eggs were compared with the monitoring data. Estimated levels were found to closely match field levels for both DDE and PCBs (the largest deviation was a 50 per cent overestimate of the concentration for DDE in peregrine falcon eggs, but a close to 1:1 correlation was

found for PCBs in both peregrine falcon eggs and bald eagle eggs, and DDE in bald eagle eggs). The modelled results of levels in double-crested cormorant eggs were found to be in close agreement with the field results from Anacapa Island (only around 20-25 per cent difference between modelled and field results), but predicted levels overestimated field levels by a factor of around 10 for Santa Barbara Island.

11.3 Summary of the QEAFDCHN model

An overview of the method is given in Table 11.2.

Table 11.2 Summary of the QEAFDCHN model

Criteria	Comment
Structure of the method	The framework for the model is available as a computer program. This framework allows user-defined aquatic food chains to be constructed, but it does not itself contain a (default) food chain. Several papers have been published showing how the model (or adaptations of the model) can be parameterised for specific food chains.
Scope of the method	The model has been used to study the behaviour of persistent organochlorine compounds (such as PCBs and DDE) in food chains in the United States. In each case, the model was adapted to the specific food chain (and in some cases, chemicals) being modelled. Overall, the method appears to be applicable to hydrophobic organic chemicals in general.
Type of method	The model is a kinetic model based on the principles of conservation of mass (mass balance model) and energy. The model can consider exposure via both sediment and water for a range of species/trophic levels including benthic organisms, plankton, forage fish, pisciverous fish and, with suitable adaptation, air-breathing mammals and birds.
Calculation method	Computer program. Details of specific applications of the models are laid out as a series of equations in the published literature.
Outputs from the method	Outputs from the model can include the following: • concentration of chemical in each species; • contaminant uptake and loss rates in each species; • information on loss rates from individual processes for some species.
Focus of the method	The model can take account of different age groups within a species. Some adaptations to the model can consider accumulation in mother's milk and the fetus of certain air-breathing mammals (although such adaptations may not be readily implemented in the QEAFDCHN framework as it stands).
Chemical-specific input parameters	The chemical-specific input parameters required for the QEAFDCHN model are summarised in Table 11.1 and include the BCF, the ratio of the energy efficiency of contaminant transfer across the gill to the efficiency of oxygen transfer across the gill, the resistance factor for transfer of each chemical from lipid to blood and the toxicant assimilation efficiency for each species. Some of the input parameters required by the QEAFDCHN framework are not altogether clear; however, the published papers generally provide values for most inputs for the chemicals considered in those studies.
Key default parameters used in the method	The QEAFDCHN framework does not contain any default parameters as such. These have to be user-defined, based on the food chain being considered. Table 11.1 outlines the main species-related and environmental-related parameters needed.
Environment considered	QEAFDCHN is a generic framework that can be tailored to consider a wide range of situations.

Criteria	Comment
How is persistence considered?	Metabolism (and other elimination processes) is included in the model. The metabolism rate can be estimated in a number of ways (see Table 11.1).
Are seasonal variations considered?	Yes. Changes in temperature, salinity and feeding pattern of the organisms with time can be incorporated in the model.
Strengths	The model has been validated in several studies. The framework is adaptable to many different aquatic food chains. Extensions to the model could be made to include air-breathing mammals and birds.
Weaknesses and limitations	The information requirements of the model are quite large, particularly if it is to be adapted for new food chains (and chemicals). Not all of the input parameters required by the QEAFDCHN framework are obvious, and sufficient information may not be available for many chemicals.
Overall assessment of whether the model could be adapted to the UK situation	The model could be adapted to the UK situation; however, this would take considerable effort.
Further work	The model as it stands is relatively difficult to use (for example, the model does not have a user-friendly interface and all the necessary modifications have to be made by editing files). More user-friendly models exist that cover similar aquatic food chains to the QEAFDCHN model, and so it is not recommended that the QEAFDCHN model is developed further for the UK situation. However, some recent papers published on the models for air-breathing mammals and birds may be of interest for the development of future models relevant to such organisms in the UK.

11.4 Evaluation against screening criteria

11.4.1 Data requirements

The chemical-related data required to run the model are relatively modest, but some of the data required may not be readily available for many types of chemical. Published papers give appropriate values mainly for PBCs (and some other organochlorine chemicals), but it may be difficult to obtain similar data for other chemicals. Overall, this may limit the usefulness of the model. A score of one is appropriate. The importance rating for this criterion is five. Therefore,

$SCORE_{DATA} = 1 \times 5 = 5$.

11.4.2 Model calibration

The model is based mainly on theoretical considerations and has generally been calibrated and validated for a limited group of chemicals (mainly PCBs) in specific food chains. The model is applicable to hydrophobic chemicals, but the range of applicability (in terms of log K_{ow} , for example) is unclear. A score of two is considered appropriate. The importance rating for this criterion is five. Therefore,

$SCORE_{CALIBRATION} = 2 \times 5 = 10$.

11.4.3 Model validation

The bioaccumulation model has been validated against field BAFs mainly for PCBs. The agreement between experimental and field data was generally found to be good for specific food chains. A score of three is considered appropriate. The importance rating for this criterion is five. Therefore,

$SCORE_{VALIDATION} = 3 \times 5 = 15$.

11.4.4 Ease of use

The model is quite complex and would require considerable experience to use, particularly if user-defined simulations were to be run. A score of one is appropriate. The importance rating for this criterion is two. Therefore,

$SCORE_{EASE} = 1 \times 2 = 2$.

11.4.5 Transparency

The underlying principles of the model are clear, but the exact calculations used are not always clear. A score of two is appropriate. The importance rating for this criterion is five. Therefore,

$SCORE_{TRANS} = 2 \times 5 = 10$.

11.4.6 Prediction uncertainty

The prediction uncertainty of this method will depend to some extent on the availability of reliable chemical-related data. If such data are available (or are estimated), the method appears to have a relatively low prediction uncertainty. However, in the absence of such data (or estimates of such data), it may not be possible to use the model reliably (precautionary assumptions may have to be made). Given that such data may not be generally available for a wide range of chemicals, a score of one is considered appropriate. The importance rating for this criterion is five. Therefore,

$SCORE_{UNCERT} = 1 \times 5 = 5$.

11.4.7 Ability to predict the concentration near the top of the food chain

The model allows predictions of concentrations in more than two trophic levels near the top of the food chain (data permitting) and so a score of three is judged appropriate. The importance rating for this criterion is four. Therefore,

$SCORE_{TOP\ FOOD} = 3 \times 4 = 12.$

11.4.8 Relevance to England and Wales

Applications of the model have typically been carried out for food chains in the United States and so are not directly relevant to the UK. It is possible for the user to define the food chain used by the model and so it would be possible to construct example food chains relevant to the UK. However, the data requirements are quite extensive and so this adaptation would not be straightforward, and would require expert knowledge of the model. A score of one is therefore considered appropriate. The importance rating for this criterion is four. Therefore,

$SCORE_{RELEVANCE} = 1 \times 4 = 4.$

11.4.9 Overall score

Using the methodology outlined in Appendix C, the overall score can be estimated as follows:

$$\begin{aligned} \text{TOTAL SCORE} &= SCORE_{DATA} + SCORE_{CALIBRATION} + SCORE_{VALIDATION} + SCORE_{EASE} + SCORE_{TRANS} + SCORE_{UNCERT} + SCORE_{TOP\ FOOD} + SCORE_{RELEVANCE} \\ &= 5 + 10 + 15 + 2 + 10 + 5 + 12 + 4 \\ &= 63. \end{aligned}$$

12 GEMCO

12.1 Introduction

The GEMCO model is a generic model for contaminants in estuaries. The model was developed by Delft Hydraulics, the French Research Institute for Exploitation of the Sea (Ifremer) and the Institute for Environmental Studies (IVM) for the European Chemical Industry Council (CEFIC) Long-Range Research Initiative (LRI).

The model (version 1.0.1 was reviewed for this work) is available on CD-ROM from the LRI contact point[17]. No documentation on the model appears to be available.

12.2 Description of model

The model consists of three input modules relating to the chemical, the emissions and the estuary respectively. The information required for each part of the model is summarised in Table 12.1.

Table 12.1 Inputs required for GEMCO model

Parameter	Comment
Chemical-specific parameters	
Molecular weight	
Log K_{ow}	
Kd	It is not entirely clear what this parameter is, but it is only used for metals. It probably represents the sediment-water partition coefficient (or similar partition coefficient).
Henry's law constant or water solubility and vapour pressure	Henry's law constant (in Pa m^3/mole) can be entered directly or estimated from the water solubility (in g/m^3) and vapour pressure (in Pa).
Log K_{oc} (organic carbon-water partition coefficient)	This can be estimated using one of the two in-built QSARs, or entered directly.
Degradation rate constants for water	Rate constants (units of day^{-1}) can be entered for biodegradation, hydrolysis and photolysis. If no data are available, a rate constant of zero is assumed.
Degradation rate constants for sediment	Rate constants (units of day^{-1}) can be entered for biodegradation, hydrolysis and photolysis. If no data are available, a rate constant of zero is assumed.
Biotransformation correction factors	These factors can be entered for zooplankton, secondary consumers, round fish, Tellina and benthic fish. Values between zero and one can be entered and if no data are available, a value of zero is used. The actual meaning of the value is unclear, but it probably reflects the metabolism of the substance (the higher the value, the more rapid the metabolism).
Bioaccumulation parameters	These are estimated by the program and cannot be altered. The values are called alpha water, beta prey and beta detritus. The meaning of the values is unclear.
Emission data	
Emission to estuarine water	Data can be entered for four point sources along the estuary.

[17] http://www.cefic-lri.org/Templates/shwProject.asp?NID=42&HID=419&S=35&PID=96.

Parameter	Comment
	The values are entered as kg/year.
Atmospheric emissions	The load from atmospheric deposition (as g/km^2/year) can be entered.
Emissions to marine water	The emission directly to the marine compartment can be entered (as kg/year).
Concentration in river	The concentration in the river flowing into the estuary can be entered (as µg/l).
Concentration in sea	The concentration in the sea can be entered (as µg/l).
Historic concentration in sediment	The concentration in sediment can be entered (as µg/g).
Estuary-specific data	
Width of estuary mouth	These parameters are used by the model to define the dilution/dispersion properties of the estuary.
Width of estuary at distance X from the mouth, where X can be user-defined	
Estuary length	
Estuary depth	
River flow rate into estuary	
Tidal range	
Tidal period	
Marine longshore current	
Temperature	
Dispersion method	This determines the method for calculating the dispersion/dilution in the estuary. Two methods are available, default and salinity. If salinity is chosen, the model uses information on the salinity in three zones at user-defined distances from the mouth of the estuary, which needs to be entered by the user.
Salinity at distance X from the mouth of the estuary	
Net sedimentation rate in estuary	
Suspended solids content	Values are entered (as mg/l) for freshwater (<8 practical salinity units (psu)), intermediate water (8 to 20 psu), saline (>20 psu) and marine water.
Particulate organic carbon (POC)	Values are entered (as mg organic carbon/l) for freshwater (<8 psu), intermediate water (8 to 20 psu), saline (>20 psu) and marine water.
Dissolved organic carbon (DOC)	Values are entered (as mg organic carbon/l) for freshwater (<8 psu), intermediate water (8 to 20 psu), saline (>20 psu) and marine water.
Fraction of organic carbon in sediment	Values are entered for freshwater (<8 psu), intermediate water (8 to 20 psu), saline (>20 psu) and marine sediments.
Mixed sediment layer thickness	Values are entered (as metres) for freshwater (<8 psu), intermediate water (8 to 20 psu), saline (>20 psu) and marine water.
Chlorophyll concentration	Values are entered (as µg/l) for freshwater (<8 psu), intermediate water (8 to 20 psu) and saline water (>20 psu).
Phytoplankton biomass	Values are entered (as mg/l) for freshwater (<8 psu), intermediate water (8 to 20 psu) and saline water (>20 psu). Values can also be estimated by the program from the chlorophyll concentration.
Zooplankton biomass	Values are entered (as mg/l) for freshwater (<8 psu), intermediate water (8 to 20 psu) and saline water (>20 psu).
Dissolved oxygen content	Values are entered (as mg/l) for freshwater (<8 psu), intermediate water (8 to 20 psu) and saline water (>20 psu).

The model contains estuary-specific information for a large number of estuaries in Europe, including major and minor estuaries in the United Kingdom. A complete list of estuaries covered in the model is given in Appendix A. As well as specific estuaries, a number of generic estuaries are included as follows:

- river-dominated estuary (yearly average, summer or winter);
- small flow, high dispersive estuary (yearly average, summer or winter);
- small flow, low dispersive estuary (yearly average, summer or winter);
- large estuary (yearly average, summer or winter).

The bioaccumulation part of the model consists of zooplankton, secondary consumers, round fish (sea bass), Tellina (bivalve molluscs) and benthic fish (dab). Details of the actual model used are not available, but it is possible that the models are based on those developed by Loizeau and Menesguen (1993) for a dab food web and Loizeau *et al*. (2001) for a sea bass food web (the authors of these papers are associated with Ifremer, who developed the biaccumulation model for GEMCO).

The Loizeau and Menesguen (1993) model considers a food chain consisting of marine water (dissolved and suspended sediment), phytoplankton/detritus, crustaceans/annelids/molluscs/ ophiuroids and dab. The model is a five-compartment steady-state model developed for the Seine estuary that was validated using data for PCBs. The Loizeau *et al*. (2001) model considers a food chain consisting of marine water (dissolved and suspended sediment), phytoplankton/detritus, crustaceans (shrimps and mysidaceans), small fish (guppies) and sea bass, and again is a steady-state (six-compartment) model. Later (dynamic) adaptations were made to this model to take into account seasonal variations and population dynamics (to allow accumulation in different age classes to be determined). The model was again validated on PCBs using data from the Seine estuary. The models are essentially extensions of the model developed by Thomann (1989) which is the basis of the QEAFDCHN model (see Chapter 11). It is not clear which parts (if any) of these models are incorporated into the GEMCO model.

Outputs from the GEMCO model can be displayed in graphical form (as a line graph or spatial map, both showing the concentration with distance down the estuary) or as a table. The tabular outputs are as follows:

- Salinity (in psu; 95th percentile, average, fifth percentile concentrations in the estuary are given, along with the concentration in marine water).
- Total water concentration (in µg/l; 95th percentile, average, fifth percentile concentrations in the estuary are given, along with the concentration in marine water).
- Dissolved water concentration (in µg/l; 95th percentile, average, fifth percentile concentrations in the estuary are given, along with the concentration in marine water).
- Suspended matter concentration (in µg/g dry weight; 95th percentile, average, fifth percentile concentrations in the estuary are given, along with the concentration in marine water).
- Sediment concentration (in µg/g dry weight; 95th percentile, average, fifth percentile concentrations in the estuary are given, along with the concentration in marine sediment).
- Zooplankton concentration (in ng/g dry weight; 95th percentile, average, fifth percentile concentrations in the estuary are given).

- Secondary consumer concentration (in ng/g dry weight; 95th percentile, average, fifth percentile concentrations in the estuary are given).
- Round fish (sea bass) concentration (in ng/g dry weight; 95th percentile, average, fifth percentile concentrations in the estuary are given).
- Tellina concentration (in ng/g dry weight; 95th percentile, average, fifth percentile concentrations in the estuary are given).
- Benthic fish (dab) concentration (in ng/g dry weight; 95th percentile, average, fifth percentile concentrations in the estuary are given).

The GEMCO program indicates that the bioaccumulation model is not valid outside the log K_{ow} range 4.5 to 10.

The model has been validated for the Scheldt and Seine estuaries, but no details appear to be available of the validation studies.

12.3 Summary of the GEMCO model

An overview of the method is given in Table 12.2.

Table 12.2 Summary of the GEMCO model

Criteria	Comment
Structure of the method	The model is an estuarine dilution/dispersion model linked to a bioaccumulation model for two estuarine food chains. The food chains consider both pelagic and benthic organisms. The model is available as a computer program.
Scope of the method	Applicable to organic chemicals with a log K_{ow} of between 4.5 and 10. Also applicable to metals. The model was developed under the CEFIC LRI program.
Type of method	Not entirely clear, but appear to be steady-state calculations.
Calculation method	Computer program.
Outputs from the method	95th percentile, average and fifth percentile concentrations for the following: • water (total and dissolved) (µg/l) • suspended matter (µg/g dry weight) • sediment (µg/g dry weight) • zooplankton (ng/g dry weight) • secondary consumers (ng/g dry weight) • Tellina (molluscs) (ng/kg dry weight) • round fish (sea bass) (ng/g dry weight) • benthic fish (dab) (ng/g dry weight) • information on the spatial variation in concentrations is available graphically.
Focus of the method	The method does not focus specifically on sensitive groups (such as young animals).
Chemical-specific input parameters	Physico-chemical properties include log K_{ow} and Henry's law constant (or water solubility and vapour pressure); organic carbon-water partition coefficient (can be estimated within the program); rate constants for degradation in water and sediment (biodegradation, hydrolysis and photolysis); and biotransformation correction factors (appear to be related to

Criteria	Comment
	metabolism) for zooplankton, secondary consumers, round fish, Tellina and benthic fish.
Key default parameters used in the method	Most of the key default parameters for the estuarine compartment can be varied. Appropriate values are available for most major and minor estuaries in the EU including the UK.
Environment considered in the method	Estuarine waters. Both generic estuaries and actual estuaries are modelled.
How is persistence considered?	Degradation in sediment and soil is included in the model. Metabolism in the various steps in the food chain appears to be taken into account via the biotransformation correction factors, but little information is available on how these are applied.
Are seasonal variations considered?	Seasonal variations can be taken into account in the generic models (versions of the generic estuaries are given for winter and summer conditions). The temperature of the specific estuaries can be adjusted.
Strengths	The program is easy to use. The properties of the estuary can easily be varied to specific situations. A large database of properties for all the major and minor estuaries in the EU and the UK is included.
Weaknesses and limitations	There does not appear to be any way of using actual accumulation data (such as actual BCF or BAF values) in the model. The food chain cannot be varied (although the one chosen appears to be appropriate to the EU and UK). Few details of the bioaccumulation model used are available. In particular, the treatment of metabolism/biotransformation in the model is unclear.
Overall assessment of whether the model could be adapted to the UK situation	The model could be used for specific estuaries in the UK directly without adaptation. The generic scenarios could easily be modified to reflect the UK situation if needed (although as the model is EU-based, the generic scenarios are also likely to be relevant to the UK).
Further work	None identified.

12.4 Evaluation against screening criteria

12.4.1 Data requirements

The model requires easily available information (or information that could be estimated) for the chemical. More complex information (such as metabolism data) can be used in the model if this is available. A score of three is appropriate. The importance rating for this criterion is five. Therefore,

$SCORE_{DATA} = 3 \times 5 = 15$.

12.4.2 Model calibration

The basis behind the actual model in GEMCO is unclear. Associated papers describing similar models are mainly based on theoretical considerations. The applicability of the model (in terms of a log K_{ow} range of one to 10) is described. A

score of two is considered appropriate. The importance rating for this criterion is five. Therefore,

$SCORE_{CALIBRATION} = 2 \times 5 = 10$.

12.4.3 Model validation

The model has been validated for some estuaries, but details of this validation are not available. A score of two is therefore appropriate. The importance rating for this criterion is five. Therefore,

$SCORE_{VALIDATION} = 2 \times 5 = 10$.

12.4.4 Ease of use

The model is easy to use and gives concentrations in the organisms at each trophic level and each exposure media, which should allow suitable BAFs to be estimated that could be used directly in setting standards (see Chapetr 15). The score for this criterion is therefore three. The importance rating for this criterion is two. Therefore,

$SCORE_{EASE} = 3 \times 2 = 6$.

12.4.5 Transparency

The underlying methods used in the bioaccumulation model are not clear and so a score of one is appropriate (however, it is probable that they are similar to methods published in the literature). The importance rating for this criterion is five. Therefore,

$SCORE_{TRANS} = 1 \times 5 = 5$.

12.4.6 Prediction uncertainty

The prediction uncertainty of this method is difficult to judge, as the underlying methods are not clear. The method can take account of metabolism data (if available) but would assume no metabolism (a precautionary approach) if such data were absent. Overall, a score of two is considered appropriate. The importance rating for this criterion is five. Therefore,

$SCORE_{UNCERT} = 2 \times 5 = 10$.

12.4.7 Ability to predict the concentration near the top of the food chain

The model allows predictions of concentrations in more than two trophic levels, including those near the bottom and top of the food chain (data permitting), and so a score of three is appropriate. The importance rating for this criterion is four. Therefore,

$SCORE_{TOP\ FOOD} = 3 \times 4 = 12$.

12.4.8 Relevance to England and Wales

The method is directly applicable to the UK, where many UK estuaries are included in the model. The method could also be adapted to the properties of other (generic) estuaries (but the food chain part of the model cannot be changed). On this basis, a score of three is proposed. The importance rating for this criterion is four. Therefore,

$SCORE_{RELEVANCE} = 3 \times 4 = 12$.

12.4.9 Overall score

Using the methodology outlined in Appendix C, the overall score can be estimated as follows:

$$\begin{aligned} \text{TOTAL SCORE} &= SCORE_{DATA} + SCORE_{CALIBRATION} + SCORE_{VALIDATION} + SCORE_{EASE} + SCORE_{TRANS} + SCORE_{UNCERT} + SCORE_{TOP\ FOOD} + SCORE_{RELEVANCE} \\ &= 15 + 10 + 10 + 6 + 5 + 10 + 12 + 12 \\ &= 80. \end{aligned}$$

It should be noted that the actual bioaccumulation model used in this method is unclear. Therefore, although some aspects of the model score well against the criteria set, this uncertainty is an important limitation in the usability of this model within the project. A lower score could possibly be justified given the lack of information on this model, or the uncertainty of the score highlighted.

13 Other models

13.1 Introduction

A number of other bioaccumulation models were identified in the initial review (Appendix D) as candidates for an in-depth review. However, these models were considered by the peer reviewers to be too complex for general use in setting standards (they are effectively expert systems with a high level of complexity). Therefore, only brief details of the main features of these models are reported here. Based on this brief review, it is concluded that these models are indeed expert systems too complex to be useful for the purposes of this project. However, all three models contain (or provide access to) databases on chemical-related and species-related information that are likely to be useful for the adaptation and parameterisation of several other models considered in this review.

13.2 ARAMS

The Army Risk Assessment Modelling System (ARAMS) is used by the United States Department of Defence and the Army to conduct risk assessments to determine safe levels and clean-up target levels for military chemicals, and to evaluate remediation alternatives. The model is freely available via the internet[18].

The modelling system integrates the multimedia fate and transport, exposure, intake and uptake and effects of the chemicals using several sub-models. These models include the Terrestrial Wildlife Exposure Model (TWEM), RAMAS Ecorisk (an ecological population model), Theoretical Bioaccumulation Potential (TBP) model, Trophic Trace (a tool for assessing the trophic transfer of sediment-associated contaminants) and Multimedia Environmental Pollutant Assessment System (MEPAS, which considers multimedia uptake by humans, including from food). ARAMS is also integrated with various databases including the Biota-Sediment Accumulation Factors (BSAF) and databases of species information (for example, databases on organism lipid contents, environmental effects, residue levels and terrestrial toxicity).

The various sub-models within the system can be run alone or in combination with other sub-models. Various default habitats are included such as desert, estuary, coniferous forest, deciduous forest, grassland/prairie, lake, marine, riparian, river, slow-moving shallow water and wetland. Other environments can be user-defined. The receptors in the model include American kestrel, American robin, American woodcock, belted kingfisher, coyote, deer mouse, eastern cottontail rabbit, little brown bat, mallard duck, meadow vole, mink, mule deer, northern short tailed shrew, osprey, red fox, red tailed hawk, western meadowlark. In addition, the model contains a database of 417 aquatic organisms that can be used in the construction of the food chain.

Details of the bioaccumulation model within the method are unclear, but it appears to be relatively simplistic, based on user-defined bioavailabilities, absorption factors and/or bioaccumulation factors for the species in question. The model predicts uptake into the target receptor (in terms of mg/kg/day) from soil, sediment, water and food.

[18] http://el.erdc.usace.army.mil/arams/.

13.3 AQUATOX

The AQUATOX model was produced by the United States Environmental Protection Agency to assist in the performance of ecological risk assessments for aquatic ecosystems. The model and manuals are freely available via the internet[19]. Details of the model are given in USEPA (2004).

The model is an ecological risk assessment model for aquatic ecosystems that takes into account the combined environmental fate and effects of toxic chemicals, and also pollutants such as nutrients and sediment. It considers several trophic levels including attached and planktonic algae, submerged aquatic vegetation, invertebrates, forage-feeding fish, bottom-feeding fish and game fish. The model simulates the transfer of biomass, energy and chemicals from one compartment of an ecosystem to another using a process-based or mechanistic model.

The environmental fate part of the model considers processes such as partitioning among organisms, suspended and sedimented detritus, suspended and sedimented inorganic sediments and water, ionisation, and loss processes such as volatilisation, photolysis, hydrolysis and microbial degradation. The effects part of the model considers acute toxicity caused by exposure to the chemical, and various indirect effects such as release of grazing and predation pressure, increase in detritus and recycling of nutrients from dead organisms, dissolved oxygen depletion resulting from increased decomposition and loss of food-base for animals.

A database of species-related data is contained within the model (all data within the database is referenced). This database covers numerous species including fish, aquatic invertebrates, benthic organisms and aquatic plants and algae.

Many outputs from the model are available including BAFs and predicted concentrations in the aquatic organisms considered. The model also has built-in routines to carry out uncertainty analysis.

The chemical-related information requirements of the model are themselves modest and are likely to be available (or could be estimated) for a large number of chemicals. These include molecular weight, acid dissociation constant, solubility, Henry's law constant, vapour pressure, log K_{ow} , sediment-water partition coefficient (which can be estimated from log K_{ow} (+pKa)), activation energy, rate constants for degradation (anaerobic degradation, aerobic degradation, hydrolysis, photolysis and oxidation), metabolism/elimination rate constant for the species considered and the LC_{50} and a parameter called the Weibull shape parameter. The model also has a user-friendly interface, but there are many variables within the model (particularly for organism-specific data) and so it requires considerable experience and expert knowledge to use (particularly if it is to be adapted to UK situations).

13.4 TRIM.FaTE

The Total Risk Integrated Methodology (TRIM.FaTE) was produced by the United States Environmental Protection Agency to assist in the performance of ecological risk assessments. The model and manuals are freely available from the internet[20].

TRIM.FaTE is a spatially explicit, compartmental mass balance model that can be used to predict pollutant concentrations in multiple environmental media (including biota) and pollutant intakes for biota. The actual food chains considered can be user-defined. The model contains information for various defined compartment types that can be

[19] http://www.epa.gov/ost/models/aquatox/.
[20] http://www.epa.gov/ttn/fera/trim_fate.html.

used to construct an ecosystem; some of these compartments contain the necessary input data for the model, others have to be input by the user. The compartment types within the model are summarised below (Table 13.1).

Table 13.1 Compartments within the TRIM.FaTE model

Abiotic compartments:	Air	
	Surface soil	
	Root zone soil	
	Vadose zone soil	
	Ground water	
	Surface water	
	Sediment	
Biotic compartments:	Aquatic plants	Macrophyte
	Benthic fauna	Benthic invertebrate
		Benthic omnivore
		Benthic carnivore
	Water column fauna	Water-column herbivore
		Water-column omnivore
		Water-column carnivore
	Semi-aquatic fauna	Piscivore (belted kingfisher, common loon, mink)
		Predator/scavenger (bald eagle)
		Aerial insectivore (tree swallow)
		Omnivore (mallard, raccoon)
	Terrestrial plants	Plant leaf
		Particle on leaf
		Plant stem
		Plant root
	Terrestrial fauna	Omnivore (American robin, white-footed mouse)
		Insectivore (black-capped chickadee)
		Predator/scavenger (long-tailed weasel, red-tailed hawk)

Terrestrial vertebrate herbivore	Black-tailed deer, bobwhite quail, long-tailed vole, meadow vole, mule deer, white-tailed deer
Terrestrial ground-invertebrate feeder	Short-tailed shrew, trowbridge shrew, American woodcock
Flying insect	Mayfly
Soil detrivore	Earthworm, soil arthropod

The model uses a system of libraries to store information related to the chemicals, compartments, composite compartments (for example, a plant is considered as consisting of leaves, stem and roots), sources and so on. The information in these libraries can be drawn on to construct various food chains. The model can be run either as a dynamic or steady-state model. The outputs from TRIM.FaTE can be used as inputs to a human ingestion exposure model (TRIM.Expo-ingestion) to estimate human exposures. The model can also carry out a sensitivity analysis and a Monte-Carlo analysis to investigate uncertainty in the predictions.

Outputs from the model include the mass of chemical, concentration of chemical and the number of moles of chemical in each compartment (all can be generated at each time step of the simulation).

Similar to the previous two models, this model is considered to be an expert system and will require considerable knowledge and experience in order to use it. The information requirements of the model are quite extensive and so, although extensive databases of chemical-, species-, and environment-related information are already included in the model, it would not be straightforward to adapt it to species or environments that are not included.

14 Results and discussion

14.1 Ranking of models and recommendations

Based on the scoring system used, the models reviewed in this report can be ranked in the following order, listed in Table 14.1.

Table 14.1 Ranking of the models reviewed

Model	Food chain	Total score
Prediction of Bioaccumulation in Aquatic Food Webs model	Aquatic	96
ECOFATE and Food Chain Bioaccumulation models	Aquatic	96
Foodweb model	Aquatic	94
Arctic Terrestrial Food-Chain Bioaccumulation model	Terrestrial	88
EU Technical Guidance Document	Aquatic	84[21]
	Terrestrial	
	Human	
GEMCO	Aquatic	80
ACC-Human	Aquatic	75[21]
	Terrestrial	
	Human	
System dynamic model	Aquatic	73[21]
	Terrestrial	
BASS/FGETS	Aquatic	73
QEAFDCHN	Aquatic	63
ARAMS	Aquatic	Not scored
	Terrestrial	
AQUATOX	Aquatic	Not scored
TRIM.FaTE	Aquatic	Not scored
	Terrestrial	
	Human	

[21] For models covering more than one food chain, a single score is given covering all food chains considered.

For the aquatic food chain, the models that rank most highly are the Prediction of Bioaccumulation in Aquatic Food Webs model (see Chapter 10) and the Food Chain Bioaccumulation model/ECOFATE (see Chapter 8). The Food Chain Bioaccumulation model/ECOFATE model provides a flexible framework for modelling the bioaccumulation of chemicals in aquatic food webs, but would need to be adapted to be representative of a UK food chain. The information requirements of the model are relatively modest and so it should be reasonably straightforward to adapt this method to the UK situation. The Prediction of Bioaccumulation in Aquatic Food Webs model is a series of simple regression-based equations. The applicability of these equations to the UK would need to be established. It is therefore recommended that both these models are further validated against datasets for the UK.

For the terrestrial food chain, the models that rate most highly are the Arctic Terrestrial Food-chain Bioaccumulation model (see Chapter 9) and the EU Technical Guidance Document (see Chapter 3). The Arctic Terrestrial Food-chain Bioaccumulation model would need be significantly adapted to be useful to the UK situation, but it is one of the few terrestrial models to consider exposure of mammalian top predators, and some of the model's findings indicate that factors other than log K_{ow} (which is normally assumed to be a reasonable predictor of bioaccumulation potential of a chemical) may be important for such organisms. Therefore, it is recommended that consideration be given to adapting the model's approach to a food chain more representative of the UK. The EU Technical Guidance Document is an established methodology used throughout the EU for risk assessment of chemicals. It could therefore be used for the UK situation without further modification. However, it could be useful to incorporate some of the recent advances in earthworm and plant models (see Chapter 3). In addition, consideration should be given to further validating these methods against UK datasets.

For human exposure via environmental routes, the two highest ranking models are the EU Technical Guidance Document (see Chapter 3) and the ACC-Human model. The above discussion on the EU TGD also applies here. The ACC-Human model would need to be adapted to the UK situation, but this should be relatively straightforward (if other fish species are required, the availability of species-specific information may limit the number of fish age classes that can be included). Therefore, it is recommended that consideration be given to adapting the ACC-Human model to a representative UK situation. In addition, consideration should be given to further validating these methods against datasets for the UK.

14.2 Other information required for modelling bioaccumulation

As can be seen from preceding sections, the amount of chemical-specific, species-specific and ecosystem-specific information required to run the bioaccumulation models varies considerably between models. Most models contain sufficient information to be run for similar chemicals, species and ecosystems to those on which they are based, but a potential problem arises over data availability if the model is run for different chemical types, or is adapted to include other species or the properties of other ecosystems. It is then useful to consider possible sources of information that would allow the models to be run for, or further adapted to, these situations. Below is a brief summary of such sources of information uncovered during the course of this study. No systematic attempt was made to locate all such sources of information, and so it is likely that further sources exist.

A key parameter for consideration of bioaccumulation in aquatic systems is often the bioconcentration factor (BCF). In this review, it has been assumed that BCF values for fish (if needed for a given model) will be available for a wide range of chemicals, either

obtained directly from experiments, or predicted from physico-chemical properties such as log K_{ow}. However, there are models available for predicting bioconcentration in fish and several of these have been reviewed by Barber (2003). As bioconcentration models are incorporated into several of the more complex aquatic food chain models, the findings of the Barber (2003) review have been taken into account in our reviews of the models.

Many of the available models require information on the rates of elimination of the chemical from the organism. These data are not routinely available for organic chemicals, although it may be possible to estimate these values in some cases. For example, Hendriks (1995) developed a series of regression equations relating the elimination rate constant for persistent organic chemicals to log K_{ow} and the size of the species for aquatic invertebrates, fish and warm-blooded animals. These rate constants were seen to represent the minimum elimination rate for the organism. Chemicals that undergo extensive metabolism would be expected to have elimination rate constants larger than these values.

Similarly, many of the models investigating uptake via food require knowledge of the uptake or assimilation efficiency of the chemical. Gobas *et al*. (1988) derived a regression relationship between the uptake efficiency from food in fish and log K_{ow} (incorporated into the Foodweb model outlined in Chapter 6) that could be useful in this respect. Similarly, Hendriks *et al*. (2001) and Traas (2004) developed a method for estimating accumulation (uptake and depuration) kinetics of organic substances as a function of the K_{ow} of the chemical and the weight, lipid content and trophic level of the species in question. These methods effectively circumvent the need for parameters such as ventilation rates and gill or gut uptake efficiencies used in some of the models (and for which data may not generally be available for a wide range of chemicals).

Hendriks *et al.* (1999) collated and reviewed over 100 allometric regression equations for estimating rate, age and density parameters for many species commonly used in ecological models. These equations may be useful when adapting a model for a new food chain or species. They include the following:

- air inhalation rate constants versus species size (weight);
- water absorption and excretion rate constants versus species size (weight);
- rate constants for average nutrient absorption or food consumption versus species size (weight);
- rate constants for maximum nutrient absorption of food consumption versus species size (weight);
- average reproduction rate constant versus species size (weight);
- maximum reproduction rate constant versus species size (weight);
- laboratory respiration rate constant versus species size (weight);
- field respiration rate constant versus species size (weight);
- mortality rate constant versus species size (weight);
- fraction assimilated of ingested food;
- fraction of assimilated food that is spent on production (net growth or production efficiency);
- maturation age versus species size (weight);
- average age versus species size (weight);

- maximum age versus species size (weight);
- population density versus species size (weight);
- biota density versus species size (weight);
- consumer size versus food size (weight).

In addition, several of the models considered in this report, such as Aquatox (Chapter 13.3), ARAMS (Chapter 13.2) and TRIM.FaTE (Chapter 13.4), contain databases of species-specific parameters that may be useful for the adaptation of other models.

14.3 Recommended approach for incorporating bioaccumulation in standards

The available models allow the concentrations in, and/or bioaccumulation factors for, various organisms within the food chain to be estimated.

A generalized scheme for considering bioaccumulation through the food chain when setting standards is shown below.

$$SC_{media} = \frac{NOEC_{predator}}{BAF_{Prey}} \quad \text{or} \quad SC_{media} = \frac{NOEC_{predator} \times Conc_{media}}{PEC_{Prey}}$$

where: SC_{media} = standard concentration for the environmental compartment being considered, such as water, sediment (where the BAF would be more correctly termed a BSAF), soil and so on.

$NOEC_{predator}$ = estimated no effect concentration or "safe concentration" in diet for the top predator or humans – this may also take account of uncertainty factors and other factors (see below).

BAF_{prey} = bioaccumulation factor for the prey organism, related to the concentration in water, sediment and soil. This could include one or more further steps in the food chain.

$Conc_{media}$ = concentration in water, sediment or soil that was assumed in the model.

PEC_{Prey} = modelled or predicted concentration in the prey resulting from exposure of the ecosystem to $Conc_{media}$.

The extrapolation of toxicity data from laboratory animals to wildlife and humans requires the consideration of suitable uncertainty and conversion factors to account for the feeding habits of wildlife (in order to convert laboratory toxicity data from daily intake rates (such as mg/kg body weight/day) to an equivalent dosage concentration in diet (such asmg/kg diet)). Methods for carrying out such extrapolations are given in the EU Technical Guidance Document (see Chapter 3), USEPA (2000) (see Chapter 2.2), Traas *et al*. (1996) and Jongbloed *et al*. (1994 and 1996) for birds and mammals (see Chapter 2.4); a comprehensive framework for a range of avian, mammalian, reptilian and amphibian species is given in Canadian Council of Ministers of the Environment (1999) (see Chapter 2.3).

The method outlined in the EU TGD for wildlife differs from the methods used in USEPA (2000), Canadian Council of Ministers of the Environment (1999) and Traas *et al.* (1996). The TGD method assumes that predicted or estimated no effect dosage in diet derived from laboratory animals is the same for all wildlife irrespective of their weight and feeding rates, whereas the other methods assume that the total exposure (in terms of mg/kg body weight/day) of the organism should be the same for all wildlife and hence the equivalent dosage in diet varies for different species of wildlife (being dependent on both body weight and daily feeding rate amongst other factors). The latter method also takes into account differences in energy content between laboratory food and food in the wild, and differences in metabolic rates between laboratory animals and wild animals. A detailed review of methods to determine NOECs and "safe concentrations" for wildlife and humans is beyond the scope of this work. However, the more factors that are accounted for qualitatively in the method, the lower the overall uncertainty factor that is generally applied. For example, the Traas *et al.* (1996) method does not use uncertainty factors at all; rather, the NOEC/safe concentration takes into account a number of dietary factors and estimates the final concentration by statistical methods. In contrast, the EU TGD method, which ignores many dietary factors, uses quite large uncertainty factors to take into account the overall uncertainty.

The available models allow BAFs or BSAFs (or the PEC_{prey} resulting from exposure of the ecosystem to a constant concentration, $Conc_{media}$) to be determined that could be used directly in this scheme. However, in reality this scheme is a simplification, because the predator may be exposed via one or more routes (for example, humans can be exposed though consuming contaminated fish, crops, meat, water and air) and the key question to be addressed is how these different routes of exposure should be considered when setting standards.

