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# A review of models and methods for ecological risk assessment

Science Report – SC030003/SR

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Steve Killeen

**Head of Science**

# Executive summary

The proposed draft Ecological Risk Assessment (ERA) framework for contaminated land assessment under Part 2A of the Environmental Protection Act 1990 may be performed in a number of tiers. Ecological information will be collected at all tiers of the framework. In early tiers a risk assessor will need to identify receptors of interest. Site walk-overs and basic desk studies will be required to identify spatial information (e.g. home ranges) and feeding habits (e.g. likely prey organisms). At later tiers a risk assessor refines the information already gathered in previous tiers (e.g. toxicity data) by interpreting data into meaningful terms at population, community, or ecosystem levels. Further assessment may extend beyond simple food-chain interpretations to include modelling impacts on food webs, perturbations to soil processes, interpreting field surveys and biomonitoring studies.

This report assesses the available ecological modelling approaches for use in the site-specific assessments.

An initial review of the available literature assessed those models that might be suitable for evaluating the effects of exposure to contaminated land on populations, communities and ecosystems. It collated information from journal publications, book articles and the Internet, including websites of universities and regulatory organisations and authorities. The initial review drew heavily on the recommendations of Pastorok *et al.* (2002), who had recently completed an in-depth assessment of the use of models in ecological risk assessment. Central Science Laboratory (CSL) were then contracted to critically evaluate the review and determine whether it adequately covers the available modelling approaches and whether the conclusions were justifiable. With a few exceptions, all the major modelling approaches that might be applicable at Tier 2 have been considered.

A detailed assessment of the shortlisted models from the initial review was performed to identify the input requirements for each model. A comparison of these requirements with information on the data that are likely to be available for a particular site, or that could be predicted or obtained from the literature, indicated that key input data would be lacking for the majority of the models. However, the EU method for predicting risk of pesticides to birds and mammals (RASTV) might be appropriate for site-specific assessments.

The RASTV approach was applied to three hypothetical contaminated sites. Using this approach it was possible to characterise the risks posed by the majority of contaminants found in one scenario. A lack of data on toxicity of contaminants to avian and amphibian species meant that it was not possible to characterise the impacts of contaminants in the other scenarios. However, by performing a series of focused experiments to address the major data gaps and/or using predictive models, this approach could in the future be used to assess the impacts of contaminants on species of interest.

Finally, a number of recommendations for making ecological assessments, based on the findings of these reports, are presented. Recommendations include the use of the RASTV model, but also to collect extra data to populate other models where appropriate and the use of new models or methods whenever they become available, if suitable data exist.

# Acknowledgements

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# Contents

# 1 Introduction

Part 2A of the Environmental Protection Act (1990) was introduced in England on 1 April 2000, and in Wales on 1 July 2001. The aim of the Act is to identify, and remediate, land with contamination considered to be posing unacceptable risks to human health or the environment (DETR 2000). The statutory definition of 'contaminated land', described in the Environmental Protection Act (1990) is:

> *any land which appears to the local authority in whose area it is situated to be in such a condition, by reason of substances on, in or under the land that:*
>
> - *significant harm is being caused or there is a significant possibility of such harm being caused; or*
> - *pollution of controlled waters is being, or is likely to be, caused.*

Under Part 2A, land can only be defined as 'contaminated land' if there is a 'significant pollutant linkage' present (i.e. there must be evidence of a 'contaminant–pathway–receptor' relationship). Although it is the responsibility of the individual local authorities to identify contaminated land, the Environment Agency aids this process by providing information and inspecting sites on behalf of the local authorities.

In this context, the Environment Agency is developing a tiered Ecological Risk Assessment (ERA). ERA may be defined as 'a process that evaluates the likelihood that adverse ecological effects may occur or are occurring as a result of exposure to one or more stressors' (USEPA 1992). The tiered risk assessment comprises a number of different levels (tiers), each providing different chemical and/or biological information about a site. Two recently completed projects by the Environment Agency (P5-063 and P5-069; Environment Agency 2004a and 2004b respectively) reviewed and tested a suite of lethal and sublethal tests that could be applied in Tiers 1 and 2 of the ERA framework. A third project (P5-091; Environment Agency 2004c) reviewed and recommended a method for deriving soil screening values for use in Tier 1 of the framework. A triad approach of using chemical, biological and ecological data is preferred for use within the ERA framework when making decisions about a site based on a weight of evidence. However, the ERA framework currently lacks significant ecological information and approaches that could be applied in Tier 2. The present project will assess and recommend ecological models for use in Tier 2 of the ERA. Full descriptions and summaries of the ERA framework are published elsewhere (see Environment Agency 2000, 2002a, 2002b, 2004a, 2004b, 2004c), and so will not be dealt with in detail here. However, since the tiered framework for ERA, together with the various outputs from each tier, are important prerequisites of Tier 2 assessments, a brief description follows.

In lower tiers, risk assessors will develop a conceptual site model (Tier 0) and gather chemical data on contaminants in the soil (Tier 1). At Tier 2 biological and ecological effects must be considered. Biological effects can be predicted using surrogate toxicity test species, possibly with body burden data. However, as yet there are no methods recommended for assessing ecological impacts. Although, therefore, Tiers 0 and 1, and certain parts of Tier 2, of the framework provide useful information for conducting an ERA (e.g. chemical information, contaminant levels in the soil, mortality, growth, behaviour etc), there remains a need to predict effects at higher levels of biological organisation. Although some preliminary ecological information is likely to have been collected at the very start of the ERA process, to identify receptors at risk of exposure to soil contamination (e.g. lists of protected species from the Wildlife and Countryside Act), a risk assessor will need to assess risk in meaningful terms at population, community, or ecosystem levels (e.g. population growth, likelihood of population decline/extinction etc). The most appropriate method for estimating population level effects is ecological modelling. Examples of outputs from ecological models that will be of use to assessors during ERA include species richness, population abundance/biomass, population growth rate, population reproductive output, population age structure etc (Pastorok *et al.* 2002).

In summary, in addition to assessing biological effects, Tier 2 will use modelling techniques to determine the effects of exposure to contamination on biota (receptors) at population, community and ecosystem levels, and to predict how different approaches to remediation might affect an ecosystem. If significant effects of contamination are predicted from Tier 2 modelling, environmental management will be required (e.g. remediation of the site).

## 1.1 Aims

This report describes the results of a study to explore the use of ecological and population models at Tier 2 of the risk assessment process. The report comprises two separate studies, Chapters 2–3, and 4–6 respectively.

**Part 1**

Part 1 was produced by the Environment Agency and was a review of available models of potential use at Tier 2 of the ERA.

**Part 2**

Part 2 was produced by the Central Science Laboratory. Specifically, the aims of Part 2 were to:

1. Critically review the Environment Agency review of ecological models presented in Chapter 3 (Chapter 4);
2. Propose modelling approaches that can be applied at Tier 2 of the risk assessment process (Chapter 5); and
3. Illustrate the application of the proposed models using data provided by the Environment Agency, including field derived species composition data, biological effects data, ecotoxicological results and data on chemical contamination (Chapter 6).

# 2 A review of ecological models for use in ecological risk assessment

## 2.1 Introduction and methods

### 2.1.1 Methods

The purpose of this report is not to assess all of the available models first hand; such an approach is beyond the scope of this project. Instead, the report draws together information, assessments and recommendations from other works produced by experts in the field of ecological modelling and ecological risk assessment (ERA).

Information sources used during the production of this report are described below.

(1) Several reviews of ecological models have been compiled and published as books. Although the emphasis of this report was to review the most recent advances in ecological modelling, with the specific remit of use in ERA, several books provided the foundation of this report. These are:

- *Ecological Modeling in Risk Assessment: Chemical Effects on Populations, Ecosystems and Landscapes* (2002) Edited by R. Pastorok, S.M. Bartell, S. Ferson and L.R. Ginzburg
- *Fundamentals of Ecological Modelling* (2001) S.E. Jørgensen
- *Handbook of Environmental and Ecological Modelling* (1996) Edited by S.E. Jørgensen, B. Halling-Sørensen and S.N. Nielsen

(2) The literature database Web of Knowledge was searched for relevant recent (2003–2005) articles on ecological modelling and risk assessment. Journals of particular relevance included *Ecological Modelling* (Elsevier) and *Environmental Toxicology and Chemistry* (SETAC Press).