One approach that could be used for humans (and wildlife) would be to consider exposure via the aquatic food chain (for example, consumption of contaminated fish and/or drinking water), the terrestrial food chain (such as consumption of contaminated crops and/or meat) and air separately. Thus, it would be possible to back-calculate to a separate standard concentration for water, sediment, soil and/or air. This approach may not, however, be precautionary if exposure of an individual occurs by more than one food chain, as the NOEC or "safe concentration" could be exceeded if all routes of exposure occur simultaneously. An alternative approach would be to use the estimated fraction that each food chain makes to the diet of the target species to adjust the standard for each medium, so that if an individual is exposed simultaneously via all food chains at standard concentrations, the total exposure would equal the NOEC or "safe concentration". A similar approach is used in USEPA (2000) for human exposure (see Chapter 2.2).

For some food chains, for example where exposure can occur via water and sediment, it is possible to combine both routes of exposure into a single standard (either for sediment or water) by assuming that the two media are in equilibrium with each other.

For the aquatic food chain, it is theoretically possible to address combined routes of exposure for predatory fish by using the TLM or IEC approach outlined in Chapter 2.3. However, such an approach is relatively new and can only be applied currently to narcotic chemicals. This may also present similar problems, as outlined above, when extrapolating back to a standard in a single medium.

Some models are steady state, whilst others can be run for time-dependent changes in input concentrations and so on. If a time-dependent model is run for a sufficient length of time using a constant input concentration, the resulting calculations will effectively be at steady state. This mode of calculation is probably the most relevant for standard setting, as it allows for long-term exposure to a constant concentration to be taken into account. However, models that carry out time-dependent calculations may also be

useful for other applications, such as determining how, and how quickly, the ecosystem may respond to changes in emission patterns resulting, for example, from the use of local control measures.

Some models can also take into account (bio)degradation of the chemical in the environment. While this may be important for the risk assessment of a chemical, it is less important for setting standards, Standards are estimated on the basis that no effects will be seen in an organism if long-term exposure of the food chain to a chemical at or below the standard concentration in a media occurs, whereas the degradation of the chemical determines the actual concentration present in the environment.

BAFs and other factors determined in the models (particularly for the aquatic compartment) can refer to either the total or dissolved concentration in water; models that do not consider sediment interactions generally refer to the dissolved concentration. Thus, any standard derived from the method would then apply to the respective total or dissolved concentration. It is possible to convert between the two by assuming equilibrium partitioning between the dissolved and particulate phase, having knowledge of the partition coefficient and suspended particulate concentration of the water system under consideration (such conversions are used in many of the models, as most assume that uptake occurs from the dissolved fraction in the water phase).

Similarly, some of the models estimate concentrations (and hence BAFs) on a lipid weight basis. These data would generally need to be converted to a whole organism basis using the lipid contents of the species in question.

In order to test this scheme, several of the models that rated highly in this review, and for which calculations were relatively straightforward to carry out, were used to derive standards for a hypothetical chemical. Details of the calculations are given in Appendix B. The resulting hypothetical standards derived for a fish-eating top predator are shown below. A NOEC or "safe concentration" of 10 mg/kg food was assumed in a wildlife top predator in each case.

EU Technical Guidance Document

Derived BAF = 4.6×10^{5} l/kg for freshwater food chain and 4.6×10^{6} for marine food chain, both related to dissolved concentration.

Derived standard = $10/4.6\times10^{5} = 2.2\times10^{-5}$ mg/l (dissolved) for freshwater food chain.

= $10/4.6\times10^{6} = 2.2\times10^{-6}$ mg/l (dissolved) for marine food chain.

ACC-Human

Derived BAF = 1.67×10^{8} l/kg lipid for cod and 5.3×10^{7} l/kg lipid for herring, both related to the dissolved concentration. Using the lipid contents for cod (4.4 per cent) and herring (3.5 per cent) in the model, these are equivalent to whole body BAFs of 7.3×10^{6} l/kg for cod and 1.9×10^{6} l/kg for herring.

Derived standard = $10/7.3\times10^{6} = 1.4\times10^{-6}$ mg/l (dissolved) for cod-eater.

= $10/1.9\times10^{6} = 5.3\times10^{-6}$ mg/l (dissolved) for herring-eater.

Prediction of Bioaccumulation in Aquatic Food Webs

The BAF determined for trophic level 4 (pisciverous fish) was 3.3×10^{8} l/kg based on the dissolved concentration in freshwater.

Derived standard = $10/3.3\times10^{8} = 3.0\times10^{-8}$ mg/l (dissolved) for freshwater food chain.

Food Chain Bioaccumulation Model (version 1.1)

The BAF determined for rainbow trout was 1.02×10^{7} l/kg based on the total concentration in water.

Derived standard = $10/1.02\times10^{7} = 9.8\times10^{-7}$ mg/l (total concentration) for freshwater food chain.

As can be seen from these example calculations, there are large differences between standards derived using the different models. This reflects differences in the food chains considered in the models (such as the length of food chain, species considered, properties of the environmental compartments), as well as assumptions made within the models. At present, it is not known which of these models gives the most reliable predictions of accumulation in food chains relevant for England and Wales. However, the range of values obtained here indicates that further investigation of the validity and predictive power of the models is needed before reliable standards can be derived.

14.4 Limitations of the method

The vast majority of modelling methods assume that the partitioning of a substance from water to a medium is a function of the lipid or organic carbon content of that medium (and hence can be related to the log K_{ow}). Such models will not necessarily apply to substances whose partitioning behaviour does not fall within such assumptions. Examples include surface active agents, substances whose partitioning behaviour may be pH-dependent (such as acids and bases), substances that adsorb onto mineral fractions of particulate matter, or those that are actively taken up by organisms. Care would have to be exercised when modelling the bioaccumulation potential of these types of substances, by careful choice of the chemical-related input parameters.

Many of the models have been developed and/or validated using only a relatively small range of chemical types (such as PCBs and other persistent organochlorine chemicals) and so the applicability of these models to other chemicals, particularly those that may be metabolised rapidly and of a relatively low log K_{ow} (below four), is unclear.

14.5 Possible problems and limitations with considering bioaccumulation in setting standards

Approaches generally consider accumulation of the parent compound through the food chain. This approach is applicable when it is the parent compound itself that causes

toxic effects in the target organism. A potential problem arises when the toxic effects are caused by metabolites of the chemical. In this case, the bioaccumulation behaviour of metabolites may not be the same as that of the parent compound.

When interpreting the results of a standard toxicity test, it is not normally important whether the toxic effects are caused by the parent compound or metabolites. For example, in a mammalian toxicity test, it is usually only necessary to know that if the animals are exposed to a constant concentration of a chemical in water, then certain effects will occur; it is not normally important to know exactly how the chemical exerts these effects inside the organism. Thus, for exposure via food of one trophic level, it would be relatively straightforward to set a standard from the results of this type of test.

However, if bioaccumulation through the food chain is taken into account the situation is less clear, as exposure of the organisms to parent compound and metabolites will depend to some extent on the metabolic capability of each step in the food chain, the bioaccumulation properties of the metabolites and those of the parent compound. In practice, however, such considerations may not be so important given that metabolic products are usually more hydrophilic than the parent compound, and so are less likely to accumulate along the food chain. Thus, organisms at the top of the food chain are likely to be exposed mainly to the parent compound rather than metabolites, and so the situation would become analogous to the simple situation outlined above.

One note of caution with regards to the use of steady-state bioaccumulation models: steady state can take a long time to reach for substances that have very high log K_{ow} values (greater than 7.5) and are slowly metabolised (Arnot and Gobas, 2004).

Several models allow Monte-Carlo simulations to be carried out to obtain information on the uncertainties of predictions; such simulations could also be carried out on other models with suitable adaptation. However, care should be taken in interpreting the results of uncertainty analyses, as error/uncertainty in the model structure is not considered in a Monte-Carlo simulation, and no comparison of model predictions with an independent dataset is made in such simulations (Arnot and Gobas, 2004). Comparing model predictions with an independent field dataset (provided sufficient data points are available) would take into account systematic errors in the model (related to both the model structure and parameters used) as well as errors and natural variability associated with the field data.

An important consideration when setting standards for bioaccumulative substances is that the more traditional media to which standards apply (such as water, sediment, air) may not be the most appropriate, owing to analytical limitations. For instance, the example calculations given in Chapter 14.3 show that the levels in water would be very low and may not be analytically determinable. Therefore, it may be more relevant to relate any standard to a concentration in a medium where the concentration could be more easily determined, such as prey items (fish, mussels, earthworms and other food items). This approach is essentially the one taken in the Canadian tissue residue guidelines (see Chapter 2.3). However, this approach in itself may present problems, as prey/food items are much more difficult (and costly) to monitor routinely than air, water and sediment, and animal welfare needs to be taken into consideration.

15 Conclusions

Following a detailed review of available bioaccumulation models, the following models are recommended for further consideration when setting environmental standards.

Aquatic food chain	Prediction of Bioaccumulation in Aquatic Food Webs model
	Food Chain Bioaccumulation/ECOFATE models
	EU Technical Guidance Document
Terrestrial food chain	Arctic Terrestrial Food-chain Bioaccumulation model
	EU Technical Guidance Document
Human food chain	EU Technical Guidance Document
	ACC-Human

All models (with the exception of the Prediction of Bioaccumulation in Aquatic Food Webs model) will need further development to parameterise them to better represent the UK situation, or to take account of recent developments. In addition, consideration should be given to validating the models against UK datasets. This validation should consider as wide a range of chemical types (and physico-chemical properties) as possible.

A framework is also presented for how the modelled bioaccumulation data could be used in deriving standards.

References

ARNOT, J. A. AND GOBAS, F.A.P.C., 2003. A generic QSAR for assessing the bioaccumulation potential of organic chemicals in aquatic food webs. QSAR and Combinatorial Science, 22, 337-345.

ARNOT, J. A. AND GOBAS, F.A.P.C., 2004. A food web bioaccumulation model for organic chemicals in aquatic ecosystems. Environmental Toxicology and Chemistry, 23, 2343-2355.

BARBER, M.C., SUÁREZ, L.A. AND LASSITER, R.R., 1988. Modelling bioconcentration of non-polar organic pollutants by fish. Environmental Toxicology and Chemistry, 7, 545-558.

BARBER, M.C., SUÁREZ, L.A. AND LASSITER, R.R., 1991. Modelling bioaccumulation of organic pollutants in fish with an application to PCBs in Lake Ontario salmonids. Canadian Journal of Fisheries and Aquatic Sciences, 48, 318-337.

BARBER, M.C., 2003. A review and comparison of models for predicted dynamic chemical bioconcentration in fish. Environmental Toxicology and Chemistry, 22, 1963-1992.

BARBER, M.C., 2005a. *Bioaccumulation and aquatic system simulator (BASS) user's manual version 2.2*. United States Environmental Protection Agency Report No. 600/R-05/XXX, Draft 24th January 2005.

BARBER, M.C., 2005b. *Bioaccumulation and aquatic system simulator (BASS) data supplement version 2.2*. United States Environmental Protection Agency Report No. 600/R-05/XXX, Draft 20th January 2005.

BRIGGS, G.G., BROMILOW, R.H. AND EVANS, A.A., 1982. Relationship between lipophilicity and root uptake and translocation of non-ionized chemicals by barley. Pesticide Science, 13, 495-504.

BROCKWAY, D.L., SMITH, P.D. AND BARBER, M.C., 1996. *PCBs in the aquatic-riparian zone of the Lake Hartwell ecosystem, South Carolina*. United States Environmental Protection Agency, National Exposure Research Laboratory, Athens (internal report; as reported in Barber, 2005a).

BROOKE, D., CROOKES, M. AND QUARTERMAN, P., 2003. *Review of methods for assessing biomagnification of chemicals*. Draft report prepared for Steve Dungey, Environment Agency, August 2003.

BURKHARD, L.P., SHEEDY, B.R., MCCAULEY, D.J. AND DEGRAEVE, G.M., 1997. Bioaccumulation factors for chlorinated benzenes, chlorinated butadienes and hexachloroethane. Environmental Toxicology and Chemistry, 16, 1677-1686.

CALAMARI, D., VIGHI, M. AND BACCI, E., 1987. The use of terrestrial plant biomass as a parameter in the fugacity model. Chemosphere, 16, 2359-2364.

CAMPFENS, J. AND MCKAY, D., 1997. Fugacity-based model of PCB bioaccumulation in complex aquatic food webs. Environmental Science and Technology, 31, 577-583.

CANADIAN COUNCIL OF MINISTERS OF THE ENVIRONMENT, 1999. *Protocol for the derivation of Canadian tissue residue guidelines for the protection of wildlife that consume aquatic biota*. Canadian Council of Ministers of the Environment, Winnipeg, Canada.

CARBONELL, G., RAMOS, C., PABLOS, M.V., ORTIZ, J.A. AND TARAZONA, J.V., 2000. A system dynamic model for the assessment of different exposure routes in aquatic ecosystems. The Science of the Total Environment, 247, 107-118.

CLARK, K.E., GOBAS, F.A.P.C. AND MACKAY, D., 1990. Model of organic uptake and clearance by fish from food and water. Environmental Science and Technology, 24, 1203-1213.

COLLINS. C., SHAW, G. AND FRYER, M.E., 2004. *Review of plant uptake models for CLEA*. Confidential Draft – May 2004. Document produced under R&D Project P5-079/4. Environment Agency, Bristol.

CONNELL, D.W. AND HAWKER, D.W., 1988. Use of polynomial expressions to describe the bioconcentration of hydrophobic chemicals by fish. Ecotoxicology and Environmental Safety, 16, 242-257.

CONNOLLY, J.P., 1991. Application of a food chain model to polychlorinated biphenyl contamination of the lobster and winter flounder food chains in New Bedford Harbor. Environmental Science and Technology, 25, 760-770.

CONNOLLY, J.P. AND GLASER, D., 2002. p,p'-DDE bioaccumulation in female sea lions of the California Channel Islands. Continental Shelf Research, 22, 1059-1078.

CONNOLLY, J.P., ZAHAKOS, H.A., BENAMAN, J., ZIEGLER, C.K., RHEA, J.R AND RUSSEL, K., 2000. A model of PCB fate in the upper Hudson River. Environmental Science and Technology, 34, 4076-4087.

CROMMENTUIJN, T., SIJM, D., DE BRUIJN, J., VAN LEEUWEN, K. AND VAN DE PLASSCHE, E., 2000. Maximum permissible and negligible concentrations for some organic substances and pesticides. Journal of Environmental Management, 58, 297-312.

CZUB, G. AND MCLACHLAN, M.S., 2004. A food chain model to predict the levels if lipophilic organic contaminants in humans. Environmental Toxicology and Chemistry, 23, 2356-2366.

DEVILLERS, J., 1998. Comparative QSAR. Taylor and Francis, Washington DC.

DI TORO, D.M., MCGRATH, J.A. AND HANSEN, D.J, 2000. Technical basis for narcotic chemicals and polycyclic aromatic hydrocarbon criteria. I. Water and tissue. Environmental Toxicology and Chemistry, 19, 1951-1970.

DOWDY, D.L AND MCKONE, T.E, 1997. Predicting plant uptake of organic chemicals from soil or air using octanol/water and octanol/air partition ratios and a molecular connectivity index. Environmental Toxicology and Chemistry, 16, 2448-2456.

DOWDY, D.L., MCKONE, T.E AND HSIEH, D.P.H., 1996. Prediction of chemical biotransfer of organic chemicals from cattle diet into beef and milk using the molecular connectivity index. Environmental Science and Technology, 30, 984-989.

ENVIRONMENT AGENCY AND DEFRA, 2002. *The contaminated land exposure assessment (CLEA) model: Technical basis and algorithms*. R&D Publication CLR 10, Environment Agency, Bristol.

ESCHER, B.I. AND HERMENS, J.L.M., 2004. Internal exposure: Linking bioavailability to effects. Environmental Science and Technology, 38, 455A-462A.

EUROPEAN COMMISSION, 2002. Draft Working Document: *Guidance Document on Risk Assessment for Birds and Mammals under Council Directive 91/414/EEC*. European Commission, Health and Consumer Protection Directorate-General,

Directorate E – Food Safety: Plant Health, Animal Health and Welfare, 25th September 2002.

EUROPEAN COMMISSION, 2003. *Technical Guidance Document on Risk Assessment in support of Commission Directive 93/67/EEC on Risk Assessment for existing substances, Commission Regulation (EC) No 1488/94 on Risk Assessment for existing substances and Directive 98/8/EC of the European Parliament and of the Council concerning the placing of biocidal products on the market*. European Commission, Joint Research Centre, EU 20418 EN, Second Edition.

EVERTS, J.W., EYS, Y., RUYS, M., PIJNENBURG, J., VISSER, H. AND LUTTIK, R., 1993. Assessing the risk of biomagnification: a physiological approach. Science of the Total Environment, Supplement, 1501-1506.

FEDERAL REGISTER, 1995. Final water quality guidance for the Great Lakes system. Federal Register, 60(56), Thursday March 23 1995, pp15365-15425.

FRASER, A.J., $BURK_{ow}$, I.C., WOLKER, H. AND MACKAY, D., 2002. Modelling biomagnification and metabolism of contaminants in harp seals of the Barents Sea. Environmental Toxicology and Chemistry, 21, 55-61.

GARTEN, JR, C.T. AND TABALKA, J.R, 1983. Evaluation of models for predicting terrestrial food chain behaviour of xenobiotics. Environmental Science and Technology, 17, 590-595.

GLASER, D. AND CONNOLLY, J.P., 2002. A model of p,p'-DDE and total PCB bioaccumulation in birds from the Southern California Bight. Continental Shelf Research, 22, 1079-1100.

GOBAS, F.A.P.C., 1993. A model for predicting the bioaccumulation of hydrophobic organic chemicals in aquatic food webs: Applications to Lake Ontario. Ecological Modelling, 69, 1-17.

GOBAS, F.A.P.C. AND MACKAY, D., 1987. Dynamics of hydrophobic organic chemical bioconcentration in fish. Environmental Toxicology and Chemistry, 6, 495-504.

GOBAS, F.A.P.C , KELLY, B.C. AND ARNOT, J.A, 2003. Quantitative structure activity relationships for predicting the bioaccumulation of POPs in terrestrial food-webs. QSAR and Combinatorial Science, 22, 329-336.

GOBAS, F.A.P.C., MUIR, D.C.G. AND MACKAY, D., 1988. Dynamics of dietary bioaccumulation and faecal elimination of hydrophobic organic chemicals in fish. Chemosphere, 17, 943-962.

HENDRIKS, A.J., 1995. Modelling non-equilibrium concentrations of microcontaminants in organisms: comparative kinetics as a function of species size and octanol-water partitioning. Chemosphere, 30, 265-292.

HENDRIKS, A.J., 1999. Allometric scaling of rate, age and density parameters in ecological models. OIKOS, 86, 293-310.

HENDRIKS, A.J., VAN DER LINDE, A., CORNELISSEN, G. AND SIJM, D T., 2001. The power of size. 1. Rate constants and equilibrium ratios for accumulation of organic substances related to octanol-water partition ratio and species weight. Environmental Toxicology and Chemistry, 21, 1399-1420.

HICKIE, B.E., MACKAY, D. AND KONING, J., 1999. Lifetime pharmaco-kinetic model for hydrophobic contaminants in marine mammals. Environmental Toxicology and Chemistry, 18, 2622-2633.

HOLLING, C.S., 1966. The functional response of invertebrate predators to prey density. Memoirs of the Entomological Society and Canada, 48, 1-86 (as quoted in Barber, 2005a).

HRUBEC, J. AND TOET, C., 1992. *Predictability of the removal of organic compounds by drinking water treatment*. RIVM Report 714301007, National Institute of Public Health and the Environment, Bilthoven, the Netherlands (as quoted in European Commission, 2003).

HUNG, H. AND MACKAY, D., 1997. A novel and simple model of the uptake of organic chemicals by vegetation from air and soil. Chemosphere, 35, 959-977.

JAGER, T., 1998. Mechanistic approach for estimating bioconcentration of organic chemicals in earthworms (Oligochaeta). Environmental Toxicology and Chemistry, 17, 2080-2090.

JAGER, T., 2003. *Worming your way into bioavailability. Modelling the uptake of organic chemicals in earthworms*. Thesis from Institute for Risk Assessment Sciences, University of Utrecht.

JAGER, T., 2004. Modelling ingestion as an exposure route for organic chemicals in earthworms (Olgochaeta). Ecotoxicology and Environmental Safety, 57, 30-38.

JAGER, T., FLEUREN, R.H.L.J., HOGENDOORN E A AND DE KORTE G, 2003. Elucidating the routes of exposure for organic chemicals in the earthworm, *Eisenia Andrei* (Oligochaeta). Environmental Science and Technology, 37, 3399-3404.

JONGBLOED, R.H., PIJNENBURG, J., MENSINK, B.J.W.G., TRAAS, T.P. AND LUTTIK, R., 1994. *A model for environmental risk assessment and standard setting based on biomagnification. Top predators in terrestrial ecosystems*. RIVM Report 719101012, National Institute of Public Health and the Environment, Bilthoven, the Netherlands, October 1994.

JONGBLOED, R.H., TRAAS, T.P. AND LUTTIK, R., 1996. A probabilistic model for deriving soil quality criteria based on secondary poisoning of top predators. II. Calculations for dichlorodiphenyltrichloroethane (DDT) and cadmium. Ecotoxicology and Environmental Safety, 34, 279-306.

KELLY, B.C. AND GOBAS, F.A.P.C., 2001. Bioaccumulation of persistent organic pollutants in lichen-caribou-wolf food chains of Canada's central and Western Arctic. Environmental Science and Technology, 35, 325-334.

KELLY, B.C. AND GOBAS, F.A.P.C., 2003. An arctic terrestrial food-chain bioaccumulation model for persistent organic pollutants. Environmental Science and Technology, 37, 2966-2974.

KELLY, B.C., GOBAS, F.A.P.C. AND MCLACHLAN M.S, 2004. Intestinal absorption and biomagnification of organic contaminants in fish, wildlife, and humans. Environmental Toxicology and Chemistry, 23, 2324-2336.

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

LIJZEN, J.P.A., BAARS, A,J., OTTE, P.F., RIKKEN, M.G.J., SWARTJES, F.A., VERBRUGGEN, E.M.J. AND VAN WEZEL, A.P., 2001. *Technical evaluation of the intervention values for soil/sediment and groundwater. Human and ecotoxicological risk assessment and derivation of risk limits for soil, aquatic sediment and groundwater*. RIVM Report 601516011/2004. Rijksinstituut voor Volksgezondheid en Milieu, Bilthoven, Netherlands.

LOIZEAU, V. AND MENESGUEN, A., 1993. A steady-state model for PCB accumulation in dab food web. Oceanological Acta, 16, 633-639.

LOIZEAU, V., ABARNOU, A., CUGIER, P., JAOUEN-MADOULET, A., LE GUELLEC, A-M. AND MENESGUEN, A., 2001. A model of PCB bioaccumulation in the sea bass food web from the seine Estuary (Eastern English Channel). Marine Pollution Bulletin, 43, 242-255.

MCCARTY, L.S. AND MACKAY, D., 1993. Enhancing ecotoxicological modelling and assessment. Environmental Science and Technology, 27, 1719-1728 (as quoted in Barber, 2005a).

MCGRATH, J.A., PARKERTON, T.P. AND DI TORO, D.M., 2004. Application of the narcosis target lipid model to algal toxicity and deriving predicted-no-effect concentrations. Environmental Toxicology and Chemistry, 23, 2503-2517.

MCLACHLAN, M.S., 1994. Model of the fate of hydrophobic contaminants in cows. Environmental Science and Technology, 28, 2407-2414.

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

MORRISON, H.A., GOBAS, F.A.P.C., LAZAR, R AND HAFFNER, G.D, 1996. Development and verification of a bioaccumulation model for organic contaminants in benthic invertebrates. Environmental Science and Technology, 30, 3377-3384.

MORRISON, H.A., GOBAS, F.A.P.C., LAZAR, R, WHITTLE, D.M. AND HAFFNER, G. D, 1997. Development and verification of a benthic/pelagic food web bioaccumulation model for PCB congeners in Western Lake Erie. Environmental Science and Technology, 31, 3267-3273.

MOSER, G.A. AND MCLACHLAN, M.S., 2002. Modelling digestive tract absorption and desorption of lipophilic organic contaminants in humans. Environmental Science and Technology, 36, 3318-3325.

MÜLLER, J.F., HAWKER, D.W. AND CONNELL, D.W., 1994. Calculation of bioconcentration factors of persistent hydrophobic compounds in the air/vegetation system. Chemosphere, 29, 623-640.

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

PATTERSON, S., MACKAY, D. AND CALAMARI, D., 1991a. Correlation of the equilibrium and kinetics of leaf-air exchange of hydrophobic organic chemicals. Environmental Science and Technology, 25, 866-871.

PATTERSON, S., MACKAY, D. AND GLADMAN, A., 1991b. A fugacity model of chemical uptake by plants from soils and air. Chemosphere, 23, 539-565.

PATTERSON, S., MACKAY, D. AND MCFARLANE, C., 1994. A model of organic chemical uptake by plants from soil and the atmosphere. Environmental Science and Technology, 28, 2259-2266.

PEREIRA, W.E., ROSTAD, C.E., CHIOU, C.T., BRINTON, T.I., BARBER, L.B., DEMCHECK, D.K. AND DEMAS, C.R., 1988. Contaminations of estuarine water, biota, and sediment by halogenated organic compounds: a field study. Environmental Science and Technology, 22, 772-778.

PETERSON, D.R., 1994. Calculating the aquatic toxicity of hydrocarbon mixtures. *Chemosphere*, 29, 2493-2506 (as quoted in Barber, 2005a).

QEA, 1999. *PCBs in the Upper Hudson River. Volume 2: A model of PCB fate, transport and bioaccumulation*. Prepared for General Electric. Quantitative Environmental Analysis, LCC, Montvale, United States (available from http://www.ge.com/en/commitment/ehs/hudson/techReport.htm).

QEA, 2001a. *Documentation Bioaccumulation Model QEAFDCHN v1.0*. Quantitative Environmental Analysis, LLC, Montvale, United States, February 2001 (available from http://www.dnr.state.wi.us/org/water/wm/lowerfox/rifs/modeldocs/e2_manual.pdf).

QEA, 2001b. *A model of PCB bioaccumulation in the Lower Fox River and Green Bay: GBFood*. Quantitative Environmental Analysis, LLC, Montvale, United States (available from http://www.dnr.state.wi.us/org/water/wm/lowerfox/rifs/feasabilitystudy.html).

RASHEVSKY, 1959. Some remarks on the mathematical theory of nutrition of fishes. *Bulletin of Mathematical Biophysics*, 21, 161-183 (as quoted in Barber, 2005a).

RIEDERER, M., 1990. Estimating partitioning and transport of organic chemicals in the foliage/atmosphere system: Discussion of a fugacity-based model. Environmental Science and Technology, 24, 829-837.

RIKKEN, M.G.J. AND LIJZEN, J.P.A., 2004. *Update of risk assessment models for the indirect human exposure*. RIVM Report 601516011/2004. Rijksinstituut voor Volksgezondheid en Milieu, Bilthoven, Netherlands.

RIKKEN, M.G.J., LIJZEN, J.P.A., AND CORNELESE, A, 2001. *Evaluation of model concepts on human exposure. Proposals for updating the most relevant exposure routes of CSOIL*. RIVM Report 711701022/2001. Rijksinstituut voor Volksgezondheid en Milieu, Bilthoven, Netherlands.

RYAN, J.A., BELL, R.M., DAVIDSON, J.D. AND O'CONNOR, G.A., 1988. Plant uptake of non-ionic organic chemicals from soils. Chemosphere, 17, 2299-2323.

SANGSTER, H., 1997. *Octanol-water partition coefficients: fundamentals and physical chemistry*. John Wiley and Sons Inc., New York.

SCHRAMM, K-W., REISCHL, A. AND HUTZINGER, O., 1987. UNITTree. A multimedia compartment model to estimate the fate of lipophilic compounds in plants. Chemosphere, 16, 2653-2663.

THOMANN, R.V., 1981. Equilibrium model of fate of microcontaminants in diverse aquatic food chains. Canadian Journal of Fisheries and Aquatic Sciences, 38, 280-296.

THOMANN, R.V., 1989. Bioaccumulation model of organic chemical distribution in aquatic food chains. Environmental Science and Technology, 23, 699-707.

THOMANN, R.V. AND CONNOLLY, J.P. 1984. Model of PCB in the Lake Michigan lake trout food chain. Environmental Science and Technology, 18, 65-71.

THOMANN, R.V., CONNOLLY, J.P. AND PARKERTON, T.F., 1992a. An equilibrium model of organic chemical accumulation in aquatic food webs with sediment interaction. Environmental Toxicology and Chemistry, 11, 615-629.

THOMANN, R.V., CONNOLLY, J.P. AND PARKERTON, T.F., 1992b. Modelling accumulation of organic chemicals in aquatic food-webs. In *Chemical Dynamics in Aquatic Ecosystems*. Editors F A P C Gobas and J A McCorquodale. Lewis Publishers, Chelsea, MI, pp153-186.

TRAAS, T.P. , 2001. *Guidance document on deriving environmental risk limits*. RIVM Report 601501 012, National Institute of Public Health and the Environment, Bilthoven, the Netherlands, June 2001.

TRAAS, T.P., LUTTIK, R. AND JONGBLOED, R.H., 1996. A probabilistic model for deriving soil quality criteria based on secondary poisoning of top predators. I. Model description and uncertainty analysis. Ecotoxicology and Environmental Safety, 34, 264-278.

TRAAS, T.P., VAN WEZEL, A.P., HERMENS, J.L.M., ZORN, M., VAN HATTUM, A.G.M. AND VAN LEEUWEN, C.J., 2004. Envrionmental quality criteria for organic chemicals predicted from internal effect concentrations and a food web model. Environmental Toxicology and Chemistry, 23, 2518-2527.

TRAPP, S., 1995. Model for uptake of xenobiotics into plants. In *Plant Contamination: Modelling and Simulation of Organic Chemical Processes*, edited by S Trapp and J C McFarlane, pp107-151. Boca Raton: Lewis Publishers.

TRAPP, S., 2000. Modelling uptake into roots and subsequent translocation of neutral and ionisable organic compounds. *Pest Management Science*, 56, 767-778.

TRAPP, S., 2002. Dynamic root uptake model for neutral lipophilic organics. Environmental Toxicology and Chemistry, 21, 203-206.

TRAPP, S., 2004. Plant uptake and transport models for neutral and ionic chemicals. Environmental Science and Pollution Research, 11, 33-39.

TRAPP, S. AND MATTHIES, M., 1995. Generic one-compartment model for uptake of organic chemicals by foliar vegetation. Environmental Science and Technology, 29, 2333-2338.

TRAPP, S. AND MATTHIES, M., 1998. *Chemodynamics and environmental modelling – an introduction*. Springer, London.

TRAPP, S., MATTHIES, M., SCHEUNERT, I. AND TOPP, E.M., 1990. Modelling the bioconcentration of organic chemicals in plants. Environmental Science and Technology, 24, 1246-1252.

TRAPP, S., RASMUSSEN, D. AND SAMSØE-PETERSEN, L., 2003. Fruit tree model for uptake of organic compounds from soil. SAR and QSAR in Environmental Research, 14, 17-26.

TRAVIS C C AND ARMS A D, 1988. Bioconcentration of organics in beef, milk and vegetation. *Environmental Science and Technology*, 22, 271-274.

USEPA, 1995a. *Great Lakes water quality initiative technical support document for wildlife criteria.* United States Environmental Protection Agency, EPA-820-B95-009.

USEPA, 1995b. *Great Lakes water quality initiative technical support document for the procedure to determine bioaccumulation factors*. United States Environmental Protection Agency, EPA-820-B95-005.

USEPA, 2000. *Methodology for deriving ambient water quality criteria for the protection of human health*. United States Environmental Protection Agency, EPA-822-B00-004.

USEPA, 2004. *AQUATOX (Release 2). Modelling environmental fate and ecological effects in aquatic ecosystem. Volume 2: Technical documentation*. United States Environmental Protection Agency, EPA-823-R-04-002, January 2004.

VAN DEN BERG, R., 1995. *Exposure of man to soil contamination. A qualitative and quantitative analysis, resulting in proposals for human-toxicological C values*. RIVM

Report 725201006/1995 (revised version of RIVM Report 725201011/1991). Rijksinstituut voor Volksgezondheid en Milieu, Bilthoven, Netherlands (in Dutch).

VAN HATTUM, B., CUNTO PONS, M.J. AND CID MONTANES, J.F., 1998. Polycyclic aromatic hydrocarbons in freshwater isopods and field-partitioning between abiotic phases. Archives of Environmental Contamination and Toxicology, 35, 257-267.

VAN LOON, W.M.G.M., VERWOERD, M.E., WIJNKER, F.G., VAN LEEUWEN, C.J., VAN DUYN, P., VAN DE GUCHTE, C. AND HERMENS, J.L.M., 1997. Estimating total body residues and baseline toxicity of complex organic mixtures in effluents and surface waters. Environmental Toxicology and Chemistry, 16, 1358-1365 (as quoted in Barber, 2005a).

VEITH, G.D., DEFOE, D.L. AND BERGSTEDT, 1979. Measuring and estimating the bioconcentration factor of chemicals in fish. Journal of the Fisheries Resources Board of Canada, 36, 1040-1048.

VOUTSAS, E., MAGOULAS, K. AND TASSIOS, D., 2002. Prediction of the bioaccumulation of persistent organic pollutants in aquatic food webs. Chemosphere, 48, 645-651.

List of abbreviations

AWQC	Ambient water quality criteria
BAF	Bioaccumulation factor
BCF	Bioconcentration factor
BFAF	Biota-food accumulation factor
BMF	Biomagnification factor
BSAF	Biota-sediment accumulation factor
BTF	Biotransfer factor
bw	Bodyweight
CEFIC	European Chemical Industry Council
DDE	Dichlorodiphenyldichloroethylene
DDT	Dichlorodiphenyltrichloroethane
DOC	Dissolved organic carbon
ERL	Environmental risk limit
EQC	Environmental quality criteria
EQS	Environmental quality standard
EUSES	European Uniform System for Evaluation of Substances
HC_5	Fifth-percentile hazardous concentration
IEC	Internal effect concentration
Ifremer	French Research Institute for Exploitation of the Sea
IVM	Institute for Environmental Studies
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)
LC_{50} / EC_{50}	Concentration that is lethal to / causes adverse effects in 50 per cent of the exposed population
LOAEL	Lowest observe adverse effect level
LRI	Long-Range Research Initiative
MPC	Maximum permissible concentration
MW	Molecular weight
NC	Negligible concentration

NOAEL	No observed adverse effect level
NOEC	No observed effect concentration
PCB	Polychlorinated biphenyl
PEC	Predicted environmental concentration
POC	Particulate organic carbon
POPs	Persistent organic pollutants
PSU	Practical salinity units
QSAR	Quantitative structure-activity relationship
r^2	Correlation coefficient
SGV	Soil guideline value
SRC_{ECO}	Ecotoxicological serious risk concentration
TDI	Tolerable daily intake
TGD	Technical Guidance Document
TLM	Target lipid model
TRG	Tissue residue guideline
TSCF	Transpiration stream concentration factor
USEPA	United States Environmental Protection Agency
wet wt	Wet weight basis
WV	Wildlife criteria value

Glossary

Adapted from USEPA (2000).

Allometric	Relative growth of a part of an organism in relation to the growth of the whole.
Benthic	Referring to organisms living close to the bottom of an ocean, sea, lake and so on.
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 the 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 concentrations 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 the 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.
Epilimnion	The upper (warmer) layer of a stratified water body.
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 (such as lipid, organic carbon) compared with chemicals of lower hydrophobicity.
Hypolimnion	The lower (colder) layer of a stratified water body.
Lipid-normalized concentration	The total concentration of a contaminant in tissue or whole organism, divided by the lipid fraction in that tissue, organism or media.
Octanol-water partition coefficient	The ratio of the concentration of a substance in the n-octanol phase to its concentration in the aqueous phase in an equilibrated two-phase octanol-water system. The value is often expressed as a base 10 logarithm value (log K_{ow}).
Organic carbon-normalized concentration	For sediments, the total concentration of a contaminant in sediment divided by the fraction of organic carbon in the sediment.
Pelagic	Referring to organisms living near to the surface in oceans, lakes and so on.
Periphyton	Aquatic organisms which are attached to, or cling to, stems and leaves of rooted plants, rocks and so on.
Phytoplankton	Vegetable plankton.
Piscivorous	Fish-eating.
Planktivorous	Feeding on plankton.
Poikilothermal	Having a variable blood temperature – cold blooded.
Uptake	The acquisition by an organism of a substance from the environment as a result of any active or passive process.
Zooplankton	Animal plankton

Appendix A – Estuaries included in GEMCO

The following estuaries are included in the GEMCO model.

Aulne
Backwater
Barthe River
Boyne
Carlingford Lough
Clyde
Corrib
Cree
Dart
Dee (Dumfries & Galloway)
Dee (Grampian)
Dee (North Wirral)
Douro
Duddon
Ebro
Elbe
Ems
Erne
Exe
Fal
Firth of Forth
Firth of Tay
Flensborg Fjord
Fowey
Gironde
Guadalquiver
Guadiana
Helford
Humber
Inverness Firth
Jucar
Kolding Fjord
Lee
Liffey
Loch Crinan
Loch Gilp
Loire
Lune
Lupawa
Lyne
Mariager Fjord
Medway
Mersey
Minho
Mondego
Morecambe Bay
Moy
Neath
Nieuwe Waterweg
Nith
Odelouca
Odra
Ouse
Po
Randers Fjord
Rechnitz River
Rhone
Ria A Coruna
Ria de Camarinas
Ria de Murosy
Noya
Ria de Pontreveda
Ria de Vigo
Ribble
Sado
Salcombe and Kingsbridge
Schelde
Seine
Severn
Shannon River
Sligo
Somme
Southhampton Water
Spey Bay
Stour
Tamar
Tees
Teifi
Tejo
Thames
The Wash
Tiber
Tinto
Tyne
Tweed
Vejle Fjord
Warnow River
Weser
Wisla
Yealm

Appendix B – Example calculations

This appendix considers how the results from several of the more highly ranking models could be used in setting standards. Calculations were carried out using mainly the default settings of each model for a hypothetical chemical. The properties of the chemical are summarised in Table B1.

Table B1 Properties of the hypothetical chemical used in the calculations

Property	Value used
Molecular weight	361 g/mole
Melting point	103°C
Boiling point	400°C
Vapour pressure at 25°C	1.19×10^{-4} Pa
Water solubility at 25°C	0.001 mg/l
Log K_{ow}	6.9
K_{oc}	4.89×10^{5} l/kg
Henry's law constant at 25°C	43 Pa m^3/mole (dimensionless version (air-water partition coefficient) = 0.018)
(Bio)degradation rate constant	0 (assumed no degradation)
Metabolism rate constant	0 (assumed no metabolism in any organism)
Toxicological value for derivation of standards for human health	1 mg/kg food
Toxicological value for derivation of standards for wildlife	1 mg/kg food

The EU Technical Guidance Document methodology was used (via the EUSES 2.0 program) assuming an emission of the substance of 1 kg/day to waste water at a local site and 1 kg/day to waste water in the regional compartment. The resulting predicted concentrations and the derived whole compartment BAFs (estimated by dividing the concentration in the organism or plant by the relevant concentration in the exposure medium) are summarised in Table B2. The concentrations predicted are meaningless; they are merely used as a way of estimating the necessary BAFs.