(3) The Internet and World Wide Web provide a great deal of information on ecological modelling, including several websites with directories of many useful models (Table 2.1).

4) Previous Environment Agency projects.

### 2.1.2 Structure of the review

This part of the report is structured as follows. The introduction (i.e. background to this project, Part 2A of the Environmental Protection Act), and the methods are presented first. There then follows a brief discussion of ERA at population level. This incorporates some specific data-related information on the tiered ERA being developed by the Environment Agency. Some brief information is then presented on modelling terminology and the use of computer software, before the reviews of the models are presented. The model review section (Chapter 3) summarises Pastorok *et al.* (2002), and is separated into sections according to the types of model being reviewed. Following the review of models, information from a similar Environment Agency project reviewing bioaccumulation models (Environment Agency 2007a, 2007b) is presented for terrestrial models. A table identifying sources of computer software for modelling is then presented, prior to summaries of a selection of published examples of some of the models identified in this review. A summary of how other countries (Canada, the USA and the Netherlands) use population modelling in risk assessment is then given, followed by a discussion of all the models described in this review. Finally, the recommendations from this review on which models should be validated are presented.

**Table 2.1 Internet and World Wide Web sources of information on ecological modelling**

| Internet/www address[1] | Site/information given |
|---|---|
| http://dino.wiz.uni-kassel.de/ecobas.html | Server for Ecological Modelling |
| http://dino.wiz.uni-kassel.de/mod-info/all.html | Register and Sources of Ecological Models |
| http://www.epa.gov/ceampubl/ceamhome.htm | USEPA Ecological Modelling Page |
| http://www.trentu.ca/cemc/ | Canadian Environmental Modelling Centre |
| http://www.isemna.org/ | International Society for Ecological Modelling |
| http://www.canadiancontent.net/dir/top/science/biology/ecology/software/ | Ecological modelling software links |
| http://www.red3d.com/cwr/ibm.html | Individual-based models |
| http://www.esd.ornl.gov/programs/SERDP/EcoModels/ | Strategic Environmental Research and Development Program (SERDP) Ecological Modelling Homepage |

[1] If websites given in Table 2.1 are no longer correct, and you are not automatically re-directed to the new address, entering the title into a search engine (e.g. http://www.google.co.uk) may help find the new address.

## 2.2 Ecological modelling

### 2.2.1 Introduction

Collecting and collating information for this review demonstrated that there is a very large amount of work being carried out on ecological modelling. Although considerable effort has been made in developing entirely new models, much modelling research has focused on the use of existing models in new applications which, due to the often-specific nature of ecological models, usually requires a certain amount of reprogramming. Modelling of ecological systems has been performed since the 1920s, but widespread use of ecological models in environmental management did not start until the 1970s, when ecotoxicological models were first developed (Jørgensen *et al.* 1996). During this time, most effort has concentrated on aquatic ecosystems, with comparatively little development of models for terrestrial ecosystems. Furthermore, development of models for terrestrial environments has been targeted at specific types of environment. One of the main reasons that soil has received little modelling attention is its heterogeneous nature. Whereas aquatic environments tend to be relatively physico-chemically homogeneous, soil can change from clay to sand to rocks over a very small spatial scale (Jørgensen *et al.* 1996). Regardless of which systems are modelled, the development and use of ecological modelling techniques has had mixed success. However, it is acknowledged that as long as models are based on sound ecological knowledge they can be powerful tools in the understanding of ecosystem function and, when applied correctly, can help provide better environmental management (Jørgensen *et al.* 1996). One such use of models for environmental management is that of ERA.

There now exists a wide range of biomonitoring and ecotoxicological testing techniques that can be applied in the terrestrial environment, but these are frequently applied at the individual or lower levels of biological organisation (Figure 1.1). Typically, the results from these types of testing techniques are hazard quotients, median lethal concentration (LC50), no observed effect concentration (NOEC) or lowest observed effect concentration (LOEC). It has long been recognised, however, that these laboratory-derived data have limited use in determining 'real world' effects (see Figure 1.1).

One of the most common problems with ecotoxicological testing and risk assessments is projecting the effects of pressures on physiological processes or individuals to higher levels of organisation. For example, if a contaminant impacts on a certain percentage of individuals, how will that affect the total population for that species? Furthermore, how will other species (e.g. predators) that rely on the species impacted initially be affected (e.g. due to loss of prey, or by consuming prey that is contaminated)? Currently, many ERAs have limited power because they do not consider population, ecosystem or landscape endpoints (Pastorok *et al.* 2002) and may, therefore, be too conservative or too precautionary. Generally, due to the complexities of factors affecting populations and ecosystems, it is not feasible to answer these questions experimentally, so mathematical models are used. Essentially ecological models predict the responses of population, ecosystem and landscape endpoints to perturbations in ecological components (Jørgensen *et al.* 1996; Pastorok *et al.* 2002), and are therefore an appropriate, alternative way of estimating impacts of contaminants at these higher levels of organisation.

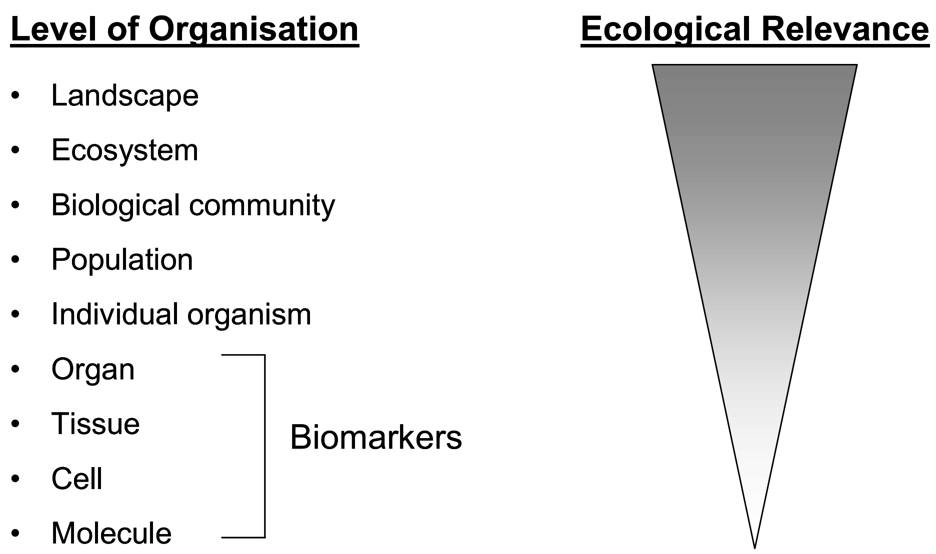


**Figure 1.1 Conceptual illustration of the contribution of biological organisation to ecological importance**

### 2.2.2 Ecological modelling in ecological risk assessment

Jørgensen *et al.* (1996) identified three main questions addressed by ERA:

(1) What is the ecological risk associated with new chemicals or products and their uses?

(2) What are the ecological impacts and risks associated with past uses of chemicals and products?

(3) What are the appropriate remediation criteria for soil, water, sediment and air; what are the most appropriate clean-up measures to reduce risk; and what is the residual risk following clean-up procedures?

Ecological modelling can address all three of these questions but, in terms of ERA for Part 2A, questions 2 and 3 are the most important. Depending on the model used, and the data available, model endpoints suitable for ERA can include (Jørgensen *et al.* 1996; Pastorok *et al.* 2002):

- abundance of individuals
- abundance of individuals of certain age classes
- spatial distribution of individuals
- spatial distribution of species
- individual characteristics (e.g. body weight)
- population growth rate
- rate of population decline
- risk of extinction
- species richness
- trophic structure
- abundance of each component in a food-web
- productivity
- metapopulation persistence
- metapopulation occupancy
- landscape occupancy patterns.