Table B2 Examples of data that can be generated from the EU Technical Guidance Document methodology

Food chain	Predicted concentrations	Derived BAF	Comment
Water to top predators	Dissolved concentration in freshwater = 1.3×10^{-3} mg/l. Dissolved concentration in marine water for predatory fish = 1.44×10^{-3} mg/l. Dissolved concentration in marine water for top predatory marine fish = 2.88×10^{-4} mg/l. Concentration in predatory freshwater fish = 603 mg/kg wet wt. Concentration in predatory marine fish = 665 mg/kg wet wt. Concentration in top predatory marine fish = 1.33×10^{3} mg/kg wet wt.	4.6×10^{5} l/kg wet wt for predatory freshwater and marine fish. 4.6×10^{6} l/kg for top predatory marine fish.	For this calculation, the concentration in water is taken as being 50 per cent from local sources and 50 per cent from regional sources for freshwater and marine predatory fish, and 10 per cent from local sources and 90 per cent from regional sources for top predatory marine fish. BAFs can also be estimated directly from BCF (4.6×10^{4} l/kg) and default BMFs (10 for predatory freshwater and marine fish, and 10×10 for top predatory marine fish). The same calculations can be done using the total concentration in water
Soil to earthworm	Concentration in soil = 8.3 mg/kg wet wt. Concentration in earthworm 83.5 mg/kg wet wt.	10.1 kg/kg	For this calculation, the concentration in soil is taken as being 50 per cent from local agricultural soil and 50 per cent from regional natural soil.
Soil to root crops	Regional concentration in soil = 0.0138 mg/kg wet wt. Regional concentration in root crops = 0.0822 mg/kg wet wt.	5.96 kg/kg	
Soil and air to grass	Region concentration in soil = 0.0138 mg/kg wet wt. Regional concentration in air = 1.6×10^{-8} mg/m^3. Regional concentration in grass = 3.18 mg/kg wet wt.	For air BAF_{air} = $3.18\times0.991/1.6\times10^{-8}$ = 1.97×10^{8} m^3/kg. For soil BAF_{soil} = $3.18\times9.45\times10^{-3}/0.0138$ = 2.18 kg/kg.	The EUSES printout gives the fraction contribution to plants via soil (9.45×10^{-3}) and air (0.991). These can then be used to separate out the overall BAF for each route of exposure.
Soil and air to leaf crops	Region concentration in soil = 0.0138 mg/kg wet wt. Regional concentration in air = 1.6×10^{-8} mg/m^3. Regional concentration in leaf crops = 3.18 mg/kg wet wt.	For air BAF_{air} = $3.18\times0.991/1.6\times10^{-8}$ = 1.97×10^{8} m^3/kg. For soil BAF_{soil} = $3.18\times9.45\times10^{-3}/0.0138$ = 2.18 kg/kg.	
Soil, air, grass and drinking water to grass to cattle/meat	Regional concentration in soil = 0.0138 mg/kg wet wt. Regional concentration in air =1.6×10^{-8} mg/m^3. Regional concentration in grass = 3.18 mg/kg wet wt. Regional concentration in drinking water = 1.6×10^{-6} mg/l. Regional concentration in meat = 6.88×10^{-4} mg/kg wet wt	For air BAF_{air} = $6.88\times10^{-4}\times2.27\times10^{-4}/1.6\times10^{-8}$ = 0.098 m^3/kg. For soil ingestion BAF_{soil} = $6.88\times10^{-4}\times$ 0.742/0.0138 = 0.037 kg/kg. For grass consumption BAF_{grass} = $6.88\times10^{-4}\times$ $0.248/3.18 = 5.4\times10^{-5}$ kg/kg. For drinking water $BAF_{drink\ water}$ = $6.88\times10^{-4}\times$ $0.0102/1.6\times10^{-6}$ = 4.4 kg/l.	The EUSES printout gives the fraction contribution via intake of grass (0.248), drinking water (0.0102), air (2.27×10^{-4}) and ingestion of soil (0.742). These can be used to separate out the contributions from each source.
Soil, air, grass and drinking water to grass to milk	Regional concentration in soil = 0.0138 mg/kg wet wt. Regional concentration in air =1.6×10^{-8} mg/m^3. Regional concentration in grass = 3.18 mg/kg wet wt.	For air BAF_{air} = $2.18\times10^{-4}\times$ $2.27\times10^{-4}/1.6\times10^{-8}$ = 0.031 m^3/kg For soil ingestion BAF_{soil} = $2.18\times10^{-4}\times$	The EUSES printout gives the fraction contribution via intake of grass (0.248), drinking water (0.0102), air (2.27×10^{-4}) and ingestion of soil (0.742). These can be used to

Food chain	Predicted concentrations	Derived BAF	Comment
	Regional concentration in drinking water = 1.6×10^{-6} mg/l. Regional concentration in milk = 2.18×10^{-4}	0.742/0.0138 = 0.012 kg/kg. For grass consumption $BAF_{grass} = 2.18\times10^{-4}\times 0.248/3.18 = 1.7\times10^{-5}$ kg/kg. For drinking water $BAF_{drink\ water} = 2.18\times10^{-4}\times 0.0102/1.6\times10^{-6} = 1.39$ kg/l.	separate out the contributions from each source.

The second model run was the ACC-Human model. As this is time-dependent, the model was run for a ten-year period as an example, although steady state may have not been reached over this period in some receptors. Chemical-specific input data were those given in Table B1, with the addition of heats of phase transfers needed by the model which were each 300 J/mole.

Concentrations in air, sea water, freshwater and soil were all assumed to be at a constant concentration of 1×10^{-6} g/m^3 throughout the model run. However, as the model considers all routes of exposure together, the model was also run assuming a concentration of 1×10^{-6} g/m^3 in each environmental compartment in turn in order to investigate the contribution from each source of exposure. The results from the model and the derived ecosystem BAFs are summarised in Table B3.

Table B3 Examples of data that can be generated from the ACC-Human model

Food chain	Predicted concentrations	Derived BAF	Comment
Seawater to fish	Concentration in seawater 1×10^{-3} mg/m^3 = 1×10^{-6} mg/l. Concentration in cod (aged 10 at start of simulation) = 1.66×10^{5} ng/g lipid = 166 mg/kg lipid. Concentration in herring (age 10 at start of simulation) = 5.33×10^{4} ng/g lipid = 53.3 mg/kg lipid.	1.67×10^{8} l/kg lipid for cod and 5.3×10^{7} l/kg lipid for herring	Data for fish of other ages are also generated.
Seawater to zooplankton	Concentration in seawater = 1×10^{-3} mg/m^3 = 1×10^{-6} mg/l. Concentration in zooplankton = 8.73×10^{4} ng/g lipid = 87.3 mg/kg lipid.	8.7×10^{7} l/kg lipid	
Seawater to seafood to human female	Concentration in seawater = 1×10^{-3} mg/m^3 = 1×10^{-6} mg/l. Concentration in human female (age 0-10 years) = 1.29×10^{4} ng/g lipid = 12.9 mg/kg lipid.	1.29×10^{7} l/kg lipid	Data are available for other human age ranges.
Seawater to seafood to human male	Concentration in seawater = 1×10^{-3} mg/m^3 = 1×10^{-6} mg/l. Concentration in human male (age 0-10 years) = 1.52×10^{4} ng/g lipid = 15.2 mg/kg lipid.	1.52×10^{7} l/kg lipid	Data available for other human age ranges.
Air to cattle feed	Concentration in air = 1×10^{-3} mg/m^3. Concentration in feed = 4.18×10^{5} pg/g fresh weight = 0.42 mg/kg fresh weight.	418 m^3/kg fresh weight	
Air to milk	Concentration in air = 1×10^{-3} mg/m^3. Concentration in milk = 2.01×10^{7} pg/g lipid = 20.1 mg/kg lipid.	2.01×10^{4} m^3/kg lipid	
Air to milk cow	Concentration in air = 1×10^{-3} mg/m^3. Concentration in milk cow = 2.01×10^{7} pg/g lipid = 20.1 mg/kg lipid.	2.01×10^{4} m^3/kg lipid	
Air to beef cattle (1-2 year old)	Concentration in air = 1×10^{-3} mg/m^3. Concentration in cattle = 2.92×10^{7} pg/g lipid = 29.2 mg/kg lipid.	2.92×10^{4} m^3/kg lipid	Data are also generated for 1-2 year old cattle.
Air to beef	Concentration in air = 1×10^{-3} mg/m^3.	5.38×10^{4} m^3/kg lipid	

Food chain	Predicted concentrations	Derived BAF	Comment
	Concentration in beef = 5.38×10^{7} pg/g lipid = 53.8 mg/kg lipid.		
Air to human female	Concentration in air = 1×10^{-3} mg/m^3. Concentration in human female (age 0-10 years) = 1.42×10^{5} ng/g lipid = 142 mg/kg lipid. Concentration in human female (age 20-30 years) = 9.07×10^{4} ng/g lipid = 90.7 mg/kg lipid.	1.42×10^{5} m^3/kg lipid for 0-10 year old. 9.07×10^{4} m^3/kg lipid for 20-30 year old.	Data for other age ranges are generated.
Air to human male	Concentration in air = 1×10^{-3} mg/m^3. Concentration in human male (age 0-10 years) = 1.65×10^{5} ng/g lipid = 165 mg/kg lipid.	1.65×10^{5} m^3/kg lipid	
Freshwater (drinking water) to milk	Concentration in freshwater = 1×10^{-6} g/m^3 = 1×10^{-3} mg/l. Concentration in milk = 39.3 pg/g lipid = 3.93×10^{-5} mg/kg lipid.	0.039 l/kg lipid	
Freshwater (drinking water) to milk cow	Concentration in freshwater = 1×10^{-6} g/m^3 = 1×10^{-3} mg/l. Concentration in milk cow = 39.3 pg/g lipid = 3.93×10^{-5} mg/kg lipid.	0.039 l/kg lipid	
Freshwater (drinking water) to beef cattle (0-1 year old)	Concentration in freshwater = 1×10^{-6} g/m^3 = 1×10^{-3} mg/l. Concentration in cattle = 39.4 pg/g lipid = 3.94×10^{-5} mg/kg lipid.	0.039 l/kg lipid	Data are also available for 1-2 year old cattle.
Freshwater (drinking water) to beef	Concentration in freshwater = 1×10^{-6} g/m^3 = 1×10^{-3} mg/l. Concentration in beef = 96.1 pg/g lipid = 9.61×10^{-5} mg/kg lipid.	0.096 l/kg lipid	
Freshwater (drinking water) to human female	Concentration in freshwater = 1×10^{-6} g/m^3 = 1×10^{-3} mg/l. Concentration in human female (0-10 year old) = 0.838 ng/g lipid = 8.38×10^{-4} mg/kg lipid.	0.838 l/kg lipid	Data are also available for other age ranges.
Freshwater (drinking water) to human male	Concentration in freshwater = 1×10^{-6} g/m^3 = 1×10^{-3} mg/l. Concentration in human male (0-10 year old) = 0.845 ng/g lipid = 8.45×10^{-4} mg/kg lipid.	0.845 l/kg lipid	Data are also available for other age ranges.
Soil to cattle feed	Concentration in soil = 1×10^{-6} g/m^3 = 1×10^{-3} mg/m^3. Assuming a soil bulk density of 1,700 kg/m^3 for wet soil, this is equivalent to a concentration of 5.9×10^{-7} mg/kg wet wt. Concentration in feed = 7.04×10^{-10} pg/g fresh wt = 7.04×10^{-16} mg/kg fresh wt.	1.2×10^{-9} kg/kg	
Soil to milk	Concentration in soil = 1×10^{-3} mg/m^3= 5.9×10^{-7} mg/kg wet wt. Concentration in milk = 3.37×10^{-8} pg/g lipid = 3.37×10^{-14} mg/kg lipid.	5.7×10^{-8} kg wet wt/kg lipid	
Soil to milk cow	Concentration in soil = 1×10^{-3} mg/m^3= 5.9×10^{-7} mg/kg wet wt. Concentration in milk cow = 3.37×10^{-8} pg/g lipid = 3.37×10^{-14} mg/kg lipid.	5.7×10^{-8} kg wet wt/kg lipid	
Soil to beef cattle (0-1 year old)	Concentration in soil = 1×10^{-3} mg/m^3= 5.9×10^{-7} mg/kg wet wt. Concentration in beef cattle = 4.86×10^{-8} pg/g lipid = 4.86×10^{-14} mg/kg lipid.	8.2×10^{-8} kg wet wt/kg lipid	Data are also available for 1-2 year old cattle.
Soil to beef	Concentration in soil = 1×10^{-3} mg/m^3= 5.9×10^{-7} mg/kg wet wt. Concentration in beef = 8.99×10^{-8} pg/g lipid = 8.99×10^{-14} mg/kg lipid.	1.5×10^{-7}	
Soil to human female	Concentration in soil = 1×10^{-3} mg/m^3= 5.9×10^{-7} mg/kg wet wt. Concentration in human female (0-10 years old) = 2.34×10^{-10} ng/g lipid = 2.3×10^{-13} mg/kg lipid.	4.0×10^{-7} kg wet wt/kg lipid	Data are also available for other age ranges.

Food chain	Predicted concentrations	Derived BAF	Comment
Soil to human male	Concentration in soil = 1×10^{-3} mg/m^3= 5.9×10^{-7} mg/kg wet wt. Concentration in human male (0-10 years old) = 2.73×10^{-10} ng/g lipid = 2.7×10^{-13} mg/kg lipid.	4.6×10^{-7} kg wet wt/kg lipid	Data are also available for other age ranges.

The Prediction of Bioaccumulation in Aquatic Food Webs method gives the following BAFs (based on the freely dissolved concentration in water and a fresh or wet weight concentration in the organisms) for a substance with a log K_{ow} of 6.9.

- Trophic level 1 (phytoplankton/zooplankton) BAF = 5.5×10^7 l/kg
- Trophic level 2 (benthic invertebrates) BAF = 7.6×10^7 l/kg
- Trophic level 3 (planktivorous fish) BAF = 1.3×10^8 l/kg
- Trophic level 4 (piscivorous fish) BAF = 3.3×10^8 l/kg

The final model used in this test was the Food Chain Bioaccumulation model version 1.1. This model was run using its default food chain and physico-chemical properties from Table B1. A concentration in water of 1×10^{-6} g/l was used. This model gives BAFs and BSAFs (on a wet weight basis and a lipid weight basis), BCF and the BMF directly. These are summarised below. BAFs relate to the dissolved concentration of the chemical in water.

Organism	**BAF_{lipid} (kg/kg lipid)**	**BAF_{fresh} (l/kg wet wt)**	**$BSAF_{lipid}$ (kg/kg lipid)**	**BSAF (kg/kg)**	**BCF (l/kg)**	**BMF (kg/kg)**
Phytoplankton	7.94×10^6	3.97×10^5				
Mysids	7.94×10^6	2.38×10^5				
Pontoporeia	2.86×10^6	8.58×10^4	4.44×10^3	6.65×10^3		
Oligochaetes	2.86×10^6	2.86×10^4	4.44×10^3	2.22×10^3		
Sculpins	1.05×10^7	8.42×10^5	8.16×10^5	6.53×10^4	1.5×10^5	6.09
Alewife	1.72×10^7	1.21×10^6	1.33×10^6	9.36×10^4	9.98×10^4	6.25
Smelt	2.80×10^7	2.24×10^6	2.17×10^6	1.74×10^5	6.17×10^4	6.11
Lake trout	7.20×10^7	1.25×10^7	5.58×10^6	9.72×10^5	4.27×10^4	7.88
Rainbow trout	7.82×10^7	1.02×10^7	6.06×10^6	7.88×10^5	3.19×10^4	6.40

Appendix C – Scoring criteria

This scoring system was developed as part of R&D project P6-020/6, *Consideration of persistence and bioaccumulation of substances in environmental standards*. The scoring system was used in this report to rank the models reviewed in terms of their suitability for deriving standards in water, sediment or soil protective of top predators and humans (aquatic environment only). A draft scoring system was circulated to the project board and peer reviewers (RIVM) in November 2004 and this revised version takes into account the comments received.

The scoring system takes into account the following aspects: model validity and quality, data requirements; ease of use; transparency; uncertainty; ability to predict the concentration near the top of the food chain; and model relevance to England and Wales.

For each criterion, the scoring scheme considers two parts. Firstly, a single number is proposed reflecting the importance of the aspect in question to the usability of the model for the project. This is deemed the 'importance rating' and is given a number between one (low importance) and five (high importance).

The second number defines three sub-groups or scoring groups for each aspect considered. A 'score' of one, two or three is given to each of these groups. The higher the score, the better the model meets the requirements of the project in terms of that criterion. For example, a model that has been extensively validated and gives reliable predictions would attract a higher score than a model that has been shown to have relatively poor predictive power.

This then allows a 'score' to be calculated for each criterion as follows:

$$SCORE_{CRITERION} = \text{IMPORTANCE RATING} \times \text{SCORE}$$

The 'total score' for each model can then be determined as follows:

$$\text{TOTAL SCORE} = SCORE_{DATA} + SCORE_{CALIBRATION} + SCORE_{VALIDATION} + SCORE_{EASE} + SCORE_{TRANS} + SCORE_{UNCERT} + SCORE_{TOP\ FOOD} + SCORE_{RELEVANCE}$$

The 'total score' can be used to rank each model in terms of its overall performance against the criteria. This ranking can be used to inform the final choice of model(s) that have potential for use in setting standards. However, expert judgement will also play an important role in the final selection.

The criteria considered are discussed below.

Data requirements

This is a key aspect with regards to the overall usefulness of a model. For the majority of chemicals only a limited dataset is available, but model users may be reluctant to carry out extensive additional testing to generate the necessary data, both on cost and animal welfare grounds. As a consequence, models that use a small amount of easily available or predictable data (such as log K_{ow} , water solubility, vapour pressure, fish bioconcentration factor) should

score more highly than those requiring large amounts of data derived from animal testing (such as uptake and metabolism rates).

However, the predictive power of models that require greater amounts of data may be higher than those based solely on relatively simple chemical properties. Ideally, if animal testing data (such as measured accumulation factors, metabolism rates, assimilation efficiencies) are available for a given substance, these should be used where possible in the model.

Balancing these two somewhat opposite needs, the scoring scheme proposed below gives the highest scores to models that require a limited input dataset, but can also take into account more complex data if available.

The following values for the scoring system are proposed for the data requirements criterion.

IMPORTANCE RATING 5

	SCORE
The model can be used with relatively simple physico-chemical properties that are usually readily available (or can be easily estimated), but more complex data can also be used if available.	3
The model requires only relatively simple physico-chemical properties that are usually readily available (or can be easily estimated).	2
The model requires data that are not routinely available for a wide range of chemicals.	1

Model calibration

One of the consequences of using a model that requires relatively little chemical-specific input data is that many of the chemical-related parameters used by the model will be estimated for the chemical in question. For example, the log K_{ow} value is often used as a surrogate to predict the adsorption properties of substances to sediment and soil, and to estimate bioaccumulation properties in the food chain. However, surrogate values may only be valid over a narrow range or for certain chemical types. Thus the reliability, and general applicability, of the modelling results depend to some extent on the accuracy of the underlying estimation methods.

Model calibration refers to the test dataset used in the development of the model. Information on the model's calibration can give insights into its quality, the scatter around its predictions (which is also related to uncertainty) and the domain of applicability.

Although this is an important criterion it is quite difficult to score, as the score will depend on the type of chemical being modelled; for example, if the underlying methods are valid for the chemical being considered, this will score differently than if the chemical's properties are outside the calibration range. For the proposed scores below, it is assumed that models which incorporate methods more applicable over a wide range of chemical types and properties should score more highly than those applicable to limited types of chemicals or ranges of properties.

However, models that have not yet been calibrated are not necessarily of poor quality; it may simply mean that the calibration details are not available. Therefore, although well-calibrated models will receive a high score, the scoring proposed ensures that uncalibrated models will not necessarily attract an overall low score in the scheme.

It is difficult to be prescriptive over the scoring here, and a degree of expert judgement is needed.

IMPORTANCE RATING 5

	SCORE
The model calibration is detailed and shows a relatively low scatter around model predictions; the domain of applicability is well-described and covers a wide range of chemical types.	3
The model calibration is detailed but the scatter and/or domain of applicability is not quantified or covers a defined range of chemical types. This score also applies in cases where no calibration has been carried out (see text above).	2
The model calibration is detailed but shows a relatively high scatter around model predictions, or the domain of applicability is limited to a specific type of chemical or not given. These models will be flagged as the results will be of limited predictive value.	1

Model validation

Validation also plays a part in overall model quality. It is difficult, however, to score since validation datasets are often scarce, and very often validation is only done in a qualitative way. Furthermore, models that have not yet been validated are not necessarily of poor quality; it may simply mean that the validation details are not available. Therefore, although well-validated models will receive a high score, the scoring proposed ensures that non-validated ones will not necessarily attract an overall low score in the scheme.

It is difficult to be prescriptive over the scoring here, and a degree of expert judgement is needed.

IMPORTANCE RATING 5

	SCORE
The model validation is demonstrated, quantified and satisfactory (for example, the scatter around predictions is about equal to that around the calibration data)	**3**
The model validation is demonstrated and satisfactory, but has been judged in a qualitative way. This score also applies in cases where no validation has been carried out (see text above).	**2**
The validation is demonstrated but the model gives inadequate predictions. These models will be flagged as they will have limited predictive power.	**1**

Ease of use

Ease of use is an important criterion when considering the overall usability of a model. Models that are user friendly and should be relatively easy to use by Environment Agency staff with some technical knowledge (such as experience of chemical risk assessment) will score more highly than those that are difficult to use. Again, the proposed scoring is somewhat subjective.

IMPORTANCE RATING 2

	SCORE
The model is available in a user-friendly format (for example, simple model, simple spreadsheet or simple equations).	3
The model is available in a format that requires some experience/knowledge to use (for example, a series of equations).	2
The model is available as an expert system that requires considerable experience to use.	1

Transparency

How transparent the model needs to be depends to some extent on the end use. For example, if the model is used without modification, there is no real need for it to be transparent as long as the underlying assumptions are understood. However, for this project it is assumed that some modifications (for example, to take account of different environmental properties and food chains) may need to be made for various end applications. Therefore, models where the calculations are transparent and can be easily modified will score more highly than models where the calculation methods are unclear and cannot be easily altered.

IMPORTANCE RATING 5

	SCORE
All of the underlying methods used in the model are clear.	3
The most important underlying methods used in the model are clear.	2
The underlying methods used in the model are not apparent.	1

Prediction uncertainty

In this review, an assessment will be made of the likely uncertainty in model predictions resulting from assumptions inherent in the model itself. This will take into account, in particular, any conservative or precautionary approaches (for example, neglecting metabolism as a removal process), and any validation studies that are apparent. For most models, it may only be possible to address the uncertainty in a qualitative way, based on our knowledge and experience.

This criterion is closely related to the model calibration and validation criteria, as models that are conservative or precautionary may have been designed to avoid “false positives” owing to the uncertainties in the underlying methods. Therefore, judgement of the trade-off between uncertainty and precautionary approaches partly depends on the insight gained through model calibration and validation studies.

IMPORTANCE RATING 5

	SCORE
Based on expert judgement, the model has low uncertainty and/or does not rely on conservative or precautionary approaches.	3
Based on expert judgement, the model has moderate uncertainty and/or relies to some extent on conservative or precautionary approaches.	2
Based on expert judgement, the model has high uncertainty and/or relies to a large extent on conservative or precautionary approaches.	1

Ability to predict the concentration near the top of the food chain

This is an important consideration for human exposure models, as one of their possible uses is to allow the Food Standards Agency to assess the potential impact on human consumers and compare with maximum permissible levels of chemicals in animals or plants used as foods; in this context, “near the top of the food chain” will be animals and plants that form part of the human diet. This criterion is also important for setting standards for organisms, in that substances with a high bioaccumulation potential will be expected to accumulate at the top of the food chain and so lead to exposure of higher organisms such as birds or predatory mammals. In this respect, models that allow concentrations (or accumulation factors) to be predicted at many different trophic levels, including organisms near the top of the food chain, will score more highly than models that generate predictions for only a few, generally lower, trophic levels. However, for some bioaccumulative substances that are biotransformed by, for example vertebrates, the highest concentrations in the food chain may occur at lower trophic levels.

Given the importance of this criterion to the Food Standards Agency, it is given a relatively high importance rating in the proposed scheme.

IMPORTANCE RATING 4

	SCORE
The model allows predictions of concentrations (or accumulation factors) in more than two trophic levels, including those near the bottom and top of the food chain.	3
The model allows predictions of concentrations (or accumulation factors) in two or fewer trophic levels near the top of the food chain.	2
The model allows predictions of concentrations (or accumulation factors) in trophic levels near the bottom of the food chain only.	1

Relevance to England and Wales

As the intention is that the model(s) will eventually be used for setting standards within England and Wales, it is important to consider whether the models are relevant to the situation in England and Wales, or could be adapted to these situations.

IMPORTANCE RATING 4

	SCORE
The model is applicable to the situation in England and Wales.	3
The model is not applicable to the situation in England and Wales but could be easily adapted.	2
The model is not applicable to the situation in England and Wales and would be difficult to adapt.	1

Summary

The scheme outlined above can be used for scoring the models reviewed in this project against a standard set of criteria. These scores can then be used to generate a ranking (or groupings) of the models in terms of their predictive ability for subsequent use by the Environment Agency, and other authorities, in the setting of standards. The diverse nature of the available models means that by necessity, scoring against many of the criteria will be subjective, but the scoring will be based on the findings obtained in the critical review.

Using this proposed system, the minimum and maximum total scores are 35 and 105

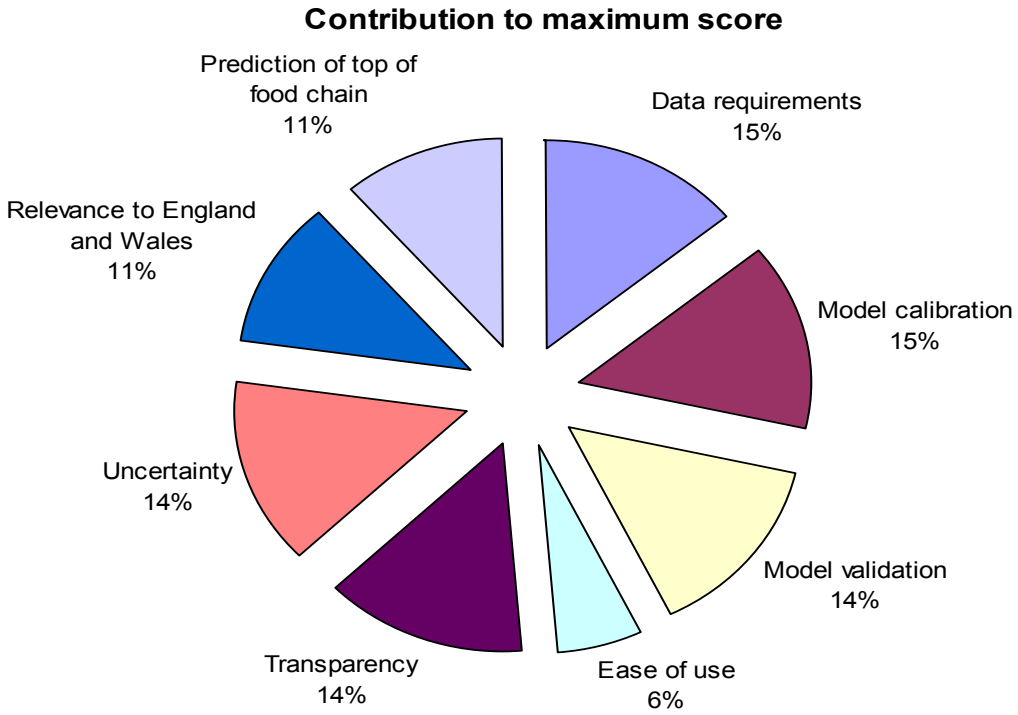


Figure C.1.: Contribution to overall score of each criterion

Appendix D – Initial review of bioaccumulation models

Introduction

This project forms part of a broader programme of work to support the Environment Agency in developing chemical standards for the protection of the environment and human health (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 role in pollution control. This project will help to provide a sound scientific basis and a transparent and consistent approach to setting standards across different functions within the Environment Agency.

Bioaccumulative substances are of concern as they have the potential to biomagnify through the food chain and affect organisms at higher trophic levels. Bioaccumulation is of particular concern when the substance is toxic and 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 account for the possibility of 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 which bioaccumulate, direct exposure via 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 future EU meetings to agree environmental quality standards for pollutants and priority substances detailed in Annexes VIII to X to the Water Framework Directive (Directive 2000/60/EC).

When setting soil standards, the Environment Agency needs to consider indirect exposure routes for organisms at the top of the terrestrial food chain. The method for considering bioaccumulation and persistence when deriving soil standards will feed into the tiered terrestrial ecological risk assessment (ERA) framework that is being developed by the Environment Agency and Defra (currently undergoing public consultation). Once finalised, this framework will be used in Part IIA of the Environmental Protection Act 1990 to assess the impacts of soil contamination on top wildlife predators; 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 as a result of some types of soil contamination are already available in the CLEA approach (Environment Agency, 2002); however, equivalent methods for determining exposure to chemicals from other routes, such as the aquatic food chain, are not generally available.

This review was commissioned by the Environment Agency to identify models suitable for taking into account the bioaccumulation of organic chemicals when setting environmental standards. This report summarises the available methods and models that could theoretically be used to

estimate or predict the bioaccumulation of a chemical through food chains. A critical review of the selected methods for their suitability in setting standards will be carried out in a future report.

A draft version of this review was prepared in October 2004 and circulated to the project board and peer reviewers (the National Institute for Public Health and the Environment (RIVM) in the Netherlands) for comment. This final version has been revised to take account of the comments received.

Approach

Types of models that could be used in standard setting

Up until recently, standards set for air, water, sediment and soil have generally been based on the potential for effects on organisms directly exposed in the media in question. However, such standards may not necessarily be protective of species (such as top predators) that consume these organisms, particularly for bioaccumulative substances. In order to take this scenario into account, it is necessary to consider bioaccumulation through the food chain when setting standards. A generalized scheme for this is shown below, which involves back-calculating from a dietary exposure concentration considered to present a low risk to a given top predator, to an equivalent concentration in the exposure medium in question (air, water, sediment or soil) that would be expected to lead to the same concentration in the top predator's food, assuming that bioaccumulation through the food chain occurs.

$$SC = \frac{NOEC_{predator}}{BAF_{prey}}$$

where SC = standard concentration for the environmental compartment being considered.

$NOEC_{predator}$ = estimated no effect concentration in diet for the top predator under consideration. This could be wildlife or humans.

BAF_{prey} = bioaccumulation factor for the prey organism, related to the concentration in water, sediment and soil. This could include one or more further steps in the food chain.

Approaches similar to this (in general terms) have been developed in the United States (such as USEPA, 1995a and 2000; Federal Register, 1995) and the Netherlands (Romijn *et al.*, 1993 and 1994; Traas *et al*., 1996 and 2001a; Jongbloed *et al.*, 1994 and 1996) that could be applied to aquatic and terrestrial food chains.

There are two key considerations in this generalized approach. Firstly, the food chains or exposure routes (and hence top predators) that can be considered are limited to a large extent by the availability of experimental data, or by models that allow the bioaccumulation of a chemical through a given food chain or exposure route to be estimated. Secondly, the top predators that can be considered are limited by the availability of experimental toxicity data, or by methods to extrapolate toxicity data from laboratory animals to wildlife.

Any model able to predict a bioaccumulation factor (for an individual organism or the whole food chain) could be used directly in the approach. In addition, any model relating a concentration in a given medium to a concentration in prey (or food) could also be used, as it would then be possible to estimate the bioaccumulation factor from the results. These criteria were used as a basis for identifying the types of models to include in this review.

Extrapolation of toxicity data from laboratory animals to wildlife requires suitable conversion factors to account for the feeding habits of the wildlife, in order to interconvert laboratory toxicity data for example, from daily intake rate (in mg/kg body weight/day) to an equivalent dosage concentration in diet (in mg/kg diet). Methods for carrying out such extrapolations are given in the TGD, Traas *et al.* (1996) and Jongbloed *et al.* (1994 and 1996) for birds and mammals; a comprehensive framework for a range of avian, mammalian, reptilian and amphibian species is given in Canadian Council of Ministers of the Environment (1999)[22].

Methods for determining human exposure to chemicals as a result of soil contamination are already available in the CLEA approach (Environment Agency and Defra, 2002). This approach estimates child and adult exposures to soil contaminants for those potentially living, working and/or playing on contaminated sites over extended timeframes, and is used in the setting of soil guideline values for the protection of these populations within the United Kingdom. The routes of exposure considered in the CLEA model include the ingestion of contaminated soil and produce (crops), inhalation of contaminated dust and vapour and absorption of the contaminant through the skin. Other models that cover primarily these routes of exposure, such as CalTOX[23] and CSOIL[24], have not been considered further as part of this project.

Information sources

Suitable models on the bioaccumulation or uptake of organic chemicals in food chains for review were located using the following methods.

- literature searches
- internet searches
- consultation with experts
- peer review.

Searching for information on bioaccumulation is problematic, in that there is a vast literature available on the subject, the majority of which would not be directly relevant to this project. Furthermore, as wide a range as possible of food chains (aquatic, sediment, terrestrial) was considered in the initial review. Searching of extensive databases such as the Chemical Abstracts Registry was therefore not practical for cost reasons, so searches of the literature were undertaken using the more limited SCIRUS and PUBMED databases. Searches were carried out for general accumulation models and also using author names from known models.

In order to complement the literature trawl, a search of the internet was also undertaken. This located a number of useful websites with information on environmental modelling, including:

[22] The TGD method differs fundamentally from the method used in Canadian Council of Ministers of the Environment (1999) and Traas *et al.* (1996) in that it assumes that the predicted or estimated no effect dosage in diet derived from laboratory animals is the same for all wildlife irrespective of their weight and feeding rates. The Canadian Council of Ministers of the Environment (1999) and Traas *et al*. (1996) methods essentially assume that the total exposure (in terms of mg/kg bodyweight/day) of the organism should be the same for all wildlife and hence the equivalent dosage in diet varies for different species of wildlife (being dependent on both body weight and daily feeding rate).

[23] CalTOX is a human exposure model for hazardous waste sites in the United States. Details are available at http://www.dtsc.ca.gov/ScienceTechnology/caltox.html.

[24] See Model reference number 14.

- The GAIA Modelbase (http://www.ess.co.at/GAIA/models.html).
- The USEPA Exposure Assessment Models website (http://www.epa.gov/ceampubl/index.htm).
- The Canadian Environmental Modelling website (http://www.trentu.ca/cemc/welcome.html).
- The Simon Fraser University modelling website (http://www.rem.sfu.ca/toxicology/models.htm).
- The Register of Ecological Models (http://www.gsf.de/UFIS/ufis/modelhom.html and http://www.wiz.uni-kassel.de/ecobas.html).
- The OECD Database on Chemical Risk Assessment Models website (http://webdomino1.oecd.org/comnet/env/models.nsf)

Along with the searches, a consultation exercise was carried out with experts in bioaccumulation models. A list of people contacted is given in Appendix D1 to this report. The intention of the consultation exercise was to identify any further models that should be considered in the review and any new models in development.

The sheer number of papers published on the bioaccumulation of chemicals means that it is difficult to be fully comprehensive in a general review of models of this type. However, the approach taken above to select suitable models should mean that at least the major models (or groups of models) available are included in the review.

Model reviews

For each of the models or methods located in the search, a preliminary review was undertaken. The objective of this initial review was to identify around ten to fifteen models showing the most promise for use in setting standards. These models would then be subject to a more detailed review at a later stage of this project.

The initial review considered the availability and form of the model (such as published paper, spreadsheet, computer program), the food chain modelled, the main types of chemicals considered in the model, the environment to which it related (a generic environment or a specific location), the data requirements of the model, its intended purpose (in particular if it were used for any regulatory purpose), and a brief assessment of the model. From these, a recommendation as to whether the model should be considered in the subsequent in-depth review was made.

Given the large numbers of models considered, the aim of this initial appraisal was not to review comprehensively the methods and data requirements, but rather to present an overall view of the main parts of the model. Thus, although brief descriptions of the data requirements and so on are given for each model, exact data requirements and details of other aspects will only become apparent in the subsequent in-depth review.

Findings

Models identified

The models reviewed in this project are summarised in Appendix D2. A total of 100 models, methods or relevant papers were identified. At this stage, the intention was to include rather than exclude, and as a result the majority of these were considered to be suitable for inclusion in the subsequent in-depth review. Where models were not considered suitable, the reasons are indicated in the individual reviews. In order to reduce the models and methods down to a more manageable number, models of a similar type (usually models by the same research groups but in some cases, models by other teams with similar features or underlying methods) were grouped together. The result of this grouping is shown in Table D1, with 23 groups of models. In addition to the models themselves, three main frameworks for incorporation of bioaccumulation into standards were identified. These are also summarised in Table D1.

For each group, a recommended example model is given for further consideration. This example either represents the most recent development of a model, or the most widely used version of a group of models. It is proposed that the in-depth review focuses on this example model, but draws on related models where relevant. The intention in the next stage of this project is to carry out an in-depth review of ten to fifteen of the models identified at this stage.

In addition to the plant models identified in this review, some pesticide leaching models (such as PESTLA[25]) contain routines for estimating uptake from soil by plants. However, as the overall focus of these models is the leaching (and degradation behaviour) of the substance in soils rather than accumulation in biota, they have not been considered further.

Table D1 Main groups of models identified

Main model/groups	Main food chain considered	Related or similar models
RIVER/FISH bioaccumulation model - Model reference number 1	Aquatic	
ACC-Human- Model reference number 2	Terrestrial Human	Model reference number 38 and 39
System dynamic model - Model reference number 8	Aquatic Terrestrial	Model reference number 59
Foodweb model - Model reference number 11	Aquatic	Model reference number 10, 20, 22 and 92
BASS/FGETS - Model reference number 19	Aquatic	
ECOFATE and Food Chain Bioaccumulation model - Model reference number 21	Aquatic	Model reference number 3 and 41
Arctic Terrestrial Food-chain Bioaccumulation model - Model reference number 29	Terrestrial	Model reference number 23 and 90
Dab food web model - Model reference number 31	Aquatic (marine)	Model reference number 32
Sediment-oligochaetes model - Model reference number 35	Aquatic	
Physiologically based toxicokinetic model for fish - Model reference number 47	Aquatic	Model reference number 30, 43, 44, 45, 46 and 81

[25] Information on the PESTLA model is given at http://eco.wiz.uni-kassel.de/model_db/mdb/pestla.html. The PESTLA model has now been superseded by the PEARL model (http://www.alterra-research.nl/pls/portal30/docs/folder/pearl/pearl/home.htm).

Main model/groups	Main food chain considered	Related or similar models
Plant model - Model reference number 51	Terrestrial Human	Model reference number 7, 9, 25, 26, 42, 49, 50 and 58
Technical Guidance Document - Model reference number 60	Aquatic Terrestrial Human	Model reference number 5, 6, 16, 17, 25, 27, 28, 52, 54 and 72
TOXFATE - Model reference number 65	Aquatic	
Plant uptake and transport model - Model reference number 69	Terrestrial	Model reference number 52, 58, 67, 68, 71, 87 and 88
Prediction of bioaccumulation in aquatic food webs - Model reference number 75	Aquatic	
QEAFDCHN – Model reference number 79	Aquatic	Model reference number 61, 62, 63, 78, 95 and 96
GEMCO - Model reference number 83	Aquatic (marine)	
Earthworm model - Model reference number 84	Terrestrial	Model reference number 27 and 28
RAMAS - Model reference number 85	Aquatic	
Terrestrial food chain model - Model reference number 89	Terrestrial Human	
ARAMS - Model reference number 91	Aquatic Terrestrial Human	
AQUATOX - Model reference number 93	Aquatic	
TRIM.FaTE - Model reference number 94	Aquatic Terrestrial Human	
Frameworks		
The Netherlands		Model reference number 18, 66 and 80 (the work of Traas *et al.* (1996) and Jongbloed *et al.* (1994 and 1996) is also relevant).
United States		Model reference number 73
Canada		Model reference number 97

Discussion

This review identified a range of models that could potentially be used to take account of bioaccumulation when setting standards. The models and methods range from simple regression equations that allow bioaccumulation factors to be estimated from physico-chemical properties, to complex multimedia models.

Of the more complex models, examples of both steady-state (fugacity) and time-dependent (kinetic) models were found. Kinetic models have the advantage that they can estimate time-dependent accumulation, which may be important when considering a one-off release to the environment rather than a continuous input. Mackay and Fraser (2000) showed that at steady state, kinetic and fugacity models are equivalent.

The most common food chain/web models unearthed by the review include fish food chains and plant food chains. Fewer models were found for terrestrial invertebrates and mammals.

Aquatic models

Of the available aquatic food chain models, it is recommended that a selection of the more developed models is taken forward for the in-depth review. The following are considered to be a representative selection covering the main model types, underlying assumptions, and complexities.

- Foodweb model - Model reference number 11
- BASS/FGETS - Model reference number 19
- ECOFATE and Food Chain Bioaccumulation - Model reference number 21
- Prediction of Bioaccumulation in Aquatic Food Webs - Model reference number 75
- QEAFDCHN - Model reference number 79
- GEMCO - Model reference number 83
- ARAMS - Model reference number 91
- AQUATOX - Model reference number 93
- TRIM.FaTE - Model reference number 94

Of the models given in Table D1 that are not proposed to be included in the in-depth review, the RIVER/FISH bioaccumulation model (Model reference number 1), the system dynamic model (Model reference number 8)[26], the dab food web model (Model reference number 31) and the TOXFATE model (Model reference number 65) all share similarities with one or more of the above models/methods chosen for review. The sediment-oligochaetes model (Model reference number 35) and the physiologically based toxicokinetic model for fish (Model reference number 47) both consider only a smaller part of the total food chains considered in the above models chosen for review. The RAMAS model (Model reference number 8) was originally included in the list of

[26] The project board highlighted this model as being of interest as it is used in the Draft Guidance Document on Risk Assessment for Birds and Mammals under Council Directive 91/414/EEC. Therefore, following the comments from the project board, this model will also be considered in the in-depth review. However, few details of the model are currently available and so the review may be limited in scope unless further details can be obtained.

models selected for in-depth review but, following comments from the peer review process, it became apparent that the accumulation parts of the model are poorly described and relatively simplistic. Therefore, it was decided that this model should not be taken forward.

Mackay and Fraser (2000) reviewed the available mechanisms and models for predicting bioaccumulation of persistent organic chemicals in fish and suggested the following tiered approach to assessing bioaccumulation:

- Tier 1. Prediction of the bioconcentration factor, using an empirical correlation relating bioconcentration factor to the octanol-water partition coefficient.
- Tier 2. Prediction of the bioaccumulation factor using a mechanistic mass balance model at steady state, such as the Gobas (1993) model (ECOFATE and Food Chain Bioaccumulation model; Model reference number 21) , in which the relevant uptake and loss processes are quantified. Such models can provide information on the relative importance of uptake via gills and food, and loss by egestion and metabolism.
- Tier 3. Prediction of the potential for biomagnification using a model of a food chain, similar to that described by Gobas (1993) (Model reference number 21) and Campfens and Mackay (1997) (Model reference number 11), but involving fish, birds and mammals.

As well as Gobas (1993) and Campfens and Mackay (1997), a number of the other models identified above could potentially be used in such a scheme.

A comparison of two steady-state aquatic food web models was carried out by Burkhard (1998). The models compared were those of Gobas (1993) (Model reference number 21) and Thomann *et al.* (1992) (Model reference number 63). No significant differences were found in the predictions obtained for substances with log K_{ow}s up to around 6.5-6.9, after which the results from the two models diverged (particularly for substances with log K_{ow} values greater than eight). Bioaccumulation factors predicted by the Gobas (1993) model were found to be in slightly better agreement with measured bioaccumulation factors determined from data from Lake Ontario, than the predictions from the Thomann *et al.* (1992) model.

The United States Environmental Protection Agency recently completed an evaluation of bioaccumulation models for aquatic ecosystems (Imhoff *et al.,* 2004). The review considered the following models: AQUATOX (Model reference number 93), BASS (mModel reference number 19), ECOFATE (Model reference number 21), QEAFDCHN (Model reference number 79), RAMAS Ecosystem (Model reference number 85), Biotic Ligand Model, the Everglades Mercury Cycling Model E-MCM and TRIM.FaTE (Model reference number 94). Of these models, the Biotic Ligand Model and E-MCM are concerned with metals and so are beyond the scope of this work. Of the others, the BASS model has been developed for both hydrophobic organic chemicals and metals and is based on the work of Barber (2001). The model uses the FGETS model (Barber *et al.,* 1991) as a precursor.

The ECOFATE model is based on the work of Gobas (1993), Gobas *et al.* (1995) and Morrison *et al.* (1997). The QEAFDCHN model is based on the work of Thomann and Connolly (1984 and 1991), Thomann (1989), Thomann *et al.* (1992a and 1992b), Connolly *et al.* (1992 and 2000). The AQUATOX and TRIM.FaTE models were developed by the United States Environmental Protection Agency; the TRIM.FaTE model uses a bioaccumulation sub-model based on Thomann (1989) and covers terrestrial and human food chains as well.

Plant models

A comparison of nine models for predicting the uptake, translocation and elimination of organic chemicals by herbaceous plants has been carried out by Collins and Fryer (2003). This looked at three regression-based models (Travis and Arms, 1988 (Model reference number 72), Topp *et al.,* 1986 (Model reference number 64) and Calamari *et al.,* 1987 (Model reference number 7)), three equilibrium or steady-state models (Trapp and Matthies, 1995 (Model reference number 60), Chiou *et al*., 2001 (Model reference number 82) and Müller *et al.,* 1994 (Model reference number 42)) and three dynamic models (Trapp, 1995 (Model reference number 52), Paterson *et al.,* 1994 (Model reference number 51) and Trapp and Matthies, 1998 (Model reference number 88)). The models were tested against experimental data for 19 different organic chemicals in seven different plant species. The authors concluded that the dynamic models were preferable for acute exposure durations and for rapidly changing environmental media, whereas the regression equations and equilibrium/steady-state models performed best when compared with data for more stable chronic exposure situations. It was also concluded that although the regression-based models could provide predictions as accurate as some of the more complex models for uptake from soil, the one evaluating the uptake of organic chemicals from air into plants (Calamari *et al.,* 1987) had relatively poor predictive power.

For the plant uptake models, a review of their potential use in the CLEA model has recently been undertaken by the Environment Agency (Collins *et al.,* 2004). This review is not yet published, but the report investigated the models of Ryan *et al.* (1988; this is the model currently used in CLEA, see Model reference number 54), Travis and Arms (1988) (Model reference number 72), Topp *et al.* (1996) (Model reference number 64), Chiou *et al.* (2001) (Model reference number 82), Trapp and Matthies (1995) (Model reference number 60) and Hung and Mackay (1997) (Model reference number 26). As this report is still in draft, the conclusions are not yet available.

Many of the plant models have been developed by the same group (Trapp and co-workers). This group has also developed a potato model (Samsøe-Petersen *et al.,* 2003) but details of this model are currently only available in Danish. A recent publication by this group (Kulháneka *et al.,* 2005) compared predictions from several of their crop-specific models (for leafy vegetables, root vegetables, potatoes, tree fruits and so on) with predictions from the Travis and Arms (1998) method for polycyclic aromatic hydrocarbons, and used these to estimate concentrations in soil that would be protective of human health.

Paterson *et al.* (1990) reviewed the mechanisms of uptake of organic chemicals by plants from soil and the atmosphere. The review concluded that the key chemical parameters likely to affect uptake are the octanol-water and octanol-air partition coefficients. The paper also contains a compilation of around 150 references to papers considering the fate of around 70 chemicals in 88 species of plants and trees. This compilation would be a useful starting point for any future validation exercise for plant uptake models.

For the plant models, as a method already exists within the CLEA method for estimating uptake into the food chain from contaminated land, and as other reviews are currently being carried out for the Environment Agency (such as Collins *et al*, 2004), it is questionable whether a further review of plant uptake models is desirable. Therefore, it is proposed not to include any of the individual plant models in the in-depth review. A number will in any case be considered as they form part of the models chosen for in-depth review in Chapter 3.2.1 and Chapter 3.2.3.

Terrestrial and other models

Of the other models available, it is proposed that the following are included in the in-depth review:

- ACC-Human - Model reference number 2
- Arctic Terrestrial Food-chain Bioaccumulation model - Model reference number 29
- Technical Guidance Document (TGD) - Model reference number 60

Of the models not chosen for in-depth review, the earthworm model (Model reference number 84) is related in some respects to (a further development of) the earthworm model already considered in the TGD method. The terrestrial food chain model (Model reference number 89) is a regression equation-based method that considers a small part of the terrestrial food chain (such as transfer in food to cattle, sheep and poultry).

Although the arctic terrestrial food-chain bioaccumulation model is not directly applicable to the United Kingdom, it is one of the few examples that address the terrestrial food chain. In addition, some interesting findings related to the bioaccumulation potential in terrestrial ecosystems have been found using this model. For example, Kelly and Gobas (2003) found that the predicted bioaccumulation potential in terrestrial ecosystems was governed not solely by log K_{ow} , but that the octanol-air partition coefficient was also important. This may be important in understanding the bioaccumulation potential of substances like decabromodiphenyl ether, which is found to be essentially absent from aquatic biota but has recently been found to occur in certain species of terrestrial birds and mammals. Therefore it is recommended that this model is included in the in-depth review with regards for its potential for modification for the United Kingdom.

It should be noted that several of the models identified for the aquatic food chain also consider the terrestrial and human food chains and the these parts of the models will also be reviewed alongside the aquatic food chain.

An evaluation of the methods used in the TGD/EUSES for assessing the indirect exposure to humans via the environment has recently been carried out (Rikken and Lijzen, 2004).

In addition it is understood that a further terrestrial food chain model is being developed for the Environment Agency (the DREAM model, Project P4A(99)11 Risk Modelling for Dioxin Releases). This model is currently undergoing a peer review process and full details are not yet available. The model is understood to focus on specific chemicals such as dioxins for which empirical relationships are available, and so may not be applicable to organic chemicals in general.

Other information

A key parameter for consideration of bioaccumulation in aquatic systems is often the fish bioconcentration factor (BCF). In this review it has been assumed that BCF values for fish will be available for a wide range of chemicals, either obtained directly from experiments, or predicted from physico-chemical properties such as log K_{ow} [27]. However, there are models available for predicting bioconcentration in fish and several of these have recently been reviewed by Barber (2003). As bioconcentration models are incorporated into several of the more complex aquatic food chain models the

[27] The TGD provides regression equations for estimating fish BCF from log K_{ow} values. ECETOC (1995) outlines several other methods that could be used.

findings of the Barber (2003) review will also need to be taken into account in any subsequent in-depth review of the food chain model.

Many of the available models require information on the rates of elimination of the chemical from the organism. These data are not routinely available for organic chemicals in general. However, it may be possible to estimate these values in some cases. For example, Hendriks (1995) developed a series of regression equations relating the elimination rate constant for persistent organic chemicals to log K_{ow} and the size of the species for aquatic invertebrates, fish and warm-blooded animals. These elimination rate constants were seen as representing the minimum elimination rate from the organism. Chemicals that undergo extensive metabolism would be expected to have elimination rate constants larger than these minimum values.

Similarly, many of the models investigating the uptake via food require knowledge of the uptake or assimilation efficiency of the chemical. Gobas *et al.* (1988) derived a regression relationship between the uptake efficiency from food in fish and the log K_{ow} (this was incorporated into a bioaccumulation model; Model reference number 22) that could be useful in this respect. Similarly, Hendriks *et al.* (2001) developed a method for estimating accumulation (uptake and depuration) kinetics of organic substances as a function of the octanol-water partition coefficient and the chemical and the weight, lipid content and trophic level of the species in question.

Recommendations

The following models have been identified for in-depth review.

- ACC-Human - Model reference number 2
- System dynamic model - Model reference number 8
- Foodweb model - Model reference number 11
- BASS/FGETS - Model reference number 19
- ECOFATE and Food Chain Bioaccumulation - Model reference number 21
- Arctic terrestrial food-chain bioaccumulation model - Model reference number 29
- Technical Guidance Document - Model reference number 60
- Prediction of bioaccumulation in aquatic food webs - Model reference number 75
- QEAFDCHN - Model reference number 79
- GEMCO - Model reference number 83
- ARAMS - Model reference number 91
- AQUATOX - Model reference number 93
- TRIM.FaTE - Model reference number 94

It is proposed that the in-depth review focuses on these example models but draws on the related models (outlined in Table D1) as relevant. The approaches used in the CLEA model will not be reviewed in detail, but will be included in the consideration of the overall conclusions and recommendations of the detailed review report.

The peer review process indicated that two of the models (the ARAMS model (Model reference number 91) and the TRIM.FaTe (Model reference number 94) consist of many modules, and probably contain many parameters, and so the overall usefulness of these models to this project may be limited as the data necessary to use the models may not be generally available for large numbers of chemicals.

Similarly the peer review process identified that the AQUATOX model (Model reference number 93) is a sophisticated, state-of-the-art model for simultaneous simulation of ecosystem dynamics and the linked mass flow of toxicants. From their experience it is not too difficult to change the food web structure within this model, but to add species that are not in the AQUATOX libraries is time consuming owing to the number of ecological parameters that need to be estimated. Therefore the overall usefulness of this model to this project may again be limited.

In order to focus the effort in the in-depth review on the models that are most likely to be useful, these three more complex models (ARAMS, TRIMFaTe and AQUATOX) will be given a lower priority in the in-depth review than the other models listed.

As well as models and methods for estimation of the bioaccumulation of chemicals in food chains, an overall approach or framework for the use of the bioaccumulation data in the setting of standards needs to be considered. It is recommended that the approaches developed in the United States (Model reference number 73), Canada

(Model reference number 97) and the Netherlands (e.g. Model reference number 18, 66 and 80 (and Traas *et al.* (1996) and Jongbloed *et al.* (1994 and 1996)) are considered in this respect. Any framework developed would also need to take into account other frameworks such as the existing CLEA framework for consideration of effects on human health and the ERA framework that is being developed for terrestrial ecological risk assessment.

References & Bibliography

ABBOTT, J.D., HINTON, S.W AND BORTON, D.L., 1995. Pilot scale validation of the RIVER/FISH bioaccumulation modelling program for non-polar hydrophobic organic compounds using the model compounds 2,3,7,8-TCDD and 2,3,7,8-TCDF. Environmental Toxicology and Chemistry, 14, 1999-2012.

ARMITAGE, J.M. AND GOBAS, F.A.P.C., in preparation. *Development and evaluation of a terrestrial food web bioaccumulation model*. Manuscript in preparation (abstract only available at the time of this review).

ARNOT, J. A. AND GOBAS, F.A.P.C., 2003. A generic QSAR for assessing the bioaccumulation potential of organic chemicals in aquatic food webs. QSAR and Combinatorial Science, 22, 337-345.

BACCI, E., CEREJEIRA, M.J, GAGGI, C., CHEMELLO, G., CALAMARI, D. AND VIGHI, M., 1990. Bioconcentration of organic chemical vapours in plant leaves: The azalea model. Chemosphere, 21, 525-535.

BARBER, M.C., 2001. *Bioaccumulation and aquatic system simulator (BASS) user's manual beta test version 2.1*. United States Environmental Protection Agency, National Exposure Research Laboratory, EPA 600/R-01/035, (available from http://www.epa.gov/athens/staff/members/barbermahlonc/bass21_manual.pdf).

BARBER, M.C., 2003. A review and comparison of models for predicting dynamic chemical bioconcentration in fish. Environmental Toxicology and Chemistry, 22, 1963-1992.

BARBER, M.C., SUÁREZ, L.A. AND LASSITER, R.R., 1991. Modelling bioaccumulation of organic pollutants in fish with an application to PCBs in Lake Ontario Salmonids. Canadian Journal of Fisheries and Aquatic Sciences, 48, 318-337.

BELL, R.M., 1992. *Higher plant accumulation of organic pollutants from soils*. United States Environmental Protection Agency Report EPA/600/R-92/138.

BIRAK, P., YURK, J., ADESHINA, F., LORBER, M., POLLARD, K., CHOUDHURY, H. AND KRONER, S., 2001. Travis and Arms revisited: a second look at a widely used bioconcentration algorithm. Toxicology and Industrial Health, 7, 163-175.

BOCKTING, G.J.M., KOOLENBRANDER, J.G.M. AND SWARTJES, F.A., 1996. *Model for the calculation of human exposure due to contaminated sediments*. RIVM Report 715810011/1996. Rijksinstituut voor Volksgezondheid en Milieu, Bilthoven, Netherlands (in Dutch, as quoted in Lijzen et al., 2001).

BRIGGS, G.G., BROMILOW. R.H. AND EVANS, A.A., 1982. Relationship between lipophilicity and root uptake and translocation of non-ionized chemicals by barley. Pesticide Science, 13, 495-504.

BRIGGS, G.G., BROMILOW. R.H. AND EVANS, A.A. AND WILLIAMS, M., 1983. Relationships between lipophilicity and the distribution of non-ionized chemicals in barley shoots following uptake by the roots. Pesticide Science, 14, 492-500.

BURKEN, J.G. AND SCHNOOR, J.L., 1998. Predictive relationships for uptake of organic contaminants by hybdrid popular trees. Environmental Science and Technology, 32, 3379-3385 (as quoted in Trapp et al., 2003).

BURKHARD, L.P., 1998. Comparison of two models for predicting bioaccumulation of hydrophobic organic chemicals in a great lakes food web. Environmental Toxicology and Chemistry, 17, 383-393.

BURKHARD, L.P., ENDICOTT, D.D., COOK, P.M., SAPPINGTON, K.G AND WINCHESTER, E.L, 2003. Evaluation of two methods for prediction of bioaccumulation factors. Environmental Science and Technology, 37, 4626-4634.

CALAMAR,I.D., VIGHI, M., AND BACCI, E., 1987. The use of terrestrial plant biomass as a parameter in the fugacity model. Chemosphere, 16, 2359-2364.

CAMPFENS, J. AND MCKAY, D., 1997. Fugacity-based model of PCB bioaccumulation in complex aquatic food webs. Environmental Science and Technology, 31, 577-583.

CANADIAN COUNCIL OF MINISTERS OF THE ENVIRONMENT, 1999. *Protocol for the derivation of Canadian tissue residue guidelines for the protection of wildlife that consume aquatic biota*. Canadian Council of Ministers of the Environment, Winnipeg, Canada. (available from http://www.ec.gc.ca/CEQG-RCQE/English/Ceqg/Tissue/default.cfm).

CARBONELL, G., RAMOS, C., PABLOS, M.V., ORTIZ, J.A. AND TARAZONA, J.V., 2000. A system dynamic model for the assessment of different exposure routes in aquatic ecosystems. The Science of the Total Environment, 247, 107-118.

CHIOU, C.T., SHENG, G. AND MANES, M., 2001. A partition-limited model for the plant uptake of organic contaminants from soil and water. Environmental Science and Technology, 35, 1437-1444.

CHROSTOWSKI, P.C. AND FOSTER, S.A., 1996. A methodology for assessing congener-specific partitioning and plant uptake of dioxins and dioxin-like compounds. Chemosphere, 32, 2285-2304.

CIUCANI, G., 2002. *Misura e previsione dell'assorbimento radicale e del trasporto xilematico di elettroliti deboli ad attivita' antiparassitaria*. PhD thesis. Universita' degli studi di Milano, Facolta' di Agraria, Dipartimento di Scienze Molecolaria Agroalimentaria (as quoted in Trapp, 2004).

CIUCANI, G., MOSBÆK, H. AND TRAPP, S., 2004. Uptake of tributyltin into willow plants. Environmental Science and Pollution Research, 11, 267-272 (as quoted in Trapp, 2004).

CLARK, K.E. AND MACKAY, D., 1991. Dietary uptake and biomagnification of four chlorinated hydrocarbons by guppies. Environmental Toxicology and Chemistry, 10, 1205-1217.

CLARK, K.E., GOBAS, F.A.P.C. AND MACKAY, D., 1990. Model of organic uptake and clearance by fish from food and water. Environmental Science and Technology, 24, 1203-1213.

COLLINS. C. AND FRYER, M.E., 2003. Model intercomparison for the uptake of organic chemicals by plants. Environmental Science and Technology, 37, 1617-1624.

COLLINS. C., SHAW, G. AND FRYER, M.E., 2004. *Review of plant uptake models for CLEA*. Confidential Draft – May 2004. Document produced under R&D Project P5-079/4. Environment Agency, Bristol.

CONNELL, D.W., 1989. Biomagnification by aquatic organisms – a proposal. Chemosphere, 19, 1573-1584.

CONNELL, D.W. AND HAWKER, D.W., 1988. Use of polynomial expressions to describe the bioconcentration of hydrophobic chemicals by fish. Ecotoxicology and Environmental Safety, 16, 242-257.

CONNELL, D.W. AND MARKWELL, R.D., 1990. Bioaccumulation in the soil to earthworm system. Chemosphere, 20, 91-100.

CONNOLLY, J.P., 1991. Application of a food chain model to polychlorinated biphenyl contamination of the lobster and winter flounder food chains in New Bedford Harbor. Environmental Science and Technology, 25, 760-770.

CONNOLLY, J.P. AND GLASER, D., 2002. p,p'-DDE bioaccumulation in female sea lions of the California Channel Islands. Continental Shelf Research, 22, 1059-1078.

CONNOLLY, J.P. AND THOMANN, R.V., 1985. *WASTOX, a framework for modelling the fate of toxic chemicals in aquatic environments, part 2: Food Chain*. United States Environmental Protection Agency, Environmental Research Laboratory, Gulf Breeze, EPA/600/4-85/040 (details of the model are available at http://www.epa.gov/gbwebdev/ged/publica/c1166.htm).

CONNOLLY, J.P., ZAHAKOS, H.A., BENAMAN, J., ZIEGLER, C.K., RHEA, J.R. AND RUSSELL, K., 2000. A model of PCB fate in the upper Hudson River. Environmental Science and Technology, 34, 4076-4087.

CROMMENTUIJN, T., SIJM, D., DE BRUIJN, J., VAN LEEUWEN, K. AND VAN DE PLASSCHE, E., 2000. Maximum permissible and negligible concentrations for some organic substances and pesticides. Journal of Environmental Management, 58, 297-312.

CZUB, G. AND MCLACHLAN, M. S., 2004a. A food chain model to predict the levels of lipophilic organic contaminants in humans. Environmental Toxicology and Chemistry, 23, in press.

CZUB, G. AND MCLACHLAN, M.S., 2004b. Bioaccumulation potential of persistent organic chemicals in humans. Environmental Science and Technology, 38, 2406-2412.

DOUBEN, P.E.T., ALCOCK, R.E. AND JONES, K.C., 1997. Congener-specific transfer of PCDD/Fs from air to cow's milk: an evaluation of current modelling approaches. Environmental Pollution, 95, 333-344.

DOWDY, D.L. AND MCKONE, T.E., 1997. Predicting plant uptake of organic chemicals from soil or air using octanol/water and octanol/air partition ratios and a molecular connectivity index. Environmental Toxicology and Chemistry, 16, 2448-2456.

DOWDY, D.L. AND MCKONE, T.E. AND HSIEH, D.P.H., 1996. Prediction of chemical biotransfer of organic chemicals from cattle diet into beef and milk using the molecular connectivity index. Environmental Science and Technology, 30, 984-989.

DROUILLARD, K.G., NORSTROM, R.J., FOX, G.A., GILMAN, A. AND PEAKALL, D.B., 2003. Development and validation of a herring gull embryo toxicokinetic model for PCBs. Ecotoxicology, 12, 55-68.

ECETOC, 1995. *The role of bioaccumulation in environmental risk assessment: The aquatic environment and related food webs*. Technical Report No. 67. European

Centre for Ecotoxicology and Toxicology of Chemicals, Brussels, Belgium, October 1995.

ENVIRONMENT AGENCY AND DEFRA, 2002. *The contaminated land exposure assessment (CLEA) model: Technical basis and algorithms*. R&D Publication CLR 10, Environment Agency, Bristol.

EUROPEAN COMMISSION, 2003. *Technical Guidance Document on Risk Assessment in support of Commission Directive 93/67/EEC on Risk Assessment for existing substances, Commission Regulation (EC) No 1488/94 on Risk Assessment for existing substances and Directive 98/8/EC of the European Parliament and of the Council concerning the placing of biocidal products on the market*. European Commission, Joint Research Centre, EU 20418 EN, Second Edition.

EVERTS, J.W., EYS, Y., RUYS, M., PIJNENBURG, J., VISSER, H. AND LUTTIK, R., 1993a. Assessing the risk of biomagnification: a physiological approach. Science of the Total Environment, Supplement, 1501-1506.

EVERTS, J.W., EYS, Y., RUYS, M., PIJNENBURG, J., VISSER, H. AND LUTTIK, R., 1993b. Biomagnification and environmental quality criteria: a physiological approach. ICES Journal of Marine Science, 50, 333-335.

FEDERAL REGISTER, 1995. Final water quality guidance for the Great Lakes system. Federal Register, 60(56), Thursday March 23 1995, pp15365-15425.

FRASER, A.J., BURK$_{ow}$, I.C., WOLKER, H. AND MACKAY, D., 2002. Modelling biomagnification and metabolism of contaminants in harp seals of the Barents Sea. Environmental Toxicology and Chemistry, 21, 55-61.

GLASER, D. AND CONNOLLY, J.P., 2002. A model of p,p'-DDE and total PCB bioaccumulation in birds from the Southern California Bight. Continental Shelf Research, 22, 1079-1100.

GOBAS, F.A.P.C., 1993. A model for predicting the bioaccumulation of hydrophobic organic chemicals in aquatic food webs: Applications to Lake Ontario. Ecological Modelling, 69, 1-17.

GOBAS, F.A.P.C., MUIR, D.C.G. AND MACKAY, D., 1988. Dynamics of dietary bioaccumulation and faecal elimination of hydrophobic organic chemicals in fish. Chemosphere, 17, 943-962.

GOBAS, F.A.P.C., ZHANG, X. AND WELLS, R., 1993. Gastrointestinal magnification: The mechanism of biomagnification and food chain accumulation of organic chemicals. Environmental Science and Technology, 27, 2855-2863.

GOBAS, F.A.P.C , KELLY, B.C. AND ARNOT, J.A, 2003. Quantitative structure activity relationships for predicting the bioaccumulation of POPs in terrestrial food-webs. QSAR and Combinatorial Science, 22, 329-336.

.HELLWEGER, F., FARLEY, K., DAMIANI, D. AND ANID, P., 2001. Mathematical modelling of toxics fate, transport and bioaccumulation using GIS. Paper presented at the 2001 ESRI International User Conference, San Diego, California, July 10, 2001 (available from http://gis.esri.com/library/userconf/proc01/professional/papers/pap866/p866. htm).

HENDRIKS, A.J., 1995. Modelling non-equilibrium concentrations of microcontaminants in organisms: comparative kinetics as a function of species size and octanol-water partitioning. Chemosphere, 30, 265-292.

HENDRIKS A J, MA W-C, BROUNS J J, DE RUITER-DIJKMAN E M AND GAST R, 1995. Modelling and monitoring organochlorine and heavy metal accumulation in soils,

earthworms, and shrews in Rhine-Delta floodplains. Archives of Environmental Contamination and Toxicology, 29, 115-127.

HENDRIKS, A.J., VAN DER LINDE, A., CORNELISSEN, G. AND SIJM, D.T., 2001. The power of size. 1. Rate constants and equilibrium ratios for accumulation of organic substances related to octanol-water partition ratio and species weight. Environmental Toxicology and Chemistry, 21, 1399-1420.

HOPE, B.K., 1995. A review of models for estimating terrestrial ecological receptor exposure to chemical contaminants. Chemosphere, 30, 2267-2287.

HUNG, H. AND MACKAY, D., 1997. A novel and simple model of the uptake of organic chemicals by vegetation from air and soil. Chemosphere, 35, 959-977.

IMHOFF, J.C., CLOUGH, J., PARK, R.A., STODDARD, A. AND HAYTER, E., 2004. *Evaluation of chemical bioaccumulation models of aquatic ecosystems*. Final report. National Exposure Research Laboratory, Office of Research and Development, United States Environmental Protection Agency.

JAGER, T., 1998. Mechanistic approach for estimating bioconcentration of organic chemicals in earthworms (Oligochaeta). Environmental Toxicology and Chemistry, 17, 2080-2090.

JAGER, T., 2003. *Worming your way into bioavailability. Modelling the uptake of organic chemicals in earthworms*. Thesis from Institute for Risk Assessment Sciences, University of Utrecht.

JAGER, T., 2004. Modelling ingestion as an exposure route for organic chemicals in earthworms (Olgochaeta). Ecotoxicology and Environmental Safety, 57, 30-38.

JAGER, D.T. AND HAMERS, T., 1997. *Estimation methods for bioaccumulation in risk assessment of organic chemicals.* RIVM Report 679102 013/1997. Rijksinstituut voor Volksgezondheid en Milieu, Bilthoven, Netherlands.

JAGER, T., FLEUREN, R.H.L.J., HOGENDOORN E A AND DE KORTE G, 2003. Elucidating the routes of exposure for organic chemicals in the earthworm, *Eisenia Andrei* (Oligochaeta). Environmental Science and Technology, 37, 3399-3404.

JONGBLOED, R.H., PIJNENBURG, J., MENSINK, B.J.W.G., TRAAS, T.P. AND LUTTIK, R., 1994. *A model for environmental risk assessment and standard setting based on biomagnification. Top predators in terrestrial ecosystems*. RIVM Report 719101012, National Institute of Public Health and the Environment, Bilthoven, the Netherlands, October 1994.

JONGBLOED, R.H., TRAAS, T.P. AND LUTTIK, R., 1996. A probabilistic model for deriving soil quality criteria based on secondary poisoning of top predators. II. Calculations for dichlorodiphenyltrichloroethane (DDT) and cadmium. Ecotoxicology and Environmental Safety, 34, 279-306.

KELLY, B.C. AND GOBAS, F.A.P.C., 2001. Bioaccumulation of persistent organic pollutants in lichen-caribou-wolf food chains of Canada's central and Western Arctic. Environmental Science and Technology, 35, 325-334.

KELLY, B.C. AND GOBAS, F.A.P.C., 2003. An arctic terrestrial food-chain bioaccumulation model for persistent organic pollutants. Environmental Science and Technology, 37, 2966-2974.

KULHÁNEKA, A., TRAPP, S., SISMILICH, M., JANKU, J. AND ZIMOVÁ, M., 2005. Crop-specific human exposure assessment for polycyclic aromatic hydrocarbons in Czech soils. Science of the Total Environment, 339, 71-80.

LAI, K.M., SCRIMSHAW, M.D. AND LESTER, J.N., 2002. Prediction of the bioaccumulation factors and body burden of natural and synthetic estrogens in aquatic organisms in the river systems. Science of the Total Environment, 289, 159-168.

LIEN, G.J., NICHOLS, J.W., MCKIM, J.M. AND GALLINAT, C.A., 1994. Modelling the accumulation of three waterborne chlorinated ethanes in fathead minnows (Pimephales promelas): A physiologically based approach. Environmental Toxicology and Chemistry, 13, 1195-1205.

LIJZEN, J.P.A., BAARS, A,J., OTTE, P.F., RIKKEN, M.G.J., SWARTJES, F.A., VERBRUGGEN, E.M.J. AND VAN WEZEL, A.P., 2001. *Technical evaluation of the intervention values for soil/sediment and groundwater. Human and ecotoxicological risk assessment and derivation of risk limits for soil, aquatic sediment and groundwater*. RIVM Report 601516011/2004. Rijksinstituut voor Volksgezondheid en Milieu, Bilthoven, Netherlands.

LOIZEAU, V. AND MENESGUEN, A., 1993. A steady-state model for PCB accumulation in dab food web. Oceanological Acta, 16, 633-639.

LOIZEAU, V., ABARNOU, A., CUGIER, P., JAOUEN-MADOULET, A., LE GUELLEC, A-M. AND MENESGUEN, A., 2001. A model of PCB bioaccumulation in the sea bass food web from the seine Estuary (Eastern English Channel). Marine Pollution Bulletin, 43, 242-255.

LORBER, M.N., CLEVERLY, D., SCAUM, J., PHILLIPS, L., SCHWEER, G. AND LEIGHTON, T., 1994. Development and validation of an air-to-beef food chain model for dioxin-like compounds. Science of the Total Environment, 156, 39-65 (as quoted in Douben et al., 1997).

LORD, K.A., BRIGGS, G.A., NEALE, M.C. AND MANLOVE, R., 1980. Uptake of pesticides from water and soil by earthworms. Pesticide Science, 11, 401-408.

LUK, G.K. AND BROCKWAY, F., 1997. Application of a polychlorinated biphenyls bioaccumulation model to Lake Ontario lake trout. Ecological Modelling, 101, 97-111.

LUTTIK, R. AND DE SNOO, G.R., 2004. Characterization of grit in arable birds to improve pesticide risk assessment. Ecotoxicology and Environmental Safety, 57, 319-329.

MACKAY, D., 1991. *Multimedia environmental models: The fugacity approach*. Michigan: Lewis Publishers Inc.

MACKAY, D. AND FRASER, A., 2000. Bioaccumulation of persistent organic chemicals: mechanisms and models. Environmental Pollution, 110, 375-391.

MARKWELL, R.D., CONNELL, D.W. AND GABRIC, A.J., 1989. Bioaccumulation of lipophilic compounds from sediments by oligochaetes. Water Research, 23, 1443-1450.

MATTHIES, M. AND BEHRENDT, H., 1995. Dynamics of leaching, uptake, and translocation: The Simulation Model Network Atmosphere-Plant-Soil (SNAPS). In *Plant Contamination: Modelling and Simulation of Organic Chemical Processes*, edited by S Trapp and J C McFarlane, pp215-243. Boca Raton: Lewis Publishers.

MCCRADY, J.K. AND MAGGARD, S.P., 1993. Uptake and photodegradation of 2,3,7,8-tetrachlorodibenzo-p-dioxin sorbed to grass foliage. Environmental Science and Technology, 27, 343-350 (as quoted in Chrostowski and Foster, 1996).

MCCRADY, J.K., MCFARLANE, C. AND LINDSTROM, F.T., 1987. The transport and affinity of substituted benzenes in soybean stems. Journal of Experimental Botany, 38, 1875-1890.

MCLACHLAN, M.S., 1994. Model of the fate of hydrophobic contaminants in cows. Environmental Science and Technology, 28, 2407-2414.

MCLACHLAN, M.S., 1995. Accumulation of PCDD/Fs in an agricultural food chain. Organohalogen Compounds, 26, 105-108 (as quoted in Douben et al., 1997).

MCLACHLAN, M.S., 1996. Bioaccumulation of hydrophobic chemicals in agricultural food chains. Environmental Science and Technology, 30, 252-259 (as quoted in Czub and McLachlan, 2004a).

MCLACHLAN, M.S., 1997. A simple model to predict accumulation of PCDD/Fs in an agricultural food chain. Chemosphere, 34, 1263-1276.

MCLACHLAN, M.S.,, WELSCH-PAUSCH, K. AND TOLLS, J., 1995. Field validation of a model of the uptake of gaseous SOC in *Lolium multiflorum* (rye grass). Environmental Science and Technology, 29, 1998-2004 (as quoted in Czub and McLachlan, 2004a).

MENESES, M., SCHUHMACHER, M. AND DOMINGO, J.L., 2002. A design of two simple models to predict PCDD/F concentrations in vegetation and soils. Chemosphere, 46, 1393-1402.

MORRISON, H.A., GOBAS, F.A.P.C., LAZAR, R AND HAFFNER, G.D, 1996. Development and verification of a bioaccumulation model for organic contaminants in benthic invertebrates. Environmental Science and Technology, 30, 3377-3384.

MORRISON, H.A., GOBAS, F.A.P.C., LAZAR, R, WHITTLE, D.M. AND HAFFNER, G. D, 1997. Development and verification of a benthic/pelagic food web bioaccumulation model for PCB congeners in Western Lake Erie. Environmental Science and Technology, 31, 3267-3273.

MORRISON, H.A., WHITTLE, D.M., METCALFE, C.D. AND MIIMI, A.J., 1999. Application of a food web bioaccumulation model for the prediction of polychlorinated biphenyl, dioxin and furan congener concentrations in Lake Ontario aquatic biota. Canadian Journal of Fisheries and Aquatic Sciences, 56, 1389-1400.

MÜLLER, J.F., HAWKER, D.W. AND CONNELL, D.W, 1994. Calculation of bioconcentration factors of persistent hydrophobic compounds in the air/vegetation system. Chemosphere, 29, 623-640.

NICHOLS, J.W., MCKIM, J.M., ANDERSEN, M.E., GARGAS, M.L., CLEWELL, III, H.J. AND ERICKSON, R.J., 1990. A physiologically based toxicokinetic model for the uptake and disposition of waterborne organic chemicals in fish. Toxicology and Applied Pharmacology, 106, 433-447.

NICHOLS, J.W., MCKIM, J.M., LIEN, G.J., HOFFMAN, A.D. AND BERTELSEN, S.L., 1991. Physiologically based toxicokinetic modelling of three chlorinated ethanes in rainbow trout (*Oncorhynchus mykiss*). Toxicology and Applied Pharmacology, 110, 374-389.

NICHOLS, J.W., MCKIM, J.M., LIEN, G.J., HOFFMAN, A.D., BERTELSEN, S.L. AND GALLINAT, C.A., 1993. Physiologically based toxicokinetic modelling of three waterborne chloroethanes in channel catfish, *Ictalurus punctatus*. Aquatic Toxicology, 27, 83-112.