To estimate all of the ecological endpoints mentioned above, a variety of specific parameters are needed, and not all will be available from the data collected in Tiers 1 and 2. It may be possible to estimate some of the missing parameters from published literature; however, it is extremely unlikely that enough suitable data will be available (either from Tiers 1 and 2, or by estimation) to model all of the endpoints outlined. Further information about all of the tests performed at Tiers 1 and 2 can be found in Environment Agency (2002a, 2002b, 2004a, 2004b, 2004c). Specifically, data provided from lower tiers of the ERA framework will include some, or all, of the following:

## Tier 1

- Soil chemical data – toxicant concentrations and comparison with soil screening values (Environment Agency 2004c).
- Microtox® – some Microtox® data might be available. Although Tier 2 is the more likely stage for Microtox® tests, Microtox® may be used as a rapid screening tool. Microtox® is a bacterial bioluminescence test (where amount of bioluminescence decreases with increasing toxicity), and the results themselves will not be useful for modelling effects on higher populations.
- Bait lamina – this test might also be used at Tier 1 as a rapid screening test. Essentially, this test puts strips of bait into the soil and subsequent examination of the strip gives a measure of the feeding activity of soil invertebrates (e.g. Environment Agency 2004b; Filzeck *et al.* 2004).

## Tier 2

- Microtox® (see description given in Tier 1).
- Microbial N mineralisation test (OECD 2000a) – this test assesses the activity of microbes in the solid by measuring how much carbon is mineralised.
- Neutral red.
- Bait lamina (see description given in Tier 1).
- Earthworm reproduction test (OECD 2000b).
- Acute springtail test (ISO 1999).

In terms of modelling the effects of contaminants on entire communities or ecosystems, one of the most important aspects to consider is the food chain. There are two main reasons why the food chain is important:

(1) Predator–prey relationships. For example, if the receptor is a prey item for other species, and its population declines or becomes extinct due to contaminant exposure, the predator species is indirectly affected by the contaminant. The alternative scenario might also occur, whereby predator numbers are reduced due to toxicant exposure thus allowing the prey species to increase its abundance. A number of 'knock on' effects may then occur on one or more species inhabiting the same system.

(2) Bioaccumulation and biomagnification. If an organism consumes contamination via its food or water it may (depending on the contaminant and organism) accumulate the contaminant in its body tissue. Thus, a prey species might have high body-burdens of a contaminant that are then transferred to the predator. By eating numerous 'contaminated' prey items the predator may also accumulate the contaminant in its tissues, thereby increasing the concentration of the contaminant at each link of the food chain (biomagnification).

Predator–prey relationships will be highlighted at the initial stage of the ERA when receptors are identified. The effects of contaminants on predator–prey relationships can then usually be estimated by modelling contaminant effects on the prey population, and by modelling effects of food availability on the predator population. By their very nature, predator–prey models have to be incredibly specific as they have to assess the availability of species ‘A’ on effects on species ‘B’. A number of models predicting the accumulation of contaminants in body tissues and along food chains are available. The Environment Agency is currently managing a project reviewing 100 bioaccumulation models, and evaluating/validating some of the most (potentially) useful [Environment Agency project reference number P6-020/6 (Environment Agency 2007a, 2007b)]. Although the bioaccumulation models under review by the Environment Agency are mostly for aquatic systems and food chains, the recommendations should be considered for any potential use for contaminated land ERA. Although food-chain models are considered in the present review, bioaccumulation models other than those recommended by Environment Agency (2007a, 2007b) are not considered.

Finally, it should be mentioned that ecological modelling for risk assessment is not without criticism. A large number of ecological models have been used to predict a range of endpoints that are linked to toxic contaminants; however, field studies confirming predicted effects are often lacking (Tannenbaum 2003). Tannenbaum (2003) states that no ill effects have been reported in birds or mammals since the creation of the USEPA Superfund program of risk assessment for contaminated soils, and argues that such risk assessments could cease without danger to wildlife. Instead, it might be more appropriate to replace risk assessment with impact assessment (Tannenbaum 2003). Such argument promotes reactive management, as opposed to predictive management (predictive management is preventative, but only if the predictions are accurate).

### 2.2.3 Modelling terminology

Within the area of ecological modelling, a number of terms are used to describe the various types or attributes of a model. A summary of the main terms is provided by Jørgensen (2001), some of which are given in Appendix 1 as they feature in many model descriptions. Although some of these terms are mutually exclusive, models can clearly include these attributes in a number of combinations. For example, a reductionist model can be either deterministic or stochastic, depending on whether or not it includes any random elements to account for natural variability within the system.

### 2.2.4 Computer software for ecological modelling

As one progresses from simple population models to more complex interaction-based ecosystem models, there is a move from simple mathematical formulae to more complex, interacting equations that are difficult and time-consuming to evaluate manually. Consequently, there are now several computer programs available that have been written specifically for certain modelling scenarios (or computer software programs that model for various scenarios depending on operator inputs).

The development of computer software in ecological modelling has both advantages and disadvantages. For example, often, the use of computer software simply requires data to be entered in the correct format and the computer then generates the modelled output. Software, therefore, simplifies the modelling process and allows non-specialists to generate modelled data. However, although this over-simplifies the process (often a program might need certain parts modified, included, omitted etc), the ease of use can be a disadvantage since the operator is not required to understand the actual mathematics involved. If data are entered in the correct format, computer software will always calculate an answer, even if the data entered are incorrect (computer programmers call this GIGO, or 'garbage in, garbage out'). There is, therefore, a responsibility of the operator to ensure that (a) data are entered correctly, and (b) that the output is 'sensible'.

## 2.3 Model reviews

Reviews and brief assessments of a number of models potentially suitable for use in ERA are presented in the following pages. The majority of assessments are based on those conclusions made by Pastorok *et al.* (2002). Models are reviewed/assessed according to the following criteria (after Pastorok *et al.* 2002):

<u>Scientific criteria</u>

| | |
|---|---|
| Realism | Does the model use key processes from the ecosystem in question? |
| Relevance | Are results realistic ERA endpoints? |
| Flexibility | Can the model be modified for different scenarios/ecosystems? |
| Treatment of uncertainty | Does the model include uncertainties such as natural variation? |
| Degree of development and consistency | Are there any errors in the model and has it been validated? |
| Ease of estimating parameters | How easy is it to use available data in the model, and how much data is required? |

<u>Political and economic criteria</u>

| | |
|---|---|
| Regulatory acceptance | Are regulatory agencies likely to accept the model? |
| Credibility | Does the model have scientific/technical credibility? |
| Resource efficiency | How much time and effort is required to run the model under normal scenarios? |

Models, or model types/classes, are graded (low, medium and high) in terms of the criteria listed above. These criteria are comprehensive, and cover the main areas that a regulator such as the Environment Agency is likely to consider (i.e. various aspects of scientific merit, whether other regulators are using the model, and resources required to run the model). These criteria are also considered to be appropriate for the main requirements for methods/models used at Tier 2 and provide, therefore, the basis of the recommendations made in this review.

### 2.3.1 Types of model considered

Several different types of ecological model exist, varying in level of organisation, spatial scale and, therefore, complexity. Many models are based around so-called 'Monte Carlo' simulations. This is a mathematical method whereby an expression is calculated many times, using randomly sampled data inputs, so that a range of possible solutions is produced. For example, one iteration of an ecological model would use randomly selected values for several model variables to calculate the output. By performing many iterations, a probability distribution of outputs is produced according to the probability distribution of the input variables. Endpoints at the individual level (survival, reproductive output etc) will have been assessed already at Tier 2 (possibly earlier). However, Tier 2 must also determine effects on whole populations and ecosystems, and there are various means by which these effects can be modelled.

**Population models**

<u>Scalar abundance</u>

Scalar abundance models estimate the number of individuals in a population and how that abundance varies with time.

<u>Life history</u>

Life-history models specifically predict the structure of age classes within a population (e.g. number of individuals of different age or life stage).

<u>Individual based</u>

These models recognise that variability occurs between individuals, and so they model each individual explicitly.

**Metapopulation models**

Metapopulation models assess various parameters of different populations of the same species that occur in the same spatial location.

**Ecosystem models**

<u>Food-web models</u>

These models predict the transfer of contaminants along a food chain.

<u>Terrestrial ecosystem models</u>

These are large-scale models that are highly complex and able to predict a range of factors affecting whole ecosystems.

**Landscape models**

Landscape models are able to predict changes in ecosystems over thousands of hectares and over hundreds of years, that is, they are able to inform us about changes in the entire landscape.

### Toxicity extrapolation models

These models take toxicity data for one biological species or chemical and extrapolate values for other biological species with the same toxicant, or the same biological species with a different toxicant.

# 3 Model reviews

The following pages report the review of available models for use in ERA.

| | |
|---|---|
| Name/type of model: | Malthusian population growth |
| Basic principles: | Malthusian population growth is a simple model for small populations, describing exponential growth rate in habitats where resources are unlimited |
| Assessment criteria: | |
| Realism | Low – this is a very simple model, lacking important complexities such as density dependence, age structure etc and lacks any stochastic components |
| Relevance | Medium – the model has a single parameter (population abundance) but can be used to identify perturbation effects of chemicals |
| Flexibility | High – this is a very simple model and can be applied to any species |
| Treatment of uncertainty | Low – this model is deterministic |
| Degree of development and consistency | High – included in several software packages, although it can be employed simply using a spreadsheet |
| Ease of estimating parameters | High – only one parameter is used and can be estimated easily, including the effects of chemicals |
| Regulatory acceptance | High – reasonable applications of this model are likely to be accepted by regulatory agencies |
| Credibility | High – Malthusian growth is an extremely well-known model, and has been used in numerous biological studies |
| Resource efficiency | High – easy to use even on a simple spreadsheet and only simple population data are required |
| Use | This model has been used in a wide variety of studies, including crustaceans, insects, birds and mammals |
| Applicable to land ERA | Yes |

| | |
|---|---|
| Name/type of model: | Logistic population growth |
| Basic principles: | Similar to Malthusian growth, except that logistic growth does not project to infinite population sizes |
| Assessment criteria: | |
| Realism | Low – although this model recognises that a population will not grow to infinite size, it still neglects environmental variability (i.e. it has no stochastic component) |
| Relevance | Medium – although modelling of population growth is useful for predicting toxicant effects, it cannot be used for risk assessments (e.g. predicting population decline, change of age structure) |
| Flexibility | Low – difficult to use between species unless species characteristics fit the two parameters of the model closely |
| Treatment of uncertainty | Low – in its simplest form, logistic growth is deterministic |
| Degree of development and consistency | High – included in many text-books, and several software packages (e.g. RAMAS®) have a logistic growth capabilities |
| Ease of estimating parameters | High – model only has two parameters and these are easy to estimate statistically |
| Regulatory acceptance | High – logistic growth modelling has been used for several years by regulatory agencies |
| Credibility | High – variations of this model have been used in a wide variety of biological studies |
| Resource efficiency | High – very easy to use, especially as this model is implemented in several software packages. Only simple population data are required |
| Use | Yeast, crustaceans, insects, birds, sheep, humans |
| Applicable to land ERA | Yes |

| Name/type of model: | Stock-recruitment population models |
|---|---|
| Basic principles: | Stock-recruitment models are similar to Malthusian growth models with the important exception that they include density dependence (whereby growth rate is a function of population abundance) |
| Assessment criteria: | |
| Realism | Medium – stock recruitment are more complex than logistic growth models as they consider density dependence within populations (both when density is too great for resources to support, and when density is so low that individuals may not encounter one another) |
| Relevance | Medium – although useful for population toxicological analyses (i.e. effects of toxicants on populations), these models have no predictive capabilities suitable for ERA (e.g. the likelihood of a decline in population numbers) |
| Flexibility | Medium – have been used across many species and have been derived for many life histories. However, they have no stochastic capabilities and have few parameters |
| Treatment of uncertainty | Low – usually deterministic |
| Degree of development and consistency | Medium – widely used in fisheries, and implemented in some software packages, but can be difficult to apply to new systems |
| Ease of estimating parameters | High – although accurate estimation of density dependence is difficult due to the lack of full experimental evaluation, estimation is relatively simple, with many published examples |
| Regulatory acceptance | High – widely used by fisheries agencies worldwide. Sensible estimations of density dependence are likely to be accepted by regulatory bodies |
| Credibility | High – widely used in academia |
| Resource efficiency | High – few resources need be invested when applying these models to new situations |
| Use | Crustaceans, zooplankton, fish, seals, and many commercial fisheries species |
| Applicable to land ERA | Yes |

| | |
|---|---|
| Name/type of model: | Stochastic differential equation models |
| Basic principles: | A variety of models based on Malthusian and other simpler models, which have added terms introduced to account for variability within the system |
| Assessment criteria: | |
| Realism | High – these models account for the natural variability, or 'noise', found in the natural environment (one of the main criticisms of deterministic models) |
| Relevance | High – predict population size at future times, and have stochastic capabilities to allow risk analyses. Model parameters can be manipulated to assess impacts of chemicals on populations |
| Flexibility | Medium – because scalar versions of these models are relatively simple they can be widely applied across different species. However, that same simplicity makes them unsuitable for teasing out more subtle information |
| Treatment of uncertainty | High – by design, these models account for variability in natural systems |
| Degree of development and consistency | Low – these types of models are not included in software packages, and are difficult to apply to new systems |
| Ease of estimating parameters | Medium – parameters may sometimes be difficult to estimate, but are usually interpretable by ecologists |
| Regulatory acceptance | High – some uses in regulatory circumstances. Agencies are particularly interested in the stochastic capabilities of these models |
| Credibility | Medium – well known by academics, but novel nature of these models means there are few published examples so far |
| Resource efficiency | Medium – extra programming is likely to be needed to apply these models to new systems |
| Use | Crustaceans, fish |
| Applicable to land ERA | Potentially |

| | |
|---|---|
| Name/type of model: | Stochastic discrete-time models |
| Basic principles: | A density-dependent model using direct numerical solutions via Monte Carlo type computer simulations. This method provides more types of statistical information about a population, including probability of decline (a critical statistic in ERA) |
| Assessment criteria: | |
| Realism | High – a variety of these models exist ranging in complexity. Their stochastic nature enables natural variability to be considered |
| Relevance | High – predict population size at future times, and have stochastic capabilities to allow risk analyses. Model parameters can be manipulated to assess impacts of chemicals on populations |
| Flexibility | Medium – because scalar versions of these models are relatively simple they can be widely applied across different species. However, that same simplicity makes them unsuitable for teasing out more subtle information. Their inclusion in computer software makes their application easy |
| Treatment of uncertainty | High – by design, these models account for variability in natural systems |
| Degree of development and consistency | Medium – These models are simple to understand. One advantage of this is that nonsense outputs are easily identifiable. Included in computer software packages |
| Ease of estimating parameters | High – can be estimated from simple census data, and are easily extracted from the literature. This is especially easy if models err on the side of conservatism. Parameters are simple to interpret |
| Regulatory acceptance | High – some uses in regulatory circumstances. Agencies are particularly interested in the stochastic capabilities of these models |
| Credibility | Medium – well known by academics, but novel nature of these models means there are few published examples so far |
| Resource efficiency | Medium – extra programming is likely to be needed to apply these models to new systems |
| Use | |
| Applicable to land ERA | Potentially |

| | |
|---|---|
| Name/type of model: | Equilibrium exposure model |
| Basic principles: | A logistic population growth model, deterministic by nature, that combines population dynamics and toxicant chemistry |
| Assessment criteria: | |
| Realism | High – examines population dynamics in terms of toxicant chemistry |
| Relevance | High – relating population level effects to toxicant concentrations means that outputs from this model are directly relevant to ERA. Dose-response inputs are used to determine population effects following exposure to toxicants |
| Flexibility | High – base population growth aspect of model can be altered according to requirements and data available, and different dose-response functions can be used. Model should be applicable to a variety of situations |
| Treatment of uncertainty | Low – deterministic equations are the basis of this model, although their simplicity might allow some variability to be modelled using Monte Carlo analyses |
| Degree of development and consistency | Low – although the model itself is easy to understand, it is not packaged in any software yet |
| Ease of estimating parameters | Medium – parameters are easily interpreted in terms of biology, although the dose-response functions might be difficult to estimate using typical toxicity test data |
| Regulatory acceptance | Medium – model has not yet been taken up for use by any regulatory agency, although each component of the model is used individually by such agencies |
| Credibility | Low – not widely known by academics, and few published works. In addition, the model's assumption that the toxicant under investigation is already at equilibrium in the environment is criticised |
| Resource efficiency | High – easy to apply to new scenarios with little extra work |
| Use | |
| Applicable to land ERA | Yes with caution |