NICHOLS, J.W., MCKIM, J.M., LIEN, G.J., HOFFMAN, A.D., BERTELSEN, S.L. AND ELONEN, C.M., 1996. A physiologically based toxicokinetic model for dermal absorption of organic chemicals by fish. Fundamental and Applied Toxicology, 31, 229-242.

NICHOLS, J.W., JENSEN, K.M., TIETGE, J.E. AND JOHNSON, R.D., 1998. Physiologically based toxicokinetic model for maternal transfer of 2,3,7,8-tetrachlorodibenzo-p-dioxin in brook trout (*Salvelinus fontinalis*). Environmental Toxicology and Chemistry, 17, 2422-2434.

NICHOLS, J.W., FITZSIMMONS, P.N., WHITEMAN, F.W., DAWSON, T.D., BABEU, L. AND JUENEMANN, J, 2004a. A physiologically based toxicokinetic model for dietary uptake of hydrophobic organic compounds by fish. I. Feeding studies with 2,2'5,5'-tetrachlorobiphenyl. Toxicological Sciences, 77, 206-218.

NICHOLS, J.W., FITZSIMMONS, P.N. AND WHITEMAN, F.W., 2004b. A physiologically based toxicokinetic model for dietary uptake of hydrophobic organic compounds by fish. II Simulation of chronic exposure scenarios. Toxicological Sciences, 77, 219-229.

OTTE, P.F., VAN ELSWIJK, M., BLEIJENBERG. M., SWARTJES, F. AND VAN DE GUCHTE, C., 2000. *Calculation of human risk limits for sediments: Discussion report*. RIZA-Wekdocument 2000. 084x. Bilthoven/Lelystad, Netherlands (in Dutch, as quoted in Lijzen et al., 2001).

PARK, S.S. AND ERSTFELD, K.M., 1997. A numerical kinetic model for bioaccumulation of organic chemicals in sediment-water systems. Chemosphere, 34, 419-427.

PATERSON, S. AND MACKAY, D., 1995. Interpreting chemical partitioning in soil-plant-air systems with a fugacity model. In *Plant Contamination: Modelling and Simulation of Organic Chemical Processes*, edited by S Trapp and J C McFarlane, pp191-214. Boca Raton: Lewis Publishers.

PATERSON, S., MACKAY, D., TAM, D. AND SHIU, W.Y., 1990. Uptake of organic chemicals by plants: A review of processes, correlations and models. Chemosphere, 21, 297-331.

PATERSON, S., MACKAY, D.,, BACCI, E. AND CALAMARI, D., 1991a. Correlation of the equilibrium and kinetics of leaf-air exchange of hydrophobic organic chemicals. Environmental Science and Technology, 25, 866-871.

PATERSON, S., MACKAY, D. AND GLADMAN, A., 1991b. A fugacity model of chemical uptake by plants from soil and air. Chemosphere, 23, 1991, 539-565.

PATERSON, S., MACKAY, D. AND MCFARLANE, C., 1994. A model of organic chemical uptake by plants from soil and the atmosphere. Environmental Science and Technology, 28, 2259-2266.

POLDER, M.D., HULZEBOS, E.M. AND JAGER, D.T., 1998. Bioconcentration of gaseous organic chemicals in plant leaves: comparison of experimental data with model predictions. Environmental Toxicology and Chemistry 17, 962-968.

QEA, 1999. *PCBs in the Upper Hudson River. Volume 2: A model of PCB fate, transport and bioaccumulation*. Prepared for General Electric. Quantitative Environmental Analysis, LCC, Montvale, United States (available from http://www.ge.com/en/commitment/ehs/hudson/techReport.htm).

QEA, 2001a. *Documentation Bioaccumulation Model QEAFDCHN v1.0*. Quantitative Environmental Analysis, LLC, Montvale, United States, February 2001 (available from http://www.dnr.state.wi.us/org/water/wm/lowerfox/rifs/modeldocs/e2_manual.pdf).

QEA, 2001b. *A model of PCB bioaccumulation in the Lower Fox River and Green Bay: GBFood*. Quantitative Environmental Analysis, LLC, Montvale, United States (available from http://www.dnr.state.wi.us/org/water/wm/lowerfox/rifs/feasabilitystudy.html).

RIEDERER. M., 1990. Estimating partitioning and transport of organic chemicals in the foliage/atmosphere system: Discussion of a fugacity-based model. Environmental Science and Technology, 24, 829-837.

RIEDERER. M., 1995. Partitioning and transport of organic chemicals between the atmospheric environment and leaves. In *Plant Contamination: Modelling and Simulation of Organic Chemical Processes*, edited by S Trapp and J C McFarlane, pp153-1900. Boca Raton: Lewis Publishers.

RIKKEN, M.G.J. AND LIJZEN, J.P.A., 2004. *Update of risk assessment models for the indirect human exposure*. RIVM Report 601516011/2004. Rijksinstituut voor Volksgezondheid en Milieu, Bilthoven, Netherlands.

RIKKEN, M.G.J., LIJZEN, J.P.A., AND CORNELESE, A, 2001. *Evaluation of model concepts on human exposure. Proposals for updating the most relevant exposure routes of CSOIL*. RIVM Report 711701022/2001. Rijksinstituut voor Volksgezondheid en Milieu, Bilthoven, Netherlands.

ROMIJN, C.A.F.M., LUTTIK, R., VAN DE MEENT, D., SLOOFF, W. AND CANTON, J. H., 1993. Presentation of a general algorithm to include effect assessment on secondary poisoning in the derivation of environmental quality criteria. 1. Aquatic food chains. Ecotoxicology and Environmental Safety, 26, 61-85.

ROMIJN, C.A.F.M., LUTTIK, R. AND CANTON, J. H, 1994. Presentation of a general algorithm to include effect assessment on secondary poisoning in the derivation of environmental quality criteria. 2. Terrestrial food chains. Ecotoxicology and Environmental Safety, 27, 107-127.

RYAN, J.A., BELL, R.M., DAVIDSON, J.D. AND O'CONNOR, G.A., 1988. Plant uptake of non-ionic organic chemicals from soils. Chemosphere, 17, 2299-2323.

SAMPLE, B.E., BEAUCHAMP, J.J., EFROYMSON, R.A., SUTER, II, G.W. AND ASHWOOD, T.L., 1998a. *Development and validation of bioaccumulation models for earthworms*. Report ES/ER/TM-220, Oak Ridge National Laboratory, prepared for the U.S. Department of Energy Office of Environmental Management, February 1998.

SAMPLE, B.E., BEAUCHAMP, J.J., EFROYMSON, R.A. AND SUTER, II, G.W., 1998b. *Development and validation of bioaccumulation models for small mammals*. Report ES/ER/TM-219, Oak Ridge National Laboratory, prepared for the US Department of Energy Office of Environmental Management, February 1998.

SAMPLE, B.E., SUTER, II, G.W.. BEAUCHAMP, J.J. AND EFROYMSON, R.A., 1999. Literature-derived bioaccumulation models for earthworms: Development and validation. Environmental Toxicology and Chemistry, 18, 2110-2120.

SAMSØE-PETERSEN, L., RASMUSSEN, D. AND TRAPP, S., 2003. *Modellering af optagelse af organiske stoffer I grøntsager og frugt.* Rapport til Miljøstyrelsen, Miljøprojekt Nr. 765 2003 Teknologiudviklingsprogrammet for jord- og grundsvandsforurening (in Danish).

SATCHIVI, N.M., STOLLER, E.W., WAX, L.M. AND BRISKIN, D.P., 2000. A nonlinear dynamic simulation model for xenobiotic transport and whole plant allocation following foliar application. I. Conceptual foundation for model development. Pesticide Biochemistry and Physiology, 68, 67-84.

SCHRAMM, K-W., REISCHL, A. AND HUTZINGER, O., 1987. UNITTree. A multimedia compartment model to estimate the fate of lipophilic compounds in plants. Chemosphere, 16, 2653-2663.

SIJM, D.T.H.M., SEINEN, W. AND OPPERHUIZEN, A., 1992. Life-cycle biomagnification study in fish. Environmental Science and Technology, 26, 2162-2174.

SMITH, D.G., CHAUDHURE, S., HEINHOLD, D. AND RUFFLE, B., 1995. An alternative approach for estimating plant uptake of dioxin vapours. Organohalogen Compounds, 24, 187-193 (as quoted in Douben et al., 1997).

SWARTJES, F.A., 2002. *Variation in calculated human exposure. Comparison of calculations with seven European human exposure models*. RIVM Report 711701030/2002, National Institute of Public Health and the Environment, Bilthoven, the Netherlands.

TARAZONA, J.V. AND VEGA, M.M., 2002. Hazard and risk assessment of chemicals for terrestrial ecosystems. Toxicology, 181-182, 187-191.

TARAZONA, J.V., FRESNO, A., AYCARD, S., RAMOS, C., VEGA, M.M. AND CARBONELL, G., 2000. Assessing the potential hazard of chemical substances for the terrestrial environment. Development of hazard classification criteria and quantitative environmental indicators. The Science of the Total Environment, 247, 151-164.

THOMANN, R.V., 1981. Equilibrium model of fate of microcontaminants in diverse aquatic food chains. Canadian Journal of Fisheries and Aquatic Sciences, 38, 280-296.

THOMANN, R.V., 1989. Bioaccumulation model of organic chemical distribution in aquatic food chains. Environmental Science and Technology, 23, 699-707.

THOMANN, R.V. AND CONNOLLY, J.P., 1984. Model of PCB in the Lake Michigan Lake Trout Food Chain. Environmental Science and Technology, 18, 65-71.

THOMANN, R.V., CONNOLLY, J.P. AND PARKERTON, T.F., 1992. An equilibrium model of organic chemical accumulation in aquatic food webs with sediment interaction. Environmental Toxicology and Chemistry, 11, 615-629.

TOPP, E., SCHEUNERT, I., ATTAR, A. AND KORTE, F., 1986. Factors affecting the uptake of ^{14}C-labelled organic chemicals by plants from soil. Ecotoxicology and Environmental Safety, 11, 219-228.

TRAAS, T.P. , 2001. *Guidance document on deriving environmental risk limits*. RIVM Report 601501 012, National Institute of Public Health and the Environment, Bilthoven, the Netherlands, June 2001.

TRAAS, T.P., LUTTIK, R. AND JONGBLOED, R.H., 1996. A probabilistic model for deriving soil quality criteria based on secondary poisoning of top predators. I. Model description and uncertainty analysis. Ecotoxicology and Environmental Safety, 34, 264-278.

TRAAS, T.P., LUTTIK, R., KLEPER, O., BEURSKENS, J.E.M., SMIT, M.D., LEONARDS, P.E.G., VAN HATTUM, A.G.M AND ALDENBERG, T., 2001b. Congener-specific model for polychlorinated biphenyl effects on otter (*Lutra lutra*) and associated sediment quality criteria. Environmental Toxicology and Chemistry, 20, 205-212.

TRAPP, S., 1995. Model for uptake of xenobiotics into plants. In *Plant Contamination: Modelling and Simulation of Organic Chemical Processes*, edited by S Trapp and J C McFarlane, pp107-151. Boca Raton: Lewis Publishers.

TRAPP, S., 2000. Modelling uptake into roots and subsequent translocation of neutral and ionisable organic compounds. *Pest Management Science*, 56, 767-778.

TRAPP, S., 2002. Dynamic root uptake model for neutral lipophilic organics. Environmental Toxicology and Chemistry, 21, 203-206.

TRAPP, S., 2004. Plant uptake and transport models for neutral and ionic chemicals. Environmental Science and Pollution Research, 11, 33-39.

TRAPP, S. AND MATTHIES, M., 1995. Generic one-compartment model for uptake of organic chemicals by foliar vegetation. Environmental Science and Technology, 29, 2333-2338.

TRAPP, S. AND MATTHIES, M., 1996. Generic one-compartment model for uptake of organic chemicals by foliar vegetation (addition/correction). Environmental Science and Technology, 30, 360-361.

TRAPP, S. AND MATTHIES, M., 1997. Modelling volatilization of PCDD/F from soil and uptake into vegetation. Environmental Science and Technology, 31, 71-74.

TRAPP, S. AND MATTHIES, M., 1998. *Chemodynamics and environmental modelling – An introduction*. Springer, London.

TRAPP, S. AND SCHWARTZ, S., 2000. Proposals to overcome limitations in the EU chemical risk assessment scheme. Chemosphere, 41, 965-971.

TRAPP, S., MATTHIES, M., SCHEUNERT, I. AND TOPP, E.M., 1990. Modelling the bioconcentration of organic chemicals in plants. Environmental Science and Technology, 24, 1246-1252.

TRAPP, S., MIGLIORANZA, K.S.B. AND MOSBAEK, H., 2001. Sorption of lipophilic organic compounds to wood and implications for their environmental fate. Environmental Science and Technology, 35, 1561-1566 (as quoted in Trapp et al., 2003).

TRAPP, S., RASMUSSEN, D. AND SAMSØE-PETERSEN, L., 2003. Fruit tree model for uptake of organic compounds from soil. SAR and QSAR in Environmental Research, 14, 17-26.

TRAVIS C C AND ARMS A D, 1988. Bioconcentration of organics in beef, milk and vegetation. *Environmental Science and Technology*, 22, 271-274.

USEPA, 1995a. *Great Lakes water quality initiative technical support document for wildlife criteria.* United States Environmental Protection Agency, EPA-820-B95-009.

USEPA, 1995b. *Great Lakes water quality initiative technical support document for the procedure to determine bioaccumulation factors*. United States Environmental Protection Agency, EPA-820-B95-005.

USEPA, 2000. *Methodology for deriving ambient water quality criteria for the protection of human health*. United States Environmental Protection Agency, EPA-822-B00-004.

USEPA, 2004. *AQUATOX (Release 2). Modelling environmental fate and ecological effects in aquatic ecosystem. Volume 2: Technical documentation*. United States Environmental Protection Agency, EPA-823-R-04-002, January 2004.

VAN DEN MEENT, D. AND DE BRUIJN, J.H.M., 1995. A modelling procedure to evaluate the coherence of independently derived environmental quality objectives for air, water and soil. Environmental Toxicology and Chemistry, 14, 177-186.

VAN DEN BERG, R, 1995. *Exposure of man to soil contamination. A qualitative and quantitative analysis, resulting in proposals for human-toxicological C values*. RIVM Report 725201006/1995 (revised version of RIVM Report 725201011/1991). Rijksinstituut voor Volksgezondheid en Milieu, Bilthoven, Netherlands (in Dutch, as reported in Lijzen et al., 2001).

VAN EIJKEREN, J.C.H., JAGER, D.T. AND SIPS, A.J.A.M., 1998. *Generic PBPK-modelling of lipophilic contaminants in the cow*. RIVM Report 679102 042. National Institute of Public Health and the Environment, Bilthoven, the Netherlands, March 1998.

VOUTSAS, E., MAGOULAS, K. AND TASSIOS, D., 2002. Prediction of the bioaccumulation of persistent organic pollutants in aquatic food webs. Chemosphere, 48, 645-651.

YANG, R., THURSTON, V., NEUMAN, J. AND RANDALL, D.J., 2000. A physiological model to predict xenobiotic concentration in fish. Aquatic Toxicology, 48, 109-117.

Appendix D1 – Consultation

The following people were consulted as part of this review.

Derek Muir	Environment Canada
J V Tarazona	INIA, Spain
Aaron Fisk	University of Georgia
F A P Gobas	Simon Fraser University, Canada
D Mackay	Trent University, Canada
Michael McLachlan	ITM, Sweden
Roy Thompson	Astrazeneca, United Kingdom
Lawrence Burkhard	United States Environmental Protection Agency
Stefan Trapp	University of Denmark
Earl Hayer	United States Environmental Protection Agency
J P Connolly	QEA, United States
David Glaser	QEA, United States
V Loizeau	IFREMER, France
John Nichols	United States Environmental Protection Agency
Ken Drouillard	University of Windsor , Canada
Katrine Borga	Norwegian Polar Institute
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Mark Clook	Project board (PSD)
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Robin Law	CEFAS, United Kingdom
Dick Sijm	RIVM, the Netherlands
Ross Norstrom	Carlton University, Canada (formerly Environment Canada)
Jan Hendriks	Nijmegen University, the Netherlands
Lise Samsoe-Petersen	DHI Water and Environment, Denmark
Jon Arnot	Trent University, Canada
Jim Smith	Centre for Ecology and Hydrology, United Kindom

Appendix D2 – Model summaries

As described in the main report, some of the models have been grouped together for the more detailed review to be carried out in the second phase of this work. In the summaries here, the recommendation field indicates when a model has been linked to another model. The link is only in one direction, from the particular model to the model example or version chosen to represent the grouping. Models are not linked to other members of the group, and the representative model is not shown as linked to any of the other members of the group.

Model reference number 1

Name of model/ method/paper	Pilot scale validation of the RIVER/FISH bioaccumulation modelling program for non-polar hydrophobic organic compounds using the model compounds 2,3,7,8-TCDD and 2,3,7,8-TCDF. J D Abbott, S W Hinton and D L Borton. *Environmental Toxicology and Chemistry*, **14**, 1995, 1999-2012.
Date of publication	1995
Availability	Published paper. The model was also reportedly available as a user-friendly computer program.
Food chain considered	Water (dissolved and particulate) → trophic level 1 (phytoplankton, zooplankton and/or small invertebrates) → trophic level 2 (small fish and/or large invertebrates) → trophic level 3 (benthic, filter and/or gape feeders) → trophic level 4 (large predatory fish). The model considers up to four trophic levels (it can be run with fewer) and predicts time-dependent chemical concentrations in up to 16 aquatic species residing in up to eight different geographical locations in a receiving water subject to up to eight point source releases of a chemical.
Types of chemicals modelled	Non-polar hydrophobic chemicals.
Environment to which it relates	Generic. The model was validated against data from the United States.
Data requirements	Log K_{ow} , assimilation efficiency and metabolism/elimination rate. The method also requires details of the food source for each trophic level (example values are given).
Purpose of model/method	Research paper.
Summary of validation studies	A validation study has been undertaken using a 2,3,7,8-TCDD and 2,3,7,8-TCDF. Details are given in this paper.
Assessment	The model appears to be reasonably flexible and could be modified for other food chains or locations. The method requires only a limited amount of chemical-specific information.
Recommendation	Candidate for in-depth review.

Model reference number 2

Name of model/ method/paper	ACC-Human The details of the model are presented in: A food chain model to predict the levels of lipophilic organic contaminants in humans. G Czub and M S McLachlan. *Environmental Toxicology and Chemistry*, **23**, 2004a, in press.
Date of publication	2004
Availability	Paper in press. The model will be made available for download in the near future from http://www.itm.su.se.
Food chain considered	Seawater → zooplankton → planktivorous fish → piscivorous fish → humans. Soil and air → grass → cattle → diary products and beef → humans. The model is a fugacity-based, non-steady state, mechanistic model. The top predator in the model is humans. The model can calculate the internal dose in humans. Parts of the model are based on early work by the same authors (such as McLachlan, 1994, 1996 and 1997 and McLachlan *et al.,* 1995 amongst others).
Types of chemicals modelled	Polychlorinated biphenyls.
Environment to which it relates	Generic. The parameters used in the model are typical for Southern Sweden.
Data requirements	The chemical-specific data requirements are not entirely clear at this stage but appear to be mainly log K_{ow} , octanol-air partition coefficients and degradation rate constants in the various media.
Purpose of model/method	Research paper.
Summary of validation studies	The model results for polychlorinated biphenyls were compared with data from the Swedish environment. An investigation of the influence of physico-chemical properties on the potential of organic chemicals to bioaccumulate in humans has also been undertaken using the model (Czub and Mc Clachlan, 2004b).
Assessment	The model considers many of the endpoints currently related to man exposed via the environment in the TGD. The chemical-specific data requirements of the model appear to be modest. The model was developed using data on polychlorinated biphenyls, but may be applicable to other chemical types. The model is developed using parameters relevant for Sweden, but could be adapted for other situations.
Recommendation	Candidate for in-depth review.

Model reference number 3

Name of model/ method/paper	A generic QSAR for assessing the bioaccumulation potential of organic chemicals in aquatic food webs. J A Arnot and F A P C Gobas. *QSAR and Combinatorial Science*, **22**, 2003, 337-345.
Date of publication	2003
Availability	Published paper.
Food chain considered	Water → trophic level 1 → trophic level 2 → trophic level 3 (fish). The method is a generic QSAR that relates the BCF and BAF for the highest trophic level to log K_{ow}. The method is a modification of the Gobas (1993) method and is presented as a series of equations.
Types of chemicals modelled	Organic chemicals.
Environment to which it relates	Canada. The method is a generic method but certain parameters were chosen to represent a food web consisting of three trophic interactions/levels under Canadian environmental conditions.
Data requirements	Log K_{ow}. The method can also use the metabolic transformation rate and can be adapted to take into account trophic dilution (this is done using a factor to represent the ability of organisms in the food web to metabolise absorbed substances).
Purpose of model/method	The method was developed as a screening tool to determine BAFs (in particular to identify when the BAF is greater than 5,000 in relation to the bioaccumulation criteria under the Canadian Environmental Protection Act 1999).
Summary of validation studies	The model was calibrated using a large BCF and BAF database.
Assessment	The method requires only few chemical-specific data. The method could be modified for other food chains or environments.
Recommendation	Candidate for in-depth review (should be reviewed in conjunction with Model reference number 21).

Model reference number 4

Name of model/ method/paper	Bioconcentration of organic chemical vapours in plant leaves: The azalea model. E Bacci, M J Cerejeira, C Gaggi, G Chemello, D Calamari and M Vighi. *Chemosphere*, **21**, 1990, 525-535.
Date of publication	1990
Availability	Published paper.
Food chain considered	Air $\rightarrow$ plants. The method consists of regression equations relating the leaf-air bioconcentration factor to log K_{ow} or to the air-water partition coefficient.
Types of chemicals modelled	Organic chemicals. The method was derived based on experimental data for 14 chemicals including alachlor, dieldrin, 3,3'4,4'-tetrachlorobenzene, 1,2,3,4-tetrachlorodibenzo-p-dioxin, DDT, DDE, α-hexachlorocyclohexane, γ-hexachlorocylcohexane, polychlorinated biphenyls, trifluralin, hexachlorobenzene, mirex, thionazin and sulfotep.
Environment to which it relates	Generic. The regression equations are specific to azalea leaves, although a suggested approach is given to make the method more generally applicable using the lipid content of the plant leaf.
Data requirements	Log K_{ow} and/or air-water partition coefficient (dimensionless Henry's law constant)
Purpose of model/method	Research paper.
Summary of validation studies	None located as part of this work.
Assessment	The method is simple to use and requires relatively little chemical-specific input data. The regression equations are, however, specific to azalea leaves and so have limited usefulness in respect to this project.
Recommendation	Not considered further.

Model reference number 5

Name of model/ method/paper	*Higher plant accumulation of organic pollutants from soils*. R M Bell. United States Environmental Protection Agency Report EPA/600/R-92/138, 1992.
Date of publication	1992
Availability	Published report. A summary of the report is available from the internet (http://www.epa.gov/cgi-bin/claritgw?op-Display&document=clserv:ORD:1501;&rank=6&template=epa).
Food chain considered	Soil → plants. The method is very similar to that used in the EU Technical Guidance Document.
Types of chemicals modelled	Organic chemicals.
Environment to which it relates	Generic; contaminated land.
Data requirements	Log K_{ow}. This is used to estimate a root concentration factor, a stem concentration factor and a transpiration stream concentration factor.
Purpose of model/method	Developed to assess the potential use of higher plants as an in situ clean-up technique for polluted soils.
Summary of validation studies	Greenhouse studies with hexachlorobenzene and a field trial (collection of, and analysis of, plants growing at dioxin contaminated sites) were carried out.
Assessment	The method presented is very similar to that given in the Technical Guidance Document. The study may contain useful validation data.
Recommendation	Candidate for in-depth review (in conjunction with Model reference number 60).

Model reference number 6

Name of model/ method/paper	Relationship between lipophilicity and root uptake and translocation of non-ionized chemicals by barley. G G Briggs, R H Bromilow and A A Evans. *Pesticide Science*, **13**, 1982, 495-504. Relationships between lipophilicity and the distribution of non-ionized chemicals in barley shoots following uptake by the roots. G G Briggs, R H Bromilow, A A Evans and M Williams. *Pesticide Science*, **14**, 1983, 492-500.
Date of publication	1982/1983
Availability	Published paper. The method is incorporated into the TGD method.
Food chain considered	Soil (pore water) → plants. The paper develops regression equations relating the uptake of chemicals in roots and shoots to the log K_{ow}.
Types of chemicals modelled	Non-ionised chemicals.
Environment to which it relates	Generic. The regression equations were developed from data from barley shoots.
Data requirements	Log K_{ow}.
Purpose of model/method	Research paper.
Summary of validation studies	The regression equations were developed using a series of O-methylcarbamoyloximes and substituted phenylureas.
Assessment	The method is easy to use and requires limited chemical-specific information. The method is incorporated into the methods used in the TGD and some other plant uptake models.
Recommendation	Candidate for in-depth review (in conjunction with Model reference number 60).

Model reference number 7

Name of model/ method/paper	The use of terrestrial plant biomass as a parameter in the fugacity model. D Calamari, M Vighi and E Bacci. *Chemosphere*, **16**, 1987, 2359-2364.
Date of publication	1987
Availability	Published paper.
Food chain considered	Soil (porewater) → plants. Air → plants. The model is a fugacity-based model and uses some of the regression equations derived by Briggs *et al.* (1982 and 1983). The model is presented as a series of equations.
Types of chemicals modelled	Organic chemicals. The paper considered the distribution of lindane, atrazine and cypermethrin.
Environment to which it relates	Generic.
Data requirements	The chemical-specific data needed include water solubility, vapour pressure and log K_{ow}. The model also needs some plant-related data. Generic values are used in the model.
Purpose of model/method	Research paper.
Summary of validation studies	A comparison of this model and eight other models for predicting the uptake, translocation and elimination of organic chemicals by herbaceous plants has been carried out by Collins and Fryer (2003).
Assessment	The model uses relatively little chemical-specific information. The model is similar in some respects to other models (such as Paterson *et al.,* 1991a, 1991b and 1994). The model would need to be computerised (spread-sheet?) for it to be used on a regular basis.
Recommendation	Candidate for in-depth review (in conjunction with Model reference number 51).

Model reference number 8

Name of model/ method/paper	A system dynamic model for the assessment of different exposure routes in aquatic ecosystems. G Carbonell, C Ramos, M V Pablos, J A Ortiz and J V Tarazona. *Science of the Total Environment*, **247**, 2000, 107-118.
Date of publication	2000
Availability	Published paper.
Food chain considered	Water and sediment → alga → cladoceran invertebrates → cladoceran-eating fish → fish-eating fish. Considers a primary producer and three levels of consumer using a generic framework.
Types of chemicals modelled	Lipophilic organic chemicals. The model was run using four theoretical "example" substances covering a range of degradation and metabolisation rates.
Environment to which it relates	Generic.
Data requirements	Two versions of the model are given. The simplified version requires information on the bioconcentration factor, the biota-food accumulation factor and the biota-sediment accumulation factor for each primary producer and consumer considered, and the degradation half-life of the substance in water (if non-continuous exposures are considered). A more complicated version of the model requires knowledge of the uptake (from water and sediment) and depuration rate constants for the substance in each species, but allows the time-dependent accumulation to be better modelled.
Purpose of model/method	Research paper.
Summary of validation studies	None located as part of this work.
Assessment	The model is simple to use but requires some data that may not be readily available for a large number of chemicals, although it may be possible to estimate these data. Could be easily modified to consider different aquatic food chains consisting of many different primary producers and consumers (in principal, the method can be easily modified for any number of primary producers and consumers).
Recommendation	Candidate for in-depth review (in conjunction with Model reference number 59).

Model reference number 9

Name of model/ method/paper	A methodology for assessing congener-specific partitioning and plant uptake of dioxins and dioxin-like compounds. P C Chrostowski and S A Foster. *Chemosphere*, **32**, 1996, 2285-2304.
Date of publication	1996
Availability	Published paper.
Food chain considered	Air (particulate phase and vapour phase) → plant. The method is presented as a series of equations. The approach takes into account photolysis. The method is based on data generated by McCrady and Maggard (1993), and the modelling approaches developed by Paterson *et al.* (1991a) and Müller *et al.* (1994). The method allows plant uptake factors to be determined.
Types of chemicals modelled	Polychlorinated dibenzo-p-dioxins and dibenzofurans.
Environment to which it relates	Generic, adapted to the situation close to a hazardous waste incinerator.
Data requirements	The chemical-specific information required is log K_{ow} , Henry's law constant and the photolysis rate constant. Plant-specific properties include the volume fractions of cuticular membrane, water, cellular lipids, carbohydrates and proteins (values are given for grass).
Purpose of model/method	Research paper to compare the contribution of dioxins and dioxin-like compounds in vegetation from direct particulate deposition and vapour phase uptake close to hazardous waste combustion sources.
Summary of validation studies	None located as part of this work.
Assessment	The method requires limited chemical-specific input data and could be adapted for other plant types and situations. The approach is similar to others (such as Patterson *et al.*, 1991a, and Müller *et al.*, 1994).
Recommendation	Candidate for in-depth review (in conjunction with Model reference number 51).

Model reference number 10

Name of model/ method/paper	Model of organic chemical uptake and clearance by fish from food and water. K E Clark, F A P C Gobas and D Mackay. *Environmental Science and Technology*, **24**, 1990, 1203-1213.
Date of publication	1990
Availability	Published paper.
Food chain considered	Water → fish. Food → fish. The model is a steady-state, fugacity-based model that describes food chain biomagnification, the dependence of fish concentrations on rates of metabolism and growth, and the effect of reduced bioavailability. The model is presented as a series of equations. The model can be run sequentially in order to represent higher trophic levels.
Types of chemicals modelled	Organic chemicals.
Environment to which it relates	Generic.
Data requirements	The chemical-specific data required include log K_{ow} and metabolism rate constants. The food chain-dependent parameters include lipid content, food lipid content, feeding rate and fish growth rate amongst others.
Purpose of model/method	Research paper.
Summary of validation studies	The model has been tested against experimental data for four chlorinated hydrocarbons obtained with guppies (Clark and Mackay, 1991).
Assessment	The model uses only a limited amount of chemical-specific information and could easily be adapted for different combinations of food and fish. The method would need to be computerised (spreadsheet?) for regular use.
Recommendation	Candidate for in-depth review (in conjunction with Model reference number 11).

Model reference number 11

Name of model/ method/paper	Foodweb model. Details of the model are given in the following paper: Fugacity-based model of PCB bioaccumulation in complex aquatic food webs. I Campfens and D Mackay. *Environmental Science and Technology*, **31**, 1997, 577-583.
Date of publication	1997 (the basic program was modified in 1998).
Availability	Published paper. A basic program implementing the model is available from the Canadian Environmental Modelling Centre, Trent University, free of charge (http://www.trentu.ca/cemc/models/Foodweb.html).
Food chain considered	Water → pelagic organism 1 → pelagic organism 2 → and so on. Sediment → benthic organism 1 → pelagic organism 2 → and so on. The model is a steady-state, fugacity-based model that can be modified to deal with as many trophic levels as required. The model can include both pelagic and benthic food chains. The model is presented as a series of equations and takes into account organism growth and metabolism. A computerised version is also available.
Types of chemicals modelled	Organic chemicals (the model was run for polychlorinated biphenyls in the paper).
Environment to which it relates	Generic.
Data requirements	The chemical-related data include log K_{ow} , molecular weight and Henry's law constant. The organism-related parameters include mass, lipid content, feeding rate, growth rate, metabolism half-life, digestion factor, fractional respiration rates, gut absorption efficiency parameters and diet amongst others (the paper gives the necessary parameters for plankton, mysids, pontoporeia, oligochaete, sculpin, alewife, smelt and salmonid based on data from Lake Ontario). The model also requires water properties such as concentration of suspended particulate matter, volume fraction of sediment solids and organic carbon content of suspended matter and sediment particles.
Purpose of model/method	Research paper.
Summary of validation studies	The original paper compared the predictions for polychlorinated biphenyls with measured data obtained from the Lake Ontario food chain. Lai *et al.* (2002) used the model to determine bioaccumulation factors for a range of natural and synthetic estrogens and compared these with literature measured data.
Assessment	The model appears to be very flexible and could be modified for a variety of food chains and water types. The model requires a few, readily available (or predictable) chemical-specific data.
Recommendation	Candidate for in-depth review.

Model reference number 12

Name of model/ method/paper	Bioaccumulation in the soil to earthworm system. D W Connell and R D Markwell. *Chemosphere*, **20**, 1990, 91-100.
Date of publication	1990
Availability	Published paper.
Food chain considered	Soil → soil pore water → earthworm. The model is a three-compartment equilibrium model. The paper contains details of regression equations relating the worm bioconcentration factor to log K_{ow} from Lord *et al.* (1980) and Markwell *et al.* (1989) and generates a further regression equation from other published data.
Types of chemicals modelled	Stable, lipophilic organic chemicals.
Environment to which it relates	Generic.
Data requirements	Log K_{ow} and K_{oc}. It also requires the lipid content of earthworms and the soil organic carbon content.
Purpose of model/method	Research paper. The method was implemented in the original version of the TGD and EUSES, but has since been superseded by the method of Jager (1998) in the revised TGD and EUSES 2.0.
Summary of validation studies	The model was validated by comparison with earthworm bioaccumulation data from the literature. The data used was mainly for crop protection products with a log K_{ow} in the range 1.0 to 6.5.
Assessment	The model is simple to use and requires only a small amount of data. The method was used in the old (1993) version of the TGD and has since been superseded.
Recommendation	Not considered further.

Model reference number 13

Name of model/ method/paper	Biomagnification by aquatic organisms – a proposal. D.W. Connell. *Chemosphere*, **19**, 1989, 1573-1584.
Date of publication	1989
Availability	Published paper.
Food chain considered	Food → Fish. The model is a theoretical equilibrium model which predicts that the biomagnification factor will be independent of, or weakly dependent on, the octanol-water partition coefficient and will be unity for all compounds when expressed on a lipid weight basis. The model is presented as a series of equations.
Types of chemicals modelled	Organic chemicals.
Environment to which it relates	Generic.
Data requirements	Log K_{ow}.
Purpose of model/method	Research paper.
Summary of validation studies	The biomagnification factors predicted by the model were compared with experimental data for a number of persistent and accumulative organochlorine compounds (such as PCBs, hexachlorobenzene).
Assessment	The model predicts that the biomagnification factor (expressed as the concentration in fish/concentration in food; both on a lipid weight basis) will be around one for all chemicals independent of log K_{ow}. However, the model does not take into account the kinetics of uptake and elimination and may not be appropriate for substances that are rapidly metabolised or are only slowly taken up by the organism. Therefore, the conclusion that the biomagnification factor should be close to one may not be appropriate for all chemicals.
Recommendation	Not considered further.

Model reference number 14

Name of model/ method/paper	CSOIL Exposure of man to soil contamination. *A qualitative and quantitative analysis, resulting in proposals for human-toxicological C values*. R van den Berg. RIVM Report 725201006/1995. Rijksinstituut voor Volksgezondheid en Milieu, Bilthoven, Netherlands (in Dutch).
Date of publication	1995 (and updated 2000)
Availability	Published reports. Further details are given in published reports Rikken and Lijzen (2004), Rikken *et al.* (2001) and Lijzen *et al.* (2001).
Food chain considered	Contaminated soil → humans. Contaminated soil → air → humans. Contaminated soil → drinking water → humans. Contaminated soil → vegetation → humans. For organic chemicals, the methods used are based on Briggs *et al.* (1982 and 1983) and Trapp and Matthies (1995).
Types of chemicals modelled	Organic chemicals, metals and inorganic compounds.
Environment to which it relates	Generic (the Netherlands).
Data requirements	Not clear, but will probably include log K_{ow} and vapour pressure.
Purpose of model/method	The model is used within the Netherlands to quantify the residential exposure to substances from contaminated soil.
Summary of validation studies	A comparison of the CSOIL method with the method used in EUSES/TGD is given in Rikken and Lijzen (2004). Swartjes (2002) carried out a comparison of CSOIL with other similar models, including the CLEA model.
Assessment	The method appears to perform the same function as the CLEA model in the United Kingdom.
Recommendation	Not considered further.

Model reference number 15

Name of model/ method/paper	SEDISOIL *Model for the calculation of human exposure due to contaminated sediments.* G J M Bockting, J G Koolenbrander M and F A Swartjes. RIVM Report 715810011/1996. Rijksinstituut voor Volksgezondheid en Milieu, Bilthoven, Netherlands.
Date of publication	1996
Availability	Details are available in published reports; other reports such as Otte *et al.* (2000), Lijzen *et al.* (2001) are also relevant.
Food chain considered	Contaminated sediment → fish → humans. The model considers a scenario, "recreational fishing", where exposure to humans occurs through own-caught fish and ingestion of sediment.
Types of chemicals modelled	Organic chemicals, metals and inorganic compounds.
Environment to which it relates	Generic (the Netherlands).
Data requirements	The chemical-specific information required includes molecular weight, solubility, acid dissociation constant, log K_{ow} , organic carbon-water partition coefficient, fish bioconcentration factor (for metals), soil-water partition coefficient (for metals) and oral absorption factor for soil.
Purpose of model/method	The model is used within the Netherlands to derive human toxicological risk limits for sediment.
Summary of validation studies	None located as part of this work.
Assessment	The main details of the method are in Dutch, but the method appears to consider equilibrium partitioning between the sediment and fish and does not incorporate bioaccumulation by other routes as such.
Recommendation	Not considered further.

Model reference number 16

Name of model/ method/paper	Predicting plant uptake of organic chemicals from soil or air using octanol/water and octanol/air partition ratios and a molecular connectivity index. D L Dowdy and T E McKone. *Environmental Toxicology and Chemistry*, **16**, 1997, 2448-2456.
Date of publication	1997
Availability	Published paper.
Food chain considered	Soil (pore water) → plant. Air → plant. The paper presents a series of regression equations estimating the bioconcentration ratio for both above ground and below ground vegetation, based on either molecular connectivity index or the log K_{ow}. Some of the data used in the regression equations are from Briggs *et al.* (1982).
Types of chemicals modelled	The chemicals considered included a range of pesticides and organochlorine compounds.
Environment to which it relates	Generic. The method is based on regression equations derived from experimental data.
Data requirements	Molecular connectivity index or log K_{ow}.
Purpose of model/method	Research paper.
Summary of validation studies	None. The method is based on regression equations derived from experimental data.
Assessment	The method uses relatively little chemical-specific data and is simple to use. The methods are similar in some respects to those already incorporated into the TGD.
Recommendation	Candidate for in-depth review (in conjunction with Model reference number 60).