| | |
|---|---|
| Name/type of model: | Deterministic age/stage-based models |
| Basic principles: | Determine survival and fecundity of individuals according to their age class or life stage |
| Assessment criteria: | |
| Realism | High – these models acknowledge that survival and reproductive output depend on life stage |
| Relevance | High – outputs provide important information for ecotoxicological risk assessments (e.g. survivorship, fecundity, population size). Parameters can be adjusted to reflect effects of toxicants |
| Flexibility | High – age classes and vital rate components can all be entered on a species-specific basis, and so the model can be applied to a variety of different scenarios |
| Treatment of uncertainty | Low – these models are deterministic, and do not account for environmental variability |
| Degree of development and consistency | High – these models are easy to understand and already feature in several software packages |
| Ease of estimating parameters | Medium – laboratory, field or published data can usually be fitted to these models, although laboratory experiments may not always provide suitable information |
| Regulatory acceptance | High – regulatory agencies use this model for ERA |
| Credibility | High – this model is well known and many published examples of its use exist |
| Resource efficiency | High – since software can be used to run this model, and suitable data are usually available, time and effort required to use this model are low |
| Use | Grass, polychaetes, nematodes, arachnids, insect, molluscs, crustaceans, reptiles, fish, mammals |
| Applicable to land ERA | Yes |

| | |
|---|---|
| Name/type of model: | Stochastic age/stage-based models |
| Basic principles: | Determine survival and fecundity of individuals according to their age class or life stage, but also account for environmental stochasticity |
| Assessment criteria: | |
| Realism | High – as for previous model, but with the added advantage of a stochastic component |
| Relevance | High – as for previous model |
| Flexibility | High – as for previous model |
| Treatment of uncertainty | High – both environmental and demographic stochasticity can be included in this model |
| Degree of development and consistency | High – as for previous model, stochastic matrix models are included in several software packages |
| Ease of estimating parameters | Medium – variability of vital rates are required, as is information on the effects of toxicants on those rates. Estimating these can be difficult, although parameters are easily interpreted in terms of biology |
| Regulatory acceptance | High – as for previous model |
| Credibility | High – as for previous model |
| Resource efficiency | Medium – software makes use of this model easy, although the various types of data required may need additional collection |
| Use | Algae, trees, molluscs, corals, reptiles, fish, mammals |
| Applicable to land ERA | Yes |

| | |
|---|---|
| Name/type of model: | RAMAS® Age and Stage models |
| Basic principles: | Computer programs using matrix models for age- and stage-structured populations |
| Assessment criteria: | |
| Realism | High – acknowledge, and model, the link between age or life stage and survival etc. Both models can include density dependence and environmental stochasticity |
| Relevance | High – endpoints include predicted population size and growth rate, as well as the likelihood of population decline or extinction. Survivorship and fecundity can be adjusted to reflect effects of toxicants |
| Flexibility | High – age classes and vital rate components can all be entered on a species-specific basis, and so the model can be applied to a variety of different scenarios |
| Treatment of uncertainty | High – both environmental and demographic stochasticity can be included in these models |
| Degree of development and consistency | High – software based, and so easy to use and apply to various scenarios. The computer programs check for invalid data, inconsistencies etc automatically |
| Ease of estimating parameters | Medium – many different parameters need to be entered into these models, and it may not be easy to obtain data for all the required parameters (although parameters are easily interpreted in terms of biology) |
| Regulatory acceptance | High – both models are widely used by regulatory agencies |
| Credibility | High – both models are well known in academia and many published examples of their use exist |
| Resource efficiency | High – some additional data may require collecting, otherwise the model is run by the computer software |
| Use | Kelp, fish, birds, mammals |
| Applicable to land ERA | Yes |

| | |
|---|---|
| Name/type of model: | RAMAS® Ecotoxicology |
| Basic principles: | Computer program using matrix models for age- and stage-structured populations, specifically addressing the effects of toxicants |
| Assessment criteria: | |
| Realism | High – explicitly models the effects of chemicals on age/stage-structured populations. Includes density dependence and environmental stochastic components |
| Relevance | High – endpoints include predicted population size and growth rate, as well as the likelihood of population decline or extinction, specifically in terms of exposure to toxicants |
| Flexibility | High – age classes and vital rate components can all be entered on a species-specific basis, and so the model can be applied to a variety of different scenarios. Dose-response and other toxicant data can also be entered in a variety of ways |
| Treatment of uncertainty | High – both environmental and demographic stochasticity are addressed |
| Degree of development and consistency | High – software based, and so easy to use and apply to various scenarios. The computer program checks for invalid data, inconsistencies etc automatically |
| Ease of estimating parameters | Medium – many different parameters need to be entered into this model, and it may not be easy to obtain data for all required (although parameters are easily interpreted in terms of biology) |
| Regulatory acceptance | High – this model is widely used by regulatory agencies |
| Credibility | High – this model is well known in academia and many published examples of its use exist |
| Resource efficiency | High – some additional data may require collecting, otherwise the model is run by the computer software |
| Use | Fish, birds, mammals |
| Applicable to land ERA | Yes |

| | |
|---|---|
| Name/type of model: | Unified Life Model (ULM) |
| Basic principles: | Similar to RAMAS® in that ULM is a computer program that applies matrix models to determine population dynamics |
| Assessment criteria: | |
| Realism | High – models age- or life-stage-structured populations and accommodates stochastic parameters |
| Relevance | High – endpoints are all useful ecotoxicological measures (population size, risk of decline etc) |
| Flexibility | High – age classes and vital rate components can all be entered on a species-specific basis, and so the model can be applied to a variety of different scenarios |
| Treatment of uncertainty | High – allows inclusion of environmental stochasticity |
| Degree of development and consistency | Medium – some programming is required, and MUST be made using specific language (examples available) |
| Ease of estimating parameters | High – laboratory, field or published data can be used to run this model |
| Regulatory acceptance | Low – no agencies currently use this model, and are unlikely to do so since additional programming is required |
| Credibility | Medium – known to some academics and a limited number of publications on the use of model are available |
| Resource efficiency | Medium – some additional programming is required to run this model, and some extra data may need to be collected |
| Use | Reptiles, birds |
| Applicable to land ERA | Potentially |

| Name/type of model: | SIMPDEL[1] |
|---|---|
| Basic principles: | Part of the ATLSS (Across Trophic Level System Simulation) computer program, this model simulates various aspects (ageing, growth, foraging, mortality etc) of populations of panthers and deer, to assess the effects of environmental impacts on these two species |
| Assessment criteria: | |
| Realism | High – model uses very detailed, species-specific parameters representing the biology of panthers and deer |
| Relevance | High – endpoints provide important information for risk assessment (population abundance and spatial distribution). Although toxicant effects are excluded from the model, inputs can be modified to estimate toxicant exposure |
| Flexibility | Low – this model is specific to the South Florida wetlands, and cannot be modified for use in other systems |
| Treatment of uncertainty | Medium – although specific stochastic components are not included, variability is accounted for in each of the parameters entered |
| Degree of development and consistency | Low – although this model is a computer program, its specificity makes it impossible to use for other systems |
| Ease of estimating parameters | Low – this model uses very detailed and complex information about specific species. Accurate estimation of all parameters is unlikely |
| Regulatory acceptance | Medium – the ATLSS system (of which SIMPDEL is a component) is used by regulatory authorities in Florida but, due to its specificity, nowhere else |
| Credibility | Low – not widely known in academia due to its specificity, and there are only a few published examples |
| Resource efficiency | Low – again, the specificity of this model requires much effort to apply it |
| Use | Deer, panthers |
| Applicable to land ERA | No |

[1] Spatially explicit individual-based simulation model of Florida panthers and white-tailed deer in the Everglades and Big Cypress landscapes

| | |
|---|---|
| Name/type of model: | SIMPSAR[1] |
| Basic principles: | Part of the ATLSS computer program, this model uses various aspects (sex, age, movement, interactions etc) of the Cape Sable seaside sparrow during the breeding season, to assess the effects of environmental impacts on this bird |
| Assessment criteria: | |
| Realism | High – model uses very detailed parameters of these sparrows during the breeding season |
| Relevance | High – as for previous model |
| Flexibility | Low – as for previous model |
| Treatment of uncertainty | Medium – as for previous model |
| Degree of development and consistency | Low – as for previous model |
| Ease of estimating parameters | Low – as for previous model |
| Regulatory acceptance | Medium – as for previous model |
| Credibility | Low – as for previous model |
| Resource efficiency | Low – as for previous model |
| Use | Cape Sable seaside sparrow |
| Applicable to land ERA | No |