Model reference number 17

Name of model/ method/paper	Prediction of chemical biotransfer of organic chemicals from cattle diet into beef and milk using the molecular connectivity index. D L Dowdy, T E McKone and D P H Hsieh. *Environmental Science and Technology*, **30**, 1996, 984-989.
Date of publication	1996
Availability	Published paper.
Food chain considered	Food → cattle (beef) → milk. The method estimates biotransfer factors relating the concentration of chemical found in animal tissues (such as beef and milk) to the daily intake. The method uses the molecular connectivity index. The method is based on a regression equation using biotransfer factors taken from the literature.
Types of chemicals modelled	A range of non-polar organic compounds including aliphatic and aromatic compounds. Polarity correction factors are given for a wide range of substituent groups including nitriles/cyanides, triazines, pyridines, nitro-compounds, ureas, acetamides, other nitrogen-containing groups (aliphatic compounds, cycloalkanes, aromatic compounds), aromatic ethers, aliphatic ethers, esters, aliphatic alcohols, carboxylic acids, carbonyl compounds, organophosphorus compounds, thiocarbonyl compounds and sulfones.
Environment to which it relates	Generic. The method is based on field data.
Data requirements	The method requires the molecular connectivity index. These are based on the molecular structure.
Purpose of model/method	Research paper.
Summary of validation studies	The method is based on a regression equation using biotransfer factors taken from the literature (mainly for pesticides). The paper compares the regression equations obtained with those determined by Travis and Arms (1988) that are used in the TGD.
Assessment	The method is relatively simple to use once the molecular connectivity index of the molecule has been determined. The calculation of the molecular connectivity index is complicated, particularly for complex molecules, but programs are available to calculate the index values.
Recommendation	Candidate for in-depth review (in conjunction with Model reference number 60).

Model reference number 18

Name of model/ method/paper	Assessing the risk of biomagnification: a physiological approach. J W Everts, Y Eys, M Ruys, J Pijnenburg, H Visser and R Luttik. *Science of the Total Environment*, Supplement, 1993a, 1501-1506. Biomagnification and environmental quality criteria: a physiological approach. J W Everts, Y Eys, M Ruys, J Pijnenburg, H Visser and R Luttik. *ICES Journal of Marine Science*, **50**, 1993b, 333-335.
Date of publication	1993
Availability	Published paper.
Food chain considered	Marine water → fish or mussel → bird. The method considers the differences in energy content between laboratory food and field food and in metabolic rate between caged laboratory birds and wild birds. A similar approach for the terrestrial environment is given in Traas *et al.* (1996).
Types of chemicals modelled	Cadmium, mercury, persistent organochlorine compounds.
Environment to which it relates	Generic.
Data requirements	Requires the BCF for fish or mussels, the energy content of laboratory food used in the toxicity tests with the chemical, the energy content of the prey species (fish or mussels), the existence metabolic rate of the laboratory bird, and the metabolic rate of the wild bird species under normal conditions and conditions of peak activity.
Purpose of model/method	Research. To stimulate further discussion and research in methods for setting standards.
Summary of validation studies	None.
Assessment	The method given is not a bioaccumulation model as such, rather a general approach that could be used to take account of bioconcentration in setting standards. The method is similar to that currently used in the Technical Guidance Document in that it relates the concentration in food to the concentration in water using a BCF, but differs in that the calculation also takes into account the assimilation efficiency of energy.
Recommendation	The general framework presented may be useful when considering an overall approach to standard setting.

Model reference number 19

Name of model/ method/paper	FGETS (Food and Gill Exchange of Toxic Substances) and BASS (Bioaccumulation and Aquatic System Sumulator). Details of the model are given in the following papers: Modelling bioaccumulation of organic pollutants in fish with an application to PCBs in Lake Ontario salmonids. M C Barber, L A Suárez and R R Lassiter. *Canadian Journal of Fisheries and Aquatic Sciences*, **48**, 1991, 318-337. *Bioaccumulation and aquatic system simulator (BASS) user's manual beta test version 2.1.* M C Barber. United States Environmental Protection Agency, National Exposure Research Laboratory, EPA 600/R-01/035, 2001.
Date of publication	1991 onwards. The latest version of the FGETS model (3.0.18) was released in September 1994. The FGETS model has been incorporated into the BASS 2.1 model (2001) which can take into account population dynamics. The BASS model is currently available as a test version.
Availability	Published paper. The FGETs model can be downloaded free of charge from http://www.epa.gov/ceampubl/fchain/fgets/index.htm. The BASS model can be obtained directly from the author.
Food chain considered	Water → fish. Food → fish. The model considers diffusive exchange across gill membranes and intestinal mucosa. The model can calculate the uptake of chemicals via water only or from food and water jointly. The model can be used assuming a constant or time-varying water concentration.
Types of chemicals modelled	The FGETS model was designed for non-ionic, non-metabolised, organic chemicals. The BASS model is designed for hydrophobic organic compounds and some metals.
Environment to which it relates	Generic.
Data requirements	The chemical-specific data needed for the FGETS model includes melting point, molar volume and log K_{ow}. The fish species-specific information required in the model includes information on gill morphometry, feeding and growth rate, and the fractional aqueous, lipid and non-lipid organic composition (typical values are included in the model for various fish species).
Purpose of model/method	The FGETS model was developed by the USEPA and can be used to analyze the bioaccumulation of chemicals under laboratory or field conditions.
Summary of validation studies	The Barber *et al.* (1991) paper compares the modelled results obtained for certain PCBs with both laboratory data and field data for Lake Ontario salmonids.
Assessment	The method appears to require only relatively little chemical-specific input data and is available in a computerised form.
Recommendation	Candidate for in-depth review.

Model reference number 20

Name of model/ method/paper	Modelling biomagnification and metabolism of contaminants in harp seals of the Barents Sea. A J Fraser, I C BurK_{ow}, H Wolker and D Mackay. *Environmental Toxicology and Chemistry*, **21**, 2002, 55-61.
Date of publication	2002
Availability	Published paper.
Food chain considered	Food (cod, pelagic crustacean (Thermisto sp.) → seal. The model is a fugacity-based model consisting of three uptake processes (crustacean ingestion, cod ingestion, and respiration) and four loss processes (egestion, growth dilution, respiration and metabolism). The model is a development of the model of Campfens and Mackay (1997) and is presented as a series of equations.
Types of chemicals modelled	Organochlorine compounds.
Environment to which it relates	Barents Sea food chain.
Data requirements	The chemical-specific data required are not altogether clear but appear to be mainly log K_{ow} and Henry's law constant. The model as used in the paper calculates metabolism half-lives from biomagnification factors derived from field data. The model also requires seal-specific parameters such as volume of an average seal, inhalation rates and feeding rates.
Purpose of model/method	The purpose of the model was to analyse field data from a simple aquatic food chain and to determine biomagnification factors and metabolic half-lives for the substances considered.
Summary of validation studies	The model was developed partly based on field data.
Assessment	The model is an example of how general fugacity models (such as that developed by Campfens and Mackay, 1997) can be modified to specific situations. The model given here is relatively specific to a particular food chain and some of the assumptions used may be specific to the group of chemicals considered. It may be possible to modify the model to make it more generally applicable; however, it is not clear at this stage what chemical-specific information would be needed for this.
Recommendation	Candidate for in-depth review (in conjunction with Model reference number 11).

Model reference number 21

Name of model/ method/paper	ECOFATE and Food Chain Bioaccumulation Model. Details are published in the following paper: A model for predicting the bioaccumulation of hydrophobic organic chemicals in aquatic food-webs: application to Lake Ontario. F A P C Gobas. *Ecological Modelling*, **69**, 1993, 1-17.
Date of publication	1993
Availability	Published paper. The programs ECOFATE and Food Chain Bioaccumulation Model are available free of charge from http://www.rem.sfu.ca/toxicology/models.htm.
Food chain considered	Water → phytoplankton/zooplankton → fish → predatory fish. Sediment → benthos → fish → predatory fish. Food web used consists of phytoplankton, zooplankton, benthos (Pontoporeia and Oligochaetes), and fish (sculpin, alewife, smelt and salmonids). The model is a steady-state model based on the toxicokinetics of chemical uptake, elimination and bioaccumulation of the individual organisms within the food web. The method is presented as a series of equations. Version 1.1 of the Food Chain Bioaccumulation Model also incorporates the work of Morrison *et al.* (1996) on benthic organisms. The ECOFATE model consists of an environmental fate model, a toxicological hazard assessment model and a human health risk assessment model, as well as the food web bioaccumulation model, and allows calculations to be carried out on a time-dependent and steady-state basis.
Types of chemicals modelled	Hydrophobic organic chemicals.
Environment to which it relates	Generic. The paper applied the model to a Lake Ontario food web.
Data requirements	The chemical-specific information includes the log K_{ow} and the total concentration in water and sediment. The model also requires the organic carbon content of suspended particulates in water and sediment, and the lipid content, weight and information on the diet of the species considered in the food chain.
Purpose of model/method	Research paper.
Summary of validation studies	The model results were compared with field data for a Lake Ontario food web. Morrison *et al.* (1997 and 1999) adapted and tested the model for PCBs in Western Lake Erie and Lake Ontario. Comparisons of the results of this model with other models have also been carried out (see Burkhard, 1998). Some of the principles behind the method have been tested experimentally by Gobas *et al.* (1993).
Assessment	The method is available in computerised form and can be adapted for different aquatic food webs. The method requires relatively little chemical-specific input data.
Recommendation	Candidate for in-depth review.

Model reference number 22

Name of model/ method/paper	Dynamics of dietary bioaccumulation and faecal elimination of hydrophobic organic chemicals in fish. F A P C Gobas, D C G Muir and D Mackay. *Chemosphere*, **17**, 1988, 943-962.
Date of publication	1988
Availability	Published paper.
Food chain considered	Water → fish. Food → fish. The model is a dynamic fugacity model. The model is presented as a series of equations.
Types of chemicals modelled	Hydrophobic organic chemicals.
Environment to which it relates	Generic.
Data requirements	The chemical-specific information required includes log K_{ow} , assimilation efficiency (can be estimated from log K_{ow} in the model) and rate constant for elimination (metabolism). The model also requires some fish-specific data including fish weight, fish volume, lipid content and feeding rate amongst others. Typical values are given for guppy, goldfish, salmon, rainbow trout and fathead minnow.
Purpose of model/method	Research paper.
Summary of validation studies	None located as part of this work.
Assessment	The model uses relatively little chemical-specific information and could readily be adapted for different fish species. The model would need to be computerised (spread-sheet?) for it to be used on a regular basis.
Recommendation	Candidate for in-depth review (in conjunction with Model reference number 11).

Model reference number 23

Name of model/ method/paper	Quantitative structure activity relationships for predicting the bioaccumulation of POPs in terrestrial food-webs. F A P C Gobas, B C Kelly and J A Arnot, *QSAR and Combinatorial Science*, **22**, 2003, 329-336.
Date of publication	2003
Availability	Published paper.
Food chain considered	Food and air $\rightarrow$ terrestrial mammal (wolves). The method is a generic QSAR that relates the BMF for a terrestrial organism (mammal) to log K_{ow} and octanol-air partition coefficient. The method is based on a theoretical model describing a terrestrial food chain.
Types of chemicals modelled	Organic chemicals.
Environment to which it relates	Canada. The method is a generic method but certain parameters were chosen to represent a food web consisting of three trophic interactions/levels under Canadian environmental conditions.
Data requirements	Log K_{ow} and octanol-air partition coefficient. The method can also use the metabolic transformation rate. The method requires several species-specific data including weight, lipid content, respiration rate, feeding rate, various excretion rates and air and dietary uptake efficiencies, amongst others. Example values are given for arctic wolves.
Purpose of model/method	The method was developed as a screening tool to determine BMFs (particularly in relation to the bioaccumulation criteria under the Canadian Environmental Protection Act 1999).
Summary of validation studies	The model was compared with field BMFs for a range of persistent organic compounds in wolves from the Canadian arctic.
Assessment	The method requires on few chemical-specific data. The method could be modified for other species.
Recommendation	Candidate for in-depth review (in conjunction with Model reference number 29).

Model reference number 24

Name of model/ method/paper	Modelling and monitoring organochlorine and heavy metal accumulation in soils, earthworms, and shrews in Rhine-Delta floodplains. A J Hendriks, W-C Ma, J J Brouns, de Ruiter- E M Dijkman and R Gast, *Archives of Environmental Contamination and Toxicology*, **29**, 115-127.
Date of publication	1995
Availability	Published paper.
Food chain considered	Soil → earthworm → shrew. A simple equilibrium model was used to predict the ratio of the concentration in earthworms to the concentration in soil. Biomagnification factors for shrews were not modelled but calculated directly from the measured data.
Types of chemicals modelled	Organochlorine chemicals (polychlorinated biphenyls, pentachlorobenzene, hexachlorobenzene, hexachlorocyclohexane, DDT and derivatives, dieldrin and heptachlorepoxide).
Environment to which it relates	Rhine-Delta.
Data requirements	Log K_{ow}. The method also requires the organic carbon content of the soil and the lipid content of earthworms and shrews.
Purpose of model/method	Research paper.
Summary of validation studies	The modelled results were compared with field data.
Assessment	The model requires relatively little chemical-specific input data. However, the model is very simplistic and appears to have limited predictive potential. The dataset, however, would be useful for validation purposes.
Recommendation	Not considered further (the dataset may be useful for validation).

Model reference number 25

Name of model/ method/paper	A review of models for estimating terrestrial ecological receptor exposure to chemical contaminants. B K Hope. *Chemosphere*, **30**, 1995, 2267-2287.
Date of publication	1995
Availability	Published paper
Food chain considered	Rainsplash → plant leaves. Soil → plant roots. Plant roots → above ground parts. Air (vapour and particulates) → plant leaves. Soil/sediment → bird/mammal/reptile/amphibian (dermal contact). Air (vapour) → bird/mammal/reptile/amphibian. Air (particulates) → humans (possibly applicable to mammals). Food → bird/mammal/reptile/amphibian. Water → aquatic plant. The paper presents a series of models and equations that can be used for different steps in the food chain. The models include those of Briggs *et al.* (1982 and 1983), Travis and Arms (1988), Paterson *et al.* (1990) and Reiderer (1990),
Types of chemicals modelled	Organic chemicals.
Environment to which it relates	Generic
Data requirements	The requirements are variable but are generally limited to log K_{ow} and Henry's law constants. Some models, particularly the dermal contact and food ingestion models, require other chemical-specific data such as dermal and dietary absorption factors and depuration rates
Purpose of model/method	The paper presents a suite of simple models that can be combined and used to estimate terrestrial wildlife exposures.
Summary of validation studies	None.
Assessment	The methods presented require only relatively few chemical-specific data. Some of the methods are also reviewed separately in this report, and some are incorporated into the TGD method.
Recommendation	Candidate for in-depth review (in conjunction with Model reference number 60 and Model reference number 51).

Model reference number 26

Name of model/ method/paper	A novel and simple model of the uptake of organic chemicals by vegetation from air and soil. H Hung and D Mackay. *Chemosphere*, **35**, 1997, 959-977.
Date of publication	1997
Availability	Published paper. The paper indicates that a BASIC computer version of the model is available from http://www.trentu.ca/envmodel, but this could not be located.
Food chain considered	Soil → vegetation. Air → vegetation. The model is a simple three-compartment fugacity model. The three compartments considered are leaf, stem (including fruits and seeds) and root. The model is presented as a series of equations. The model is a simplification of the dynamic model of Paterson *et al.* (1994).
Types of chemicals modelled	Organic chemicals.
Environment to which it relates	Generic.
Data requirements	The model needs a variety of partition coefficients such as soil-water, root-water, stem-water, leaf-water and air-water partition coefficient. Methods are given to estimate many of these partition coefficients from log K_{ow} in the absence of data. The model can also take into account metabolism in the plant, but assumes for most substances this is very slow. The model uses a number of plant-specific data such as the sap, air and water flow rates, growth rate and the lipid content; example values are given for soybean.
Purpose of model/method	Research paper.
Summary of validation studies	The model results were compared with experimental data for uptake of ^{14}C-bromacil by soybean under hydroponic conditions.
Assessment	The model is relatively simple to use and requires little chemical-specific information at a basic level (although experimental partitioning data can be used in the model if available). The model could be readily adapted to take account of specific plant and soil parameters.
Recommendation	Candidate for in-depth review (in conjunction with Model reference number 51).

Model reference number 27

Name of model/ method/paper	Mechanistic approach for estimating bioconcentration of organic chemicals in earthworms (Oligochaeta). T Jager, *Environmental Toxicology and Chemistry*, **17**, 1998, 2080-2090.
Date of publication	1998
Availability	Published paper.
Food chain considered	Soil $\rightarrow$ earthworm. The paper describes a generic equilibrium model for predicting the uptake and accumulation of chemicals in earthworms from soil. The method is presented as a series of equations.
Types of chemicals modelled	Organic chemicals.
Environment to which it relates	Generic.
Data requirements	Log K_{ow} and soil organic carbon partition coefficient. The species-dependent data includes the water and lipid content of worms (typical values are given).
Purpose of model/method	Research paper. The method has since been incorporated into the TGD method.
Summary of validation studies	A comparison was made between predicted and experimental bioconcentration factors for a range of neutral organic compounds and chlorophenols, covering a log K_{ow} range of -0.47 to 8.0
Assessment	The method is easy to use and requires relatively little chemical-specific input data. The method is incorporated into the TGD.
Recommendation	Candidate for in-depth review (in conjunction with Model reference number 60 and Model reference number 84).

Model reference number 28

Name of model/ method/paper	*Estimation methods for bioaccumulation in risk assessment of organic chemicals*. D T Jager and T Hamers. RIVM Report 679102 013/1997. Rijksinstituut voor Volksgezondheid en Milieu, Bilthoven, Netherlands.
Date of publication	1997
Availability	Published report.
Food chain considered	Water → fish (excluding food uptake). Soil → earthworms. Soil → plant. The paper considers a general approach to modelling bioaccumulation. Specific example steady-state models are given for bioconcentration in fish and uptake from soil in plants and earthworms. The models are presented as a series of equations.
Types of chemicals modelled	Organic chemicals.
Environment to which it relates	Generic.
Data requirements	Generally log K_{ow}. Information on metabolism rates can also be incorporated. The models also require some species-specific information (such as lipid and water contents). Example values for various species and recommended generic values are given.
Purpose of model/method	Research paper.
Summary of validation studies	The paper compares the modelled results with those obtained using the methods outlined in the TGD (1996 version).
Assessment	The methods require only a limited amount of chemical-specific information and could be modified relatively easily for different species. The models would need to be computerised (spreadsheet) for routine use. The methods are very similar to those derived elsewhere.
Recommendation	Candidate for in-depth review (in conjunction with Model reference number 60 and Model reference number 84).

Model reference number 29

Name of model/ method/paper	An arctic terrestrial food-chain bioaccumulation model for persistent organic pollutants. B C Kelly and F A P C Gobas. *Environmental Science and Technology*, **37**, 2003, 2966-2974.
Date of publication	2003
Availability	Published paper.
Food chain considered	Air and snowpack melt water → lichen and willows → caribou → wolf. The model consists of a series of mechanistic equations and comprises an air-to-vegetation distribution model and a two-compartment bioaccumulation model for terrestrial organisms. The model has been developed based on empirical data for this food chain published by Kelly and Gobas (2001).
Types of chemicals modelled	Persistent organic pollutants.
Environment to which it relates	Generic arctic food chain.
Data requirements	The chemical-specific data required include vapour pressure, log K_{ow} , octanol-air partition coefficients, Henry's law constant and information on the metabolic transformation potential. The organism-specific parameters needed for the model were based on known values for the food chain considered and included lipid contents, lung ventilation rates and feeding rates amongst others.
Purpose of model/method	Research paper.
Summary of validation studies	The model predictions for 25 substances were compared with field data on the levels in caribou and wolves from the Canadian Arctic.
Assessment	The chemical-specific requirements of the model are modest. The model is specific to the arctic food chain considered. It would be possible to construct a similar model for other food chains, although a significant amount of information on the food chain would need to be obtained. The model would need to be computerised (spread sheet?) to be used on a routine basis.
Recommendation	Candidate for in-depth review.

Model reference number 30

Name of model/ method/paper	Modelling the accumulation of three waterborne chlorinated ethanes in fathead minnows (Pimephales promelas): A physiologically based approach. G J Lien, J W Nichols, J M McKim and C A Gallinat. *Environmental Toxicology and Chemistry*, **13**, 1994, 1195-1205.
Date of publication	1994
Availability	Published paper.
Food chain considered	Water → gills → fish. Water → skin → fish. The model is a physiologically based toxicokinetic model (PBTK) and is similar in principle to other models by the same group (Nichols *et al.,* 1990, 1998 and 2004a). The model is presented as a series of equations.
Types of chemicals modelled	Non-polar, non-metabolized organic chemicals. The model is designed for substances of low to moderate hydrophobicity (example calculations are given for 1,1,2,2-tetrachloroethane, pentachloroethane and hexachloroethane).
Environment to which it relates	Generic. The model is based on properties of fathead minnows and is designed for small fish.
Data requirements	The chemical-specific data required by the model include several blood-water and tissue-blood partition coefficients. The fish-related data used include oxygen consumption rates, fractional volumes of carcass, viscera and fat in the fish and the fractional blood flows to carcass, viscera, fat and skin (values are given for fathead minnow).
Purpose of model/method	Research paper.
Summary of validation studies	The modelled data for 1,1,2,2-tetrachloroethane, pentachloroethane and hexachloroethane were compared with experimentally derived data.
Assessment	The model is quite complex and would require computerisation (spread sheet?) in order to be routinely used. The model requires some chemical-specific data that is unlikely to be routinely available for a wide range of substances, which may limit its general applicability.
Recommendation	Candidate for in-depth review (in conjunction with Model reference number 47).

Model reference number 31

Name of model/ method/paper	A steady-state model of PCB accumulation in dab food web. V Loizeau and A Menesguen. *Oceanologica Acta*, **16**, 1993, 633-639.
Date of publication	1994
Availability	Published paper.
Food chain considered	Marine water (dissolved and sediment) → phytoplankton/detritus → crustaceans; annelids; molluscs; ophiuroids → dab. The model is a five-compartment steady-state model. The model is an extension of the Thomann (1989) approach. A similar model has also been developed by the same authors for a sea bass food web (Loizeau *et al.,* 2001).
Types of chemicals modelled	Polychlorinated biphenyls (PCBs).
Environment to which it relates	Seine Estuary (Eastern English Channel).
Data requirements	Not clear. Insufficient information is presented to make an assessment.
Purpose of model/method	Research paper.
Summary of validation studies	The model was validated using samples collected from the Seine Estuary.
Assessment	The model appears to use quite a lot of information on the main physical and biological characteristics of the Seine Estuary and so is specific to this location. The model appears to be similar to other steady-state models and may be too specific to a given food chain to be used directly in this project. However, it may be possible to adapt it to other food chains. The model may also contain useful information on organisms, such as feeding rates and respiration rates, which could be used in other models.
Recommendation	Candidate for in-depth review.

Model reference number 32

Name of model/ method/paper	A model of PCB bioaccumulation in the sea bass food web from the Seine Estuary (Eastern English Channel). V Loizeau, A Abarnou, P Cugier, A Jaouen-Madoulet, A-M Le Guellec and A Menesguen. *Marine Pollution Bulletin*, **43**, 2001, 242-255.
Date of publication	2001
Availability	Published paper.
Food chain considered	Marine water → phytoplankton/detritus → crustaceans (shrimps and mysidaceans) → small fish (guppies) → sea bass. The model is a steady-state model and considers six biotic compartments as well as water (the dissolved concentration and the concentration in suspended particulate matter (detritus and phytoplankton)). Later (dynamic) adaptations of the model take into account seasonal variations and population dynamics, to allow accumulation in different age classes to be determined. A similar model has also been developed by the same authors for the dab food web (Loizeau and Menesguen, 1993).
Types of chemicals modelled	Polychlorinated biphenyls (PCBs).
Environment to which it relates	Seine Estuary (Eastern English Channel).
Data requirements	Not clear. Insufficient information is given to make an assessment.
Purpose of model/method	Research paper.
Summary of validation studies	The model was validated using samples collected from the Seine Estuary. These were analysed for 17 selected PCB congeners and the concentrations found were compared with the predicted concentration.
Assessment	The model (in particular the later dynamic versions) appears to use quite a lot of information on the physical and biological characteristics of the Seine Estuary and so is specific to this location. The model appears to be similar to other steady-state models and may be too specific to a given food chain to be used directly in this project. However, it may be possible to adapt it to other food chains. The model may also contain useful information on organisms, such as feeding and respiration rates, which could be used in other models.
Recommendation	Candidate for in-depth review (in conjunction with Model reference number 31).

Model reference number 33

Name of model/ method/paper	Uptake of pesticides from water and soil by earthworms. K A Lord, G A Briggs, M C Neale and R Manlove. *Pesticide Science*, **11**, 1980, 401-408.
Date of publication	1980
Availability	Published paper
Food chain considered	Soil → earthworms. (Pore) water → earthworms. The paper presents a regression equation relating the bioconcentration factor for worms (the distribution between worm solid and water) to the log K_{ow}. The results are based on experiments with whole and macerated worms.
Types of chemicals modelled	Pesticides.
Environment to which it relates	Generic.
Data requirements	Log K_{ow}.
Purpose of model/method	Research paper.
Summary of validation studies	None located as part of this work.
Assessment	The method is simple to use and is in principle similar to the method currently used in the TGD. The data were used in the development of the Connell and Markwell (1990) model that was incorporated into the original version of the TGD. This method has since been superseded by the method of Jager (1998) in the revised TGD and EUSES.
Recommendation	Not considered further.

Model reference number 34

Name of model/ method/paper	Application of a polychlorinated biphenyls bioaccumulation model to Lake Ontario lake trout. G K Luk and F Brockway. *Ecological Modelling*, **101**, 1997, 97-111.
Date of publication	1997
Availability	Published paper.
Food chain considered	Water → food → lake trout. The model is a bioenergetics-based accumulation model. The model is presented as a series of equations.
Types of chemicals modelled	Polychlorinated biphenyls.
Environment to which it relates	Lake Ontario.
Data requirements	The exact chemical-specific parameters required are not entirely clear from the paper. The model requires a relatively large amount of species-specific data including several food assimilation, growth and metabolism parameters.
Purpose of model/method	Research paper.
Summary of validation studies	The modelled results for PCB congeners 101 and 153 were compared with field data from a Lake Ontario food chain.
Assessment	The model is specific to a Lake Ontario food chain. It would be possible to modify the method to be applicable to other food chains, but this would require a large amount of species-specific information.
Recommendation	Not considered further.

Model reference number 35

Name of model/ method/paper	Bioaccumulation of lipophilic compounds from sediments by oligochaetes. R D Markwell, D W Connell and A J Gabric. *Water Research*, **23**, 1989, 1443-1450.
Date of publication	1989
Availability	Published paper.
Food chain considered	Sediment (pore water) → oligochaete. The paper presents a regression equation relating the bioconcentration factor to log K_{ow}. The data were taken from laboratory experiments with *Tubifex tubifex* and *Limnodilus hoffmeisteri*. The method considers the bioaccumulation in oligochaete to take place via two partitioning processes, sediment to interstitial (pore) water and interstitial water to oligochaete.
Types of chemicals modelled	Chlorinated hydrocarbons.
Environment to which it relates	Generic.
Data requirements	Log K_{ow}.
Purpose of model/method	Research paper.
Summary of validation studies	The method is based on a regression analysis of experimental data.
Assessment	The method is easy to use and requires only minimal chemical-specific information.
Recommendation	Candidate for in-depth review.

Model reference number 36

Name of model/ method/paper	Dynamics of leaching, uptake, and translocation: The Simulation Model Network Atmosphere-Plant-Soil (SNAPS). M Matthies and H Behrendt. In *Plant Contamination: Modelling and Simulation of Organic Chemical Processes* (editors S Trapp and J C McFarlane), pp215-243. Boca Raton: Lewis Publishers.
Date of publication	1995
Availability	Published paper.
Food chain considered	Soil → plant. Air → plant. SNAPS is a system of simulation models that considers the behaviour of chemicals in soils, their uptake into plants, and their exchange with the atmosphere and groundwater. The model is based on the water dynamics in soil and plants during the vegetation period and includes a soil-water model (SWACRO), a soil chemical transport model and a plant fate model. The plant fate model is that given in Trapp (1995).
Types of chemicals modelled	Organic chemicals. The model was run with three pesticides (carbofuran, isoproturon and terbuthylazine).
Environment to which it relates	Generic.
Data requirements	The chemical-specific data needed include water solubility, vapour pressure, log K_{ow} , half-life in soil, half-life in plants, transpiration stream concentration factor and soil application rates. It also requires information on soil properties, agricultural practice and climate data, crop properties.
Purpose of model/method	Research paper.
Summary of validation studies	None.
Assessment	The plant uptake part of the model is essentially the same as that given in Trapp (1995) that is included in the TGD. The other parts of the model relate mainly to the prediction of the behaviour and transport of chemicals in soils.
Recommendation	Not considered further.

Model reference number 37

Name of model/ method/paper	The transport and affinity of substituted benzenes in soybean stems. J K McCrady, C McFarlane and F T Lindstrom. *Journal of Experimental Botany*, **38**, 1987, 1875-1890.
Date of publication	1987
Availability	Published paper.
Food chain considered	Transpiration stream → plant stem. A theoretical mass transport model is given to describe the adsorption in the xylem tissue. A regression equation relating the accumulation factor to log K_{ow} is given.
Types of chemicals modelled	Non-ionised substituted benzenes (log K_{ow} around 1.5 to 5.0).
Environment to which it relates	Soybean plants.
Data requirements	Log K_{ow}.
Purpose of model/method	Research paper.
Summary of validation studies	The method was fitted to experimental data obtained using a positive pressure perfusion technique with isolated stem segments.
Assessment	The method only allows the uptake into/transport in stems to be estimated. This process is considered in many other of the plant uptake models (including the TGD) and so this paper may be most useful for validation of, or incorporation into, other models.
Recommendation	Not considered further (may be useful for validation purposes).

Model reference number 38

Name of model/ method/paper	Model of the fate of hydrophobic contaminants in cows. M S McLachlan. *Environmental Science and Technology*, **28**, 1994, 2407-2414.
Date of publication	1994
Availability	Published paper. The model has since been incorporated into the ACC-Human model (Czub and McClachlan, 2004a).
Food chain considered	Food → cow → milk The model is a fugacity-based model that describes the fate of organic chemicals in lactating cows. The model is presented as a series of equations representing both steady-state and non-steady state conditions.
Types of chemicals modelled	Organic chemicals.
Environment to which it relates	Generic.
Data requirements	The chemical-specific data requirements appear to be mainly log K_{ow}. The model also requires the contaminant ingestion rate and the milk transfer coefficient
Purpose of model/method	Research paper.
Summary of validation studies	A comparison of modelled and experimental data was carried out for PCB 138.
Assessment	The model requires only a limited amount of chemical-specific data. The model has recently been incorporated into the ACC-Human model.
Recommendation	Candidate for in-depth review (in conjunction with Model reference number 2).

Model reference number 39

Name of model/ method/paper	A simple model to predict accumulation of PCDD/Fs in an agricultural food chain. M S McLachlan. *Chemosphere*, **34**, 1997, 1263-1276.
Date of publication	1994
Availability	Published paper. Some of the principles of the model have since been incorporated into the ACC-Human model (Czub and McClachlan, 2004a).
Food chain considered	Air→ plant → cow (meat) → milk. Soil → plant → cow (meat) → milk. The model is presented as a series of equations that are specific to the chemicals being modelled.
Types of chemicals modelled	Polychlorinated dibenzofurans and dibenzo-p-dioxins.
Environment to which it relates	Generic.
Data requirements	The model uses equations/assumptions specific to polychlorinated dibenzofurans and dibenzo-p-dioxins.
Purpose of model/method	Research paper.
Summary of validation studies	A comparison of modelled and experimental data was carried out using field data from Germany.
Assessment	The model is specific to the polychlorinated dibenzofurans and dibenzo-p-dioxins. Some of the principles used in the model have recently been incorporated into the ACC-Human model.
Recommendation	Candidate for in-depth review (in conjunction with Model reference number 2).

Model reference number 40

Name of model/ method/paper	A design of two simple models to predict PCDD/F concentrations in vegetation and soils. M Meneses, M Schuhmacher and J L Domingo. *Chemosphere*, **46**, 2002, 1393-1402.
Date of publication	2002
Availability	Published paper.
Food chain considered	Soil → vegetation. Air (vapour and particulate phase) → vegetation. The model considers vapour-phase absorption, dry particle deposition, wet particle deposition and uptake via roots. The model is presented as a series of equations.
Types of chemicals modelled	Chlorinated dibenzo-p-dioxins and dibenzofurans.
Environment to which it relates	Generic.
Data requirements	The chemical-specific data required include log K_{ow} , Henry's law constant, deposition velocity, volumetric washout fraction, root uptake bioconcentration factor, and the fraction adsorbed to particles in air.
Purpose of model/method	Research paper.
Summary of validation studies	The method was validated using measured data on chlorinated dibenzo-p-dioxins and dibenzofurans.
Assessment	Some of the chemical-specific parameters will not be available for a large number of chemicals. This limits the general applicability of the model.
Recommendation	Not considered further.

Model reference number 41

Name of model/ method/paper	Development and verification of a bioaccumulation model for organic contaminants in benthic invertebrates. H A Morrison, F A P C Gobas, R Lazar and G D Haffner. *Environmental Science and Technology*, **30**, 1996, 3377-3384.
Date of publication	1996
Availability	Published paper.
Food chain considered	Sediments → [food such as plankton and suspended solids] → invertebrates. The model is a non-equilibrium steady-state model to predict the bioaccumulation of organic chemicals by filter feeding and detritivorous benthic invertebrates. The model is presented as a series of equations. The method has been incorporated into the ECOFATE/Food Chain Bioaccumulation Model.
Types of chemicals modelled	Organic chemicals.
Environment to which it relates	Generic.
Data requirements	The chemical-specific information required includes log K_{ow} , organic carbon-water partition coefficient. The paper contains details of the necessary species-specific parameters for a generic benthic invertebrate, Gammarus sp., crayfish, zebra mussel and caddisfly larvae.
Purpose of model/method	Research. The method was contrasted with the equilibrium partitioning approach.
Summary of validation studies	The modelled results were compared with field data on PCB levels in various benthic invertebrate species in western Lake Erie.
Assessment	The method requires only a limited amount of chemical-specific information. The modelling approach could be modified for other food chains/invertebrates. The model would need to be computerised (spreadsheet?) for routine use.
Recommendation	Candidate for in-depth review (in conjunction with Model reference number 21).

Model reference number 42

Name of model/ method/paper	Calculation of bioconcentration factors of persistent hydrophobic compounds in the air/vegetation system. J F Müller, D W Hawker and D W Connell. *Chemosphere*, **29**, 1994, 623-640.
Date of publication	1994
Availability	Published paper.
Food chain considered	Air → plant. The model uses a fugacity approach.
Types of chemicals modelled	Organic chemicals.
Environment to which it relates	Generic.
Data requirements	The chemical-specific information needed is log K_{ow} and Henrys' law constant. The model also needs plant-specific data such as the volume fractions of the individual phases in the leaf. Values are given in the paper for spruce needles, azalea leaves and grass leaves.
Purpose of model/method	Research paper. The aim of the model is to predict leaf-atmosphere partition coefficients.
Summary of validation studies	The model was evaluated using laboratory-based experimentally determined partition coefficients for a group of mainly chlorohydrocabons.
Assessment	The model could be easily adapted for other plants if the relevant properties of the plant were available. The paper gives the necessary overall equation to estimate the leaf-atmosphere partition coefficient. The chemical-specific data requirements of the model are modest.
Recommendation	Candidate for in-depth review (in conjunction with Model reference number 51).

Model reference number 43

Name of model/ method/paper	A physiologically based toxicokinetic model for the uptake and disposition of waterborne organic chemicals in fish. J W Nichols, J M McKim, M E Andersen, M L Gargas, H J Clewell III and R J Erickson. *Toxicology and Applied Pharmacology*, **106**, 1990, 433-447.
Date of publication	1990
Availability	Published paper.
Food chain considered	Water → gills → fish. The model is a physiologically based toxicokinetic model (PBTK) and is similar in principle to other models by the same group (Lien *et al.,* 1994; Nichols *et al.,* 1991, 1998 and 2004a). The model is presented as a series of equations.
Types of chemicals modelled	Organic chemicals (example calculations are given for pentachloroethane).
Environment to which it relates	Generic. Parameters are given in the paper relevant for rainbow trout.
Data requirements	The chemical-specific data required by the model include several tissue-blood partition coefficients and the blood-water partition coefficient. The fish-related data used include oxygen consumption rates, volumes of the compartments within the fish (such as liver, kidney, fat, poorly perfused compartment and richly perfused compartment) and the blood flows to these compartments amongst others (typical values are given for rainbow trout).
Purpose of model/method	Research paper.
Summary of validation studies	The modelled data for pentachloroethane were compared with experimentally derived data.
Assessment	The model is quite complex and would require computerisation (spread sheet?) in order to be routinely used. The model requires some chemical-specific data that are unlikely to be routinely available for a wide range of substances, which may limit its general applicability.
Recommendation	Candidate for in-depth review (in conjunction with Model reference number 47).

Model reference number 44

Name of model/ method/paper	Physiologically based toxicokinetic modelling of three chlorinated ethanes in rainbow trout (Oncorhynchus mykiss). J W Nichols, J M McKim, G J Lien, A D Hoffman and S L Bertelsen. *Toxicology and Applied Pharmacology*, **110**, 1991, 374-389.
Date of publication	1991
Availability	Published paper.
Food chain considered	Water → gills → fish. The model is a physiologically based toxicokinetic model (PBTK) and is similar in principle to other models by the same group (Lien *et al.,* 1994; Nichols *et al.,* 1990, 1998 and 2004a). The model is presented as a series of equations. A similar model for channel catfish has also been developed (Nichols *et al.,* 1993).
Types of chemicals modelled	Organic chemicals (example calculations are given for 1,1,2,2-tetrachloroethane, pentachloroethane and hexachloroethane).
Environment to which it relates	Generic. Parameters are given in the paper relevant for rainbow trout. A similar model for channel catfish has also been developed (Nichols *et al.,* 1993).
Data requirements	The chemical-specific data required by the model include several tissue-blood partition coefficients and the blood-water partition coefficient. The fish-related data used include oxygen consumption rates, volumes of the compartments within the fish (such as liver, kidney, fat, poorly perfused compartment and richly perfused compartment) and the blood flows to these compartments amongst others (typical values are given for rainbow trout).
Purpose of model/method	Research paper.
Summary of validation studies	The modelled data for 1,1,2,2-tetrachloroethane, pentachloroethane and hexachloroethane were compared with experimentally derived data.
Assessment	The model is quite complex and would require computerisation (spread sheet?) in order to be routinely used. The model requires some chemical-specific data that are unlikely to be routinely available for a wide range of substances, which may limit its general applicability.
Recommendation	Candidate for in-depth review (in conjunction with Model reference number 47).

Model reference number 45

Name of model/ method/paper	A physiologically based toxicokinetic model for dermal absorption of organic chemicals by fish. J W Nichols, J M McKim, G J Lien, A D Hoffman, S L Bertelsen and C M Elonen. *Fundamental and Applied Toxicology*, **31**, 1996, 229-242.
Date of publication	1996
Availability	Published paper.
Food chain considered	Water → gills → fish. Water → skin → fish. The model is a physiologically based toxicokinetic model (PBTK) and is similar in principle to other models by the same group (Lien *et al.,* 1994; Nichols *et al.,* 1990, 1991, 1998 and 2004a). The model is presented as a series of equations.
Types of chemicals modelled	Non-polar, non-metabolized organic chemicals (example calculations are given for 1,1,2,2-tetrachloroethane, pentachloroethane and hexachloroethane).
Environment to which it relates	Generic. Parameters are given in the paper relevant for rainbow trout and channel catfish.
Data requirements	The chemical-specific data required by the model include several tissue-blood partition coefficients, blood-water partition coefficients and skin-water partition coefficients. The fish-related data used include oxygen consumption rates, volumes of the compartments within the fish (such as liver, kidney, fat, poorly perfused compartment, richly perfused compartment, and skin) and the blood flows to these compartments amongst others (typical values are given for rainbow trout and channel catfish).
Purpose of model/method	Research paper.
Summary of validation studies	The modelled data for 1,1,2,2-tetrachloroethane, pentachloroethane and hexachloroethane were compared with experimentally derived data.
Assessment	The model is quite complex and would require computerisation (spread sheet?) in order to be routinely used. The model requires some chemical-specific data that are unlikely to be routinely available for a wide range of substances, which may limit its general applicability.
Recommendation	Candidate for in-depth review (in conjunction with Model reference number 47).

Model reference number 46

Name of model/ method/paper	Physiologically based toxicokinetic model for maternal transfer of 2,3,7,8-tetrachlorodibenzo-p-dioxin in brook trout (Salvelinus fontinalis). J W Nichols, K M Jensen, J E Tietge and R D Johnson. *Environmental Toxicology and Chemistry*, **17**, 1998, 2422-2434.
Date of publication	1998
Availability	Published paper.
Food chain considered	Food → female fish → ovaries/developing eggs Water → female fish → ovaries/developing eggs The model is a physiologically based toxicokinetic model (PBTK) and is an extension of an earlier model by the same author (Nichols *et al.,* 1990). The model is presented as a series of equations.
Types of chemicals modelled	The model was developed using data from feeding studies with 2,3,7,8-tetrachlorodibenzo-p-dioxin.
Environment to which it relates	Generic.
Data requirements	The model requires a large amount of chemical-specific data including several blood-water and tissue-blood partition coefficients. The fish-related data used are extensive and values are given for brook trout.
Purpose of model/method	Research paper.
Summary of validation studies	The model was fitted to laboratory-derived data for 2,3,7,8-tetrachlorodibenzo-p-dioxin.
Assessment	The model is quite complex and would require computerisation (spread sheet?) in order to be routinely used. The model requires a large amount of chemical-specific and species-specific data which may limit its general applicability.
Recommendation	Candidate for in-depth review (in conjunction with Model reference number 47).

Model reference number 47

Name of model/ method/paper	A physiologically based toxicokinetic model for dietary uptake of hydrophobic organic compounds by fish. I. Feeding studies with 2,2'5,5'-tetrachlorobiphenyl. J W Nichols, P N Fitzsimmons, F W Whiteman, T D Dawson, L Babeu and J Juenemann. *Toxicological Sciences*, **77**, 2004a, 206-218.
Date of publication	2004
Availability	Published paper.
Food chain considered	Water → fish. Food → fish. The model is a physiologically based toxicokinetic model (PBTK) and is an extension of an earlier model by the same author (Nichols *et al.,* 1990, 1991 and 1993). The model is presented as a series of equations.
Types of chemicals modelled	The model was developed using data from feeding studies with 2,2',5,5'-tetrachlorobiphenyl.
Environment to which it relates	Generic.
Data requirements	The model requires a large amount of chemical-specific data including several blood-water, tissue-blood and lumen-tissue partition coefficients and several digestion parameters and gut permeability coefficients. The fish-related data used are extensive and values are given for rainbow trout.
Purpose of model/method	Research paper.
Summary of validation studies	The model was developed using data for 2,2',5,5'-tetrachlorobiphenyl. A modelling simulation for this substance was carried out by Nichols *et al.* (2004b).
Assessment	The model is quite complex and would require computerisation (spread sheet?) in order to be routinely used. The model requires a large amount of chemical-specific data which may limit its general applicability.
Recommendation	Candidate for in-depth review.

Model reference number 48

Name of model/ method/paper	A numerical kinetic model for bioaccumulation of organic chemicals in sediment-water systems. S S Park and K M Erstfeld. *Chemosphere*, **34**, 1997, 419-427.
Date of publication	1997
Availability	Published paper (the paper indicates that a computerised version BASWIM was used for the calculations).
Food chain considered	Water → fish. Sediment → fish. The method is a kinetic model based on a three-compartment system.
Types of chemicals modelled	Organic chemicals.
Environment to which it relates	Generic.
Data requirements	The chemical-specific data include log K_{ow} (or fish BCF), sediment-water partition coefficient, degradation/volatilisation rate, rate of uptake from water and sediment.
Purpose of model/method	Research paper.
Summary of validation studies	The model was validated using experimental data for chlordane with goldfish in the presence of sediment.
Assessment	The model mainly considers bioconcentration processes.
Recommendation	Not considered further.

Model reference number 49

Name of model/ method/paper	A fugacity model of chemical uptake by plants from soil and air. S Paterson, D Mackay and A Gladman. *Chemosphere*, **23**, 1991b, 539-565.
Date of publication	1991
Availability	Published paper.
Food chain considered	Soil → plant. Air → plant. The model is a three-compartment (root, stem and leaf) plant fugacity model. The model incorporates some of the correlations derived by Briggs *et al.* (1982 and 1983) and Bacci *et al.* (1990). The model is presented as a series of equations.
Types of chemicals modelled	Organic chemicals. Example calculations are given for hexachlorobenzene, 2,4-D, 1,2,4-dichlorobenzene and hexachlorobiphenyl.
Environment to which it relates	Generic.
Data requirements	The chemical-specific data include solubility, vapour pressure and log K_{ow}. The model also requires various plant properties (the properties relevant to soybean are used in the paper).
Purpose of model/method	Research paper.
Summary of validation studies	None located as part of this work.
Assessment	The model uses relatively little chemical-specific information. The model is similar in some respects to other models produced by this group (such as Paterson *et al.,* 1994). The model would need to be computerised (spread-sheet?) for it to be used on a regular basis.
Recommendation	Candidate for in-depth review (in conjunction with Model reference number 51).

Model reference number 50

Name of model/ method/paper	Correlation of the equilibrium and kinetics of leaf-air exchange of hydrophobic organic chemicals. S Paterson, D Mackay, E Bacci and D Calamari, 1991a, *Environmental Science and Technology*, **25**, 866-871.
Date of publication	1991
Availability	Published paper.
Food chain considered	Air → plant. The paper presents correlations for the leaf-air bioconcentration factor and the leaf clearance rate constant based on a simple fugacity model.
Types of chemicals modelled	Hydrophobic organic chemicals.
Environment to which it relates	Generic.
Data requirements	The chemical-specific data include log K_{ow} and octanol-air partition coefficients (can be estimated from log K_{ow} and Henry's law constant). The method also requires the volume fractions of air, water and octanol-equivalents in the leaf.
Purpose of model/method	Research paper.
Summary of validation studies	The predicted leaf-air bioconcentration factors and leaf clearance rates were compared against experimental data obtained for a range of mainly hydrophobic organohalogen compounds (log K_{ow} range 1.2-6.9).
Assessment	The model uses relatively little chemical-specific information. The model is similar in some respects to other models produced by this group (such as Paterson *et al.,* 1991b and 1994).
Recommendation	Candidate for in-depth review (in conjunction with Model reference number 51).

Model reference number 51

Name of model/ method/paper	A model of organic chemical uptake by plants from soil and the atmosphere. S Patterson, D Mackay and C McFarlane. *Environmental Science and Technology*, **28**, 1994, 2259-2266. A similar model is presented in Paterson and Mackay (1995).
Date of publication	1994
Availability	Published paper. The paper indicates that a BASIC computer version of the model is available from the author (it is not known if this is still the case).
Food chain considered	Soil → vegetation. Air → vegetation. The model is a three-compartment fugacity-based mass balance model. The three compartments considered are root, stem and foliage. The model considers diffusion and bulk flow of chemical between soil and root, transport within the plant in the phloem and transpiration streams, exchange between foliage and air and between soil and air, and metabolism and growth. The model is presented as a series of equations. A simplified version of the model has been published by Hung and Mackay (1997).
Types of chemicals modelled	Organic chemicals. Example calculations were carried out for bromacil, 2,4-D, dichlorobenzonitrile and hexachlorobiphenyl.
Environment to which it relates	Generic.
Data requirements	The model is presented as a series of D-values representing transport and transformation processes. These D-values are estimated from physico-chemical properties of the substance and the flow rates in the plants. The chemical properties needed include Henry's law constant, octanol-water partition coefficient and a number of partition coefficients. Some of these partition coefficients can be estimated from, for example, log K_{ow} , but the paper indicates that experimental values are preferred. The model also requires information on the volume of composition (water and lipid content) of the various parts of the plant (typical values are given for soybean).
Purpose of model/method	Research paper. The model is primarily designed to be fitted to experimental data. The model is not designed to be applied to perennial vegetation such as trees which may be exposed for periods of years and which may contain a substantial amount of non-viable tissues.
Summary of validation studies	The model results were compared with experimental data for uptake of ^{14}C-bromacil by soybean under hydroponic conditions.
Assessment	The model is relatively complex and requires a large amount of chemical- and plant-specific data. Typical values for the plant-specific data are given in the paper and these data could easily be modified to take into account the properties of other plant types.
Recommendation	Candidate for in-depth review.

Model reference number 52

Name of model/ method/paper	PlantX. Generic one-compartment model for uptake of organic chemicals by foliar vegetation. S Trapp and M Matthies. *Environmental Science and Technology*, **29**, 1995, 2333-2338. Generic one-compartment model for uptake of organic chemicals by foliar vegetation (addition/correction). S Trapp and M Matthies. *Environmental Science and Technology*, **30**, 1996, 360-361. Further information is given in Trapp (1995).
Date of publication	1995
Availability	Computer model available free of charge from internet (http://www.er.dtu.dk/homepages/stt/). Details are given in published papers.
Food chain considered	Air → plant. Soil (pore water) → plant. The model is a fugacity-based model to estimate the uptake of chemicals by vegetation from air and via soil pore water. The method takes into account the diffusive exchange of chemicals between soil and roots in water and air pores, transfer into roots with the transpiration stream, translocation in the plant with the transpiration stream, partitioning into the stem, transport with the assimilation stream, diffusive exchange between air and leaf via stomata and cuticle, metabolism and dilution by growth.
Types of chemicals modelled	Organic chemicals.
Environment to which it relates	Generic.
Data requirements	The minimum chemical-specific information include the log K_{ow} , air-water partition coefficient (or dimensionless Henry's law constant) and molecular weight. The metabolism rate can also be included if available. The model also requires some plant-specific data (typical values are given in the program).
Purpose of model/method	Research paper. The model has since been implemented in EUSES and the TGD, using plant properties from Riederer (1990) and Trapp and Matthies (1995).
Summary of validation studies	A validation study of the air uptake part of the model has been carried out (Polder *et al.,* 1998). A comparison of the results for carbofuran and bromacil with experimental studies, and a sensitivity analysis, is included in Trapp (1995).
Assessment	This method is currently implemented in the TGD.
Recommendation	Candidate for in-depth review (in conjunction with Model reference number 60 and Model reference number 69).

Model reference number 53

Name of model/ method/paper	Estimating partitioning and transport of organic chemicals in the foliage/atmosphere system: Discussion of a fugacity-based model. M Riederer. *Environmental Science and Technology*, **24**, 1990, 829-837. A similar model also appears in Riederer (1995).
Date of publication	1990
Availability	Published papers.
Food chain considered	Air → plant. The paper describes a fugacity-based model to estimate the uptake of chemicals by vegetation from air. The model uses "typical" properties of a leaf (which are based on those for *Brassica oleracea*). Properties relevant to other plant types (such as European Beech *Fagus sylvatica*) are given in Riederer (1995).
Types of chemicals modelled	Organic chemicals including methanol, phenol, nitrophenols, 2,4-D, atrazine, 2,4,5-T, pentachlorophenol, hexachlorobenzene, perylene and DEHP.
Environment to which it relates	Generic.
Data requirements	The model requires the log K_{ow} , water solubility, saturation vapour pressure and the cuticle-water partition coefficient.
Purpose of model/method	Research paper. The model can be used to estimate the equilibrium concentration in different leaf tissues, the air-to-vegetation bioconcentration equilibrium and to identify the compartments of preferential accumulation within the leaves. The method was implemented in USES version 1.0 but was superseded by the method of Trapp and Matthies (1995) for EUSES.
Summary of validation studies	A validation study has been carried out by Polder *et al.,* (1998).
Assessment	The model could be easily adapted for other plants if the relevant properties of the plant were available. The paper presents the necessary equations to carry out the calculations, but in order to make the model more readily usable, they would need to be implemented in a computer (spread sheet?) programme. The chemical-specific data requirements of the model are modest; however, the need for a cuticle-water partition coefficient may limit the general usefulness of the method, although the paper indicates that it is possible to estimate this from fundamental properties. The method was implemented in USES version 1.0 but was superseded by the method of Trapp and Matthies (1995) for EUSES and the current TGD.
Recommendation	Not considered further.

Model reference number 54

Name of model/ method/paper	Plant uptake of non-ionic organic chemicals from soils. J A Ryan, R M Bell, J D Davidson and G A O'Connor. *Chemosphere*, **17**, 1988, 229-2323.
Date of publication	1988
Availability	Published paper.
Food chain considered	Soil → plant. Air → plant. The method is essentially very similar to that implemented in the TGD. The method consists of a series of equations that allow the root concentration factor, the stem concentration factor and the transpiration stream concentration factor to be estimated from log K_{ow}. These equations are based on the work of Briggs *et al.* (1982 and 1983). The paper also considers the significance of uptake from air based on the work of Topp *et al.* (1986).
Types of chemicals modelled	Plant protection products, PCBs, halogenated aliphatic hydrocarbons, halogenated ethers, monocyclic aromatic hydrocarbons, phthalate esters, polycyclic aromatic hydrocarbons and miscellaneous other compounds.
Environment to which it relates	Generic.
Data requirements	Log K_{ow} , degradation half-life in soil and Henrys' law constant.
Purpose of model/method	Research paper. The intention was to provide a procedure for grouping chemicals by their relative potential for plant uptake rather than predict concentrations in plants in the field.
Summary of validation studies	None.
Assessment	The method is similar to that implemented in the TGD.
Recommendation	Candidate for in-depth review (in conjunction with Model reference number 60).

Model reference number 55

Name of model/ method/paper	*Development and validation of bioaccumulation models for earthworms.* B E Sample, J J Beauchamp, R A Efroymson, G W Suter II and T L Ashwood. Report ES/ER/TM-220, Oak Ridge National Laboratory, prepared for the US Department of Energy Office of Environmental Management, February 1998a. [Some results also published in Sample *et al.,* 1999].
Date of publication	1998
Availability	Published report (available from http://www.esd.ornl.gov/programs/ecorisk/documents/tm220.pdf)
Food chain considered	Soil → earthworms. A series of regression-based equations have been derived relating the concentration of a given substance in earthworms (whole body) to the concentration in soil.
Types of chemicals modelled	Mainly metals but also two organic chemicals, tetrachlorodibenzo-p-dioxin (TCDD) and polychlorinated biphenyls (PCBs).
Environment to which it relates	Based on field data from the United States and several other countries (including United Kingdom).
Data requirements	Concentration in soil (soil pH is also required for some of the metals). The model is based on a regression equation derived from the reported chemical concentrations in co-located earthworm samples and soil samples. Regression equations were derived for individual metals and also TCDD and PCBs.
Purpose of model/method	The purpose of the model was to facilitate more accurate estimation of contaminant exposure experienced by predatory wildlife on the Oak Ridge Reservation and at other contaminated sites.
Summary of validation studies	A validation exercise was carried out using field data from six studies covering Spain, United Kingdom and the United States. There was sufficient information to carry out the validation exercise for the PCB and metal equations, but no validation of the TCDD equations was possible.
Assessment	The equations derived are substance-specific and not generally applicable to other substances. The method, therefore, has limited use in this project. The report does, however, contain a useful dataset for validation of other models.
Recommendation	Not considered further (may be useful for validation).

Model reference number 56

Name of model/ method/paper	*Development and validation of bioaccumulation models for small mammals.* B E Sample, J J Beauchamp, R A Efroymson and G W Suter II. Report ES/ER/TM-219, Oak Ridge National Laboratory, prepared for the US Department of Energy Office of Environmental Management, February 1998b.
Date of publication	1998
Availability	Published report (available from http://www.esd.ornl.gov/programs/ecorisk/documents/tm219.pdf)
Food chain considered	Soil → small mammals (including insectivores, herbivores and omnivores). A series of regression-based equations relating the concentration of a given chemical in the small mammal (whole body) to the concentration in soil have been derived.
Types of chemicals modelled	Mainly metals but also two organic chemicals, tetrachlorodibenzo-p-dioxin (TCDD) and tetrachlorodibenzofuran (TCDF).
Environment to which it relates	Based on field data from the United States and three other countries.
Data requirements	Concentration in soil. The model is based on a regression equation derived from the reported chemical concentrations in co-located small mammal and soil samples. Regression equations were derived for individual metals and also TCDD (a general equation and a more specific one for omnivores) and TCDF (a general equation only).
Purpose of model/method	The purpose of the model was to facilitate more accurate estimation of contaminant exposure experienced by predatory wildlife on the Oak Ridge Reservation and at other contaminated sites.
Summary of validation studies	There were insufficient data to validate the model for the organic chemicals considered. Validation studies were carried out for the metals considered, depending on the availability of suitable data.
Assessment	The equations derived are substance-specific and not generally applicable to other substances. The method, therefore, has limited use in this project. The report does, however, contain a useful dataset for validation of other models.
Recommendation	Not considered further (may be useful for validation).

Model reference number 57

Name of model/ method/paper	ERMESSE The model is described in the following paper: A non-linear dynamic simulation model for xenobiotic transport and whole plant allocation following foliar application. I. Conceptual foundation for model development. Satchivi N M, Stoller E W, Wax L M and Briskin D P, 2000, *Pesticide Biochemistry and Physiology*, **68**, 67-84.
Date of publication	2000
Availability	Published paper
Food chain considered	Foliar application → plant (leaves, roots and so on). The model is a dynamic, non-linear simulation model describing the whole plant transport and distribution following foliar application. The model is presented as a series of equations.
Types of chemicals modelled	Organic chemicals (the model is presented in the paper as a theoretical model with no examples).
Environment to which it relates	Generic.
Data requirements	The chemical-specific parameters include log K_{ow} , molar volume and acid dissociation constant. The method also requires several plant anatomical, physiological and biochemical characteristics.
Purpose of model/method	Research paper.
Summary of validation studies	None.
Assessment	Foliar application is less relevant to this project than exposure via other routes.
Recommendation	Not considered further.

Model reference number 58

Name of model/ method/paper	UNITTree. A multimedia compartment model to estimate the fate of lipophilic compounds in plants. K-W Schramm, A Reischl and O Hutzinger. *Chemosphere*, **16**, 1987, 2653-2663.
Date of publication	1987
Availability	Published paper
Food chain considered	Soil (pore water) → plant. Air (vapour and particulates) → plant. The model is a dynamic fugacity model for spruce (*Picea abies*) and has compartments relating to air, needlewater, stemwater, rootwater, soil pore water, needle dry-mass, wood dry-mass, root dry-mass, soil dry-mass, wax and airborne particulates. The model is presented as a series of equations.
Types of chemicals modelled	Lipophilic organic chemicals. Example calculations were given for 2,4-dichlorophenol, 2,3,7,8-tetrachlorodibenzo-p-dioxin, simazine, hexachlorobenzene and lindane.
Environment to which it relates	Generic.
Data requirements	The chemical-specific data required include vapour pressure, Henry's law constant, organic carbon-water partition coefficient and log K_{ow}. The plant-specific information needed includes the volumes, densities, organic carbon contents, surface areas and porosities of the various compartments considered (values are given for 15-year old spruce trees).
Purpose of model/method	Research paper. The model was used to describe the distribution in 15-year old spruce.
Summary of validation studies	None.
Assessment	The model uses relatively little chemical-specific information and could be modified for other plant types provided the appropriate plant-specific information is available (this may be necessary in terms of the overall aims of this project, as spruce trees are not directly relevant for food-chain exposure). The model would need to be computerised (spread-sheet?) for it to be used on a regular basis. The model appears in principle to be similar to other plant models.
Recommendation	Candidate for in-depth review (in conjunction with Model reference number 69).

Model reference number 59

Name of model/ method/paper	Hazard and risk assessment of chemicals for terrestrial ecosystems. J V Tarazona and M M Vega. *Toxicology*, **181-182**, 2002, 187-191.
Date of publication	2002
Availability	Published paper.
Food chain considered	Provides a holistic conceptual framework/model for terrestrial (and aquatic) ecosystems. However, little detail is provided. Tarazona *et al.* (2000) developed another framework for hazard estimation for the terrestrial environment. This method considered the exposure through soil, through air and through food and proposed use of persistence and bioaccumulation potentials as 'modifiers' for the hazard identification.
Types of chemicals modelled	Organic chemicals.
Environment to which it relates	Generic.
Data requirements	Not clear.
Purpose of model/method	To improve risk assessment methodologies for the terrestrial compartment.
Summary of validation studies	None located as part of this work.
Assessment	The paper mentions an unpublished system dynamic model (BIOMAG). The author has been contacted as part of this study, but no details have been received. A more detailed scheme for an aquatic food chain by this group is given in Carbonnell *et al.* (2000)
Recommendation	Candidate for in-depth review (in conjunction with Model reference number 8).

Model reference number 60

Name of model/ method/paper	TGD. *Technical Guidance Document on Risk Assessment in support of Commission Directive 93/67/EEC on Risk Assessment for existing substances, Commission Regulation (EC) No 1488/94 on Risk Assessment for existing substances and Directive 98/8/EC of the European Parliament and of the Council concerning the placing of biocidal products on the market.* European Commission, Joint Research Centre, EU 20418 EN, Second Edition, 2003.
Date of publication	2003
Availability	Available as a published report and as a computer model (EUSES 2.0). Both of these are available free of charge from http://ecb.jrc.it/existing-chemicals/.
Food chain considered	Freshwater → freshwater fish → predator Food → freshwater fish → predator Marine water → marine fish → predator → top predator Food → marine fish → predator → top predator Soil → earthworms → predator Freshwater → fish → humans Air → plant → humans. Air → plant → cattle → milk → humans. Soil → plant → humans. Soil → plant → cattle → milk → humans. The methods are presented as a series of equations. The methods are also implemented in the EUSES 2.0 program. The methods are based on the following work/models: Briggs *et al.* (1982), Jager (1998)[28], Riederer (1990), Trapp and Matthies (1995), Trapp (1995) and Travis and Arms (1988).
Types of chemicals modelled	Organic chemicals.
Environment to which it relates	Generic
Data requirements	The main chemical-specific data required are log K_{ow} , fish BCF and worm BCF (both can be estimated from log K_{ow}), water solubility, vapour pressure and Henry's law constant.
Purpose of model/method	The method is used in the risk assessment of new and existing chemicals and biocides in the EU.
Summary of validation studies	None located as part of this work (see the individual reviews for validation of the individual components of the system).
Assessment	The method is relatively easy to use and is used widely within the EU for the risk assessment of chemicals.
Recommendation	Candidate for in-depth review.

[28] Earlier versions of the TGD/EUSES included method from Connell and Markwell (1990) for the earthworm food chain. This has now been superseded by the method from Jager (1998) in the current version of the TGD.

Model reference number 61

Name of model/ method/paper	Bioaccumulation model of organic chemical distribution in aquatic food chains. R V Thomann. *Environmental Science and Technology*, **23**, 1989, 699-707.
Date of publication	1989
Availability	Published paper.
Food chain considered	Water → phytoplankton → zooplankton → small fish → top predator (fish). The model considers a generic aquatic food chain. The method is based on consideration of the kinetics of uptake and elimination, and considers growth dilution. The model is presented as a series of equations representing the steady-state situation. The model allows bioconcentration factors and bioaccumulation factors to be estimated for various parts of the food chain.
Types of chemicals modelled	Organic chemicals.
Environment to which it relates	Generic.
Data requirements	Log K_{ow}. This is used to estimate a number of parameters within the model such as uptake efficiency from water, excretion rate and assimilation efficiency from food. The method also needs certain species-specific data such as lipid contents, total weight of organisms in the trophic level, assimilation efficiencies; typical values for these are presented in the paper.
Purpose of model/method	Research paper. The model is an extension of a previously developed steady-state model (Thomann, 1981).
Summary of validation studies	A comparison was made between the bioaccumulation factors predicted for predatory fish with field data for several organochlorine substances.
Assessment	The method requires a limited amount of chemical-specific information and could be adapted to other food chains as long as the species-specific parameters are known. The model may need to be computerised (spread sheet?) if it is to be routinely used. This model has been used as the basis of development of further models such as Thomann *et al.,* 1992.
Recommendation	Candidate for in-depth review (in conjunction with Model reference number 79).

Model reference number 62

Name of model/ method/paper	Model of PCB in the Lake Michigan lake trout food chain. R V Thomann and J P Connolly. *Environmental Science and Technology*, **18**, 1984, 65-71.
Date of publication	1984
Availability	Published paper.
Food chain considered	Water → phytoplankton/detrital organic matter → *Mysis reticulata* → alewife (*Alosa pseudoharengus*) → lake trout (*Salvelinus namaycush*). The model is an age-dependent food chain model that considers species bioenergetics and exposure through water and food.
Types of chemicals modelled	Polychlorinated biphenyls (PCBs).
Environment to which it relates	Lake Michigan.
Data requirements	Growth rates and respiration rates of the organisms (given in the paper for the organisms considered), the assimilation efficiency from food of the substance ("default" values are given for PCBs for *Mysis*, alewife and lake trout), and a bioconcentration factor for phytoplankton, *Mysis*, alewife and lake trout.
Purpose of model/method	Research paper to model the concentrations of PCBs in fish from Lake Michigan.
Summary of validation studies	The model was 'calibrated' using the observed PCB concentrations in lake trout and alewife from Lake Michigan from 1971.
Assessment	The model is specific to the chemicals and food chain considered. The model is outlined in equation form, and so it should be possible to adapt the theory for other situations. In its current form the model is not easy to use, and the data needed, particularly BCFs, assimilation efficiencies and organism growth and respiration rates, for all parts of the food chain, are extensive. Overall, this means that, in the absence of easy methods to predict these parameters to adapt the model to other situations, the model may be of limited use within this project. However, this model is related to other models by the same group, such as Thomann *et al.* (1992), Connolly (1991), Connolly *et al.* (2000), Connolly and Glaser (2002) and Glaser and Connolly (2002).
Recommendation	Candidate for in-depth review (in conjunction with Model reference number 79).

Model reference number 63

Name of model/ method/paper	An equilibrium model of organic chemical accumulation in aquatic food webs with sediment interaction. R V Thomann, J P Connolly and T F Parkerton. *Environmental Toxicology and Chemistry*, **11**, 1992, 615-629.
Date of publication	1992
Availability	Published paper. The model used is available as the QEAFDCHN model.
Food chain considered	Water, sediment and phytoplankton → benthic invertebrate and zoo plankton → forage fish → pisciverous fish. The model is a five-compartment steady-state food web model that includes a benthic invertebrate compartment. Exposure of benthic organisms occurs via ingestion of particulate contaminants associated with sediment and overlying phytoplankton and via interstitial and overlying water. Higher organisms in the food web (such as fish) are exposed via ingestion of food and through water. The model is presented as a series of equations.
Types of chemicals modelled	Organic chemicals.
Environment to which it relates	Generic. Some of the parameters within the model are based on data for Lake Ontario.
Data requirements	The model requires information on the BCF, uptake and excretion rates and chemical assimilation efficiency for the routes of exposure and organisms considered. Methods are given to relate some of these parameters to log K_{ow}. In addition, the model needs information on the growth rates, lipid contents and respiration rates and feeding preferences of the organisms considered (typical values are given in the paper for a Lake Ontario food chain) and organic carbon content of the water.
Purpose of model/method	Research paper.
Summary of validation studies	The model was validated using field data from Lake Ontario for an amphipod-sculpin food chain. The model has also been applied to PCBs in the upper Hudson River (Connolly *et al.,* 2000). Burkhard (1998) carried out a comparison of the results from this model with those obtained using the model of Gobas (1993).
Assessment	The model considers exposure via the sediment and water phase as well as food. The model is generic in nature and so could be relatively easily modified for different food webs, provided the necessary species-dependent data are available. The model requires quite a lot of chemical-specific input data, but the paper provides methods to estimate much of this data from log K_{ow} in the absence of actual data.
Recommendation	Candidate for in-depth review (in conjunction with Model reference number 79).

Model reference number 64

Name of model/ method/paper	Factors affecting the uptake of ^{14}C-labelled organic chemicals by plants from soil. E Topp, I Scheunert, A Attar and F Korte. *Ecotoxicology and Environmental Safety*, **11**, 1986, 219-228.
Date of publication	1986
Availability	Published paper.
Food chain considered	Soil → plant. Air → plant. The paper presents a series of regression equations relating the plant concentration factor determined over seven days in barley and cress seedlings, to physicochemical and structural properties of the chemicals considered. Good correlations were obtained with the data for barley, but the correlations obtained with cress were generally poor.
Types of chemicals modelled	The regression equations were derived using 16 substances including benzene, 1,4-dichlorobenzene, atrazine, pentachlorophenol, 1,2,4-trichlorobenzene, kelevan, 1,2,3,5-tetrachlorobenzene, kepone, di(2-ethylhexyl)phthalate, dieldrin, pentachlorobenzene, 2,4,6,2',4'-pentachlorobiphenyl, hexachlorobenzene, p,p'-DDT, and two pigments.
Environment to which it relates	Generic. The regression equations are derived from data obtained in a laboratory setting.
Data requirements	Regression equations are given relating the plant concentration factors to soil-organic carbon partition coefficient, log K_{ow} , volatilisation from soil and molecular weight.
Purpose of model/method	Research paper.
Summary of validation studies	A comparison of this model with eight other models for predicting the uptake, translocation and elimination of organic chemicals by herbaceous plants has been carried out by Collins and Fryer (2003).
Assessment	The methods are simple and require only small amounts of easily obtainable chemical-specific information to use. The data relate to only a relatively short exposure period and may not correspond to steady-state situations and so the methods may have limited predictive power.
Recommendation	Not considered further.

Model reference number 65

Name of model/ method/paper	TOXFATE
Date of publication	1990
Availability	Available free of charge via the internet from http://www.butx.com/halfon/index.html.
Food chain considered	Water → plankton → small fish → large fish. Sediment → benthos. The model can be run as a steady-state or dynamic model. The model calculates the concentration in water, sediment, suspended sediment, benthos, plankton, small fish and large fish.
Types of chemicals modelled	Organic chemicals (mainly organochlorine chemicals).
Environment to which it relates	Great Lakes food chain.
Data requirements	The chemical-specific information required includes molecular weight, Henry's law constant (or vapour pressure and solubility), organic carbon-water partition coefficient, log K_{ow} , and the photolysis rate. The program also requires information on the food chain (files are provided for Lake Ontario).
Purpose of model/method	Research
Summary of validation studies	Several papers have been published.
Assessment	The method requires only a limited amount of chemical-specific data. However, the models are specific to the Great Lakes and would need some modification to be used for other food chains. A computer version of the model is freely available.
Recommendation	Candidate for in-depth review.

Model reference number 66

Name of model/ method/paper	*Guidance document on deriving environmental risk limits.* T P Traas (editor), with contributions from J H M de Bruijn, D T Jager, D F Kalf, B J W G Mensink, M H M M Montforts, D T H M Sijm, C E Smit, P L A van Vlaardingen, E M J Verbruggen and A P van Wezel. RIVM Report 601501 012, National Institute of Public Health and the Environment, Bilthoven, the Netherlands, June 2001a.
Date of publication	2001
Availability	Published report (available from http://www.rivm.nl/bibliotheek/rapporten/601501012.pdf). A similar method for water and soil food chains is presented in Crommentuijn *et al.* (2000).
Food chain considered	Water → fish → predator (bird/mammal). Water → mussel → predator. Sediment → prey → predator. Soil → earthworm → predator. The report outlines a methodology for deriving environmental risk limits (ERLs) for the Netherlands. The accumulation potential in top predators is considered for certain substances. The method is similar to that used in the TGD. The method essentially uses the BCF for fish, mussels and worms to back-calculate from a no effect concentration in mammals or birds to an equivalent concentration in water or soil. The sediment concentration is similarly estimated using the biota-to-sediment accumulation factor (BSAF).
Types of chemicals modelled	Substances with log K_{ow} greater than three, with low degradation rates or with high accumulation rates.
Environment to which it relates	The Netherlands.
Data requirements	Log K_{ow} , K_{oc}, BCF, BSAF. Methods are given for estimating BCFs for fish, mussels and earthworms from log K_{ow} , and for estimating BSAFs from BCFs and K_{oc}.
Purpose of model/method	Guidance document for deriving ERLs in the Netherlands for water, groundwater, soil, sediment and air. The method considers the accumulation potential in top predators for substances with log K_{ow} greater than three, with low degradation rates or with high accumulation rates. The ERLs serve as advisory values in the setting of environmental quality standards (EQSs) by the Government and for various policy purposes.
Summary of validation studies	None located as part of this work.
Assessment	A generic method requiring only a small amount of data that could easily be adapted to the United Kingdom. The method considers relatively simple food chains and exposure via the water (or pore water) phase.
Recommendation	Candidate for in-depth review.

Model reference number 67

Name of model/ method/paper	Modelling uptake into roots and subsequent translocation of neutral and ionisable organic compounds. Trapp S. *Pest Management Science*, **56**, 2000, 767-778.
Date of publication	2000
Availability	Published paper
Food chain considered	Soil → plant roots → plant shoots. The paper considers both equilibrium and dynamic (steady-state) models. The methods allow a root concentration factor and transpiration stream concentration factor to be determined. The models are presented as a series of relatively simple equations.
Types of chemicals modelled	Neutral and ionisable organic chemicals.
Environment to which it relates	Generic.
Data requirements	The chemical-specific data include log K_{ow} , pKa and the valency number. The method also requires the pH and chemical concentration in soil, and various plant properties such as root and xylem volumes and surface areas, transpiration rates, growth rates, water fractions, lipid fractions and pHs of various parts of the plant (typical values are given mainly based on soy beans).
Purpose of model/method	Research paper.
Summary of validation studies	The results were compared against experimentally-derived data for a range of neutral, weakly acidic and weakly basic substances.
Assessment	The methods require only a limited amount of chemical-specific data and could be modified for various plants and soil types. The outputs from the approach (the root concentration factor and transpiration stream concentration factor) could be used in the current methodology given in the TGD. The method covers both neutral and weakly acidic and basic organic chemicals.
Recommendation	Candidate for in-depth review (in conjunction with Model reference number 69).

Model reference number 68

Name of model/ method/paper	Dynamic root uptake model for neutral lipophilic organics. S Trapp. *Environmental Toxicology and Chemistry*, **21**, 2002, 203-206.
Date of publication	2002
Availability	Published paper and spreadsheet model. The spreadsheet model is available free of charge from http://www.er.dtu.dk/homepages/stt.
Food chain considered	Soil → plant roots. The model considers the rate of diffusion of the chemical into roots, using carrots as an example. The model is presented as a series of equations. A spreadsheet version of the carrot model is also available.
Types of chemicals modelled	Neutral lipophilic organic chemicals.
Environment to which it relates	Generic
Data requirements	The method requires log K_{ow} and Henry's law constant as the chemical-specific data. Plant-specific data include the water content, lipid content, density, transpiration stream flow, growth rate and root radius (example/generic values are given).
Purpose of model/method	Developed as an alternative to the equilibrium approach currently used in the TGD.
Summary of validation studies	Predictions from the dynamic method and equilibrium method used in the TGD were compared with experimental data for benzo[a]pyrene, polychlorinated biphenyls and chlorobenzenes generated with carrots. The equilibrium approach was found to predict the concentrations in the peels, but the dynamic model was superior for predicting the concentrations in carrot cores and whole carrots.
Assessment	The method is relatively simple to use, and appears to have some advantages in terms of predictive power over the method currently used in the TGD.
Recommendation	Candidate for in-depth review (in conjunction with Model reference number 69).

Model reference number 69

Name of model/ method/paper	Plant uptake and transport models for neutral and ionic chemicals. S Trapp. *Environmental Science and Pollution Research*, **11**, 2004, 33-39.
Date of publication	2004
Availability	Published paper and spreadsheet model. The model is available free of charge from http://www.er.dtu.dk/homepages/stt.
Food chain considered	Soil pore water → plant. The model is a 10-compartment model for uptake and fate of weak electrolytes in whole plants. It considers the speciation of the compounds in external solution, cytoplasm, vacuole, phloem and xylem.
Types of chemicals modelled	Weak electrolytes.
Environment to which it relates	Generic.
Data requirements	The chemical-specific information includes log K_{ow} , details of whether the substance is an acid or a base, acid dissociation constant (pKa) and valency. The model also requires many plant-specific parameters (typical values are included in the model).
Purpose of model/method	Research paper.
Summary of validation studies	The model has been tested with TBT (Ciucani, 2002; Ciucani, 2003)
Assessment	The model requires only a limited amount of chemical-specific information. The model is relatively easy to use (spreadsheet available). Some of the model outputs show the distribution of the chemical within the various compartments of the plant and so may require further interpretation to be useful to this project.
Recommendation	Candidate for in-depth review.

Model reference number 70

Name of model/ method/paper	Modelling volatilization of PCDD/F from soil and uptake into vegetation. S Trapp and M Matthies. *Environmental Science and Technology*, **31**, 1997, 71-74.
Date of publication	1997
Availability	Published paper.
Food chain considered	Soil → air → plant leaves. The model is an equilibrium model based on diffusion/dispersion equations. The model is presented as a series of equations.
Types of chemicals modelled	Chlorinated dibenzofurans and dibenzon-p-dioxins (example calculations are given for 2,3,7,8-tetrachlorodibenzo-p-dioxin).
Environment to which it relates	Generic.
Data requirements	The chemical-specific data required include molar mass, log K_{ow} , organic carbon-water partition coefficient, plant-air partition coefficient and Henry's law constant.
Purpose of model/method	Research.
Summary of validation studies	None located as part of this work.
Assessment	The method is specific to chlorinated dibenzofurans and dibenzon-p-dioxins, for which the necessary partitioning and volatilisation data are available. Other, more generally applicable plant uptake models are available from the same authors, such as Plant X (Trapp and Matthies, 1995 and 1996).
Recommendation	Not considered further.