[1] Spatially explicit object oriented simulation model for the Cape Sable seaside sparrow in the Everglades and Big Cypress landscapes

| | |
|---|---|
| Name/type of model: | Ecobeaker |
| Basic principles: | Computer program, designed as a teaching tool, that models ecological processes |
| Assessment criteria: | |
| Realism | High – spatially explicit and incorporates a range of key environmental factors/processes |
| Relevance | High – endpoints are of use to ERA, including abundance and spatial distribution of species, and effects of exposure to toxicants |
| Flexibility | High – allows number of species, mortality, fecundity etc to be varied. Can be used for a wide variety of scenarios |
| Treatment of uncertainty | Medium – demographic and spatial environmental variability can be included in each run of the model, but parameter uncertainties cannot be addressed |
| Degree of development and consistency | High – well-supported computer software package, which can be applied to new systems easily |
| Ease of estimating parameters | Medium – depends on how complex the user wants the model to be. The more parameters that are included, the more difficult it is to find suitable data for all parameters |
| Regulatory acceptance | Low – not known to be used by regulatory agencies |
| Credibility | Low – although well known in academia, there are no published examples of this model |
| Resource efficiency | Medium – when applied to new scenarios a small amount of re-programming is required |
| Use | Teaching only |
| Applicable to land ERA | Yes |

| | |
|---|---|
| Name/type of model: | ECOTOOLS |
| Basic principles: | Programming software that allows the user to modify parameters for individuals in ecological models |
| Assessment criteria: | |
| Realism | High – the software allows modifications to be made to model individuals more specifically. A variety of parameters can be changed |
| Relevance | High – endpoints are usually population abundance and spatial distribution, and can include toxicant effects |
| Flexibility | Medium – by design, this software allows models to be modified to accommodate new systems. However, it is principally designed for small populations |
| Treatment of uncertainty | High – stochasticity can be incorporated by including Monte Carlo simulations |
| Degree of development and consistency | Low – this is programming software, and the user must be familiar with the C++ programming language. Some of the support literature is available only in German |
| Ease of estimating parameters | Medium – depends on how complex the user wants the model to be. The more parameters that are included, the more difficult it is to find suitable data for all parameters |
| Regulatory acceptance | Low – no agencies currently use this model, and they are unlikely to do so since programming is required |
| Credibility | Low – not well known in academia, and few published examples exist |
| Resource efficiency | Low – programming, including validation and de-bugging, is always required |
| Use | Models for insect, fish and birds have been modified successfully |
| Applicable to land ERA | Yes |

| | |
|---|---|
| Name/type of model: | GAPPS |
| Basic principles: | Constructs density-dependent, individual-based models for single populations of low abundance, lengthy parental care or complex age structure |
| Assessment criteria: | |
| Realism | Low – comparatively poor detail. Neither spatially nor toxicant explicit |
| Relevance | High – population abundance is the main endpoint, and survival/fecundity parameters can be modified to assess toxicant impacts |
| Flexibility | Medium – only useful for vertebrates using age-specific variables |
| Treatment of uncertainty | Medium – demographic stochasticity is implemented in this model, but environmental stochasticity is not |
| Degree of development and consistency | Medium – DOS-based software, with all associated limitations |
| Ease of estimating parameters | High – parameters such as survival and fecundity can be estimated easily from lab, field or published data |
| Regulatory acceptance | Low – not used by regulatory agencies |
| Credibility | Low – few published examples of this model's use |
| Resource efficiency | Medium – when applied to new scenarios a small amount of re-programming is required |
| Use | Large mammals |
| Applicable to land ERA | In limited cases |

| | |
|---|---|
| Name/type of model: | Occupancy models (incidence function) |
| Basic principles: | Predict whether a species is present in a particular habitat patch, based on a single census. Predictions are then used to assess likelihood of metapopulation persistence |
| Assessment criteria: | |
| Realism | Low – only include geographic factors (size and distance between patches), and do not account for population dynamics or parameters |
| Relevance | Low – metapopulation persistence is the endpoint, and not related to physical or chemical impacts |
| Flexibility | Medium – only use a few species-specific factors so could be used for a variety of systems |
| Treatment of uncertainty | High – assess variability in whether a patch is occupied or not |
| Degree of development and consistency | Medium – not currently implemented in any computer software, although the model itself is simple and could be incorporated into software or spreadsheets quite easily |
| Ease of estimating parameters | Medium – some parameters are not easily estimated from typical population datasets |
| Regulatory acceptance | Low – not known to be used by regulatory agencies, and unlikely to be taken up for formal environmental management |
| Credibility | Medium – these models are used in academia, and 100 or so publications exist describing the models in a variety of systems |
| Resource efficiency | Low – extra data are usually required, and to apply to new systems requires extra programming and validation |
| Use | Insects, amphibians |
| Applicable to land ERA | Yes |

| Name/type of model: | Occupancy models (state transition) |
|---|---|
| Basic principles: | Similar to previous model, except that data from at least two annual censuses are required, instead of just one. The extra data allow for prediction of vacant or occupied patches in relation to colonisation and extinction |
| Assessment criteria: | |
| Realism | Low – as for previous model |
| Relevance | Low – as for previous model |
| Flexibility | Medium – as for previous model |
| Treatment of uncertainty | High – as for previous model |
| Degree of development and consistency | Medium – as for previous model |
| Ease of estimating parameters | Medium – as for previous model |
| Regulatory acceptance | Low – as for previous model |
| Credibility | Medium – as for previous model |
| Resource efficiency | Low – as for previous model |
| Use | Amphibians, birds |
| Applicable to land ERA | Yes |

| | |
|---|---|
| Name/type of model: | RAMAS® Metapop |
| Basic principles: | Computer program using structured metapopulation models, which include population dynamics within each habitat patch |
| Assessment criteria: | |
| Realism | High – incorporates a wide range of population dynamics including population structure, density dependence, survival, fecundity and dispersal as well as environmental fluctuations |
| Relevance | High – endpoints are useful ecotoxicological indicators (e.g. abundance, risk of decline or extinction etc). Metapop can implicitly model perturbations such as pollution, habitat degradation, hunting etc |
| Flexibility | High – this model has many parameters than can be altered according to different systems. However, it is not suitable for species with complex social interactions |
| Treatment of uncertainty | High – incorporates natural variability in all of its population parameters |
| Degree of development and consistency | High – this model is part of the RAMAS® software, and is therefore easy to use and has good support. The computer program checks for invalid data, inconsistencies etc automatically |
| Ease of estimating parameters | Medium – requires many different types of data; however, these can usually be obtained from field or published data |
| Regulatory acceptance | High – widely used by regulatory authorities |
| Credibility | High – widely known in academia, and well-published |
| Resource efficiency | High – application to new systems requires no further programming (although may require additional data) |
| Use | Plants, molluscs, amphibians, reptiles, fish, birds, mammals |
| Applicable to land ERA | Yes |

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|---|---|
| Name/type of model: | RAMAS® GIS |
| Basic principles: | As previous model, but also links GIS-based landscape data to the types of habitats required by the wildlife in question, as well as modelling habitat–wildlife relationships |
| Assessment criteria: | |
| Realism | High – as for previous model, but with the advantage of GIS data |
| Relevance | High – as for previous model |
| Flexibility | High – as for previous model |
| Treatment of uncertainty | High – as for previous model |
| Degree of development and consistency | High – as for previous model |
| Ease of estimating parameters | Medium – as for previous model |
| Regulatory acceptance | High – as for previous model |
| Credibility | High – as for previous model |
| Resource efficiency | High – as for previous model |
| Use | Insects, birds |
| Applicable to land ERA | Yes |

| | |
|---|---|
| Name/type of model: | VORTEX |
| Basic principles: | Computer program that models metapopulation scenarios, based on the behaviour and fate (according to age, sex, social status etc) of individuals |
| Assessment criteria: | |
| Realism | High – incorporates a wide range of biologically and ecologically important characteristics that can be entered in various combinations |
| Relevance | High – endpoints are useful ecotoxicological indicators (e.g. abundance, risk of decline or extinction etc). VORTEX can implicitly model perturbations such as pollution, habitat degradation, hunting etc |
| Flexibility | Medium – flexible in the sense that many of the parameters can be modified by the user. However, VORTEX is not suitable for highly fecund or abundant species |
| Treatment of uncertainty | High – natural variability of population characteristics is considered |
| Degree of development and consistency | High – this model is computer software, and is therefore easy to use and has good support. The computer program checks for invalid data, inconsistencies etc automatically |
| Ease of estimating parameters | Medium – requires a lot of data, so getting all data may be difficult for certain scenarios |
| Regulatory acceptance | Medium – not known to be used by regulatory agencies, but is likely to be taken up in future |
| Credibility | High – well known in academia and is widely used |
| Resource efficiency | High – application to new systems requires no further programming (although some features may need additional equations). May require additional data |
| Use | Birds, mammals |
| Applicable to land ERA | Yes |

| | |
|---|---|
| Name/type of model: | ALEX |
| Basic principles: | Generic computer model for metapopulations |
| Assessment criteria: | |
| Realism | High – incorporates a wide range of population dynamics including population structure, density dependence, survival, fecundity and dispersal as well as environmental fluctuations. Does not allow stage structure |
| Relevance | High – endpoints are useful ecotoxicological indicators (e.g. abundance, risk of decline or extinction etc). ALEX can implicitly model perturbations such as pollution, habitat degradation, hunting etc |
| Flexibility | Medium – can be applied to various scenarios, but lack of stage-structure capabilities means it may not be suitable for some species (e.g. many plants) |
| Treatment of uncertainty | High – natural variability of population characteristics is considered |
| Degree of development and consistency | Medium – easy to use computer software, but may require additional programming |
| Ease of estimating parameters | Medium – requires a lot of data, so getting all data may be difficult for certain scenarios |
| Regulatory acceptance | Medium – not known to be used by regulatory agencies, but is likely to be taken up in future |
| Credibility | High – well known in academia and is widely used |
| Resource efficiency | Medium – application to new systems requires no further programming (although some features may need additional equations). May require additional data. May need author's permission to use |
| Use | Marsupials |
| Applicable to land ERA | Potentially |

| | |
|---|---|
| Name/type of model: | Predator–prey |
| Basic principles: | Many models of this type exist, modelling the constraints on the abundance of a population depending on whether prey or predators are present |
| Assessment criteria: | |
| Realism | Medium – these models tend to focus on relationship between predator and prey, without relating to ecology of system |
| Relevance | Medium – endpoints are generally abundance of predator, prey or both. Do not model toxicant effects |
| Flexibility | Low – many of these models make assumptions that are not applicable to other systems |
| Treatment of uncertainty | Low – these models are deterministic |
| Degree of development and consistency | Medium – some software packages incorporate these models, but they are inconsistent and not easy to understand |
| Ease of estimating parameters | Medium – require parameters for both predator and prey simultaneously, which is not always easy. Feeding rates are clearly important in these models, but not easily estimated |
| Regulatory acceptance | Low – not used in isolation by regulatory agencies, although may form components of larger scale models |
| Credibility | High – these models are widely known, and there are numerous published examples of their use |
| Resource efficiency | Medium – although software is available to run these models extra data are often required |
| Use | A wide range of fauna has been modelled including bacteria, algae, crustaceans, insects, arachnids, fish, mammals, humans |
| Applicable to land ERA | No |

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|---|---|
| Name/type of model: | Population-dynamic food-chain |
| Basic principles: | Use differential equation forms of predator–prey models to assess the impacts of chemicals |
| Assessment criteria: | |
| Realism | Medium – although these models include predation and food-chain transfer of toxicants, their requirement to include predator–prey models limits them since it is not known which model is most appropriate |
| Relevance | High – endpoints are important ecotoxicological data such as population size of all included species, toxicant levels in all species as well as in the environment |
| Flexibility | High – parameters are specific to individual species and food-chain relationships, but any predator–prey model can be used. A variety of dose-response functions can be used |
| Treatment of uncertainty | High – natural variability and variability between interactions are accounted for |
| Degree of development and consistency | High – included in several software packages, including RAMAS® Ecosystem |
| Ease of estimating parameters | Medium – because this model uses many specific data it may be difficult to obtain all required data |
| Regulatory acceptance | Low – not used by any regulatory agency |
| Credibility | Low – this model is comparatively new and there are few published examples of its use |
| Resource efficiency | Medium – although software implementation of this model means that no programming is required, additional data may need to be collected to run the model |
| Use | Molluscs, crustaceans |
| Applicable to land ERA | Yes with caution |

| | |
|---|---|
| Name/type of model: | RAMAS® Ecosystem |
| Basic principles: | Part of the RAMAS® modelling software package. Incorporates the effects of toxic chemicals on predator–prey relationships |
| Assessment criteria: | |
| Realism | Medium – uses specific predator–prey models, thereby making all the assumptions included in those models, which may not accurately represent the system in question |
| Relevance | High – endpoints are all important ecotoxicological data (population size, risk of decline or extinction etc) and can incorporate toxic effects |
| Flexibility | High – a choice of three predator–prey models, and three dose-response functions is available |
| Treatment of uncertainty | High – natural variability is included. |
| Degree of development and consistency | High – as with other components of RAMAS®, this program is easy to use and well supported |
| Ease of estimating parameters | Medium – requires parameters for several species simultaneously, which is not always easy. Feeding rates are important in this model, but not easily estimated |
| Regulatory acceptance | Low – not currently used by regulatory agencies |
| Credibility | Low – few published examples of this model exist |
| Resource efficiency | High – this computer program requires no further programming, although extra data may need to be collected |
| Use | Birds |
| Applicable to land ERA | Yes |

| | |
|---|---|
| Name/type of model: | Populus |
| Basic principles: | Computer program that uses differential equations to model various trophic relationships, from single interactions to whole food webs |
| Assessment criteria: | |
| Realism | Medium – uses specific predator–prey models, thereby making all the assumptions included in those models, which may not accurately represent the system in question |
| Relevance | Medium – endpoints are important ecological data (e.g. population size(s)). Toxicant effects are not explicitly modelled, but can be incorporated by varying input data |
| Flexibility | High – number of species and interactions can be varied. Any predator–prey model can be incorporated |
| Treatment of uncertainty | Low – this program is deterministic |
| Degree of development and consistency | High – this program is easy to use and well supported |
| Ease of estimating parameters | Medium – requires parameters for several species simultaneously, which is not always easy. Feeding rates are important in this model, but not easily estimated |
| Regulatory acceptance | Low – not currently used by regulatory agencies |
| Credibility | Low – no known published examples of this model exist |
| Resource efficiency | Medium – this computer program may require further programming, and extra data may need to be collected |
| Use | Teaching only |
| Applicable to land ERA | Yes |

| | |
|---|---|
| Name/type of model: | ECOTOX |
| Basic principles: | DOS-based computer program that uses differential equations to model the effects of toxicants in food chains/webs |
| Assessment criteria: | |
| Realism | Medium – uses specific predator–prey models, thereby making all the assumptions included in those models, which may not accurately represent the system in question |
| Relevance | Medium – endpoints are important ecological data (e.g. population size(s)). Toxicant effects are not explicitly modelled, but can be incorporated by varying input data |
| Flexibility | High – number of species and interactions can be varied. Only one[1] predator–prey model can be incorporated, but toxicant effects are modelled explicitly |
| Treatment of uncertainty | Low – this model is deterministic |
| Degree of development and consistency | Medium - DOS based so not as 'user-friendly' as some software packages |
| Ease of estimating parameters | Medium – requires parameters for several species simultaneously, which is not always easy. Feeding rates are important in this model, but not easily estimated |
| Regulatory acceptance | Low – not currently used by regulatory agencies |
| Credibility | Low – few published examples of this model exist |
| Resource efficiency | Medium – this computer program may require further programming, and extra data may need to be collected |
| Use | Aquatic food chains, fish |
| Applicable to land ERA | Yes |