Model reference number 71

Name of model/ method/paper	Fruit tree model for uptake of organic compounds from soil. S Trapp, D Rasmussen and L Samsøe-Petersen. *SAR and QSAR in Environmental Research*, **14**, 2003, 17-26.
Date of publication	2003
Availability	Published paper and spreadsheet model. The spreadsheet model is available free of charge from http://www.er.dtu.dk/homepages/stt.
Food chain considered	Soil (pore water) → tree (stem) → fruit. The model is a steady-state mass balance model that considers xylem and phloem transport to fruits through the stem. The model draws on earlier work by Trapp *et al.* (2001) and Burken and Schnoor (1998). The model is presented as a series of equations. A spreadsheet version of the model is also available.
Types of chemicals modelled	Polar and non-polar organic chemicals.
Environment to which it relates	Generic.
Data requirements	The model requires the log K_{ow} and an estimate of the metabolism half-life. The tree-specific data used in the model include transpiration rate, growth rate and water flux, dry matter content of fruits and the dry wood content of the tree stand; typical values are given in the paper. The model also uses certain soil properties, such as organic carbon content, water content, gas content and density; the examples given in the paper used the properties of a Danish Reference soil.
Purpose of model/method	Research paper.
Summary of validation studies	The results from the model were validated for very liphophilic substances (log K_{ow} above five) using field data for two chlorinated dibenzo-p-dioxins and two polycyclic aromatic compounds. A sensitivity analysis was also undertaken to investigate the sensitivity of the model to various input parameters. The results of the model are compared to those obtained using the Travis and Arms (1988) method.
Assessment	The model is relatively easy to use and could be easily adapted for differing soil or fruit types. The model ideally requires a metabolism half-life for each substance considered; this data may not always be readily available (nor easy to predict), but could be used assuming effectively no metabolism in the absence of information.
Recommendation	Candidate for in-depth review (in conjunction with Model reference number 69).

Model reference number 72

Name of model/ method/paper	Bioconcentration of organics in beef, milk, and vegetation. C C Travis and A D Arms. *Environmental Science and Technology*, **22**, 1988, 271-274.
Date of publication	1988
Availability	Published paper. The method is implemented in the EUSES model.
Food chain considered	Food → cattle Food → milk Soil → plants (above ground parts). The model is a series of regression equations relating the accumulation factor, termed biotransfer factor in the paper, to log K_{ow}.
Types of chemicals modelled	Organic chemicals (mainly plant protection products) with log K_{ow} values in the approximate range 1.2 to 9.4 (the range varies for each food chain considered).
Environment to which it relates	Generic. The model is based on experimental data but does not take into account any media-specific factors (such as soil organic carbon).
Data requirements	Log K_{ow}.
Purpose of model/method	Research paper. The method is used in the TGD.
Summary of validation studies	Several studies have been carried out to investigate the validity of this method, such as Birak *et al.* (2001) and Trapp and Schwartz (2000).
Assessment	This forms part of the methodology that is currently used in the TGD to assess human exposure via the food chain. The method allows an accumulation factor for uptake from food into cattle (beef) and milk, and uptake from soil into plants, to be determined. These factors can then be used to estimate the concentration in plants and the subsequent concentration in cattle eating the plants from a concentration in soil. The method is simple to use.
Recommendation	Candidate for in-depth review (in conjunction with Model reference number 60).

Model reference number 73

Name of model/ method/paper	*Methodology for deriving ambient water quality criteria for the protection of human health*. United States Environmental Protection Agency, EPA-822-B00-004.
Date of publication	2000
Availability	Report available via the internet (http://www.epa.gov/waterscience/humanhealth/method/method.html).
Food chain considered	Water → fish and shellfish → humans. The approach considers four trophic levels within the food chain. The report provides a tiered hierarchy of methods for deriving bioaccumulation factors for the above food chain. A similar approach has also been developed for wildlife (USEPA, 1995a and 1995b; Federal Register, 1995).
Types of chemicals modelled	All chemicals, including inorganic and organometallic. Some methods are applicable to all chemical types, other methods given (such as the estimation of BAF from sediment accumulation factors) are only appropriate for non-ionic, moderately to highly hydrophobic, chemicals. A flow chart is provided to help select the most appropriate method.
Environment to which it relates	Generic.
Data requirements	Requires BCFs (predicted from log K_{ow} using log BCF = 0.85 x log K_{ow} – 0.70 if measurements are not available), and a BAF. The method can use measured BAFs from field studies, BAFs predicted from sediment accumulation factors, BAFs predicted from laboratory-measured BCFs or BAFs predicted from log K_{ow}. The method also requires fish consumption rates.
Purpose of model/method	Deriving ambient water quality criteria to protect human health in the United States under Chapter 304(a) of the Clean Water Act. A similar approach has been developed for wildlife criteria for the Great Lakes Water Quality Initiative (USEPA, 1995a and 1995b).
Summary of validation studies	Burkhard *et al.* (2003) carried out a comparison of two of the methods given for estimating BAFs (estimation from sediment accumulation factors and estimation from log K_{ow}) with field data for PCBs.
Assessment	A generic method based on theoretical considerations. The method uses a relatively small amount of data, although measured BAFs are unlikely to be available for a wide range of substances. In the absence of data, the method defaults to the use of log K_{ow}. The method could be readily adapted to the situation in the United Kingdom.
Recommendation	The general framework presented may be useful when considering an overall approach to standard setting.

Model reference number 74

Name of model/ method/paper	*Generic PBPK-modelling of lipophilic contaminants in the cow*. J C H. van Eijkeren, D T Jager and A J A M Sips. RIVM Report 679102 042. National Institute of Public Health and the Environment, Bilthoven, the Netherlands, March 1998
Date of publication	1998
Availability	Published report (available from http://www.rivm.nl/bibliotheek/rapporten/679102042.pdf).
Food chain considered	Food → cow → milk. The model is a physiologically based pharmacokinetic model. The model considers two functional organ compartments (blood and liver) and three aggregated compartments: the slowly perfused (muscle, skin and bone); the richly perfused (intestines, kidney) and the fat compartment. The model represents a cow with a lifetime of five years and three lactating periods, starting after parturition at the age of 2, 3 and 4 years. Its initial weight is 75 kg and its weight at maturity is 600 kg. The model is given as a series of differential equations.
Types of chemicals modelled	Organic chemicals.
Environment to which it relates	Generic.
Data requirements	Log K_{ow} , gastrointestinal absorption, partition coefficients between blood and the various organs, liver clearance rate.
Purpose of model/method	Investigation of an alternative to the methods used in the TGD for predicting concentrations in meat and milk.
Summary of validation studies	None located as part of this work.
Assessment	The model requires a large number of parameters. Its usefulness to this project is limited by lack of specific or generic information on the distribution of chemicals between blood, organs and milk fat, metabolism in the liver and absorption from the intestine.
Recommendation	Not considered further.

Model reference number 75

Name of model/ method/paper	Prediction of the bioaccumulation of persistent organic pollutants in aquatic food webs. E Voutsas, K Magoulas and D Tassios. *Chemosphere*, **48**, 2002, 645-651.
Date of publication	2002
Availability	Published paper. The complete dataset used was reported to be available via the internet (http://ttpl.chemeng.ntua.gr/pdf/baf/pdf), although this link does not appear to currently work.
Food chain considered	Water → trophic level 1 → trophic level 2 → trophic level 3 → trophic level 4. The model is a series of regression equations relating the bioaccumulation factor (log BAF) to log K_{ow} for four trophic levels within an aquatic food chain. The actual species considered within each trophic level is not defined in the paper.
Types of chemicals modelled	The regression equations are based on field data for between 94 and 352 non-ionic chemicals.
Environment to which it relates	Generic. The equations are based on field data from the published literature and are based on estimates of the freely dissolved concentration in water or the total concentration in water.
Data requirements	Log K_{ow}.
Purpose of model/method	Research paper.
Summary of validation studies	The equations were validated using field data for chemicals that were not included in the regression dataset.
Assessment	The method is very easy to use and uses the minimum of chemical-specific input data. The paper indicates that the correlations provide an estimate of bioaccumulation, typically within an order of magnitude. The paper lacks detail over exactly what organisms are considered in each trophic level (although this may be evident from the supplementary information).
Recommendation	Candidate for in-depth review.

Model reference number 76

Name of model/ method/paper	A physiological model to predict xenobiotic concentration in fish. R Yang, V Thurston, J Neuman and D J Randall. *Aquatic Toxicology*, **48**, 2000, 109-117.
Date of publication	2000
Availability	Published paper
Food chain considered	Water → fish. The model is a physiologically based toxicokinetic (PBTK) model that considers uptake into fish, mainly from water via the gills. This process is related in the model to oxygen uptake by the fish.
Types of chemicals modelled	Non-metabolised organic chemicals including di-2-ethylhexyl phthalate, DDT, sodium dodecylbenzene sulfonate, ethyenediamine tetraacetic acid, DDT, tetradecylheptaethoxylate, tetrachlorobenzene and tetrachloroguaiacol.
Environment to which it relates	Generic.
Data requirements	Oxygen uptake rate of the fish (used to determine the uptake rate and depuration rate constant of the chemical in the fish).
Purpose of model/method	Research paper.
Summary of validation studies	The predicted time-dependent accumulation of the substances modelled was compared with experimental data.
Assessment	The method considers that uptake from food plays only a minor role in determining the total body burden. This means that the method essentially only considers the time-dependent bioconcentration process. As actual bioconcentration factors are available for a reasonably large number of substances (and in the absence of experimental data, various simple methods are already available for predicting bioconcentration factors), the method is not considered further as part of this project.
Recommendation	Not considered further.

Model reference number 77

Name of model/ method/paper	Bird model Details of the model were obtained as a personal communication from Ross Norstrom.
Date of publication	Not yet available.
Availability	Not yet available.
Food chain considered	Food → bird (embryo, chick and adult). The model is a bioenergetic/pharmacokinetic model in which energy requirements of the bird (herring gulls) are estimated using empirical equations as a function of ambient temperature, photoperiod, foraging costs, growth and egg production. The model is still under development. The model is being developed as a spreadsheet model.
Types of chemicals modelled	Organochlorine compounds, including PCBs.
Environment to which it relates	Generic. The model has been developed for herring gulls in the Great Lakes.
Data requirements	Not clear at this stage.
Purpose of model/method	Research paper.
Summary of validation studies	Parts of the model have been validated. Other parts are still undergoing development.
Assessment	The model will not be available until the development work is completed and published. The model is being developed for herring gulls, but could be adapted for other species and different feeding strategies.
Recommendation	Not considered further at this stage owing to lack of available detail.

Model reference number 78

Name of model/ method/paper	Application of a food chain model to polychlorinated biphenyl contamination of the lobster and winter flounder food chains in New Bedford Harbor. J P Connolly. *Environmental Science and Technology*, **25**, 1991, 760-770.
Date of publication	1991
Availability	Published paper. The model used is available as the QEAFDCHN model.
Food chain considered	Water and plankton → clam and mussel → crab → lobster. Sediment → polychaetes and other benthic invertebrates → crab → lobster and flounder. The model is a mass balance, steady-state model. The model is presented as a series of equations.
Types of chemicals modelled	Polychlorinated biphenyls.
Environment to which it relates	Generic. The model was applied to New Bedford Harbour.
Data requirements	The model requires information on the BCF, uptake and excretion rates and chemical assimilation efficiency for the routes of exposure and organisms considered. Methods are given to relate some of these parameters to log K_{ow}. In addition, the model needs information on the growth rates, lipid contents and respiration rates of the organisms considered (typical values are given).
Purpose of model/method	Research paper.
Summary of validation studies	The model results were compared against field data for PCBs.
Assessment	The model considers exposure via the sediment and water phase as well as food. The model is generic in nature and so could be relatively easily modified for different food webs, provided the necessary species-dependent data are available. The model requires quite a lot of chemical-specific input data, but the paper provides methods to estimate some of these from log K_{ow} in the absence of actual data.
Recommendation	Candidate for in-depth review (in conjunction with Model reference number 79).

Model reference number 79

Name of model/ method/paper	QEAFDCHN The model is described in: *Documentation Bioaccumulation Model QEAFDCHN v1.0*. QEA, Quantitative Environmental Analysis, LLC, Montvale, United States, February 2001a.
Date of publication	2001
Availability	The QEAFDCHN v1.0 model is available from QEA. The model is based on the work of Connolly and co-workers. An earlier model based on work of the same authors called WASTOX (Connolly and Thomann, 1995) has also been developed and has been integrated into a model called GISTOX (Hellweger *et al.,* 2001).
Food chain considered	Water and sediment → food → predator. The model is flexible and can be easily adapted for different food chains. It can be run as a steady-state or dynamic model, and can take into account age-dependent accumulation and time-dependent effects such as migration. The model is currently being updated to include contaminant loss to birds eggs as described in Glaser and Connolly (2002) and contaminant loss to fetus production and to lactation from female sea lions as described in Connolly and Glaser (2002) (personal communication from D Glaser).
Types of chemicals modelled	Organic chemicals.
Environment to which it relates	Generic (model parameters can easily be adjusted for specific situations).
Data requirements	The chemical-specific information required includes log K_{ow} , BCF, the ratio of the efficiency of contaminant transfer across the gill to the efficiency of oxygen transfer across the gill, and the resistance factor for transfer of the chemical from lipid to blood and the chemical assimilation efficiency. The method also requires the chemical uptake and elimination rate (these can be estimated form log K_{ow} or BCF in the absence of data). The species-specific information required includes respiration rate, growth rate, food assimilation efficiency, the protein and lipid content of the organism, details of the food and the age/size classes for the species considered, amongst others.
Purpose of model/method	Research. The model has been used for studies of PCBs at several locations in the United States (see below).
Summary of validation studies	The model has been used in several studies such as Thomann and Connolly (1984), Thomann *et al.* (1992), Connolly (1991), Connolly *et al.* (2000), Connolly and Glaser (2002), Glaser and Connolly (2002), QEA (1999 and 2001b).
Assessment	The model is very adaptable and has been used to model accumulation in a range of food chains. The model is available in computerised form.
Recommendation	Candidate for in-depth review.

Model reference number 80

Name of model/ method/paper	A probabilistic model for deriving soil quality criteria based on secondary poisoning of top predators. I. Model description and uncertainty analysis. T P Traas, R Luttik and R H Jongbloed. *Ecotoxicology and Environmental Safety*, **34**, 1996, 264-278.
Date of publication	1996
Availability	Published paper
Food chain considered	Soil → food (plants, earthworms, insects) → birds and mammals. The method considers the differences in energy content between laboratory food and field food and in metabolic rate between caged laboratory birds and wild birds. A similar approach for the aquatic environment is given in Everts *et al.* (1993a and 1993b).
Types of chemicals modelled	The method has been applied to DDT and cadmium (Jongbloed *et al.,* 1996).
Environment to which it relates	Generic.
Data requirements	Requires the overall bioaccumulation factor (BAF) for the food species of concern (relating the concentration of the chemical in the food species to the concentration in soil). Other information required includes the energy content of laboratory food used in toxicity tests with the chemical, the energy content of the food species (in the field), the metabolic rate of the laboratory bird or mammal used in the toxicity tests and the metabolic rate of the wild bird or mammalian species considered.
Purpose of model/method	Research.
Summary of validation studies	None.
Assessment	The method given is not a bioaccumulation model as such, rather a general approach that could be used to take account of bioaccumulation in setting standards. The method relates the concentration in food for the predator to the concentration in soil using a BAF, taking into account the differences in energy content and metabolic rates between the laboratory situation and the field situation.
Recommendation	The general framework presented may be useful when considering an overall approach to standard setting.

Model reference number 81

Name of model/ method/paper	Life-cycle biomagnification study in fish. D T H M Sijm, W Seinen and A Opperhuizen. *Environmental Science and Technology*, **26**, 1992, 2162-2174.
Date of publication	1992
Availability	Published paper.
Food chain considered	Food → fish. The paper presents a kinetic model taking into account biotransformation, life-stage, sex and growth of fish. The model is presented as a series of equations.
Types of chemicals modelled	Hydrophobic organic chemicals, such as polychlorinated biphenyls.
Environment to which it relates	Generic.
Data requirements	The chemical-specific information required includes the uptake efficiency and elimination rate constant. The species-specific information required includes the growth rate constant and feeding rate.
Purpose of model/method	Research paper.
Summary of validation studies	The model was used to analyse laboratory accumulation data for polychlorinated biphenyls in the guppy.
Assessment	The model considers the differences between different lifestages of fish. The model would need to be computerised (spreadsheet) for routine use. The model as it stands requires knowledge of the uptake and depuration rates for each chemical.
Recommendation	Candidate for in-depth review.

Model reference number 82

Name of model/ method/paper	A partition-limited model for the plant uptake of organic contaminants from soil and water. C T Chiou, G Sheng and M Manes. *Environmental Science and Technology*, **35**, 2001, 1437-1444.
Date of publication	2001
Availability	Published paper.
Food chain considered	Soil (pore water) → plant. The model is a general equilibrium model that relates the concentration in a given plant part to the concentration in the external soil (pore water) by means of a partition coefficient between plant organic matter and water.
Types of chemicals modelled	Non-polar organic compounds.
Environment to which it relates	Generic.
Data requirements	The main chemical-specific requirements are a plant organic matter-water partition coefficient. The method also requires knowledge of the weight fraction of organic matter and water in the plant and the soil organic carbon content.
Purpose of model/method	Research paper.
Summary of validation studies	The model was used to fit experimental data for barley, carrots and radishes.
Assessment	The method requires a plant organic matter-water partition coefficient. This type of data is not routinely available for chemicals in general (although other plant models are available that estimate this type of parameter) and so this would limit the general usefulness of this approach to this project.
Recommendation	Not considered further.

Model reference number 83

Name of model/ method/paper	GEMCO Generic Estuary Model for Contaminants.
Date of publication	2003
Availability	The model was developed under the CEFIC Long-Range Research Initiative (LRI). The model is available on CD.
Food chain considered	Estuarine sediment and water → phytoplankton → mollusk and crustacean → fish. The model considers a simplified food web consisting of sediment and phytoplankton, and a predator and prey organism. The model estimates the concentrations in water, suspended solids, sediments, zooplankton, benthic fish and pelagic fish.
Types of chemicals modelled	Organic chemicals and metals.
Environment to which it relates	The model has been developed for European estuaries (contains data relevant to around 100 estuaries).
Data requirements	Not clear at this stage, but appears to require only relatively limited amounts of chemical-specific data. Site-specific data are included in the model for around 100 estuaries in Europe and four default estuary types.
Purpose of model/method	The model was developed under the CEFIC Long-Range Research Initiative (LRI).
Summary of validation studies	The model has been validated for the Scheldt and Seine estuaries.
Assessment	The model is directly applicable to the situation in Europe. A computerised version of the model has been developed.
Recommendation	Candidate for in-depth review.

Model reference number 84

Name of model/ method/paper	Elucidating the routes of exposure for organic chemicals in the earthworm, *Eisenia andrei* (Oligochaeta). T Jager, R H L J Fleuren, E A Hogendoorn and G De Korte. *Environmental Science and Technology*, **37**, 2003, 3399-3404. Modelling ingestion as an exposure route for organic chemicals in earthworms (Oligochaeta). T Jager. *Ecotoxicology and Environmental Safety*, **57**, 2004, 30-38. *Worming your way into bioavailability. Modelling the uptake of organic chemicals in earthworms*. D T Jager, 2003. Thesis from Institute for Risk Assessment Sciences, University of Utrecht.
Date of publication	2003/2004
Availability	Published paper.
Food chain considered	Soil pore water → earthworm. Food → earthworm. The model is a three-compartment, steady-state, mass balance model and is presented as a series of equations.
Types of chemicals modelled	Organic chemicals (chlorinated benzenes and polychlorinated biphenyls).
Environment to which it relates	Generic.
Data requirements	The chemical-specific data required include log K_{ow}. The species-specific data required include information on the feeding process (typical values are given for *Eisenia andrei*).
Purpose of model/method	Research paper.
Summary of validation studies	The model was calibrated using/compared with experimental data for 1,2,3,4-tetrachlorobenzene, hexachlorobenzene and PCB 153.
Assessment	The model requires only a limited amount of chemical-specific information and could readily be adapted for other species. The model would need to be computerised (spreadsheet?) for routine use. Earlier work by this author is incorporated into the method currently used in the TGD.
Recommendation	Candidate for in-depth review.

Model reference number 85

Name of model/ method/paper	RAMAS Ecosystem (a companion model RAMAS Ecotoxicology is also available).
Date of publication	Unknown.
Availability	Available for purchase from http://www.ramas.com/ecotox.htm.
Food chain considered	Water → algae → zooplankton → fish. The model allows specific food chains or webs to be constructed. The model considers population dynamics and toxicant kinetics. It is also possible to carry out Monte-Carlo simulations to investigate uncertainties in the results.
Types of chemicals modelled	Organic chemicals.
Environment to which it relates	Generic.
Data requirements	Not clear at this stage.
Purpose of model/method	For use in ecological risk assessment.
Summary of validation studies	None located as part of this work.
Assessment	The model is commercially available (fee payable) and can take into account population dynamics. Uncertainties in the model predictions can also be readily investigated. Although the exact details of the model are not clear at this stage, the model appears to be adaptable to different food chains/scenarios.
Recommendation	Candidate for in-depth review.

Model reference number 86

Name of model/ method/paper	Congener-specific transfer of PCDD/Fs from air to cow's milk: an evaluation of current modelling approaches. P E T Douben, R E Alcock and K C Jones. *Environmental Pollution*, **95**, 1997, 333-344.
Date of publication	1997
Availability	Published paper.
Food chain considered	Air → plant → cow → milk. The paper considers three different approaches: an equilibrium partitioning approach, a deposition velocity approach and a scavenging approach, developed by Lorber *et al.* (1994), Smith *et al.* (1995) and McLachlan (1995).
Types of chemicals modelled	Polychlorinated dibenzo-p-dioxins and dibenzofurans.
Environment to which it relates	Generic.
Data requirements	The chemical-specific data required includes vapour pressure, air-to-leaf transfer coefficient and milk bioconcentration factor.
Purpose of model/method	Research paper.
Summary of validation studies	The modelled results were compared against measured data for the United Kingdom.
Assessment	The model requires several chemical-specific parameters that may not be readily available for large numbers of chemicals. This would limit the general applicability of the method.
Recommendation	Not considered further.

Model reference number 87

Name of model/ method/paper	Modelling the bioconcentration of organic chemicals in plants. S Trapp, M Matthies, I Scheunert and E M Topp. *Environmental Science and Technology*, **24**, 1990, 1246-1252.
Date of publication	1990
Availability	Published paper.
Food chain considered	Air → plant. Soil (pore water) → plant. The model is a fugacity-based model and is presented as a series of equations. The model was developed for barley.
Types of chemicals modelled	Atrazine, dieldrin, chlorinated benzenes, PCBs and DDT.
Environment to which it relates	Generic.
Data requirements	The chemical-specific information required includes log K_{ow} , organic carbon-water partition coefficient, Henry's law constant and molecular weight. The model also requires several plant-specific data (values are given for barley).
Purpose of model/method	Research paper.
Summary of validation studies	The model was tested against laboratory data for atrazine, dieldrin, chlorinated benzenes, PCBs and DDT.
Assessment	The model requires only a relatively small amount of chemical-specific data and could be adapted for other plants as long as the relevant properties are available. The model would need to be computerised (spreadsheet?) for routine use.
Recommendation	Candidate for in-depth review (in conjunction with Model reference number 69).

Model reference number 88

Name of model/ method/paper	CemoS The manual for the model is published as: *Chemodynamics and environmental modelling - An introduction*. S Trapp and M Matthies. Springer, London, 1998.
Date of publication	1998 (onwards).
Availability	Published manual and computer model. The model (ComoS2 currently as a beta version) is also available for download free of charge from http://www.usf.uni-osnabrueck.de/projects/CemoS/download.en.html.
Food chain considered	Air → plant. Soil → plant. Plus a generic food chain model. The CemoS program contains six different models involving chemical fate simulation in air, water, soil and plants after single or continuous emissions for point and diffusive sources. The program contains a food chain model (Cemos_chain) consisting of three levels, a producer and two consumers, and a plant uptake model (Cemos_plant).
Types of chemicals modelled	Organic chemicals.
Environment to which it relates	Generic.
Data requirements	Not clear at this stage.
Purpose of model/method	Research. The model is intended for the prediction of exposure to hazardous chemicals released to the environment.
Summary of validation studies	None located as part of this work.
Assessment	The model is available as a computer program and can be readily modified for different scenarios. The plant uptake parts are based on various work published by Trapp and Matthies. The model also contains a generic three-level food chain model.
Recommendation	Candidate for in-depth review (in conjunction with Model reference number 69).

Model reference number 89

Name of model/ method/paper	Evaluation of models for predicting terrestrial food chain behaviour of xenobiotics. C T Garten Jr and J R Trabalka, 1983. *Environmental Science and Technology*, **17**, 590-595.
Date of publication	1983
Availability	Published paper
Food chain considered	Food → ruminant fat. Food → non-ruminant fat. Food → bird (poultry) fat. The paper presents a series of regression equations relating the bioaccumulation factor for terrestrial vertebrates to log K_{ow} or water solubility. The results are based on an extensive literature search of earlier published work.
Types of chemicals modelled	Organic chemicals (mainly organochlorine compounds and pesticides), covering a log K_{ow} range of -3.05 to 7.05.
Environment to which it relates	Generic.
Data requirements	Water solubility or log K_{ow}.
Purpose of model/method	Research paper. The method is incorporated into the model risk assessment scheme for top predators in the Netherlands proposed by Jongbloed *et al.* (1994).
Summary of validation studies	None. The method is based on a regression equation derived from experimental data.
Assessment	The method is simple to use and allows accumulation factors for vertebrates such as cattle, sheep and poultry to be estimated.
Recommendation	Candidate for in-depth review.

Model reference number 90

Name of model/ method/paper	*Development and evaluation of a terrestrial food web bioaccumulation model*. Armitage J M and Gobas F A P C. Manuscript in preparation (abstract only available at the time of this review).
Date of publication	Not yet published.
Availability	Not yet available.
Food chain considered	Soil → invertebrates → predators. The model is a steady-state bioaccumulation model.
Types of chemicals modelled	Organic.
Environment to which it relates	Generic.
Data requirements	Not yet clear but appears to include log K_{ow} and octanol-air partition coefficient.
Purpose of model/method	Research paper.
Summary of validation studies	Comparisons are made between experimental/observed and predicted biota-soil accumulation factors and biomagnification factors. The sensitivity of the model to the key input parameters is also being investigated.
Assessment	The model is not yet available, but appears to consider a food chain that is useful to this project.
Recommendation	Candidate for in-depth review (in conjunction with Model reference number 29).

Model reference number 91

Name of model/ method/paper	ARAMS Army Risk Assessment Modelling System
Date of publication	ARAMS v1.2 - Released June 2004
Availability	The ARAMS model is available free of charge from http://www.wes.army.mil/el/arams/arams.html.
Food chain considered	Aquatic food chain. Terrestrial food chain. Human food chain. The modelling system integrates the multimedia fate/transport, exposure, intake/uptake, and effects of military relevant compounds. The model contains several sub-models such as: the Terrestrial Wildlife Exposure Model (TWEM), RAMAS Ecorisk (an ecological population model), Theoretical Bioaccumulation Potential (TBP) model, Trophic Trace (a tool for assessing the trophic transfer of sediment-associated contaminants) and Multimedia Environmental Pollutant Assessment System (MEPAS; considers multimedia uptake by humans (including food). It also has databases of chemical and species information, such as a BSAF database. The model can be used for steady-state calculations and some sub-models also allow time-dependent analysis.
Types of chemicals modelled	Metals and organic chemicals (such as pesticides, PCBs, polycyclic aromatic compounds).
Environment to which it relates	Generic. The model was designed for military purposes but can be adapted for various food webs and food chains.
Data requirements	Not clear at the moment.
Purpose of model/method	Used by the US Department of Defence and the Army to conduct risk assessments to determine safe levels and clean-up target levels for military relevant compounds, and to evaluate remediation alternatives to provide the most cost-effective approach to reach target levels.
Summary of validation studies	None.
Assessment	The model appears to consider many different terrestrial species and routes of exposure. The model is freely available. The model incorporates many sub-models, though it has not been possible to review all of these as part of this screening exercise. As a result, it is difficult to assess the actual data requirements and capabilities of the overall model.
Recommendation	Candidate for in-depth review.

Model reference number 92

Name of model/ method/paper	Bioaccumulation Fish Model The background to the model is given in: *Multimedia environmental models*. D Mackay, 1991. Lewis Publishers Inc., Michigan.
Date of publication	1991
Availability	Model available for download from Canadian Environmental Modelling Centre, Trent University, free of charge (http://trentu.ca/cemc/models/Fish.html).
Food chain considered	Water → fish. Food → fish. The model is a steady-state model that considers uptake via respiration through the gills and food consumption.
Types of chemicals modelled	Organic chemicals.
Environment to which it relates	Generic.
Data requirements	The main chemical-specific data required include the log K_{ow}. Other information required the metabolism rate and the lipid content of fish.
Purpose of model/method	Research paper.
Summary of validation studies	None located as part of this work.
Assessment	The model is simple to use, but only considers a relatively simplistic food chain compared with other aquatic food chain models that are available. The model is available in a computerised form. The model could be adapted to various fish species.
Recommendation	Candidate for in-depth review (in conjunction with Model reference number 11).

Model reference number 93

Name of model/ method/paper	AQUATOX Details of the model are given in: *AQUATOX (Release 2)*. *Modelling environmental fate and ecological effects in aquatic ecosystems*. *Volume 2: Technical documentation*. United States Environmental Protection Agency, EPA-823-R-04-002, January 2004.
Date of publication	2004 (AQUATOX Version 2.0).
Availability	The model and manuals are available for download free of charge from the United States Environmental Protection Agency website (http://www.epa.gov/ost/models/aquatox/).
Food chain considered	Water and sediment → plants → invertebrates → fish. The AQUATOX model is an ecological risk assessment model that takes into account the combined environmental fate and effects of toxic chemicals and also pollutants such as nutrients and sediment. It considers several trophic levels including attached and planktonic algae and submerged aquatic vegetation, invertebrates, and forage, bottom-feeding and game fish.
Types of chemicals modelled	Organic chemicals.
Environment to which it relates	Generic. The model has been implemented for streams, rivers, ponds, lakes and reservoirs.
Data requirements	Not clear at this stage.
Purpose of model/method	The model was produced by the United States Environment Protection Agency to assist in the performance of ecological risk assessments for aquatic ecosystems.
Summary of validation studies	Details of validation studies are given at http://www.epa.gov/ost/models/aquatox/.
Assessment	A computerised version of the model is available. The model appears to be comprehensive and can be adapted for different scenarios, including different complexities of food webs.
Recommendation	Candidate for in-depth review.

Model reference number 94

Name of model/ method/paper	TRIM.FaTE TRIM stands for Total Risk Integrated Methodology.
Date of publication	2003 (TRIM.FaTE version 3.3).
Availability	The model and manuals are available for download free of charge from the United States Environmental Protection Agency website (http://www.epa.gov/ttn/fera/trim.fate.html).
Food chain considered	Aquatic food chains. Terrestrial food chains. Human food chains. The actual food chains can be user-defined. Compartment types that can be considered (with examples) include aquatic plant, benthic invertebrate, benthic omnivore, benthic carnivore, water-column herbivore, water-column omnivore, water-column carnivore, semi-aquatic piscivore (kingfisher, common loon, mink), semi-aquatic predator/scavenger (bald eagle), semi-aquatic aerial insectivore (tree swallow), semi-aquatic omnivore (mallard, raccoon), terrestrial plants, terrestrial omnivore (robin, white-footed mouse), terrestrial insectivore (black-capped chickadee), terrestrial predator/scavenger (weasel, red-tailed hawk), terrestrial vertebrate herbivore (quail, vole, deer), terrestrial ground-invertebrate feeder (shrew, woodcock), flying insect (mayfly) and soil detrivore (earthworm, arthropod). TRIM.FaTE is a spatially explicit, compartmental mass balance model. The model can predict pollutant concentrations in multiple environmental media, including biota, and pollutant intakes for biota. The outputs from TRIM.FaTE can also be used as inputs to a human ingestion exposure model (TRIM.Expo-ingestion), to estimate human exposures.
Types of chemicals modelled	Organic.
Environment to which it relates	Generic.
Data requirements	Not clear at present.
Purpose of model/method	The model was produced by the United States Environmental Protection Agency to assist with ecological risk assessments.
Summary of validation studies	Details of validation studies are given at (http://www.epa.gov/ttn/fera/trim.fate.html).
Assessment	A computerised version of the model is available. The model appears to be adaptable for different scenarios and food webs. Some of the species included in the model may not be directly relevant to the United Kingdom.
Recommendation	Candidate for in-depth review.

Model reference number 95

Name of model/ method/paper	p,p'-DDE bioaccumulation in female sea lions of the California Channel Islands. J P Connolly and D Glaser. *Continental Shelf Research*, **22**, 2002, 1059-1078.
Date of publication	2002
Availability	Published paper.
Food chain considered	Sediments → fish → female sea lions → milk and fetus. The model is a time-variable, age-dependent, physiologically based toxicokinetic model for female sea lions. The model is an application of the QEAFDCHN model.
Types of chemicals modelled	DDE.
Environment to which it relates	Southern California Bight.
Data requirements	Not totally clear at this stage but includes log K_{ow} , dietary assimilation efficiency and elimination half-life. The species-specific parameters include information on growth rate, metabolic rate, pup production, lactation and feeding habits.
Purpose of model/method	Research. To investigate if contaminated sediments were the principal source of DDE in sea lions from the area.
Summary of validation studies	The model used field-measured prey contamination levels.
Assessment	The model is an application of the QEAFDCHN model. Although this food chain is not directly relevant to the United Kingdom, it may be useful in considering how the QEAFDCHN model could be adapted to different scenarios.
Recommendation	Candidate for in-depth review (in conjunction with Model reference number 79).

Model reference number 96

Name of model/ method/paper	A model of p,p'-DDE and total PCB bioaccumulation in birds from the Southern California Bight. D Glaser and J P Connolly. *Continental Shelf Research*, **22**, 2002, 1079-1100.
Date of publication	2002
Availability	Published paper.
Food chain considered	Food → peregrine falcon, bald eagle and cormorant → eggs. The model is a dynamic, mechanistic, bioenergetics-based accumulation model.
Types of chemicals modelled	DDE and total PCBs.
Environment to which it relates	Southern California Bight.
Data requirements	The chemical-specific data are not totally clear at this stage but include log K_{ow} , metabolism rate and concentration in food. The species-specific data include respiration rate, growth rate, body composition (lipid content) and details of diet. Values are given for peregrine falcon, bald eagle and double-crested cormorant.
Purpose of model/method	Research. To investigate the pathways of DDE and PCB transfer to three species of birds.
Summary of validation studies	The modelled results were compared with field data.
Assessment	The model is an application of the QEAFDCHN model. Although this food chain is not directly relevant to the United Kingdom, it may be useful in considering how the QEAFDCHN model could be adapted to different scenarios.
Recommendation	Candidate for in-depth review (in conjunction with Model reference number 79)

Model reference number 97

Name of model/ method/paper	*Protocol for the derivation of Canadian tissue residue guidelines for the protection of wildlife that consume aquatic biota.* Canadian Council of Ministers of the Environment, Winnipeg, Canada, 1999 (available from http://www.ec.gc.ca/CEQG-RCQE/English/Ceqg/Tissue/default.cfm).
Date of publication	1999
Availability	Published report.
Food chain considered	Aquatic biota (food) → wildlife (birds, terrestrial/aquatic mammals). The method is not strictly a bioaccumulation model, rather it is a framework for use in setting standards for the protection of wildlife. In particular, the method includes a back-calculation from mammalian and avian toxicological data to a concentration in food that is protective of the species in question.
Types of chemicals modelled	Organic chemicals.
Environment to which it relates	Generic. Some of the species considered in the method are native to Canada.
Data requirements	The species-specific information required includes body weight and food ingestion rate (values are given for a large range of species).
Purpose of model/method	Setting of tissue residue guidelines in Canada.
Summary of validation studies	None located as part of this work.
Assessment	The method given is not a bioaccumulation model as such, rather a general approach that could be used to take account of food intake (or bioaccumulation) in setting standards for wildlife.
Recommendation	The general framework presented may be useful when considering an overall approach to standard setting.

Model reference number 98

Name of model/ method/paper	Development and validation of a herring gull embryo toxicokinetic model for PCBs. K G Drouillard, R J Norstrom, G A Fox, A Gilman and D B Peakall. *Ecotoxicology*, **12**, 2003, 55-68.
Date of publication	2003
Availability	Published paper.
Food chain considered	Bird eggs. The model is a toxicokinetic model that predicts the distribution of a chemical between the yolk and embryo tissue in developing eggs. The model is presented as a series of equations.
Types of chemicals modelled	PCBs
Environment to which it relates	Herring gull eggs.
Data requirements	The model uses the change in distribution in the lipid content in eggs with age (growth). The model assumes that the PCBs are entirely associated with the lipid phase of the egg.
Purpose of model/method	Research paper.
Summary of validation studies	The model was parameterized/calibrated using field data.
Assessment	The model predicts the distribution of PCBs within a developing egg and so is of limited use to this project.
Recommendation	Not considered further.

Model reference number 99

Name of model/ method/paper	Congener-specific model for polychlorinated biphenyl effects on otter (*Lutra lutra*) and associated sediment quality criteria. T P Traas, R Luttik, O Klepper, J E M Beurskens, M D Smit, P E G Leonards, A G M van Hattum and T Aldenberg. *Environmental Toxicology and Chemistry*, **20**, 2001b, 205-212.
Date of publication	2001
Availability	Published paper.
Food chain considered	Sediment → fish → otters. The model considers the equilibrium between sediment and fish, and fish and otters.
Types of chemicals modelled	PCBs.
Environment to which it relates	Generic (the modelling was carried out for several locations in the Netherlands).
Data requirements	The chemical-specific information used by the method uses sediment-biota accumulation factors for different fish species and fish-to-otter biomagnification factors.
Purpose of model/method	Prediction of effects on adult otters for several locations in the Netherlands and to derive sediment quality criteria.
Summary of validation studies	None located as part of this work.
Assessment	The method requires knowledge of sediment-biota accumulation factors for fish and fish-to-otter biomagnification factors. As these factors (particularly the fish-to-otter biomagnification factors) are not generally available for a wide range of chemicals, this would limit the general applicability of the method.
Recommendation	Not considered further.

Model reference number 100

Name of model/ method/paper	Characterization of grit in arable birds to improve pesticide risk assessment. R Luttik and G R de Snoo. *Ecotoxiology and Environmental Safety*, **57**, 2004, 319-329.
Date of publication	2004
Availability	Published paper.
Food chain considered	Grit (soil) → birds. The method considers the exposure of birds (and small mammals) to granular pesticides.
Types of chemicals modelled	Granular pesticide formulations.
Environment to which it relates	Generic (example calculations are given for a granular pesticide formulation used in the Netherlands).
Data requirements	The information required includes the pesticide formulation application rate, the particle size distribution and the incorporation efficiency of the granules in the soil.
Purpose of model/method	Research paper. The aim of the paper was to improve pesticide risk assessment.
Summary of validation studies	None located as part of this work.
Assessment	The method is specific to the application of granular pesticides to soil and so is not generally applicable to a wide range of chemicals.
Recommendation	Not considered further.

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