[1] Holling (1966)

| | |
|---|---|
| Name/type of model: | Short Grass Prairie Model |
| Basic principles: | Energy-flow model using a structured series of difference equations. Considers predator–prey interactions, food webs, life stage, productivity and bioenergetics |
| Assessment criteria: | |
| Realism | Low – this is a specific model for a limited ecosystem and does not consider seasonality |
| Relevance | Medium – biomass can be calculated, which is relevant to ERA. However, the physical or chemical (toxicant) disturbance cannot be modelled |
| Flexibility | High – although this model is designed for prairies, it could be used for any grassland system |
| Treatment of uncertainty | Low – the model is deterministic |
| Degree of development and consistency | Medium – although not currently implemented in any software, relevant equations have been devised to allow programming |
| Ease of estimating parameters | High – the model has only a few parameters and these can be obtained easily |
| Regulatory acceptance | Low – this model is not used by regulatory agencies |
| Credibility | Low – this model is not widely known or used |
| Resource efficiency | High – although not available as a computer program, this model is easy to apply to any grassland system |
| Use | Grass species, insects, birds |
| Applicable to land ERA | Limited use |

| | |
|---|---|
| Name/type of model: | SAGE |
| Basic principles: | Modular model that predicts effects of $SO_2$ pollution on grassland ecosystems (soil, plants and ruminants) |
| Assessment criteria: | |
| Realism | High – the various modules of this model cover most of the important processes occurring in the ecosystem |
| Relevance | High – endpoints include grassland productivity and effects on grazers |
| Flexibility | High – can be used to model several air pollutants, and can be applied to any grassland ecosystem |
| Treatment of uncertainty | Low – deterministic |
| Degree of development and consistency | Low – not available as software, and information not available to write code. The model has, however, been validated |
| Ease of estimating parameters | Low – due to the number of detailed modules incorporated in this model, obtaining all of the required data is difficult |
| Regulatory acceptance | Low – this model is not used by regulatory agencies |
| Credibility | Medium – following good initial use, no further use or development has been undertaken |
| Resource efficiency | Low – requires much work to set up all of the required parameters, particularly since the model is not available as software |
| Use | Grassland species. Specifically air pollution effects |
| Applicable to land ERA | Yes |

| | |
|---|---|
| Name/type of model: | SPUR |
| Basic principles: | Modular approach to predicting interactions among soils, plants and grazers. However, modules are integrated into the overall SPUR software package |
| Assessment criteria: | |
| Realism | High – models plant carbon accumulation and its availability to grazers. All factors affecting these processes are accounted for |
| Relevance | Medium – although providing some endpoints suitable for ERA (e.g. productivity) it does not model physical or chemical (toxicant) disturbance |
| Flexibility | High – this model could be applied to any grassland ecosystem |
| Treatment of uncertainty | Low – deterministic |
| Degree of development and consistency | High – the integrated SPUR model is available as software |
| Ease of estimating parameters | Low – due to the modular structure of this model, which requires large amounts of data, estimating all parameters is likely to be difficult |
| Regulatory acceptance | High – SPUR is issued by the US Department of the Interior, and is therefore endorsed by US regulatory agencies |
| Credibility | High – well known, and many published examples of this model are available |
| Resource efficiency | Low – due to the site-specific, modular structure of this model a large amount of data must be entered (although implementation as software makes this easier) |
| Use | Multiple grassland species |
| Applicable to land ERA | Limited use |

| | |
|---|---|
| Name/type of model: | Multi-Timescale Community Dynamics |
| Basic principles: | Predicts community dynamics by combining outputs from a population dynamic model and a biogeographic model |
| Assessment criteria: | |
| Realism | Low – tends to underpredict species turnover (change in composition due to immigration or extinction) |
| Relevance | Medium – cannot be directly applied to ERA as it does not account for toxic effects; however, this model may provide some useful ecological information |
| Flexibility | High – could potentially be applied to any system that involves barriers (physical, spatial or temporal) that restrict interactions between wildlife communities |
| Treatment of uncertainty | Low – deterministic |
| Degree of development and consistency | Medium – although not currently implemented in computer software, information does exist to allow programming of this model |
| Ease of estimating parameters | Medium – receptors are defined as distinct populations, therefore can be treated as independent groups |
| Regulatory acceptance | Low – not used by regulatory agencies |
| Credibility | Medium – these models are not well published, although the algorithms from which they are derived are well accepted |
| Resource efficiency | Medium – may need some programming to implement these models |
| Use | Birds |
| Applicable to land ERA | No |

| | |
|---|---|
| Name/type of model: | Modified SWARD |
| Basic principles: | Models the equilibrium between primary producers and consumers in a grassland ecosystem. These two components are modelled separately and then combined |
| Assessment criteria: | |
| Realism | High – considers many important ecological factors including bioenergetics and factors that affect primary production (e.g. nutrients) |
| Relevance | Medium – although this model provides suitable ecological endpoints such as productivity, it does not explicitly predict effects of physical or chemical (toxicant) disturbances |
| Flexibility | High – could be applied to any grassland ecosystem with minimal effort |
| Treatment of uncertainty | Low – deterministic |
| Degree of development and consistency | Low – not available as software |
| Ease of estimating parameters | Low – this model has many parameters that each require site-specific data |
| Regulatory acceptance | Low – not used by regulatory agencies |
| Credibility | Medium – although not well known in its own right, this model is based on accepted ecological modelling approaches |
| Resource efficiency | Medium – some programming and extra data are likely to be required |
| Use | Multiple grassland species, sheep |
| Applicable to land ERA | Potentially |

| | |
|---|---|
| Name/type of model: | Wildlife–Urban Interface Model |
| Basic principles: | Models the effects of agricultural and urban development on vegetation cover and use of habitats by wildlife. Specifically predicts the probability of certain bird species occurring following changes in land use |
| Assessment criteria: | |
| Realism | Medium – extrapolates probability of occurrence from historical land use and subsequent impacts on bird populations |
| Relevance | Medium – probability of occurrence is a useful ERA endpoint, and indeed the model was designed to predict effects of anthropogenic habitat disturbance. However, does not consider toxicant effects and incorporating this in the model could be difficult |
| Flexibility | Medium – could be applied to most temperate urban/agricultural scenarios |
| Treatment of uncertainty | Medium – estimates probability of occurrence, but estimates single values instead of density functions |
| Degree of development and consistency | Medium – not available as software, although the code is available |
| Ease of estimating parameters | Medium – essentially requires many data to estimate habitat requirements of a number of plants and birds, but these may not all be required |
| Regulatory acceptance | Low – not used by regulatory agencies |
| Credibility | Low – not used in ecological studies |
| Resource efficiency | High – based on empirical relationships |
| Use | Multiple terrestrial plant (not tree) and bird species |
| Applicable to land ERA | Potentially |

| | |
|---|---|
| Name/type of model: | STEPPE |
| Basic principles: | A gap-dynamic model that predicts grassland productivity according to available resources. Can be used to predict recovery; but only for single species |
| Assessment criteria: | |
| Realism | Medium – models species-specific growth, inter-species competition and species recruitment |
| Relevance | High – models grassland productivity, which is a suitable ERA endpoint. Physical and chemical impacts are entered by the modeller (i.e. not modelled), although toxicant influence could be incorporated into the seed production and recruitment function |
| Flexibility | Low – model is specific to a semi-arid environment, thus water availability (rain) controls growth. Can only model single species |
| Treatment of uncertainty | Low – deterministic |
| Degree of development and consistency | Medium – not available as pre-written software, although information is available to write in programming code |
| Ease of estimating parameters | Medium – requires only three parameters |
| Regulatory acceptance | Low – not used by regulatory agencies |
| Credibility | Medium – uses common algorithms and modelling structure |
| Resource efficiency | Medium – few parameters are needed, but the model requires site-specific information |
| Use | Multiple grassland plant species |
| Applicable to land ERA | Potentially |

| | |
|---|---|
| Name/type of model: | LANDIS |
| Basic principles: | Spatially explicit (GIS-based) model for predicting changes in forest landscape/structure over large areas and time-spans. Able to model disturbances (such as fire) and subsequent succession |
| Assessment criteria: | |
| Realism | High – considers many important forestry landscape processes, including natural (wind, fire, succession) and anthropogenic (management). Effects of processes are predicted according to specific life-history information |
| Relevance | High – can predict changes in forest landscapes over hundreds of years and/or thousands of hectares. A number of ecologically important endpoints are modelled; toxicant impacts could be incorporated |
| Flexibility | High – as long as life history and initial conditions are known, any forest landscape can be modelled |
| Treatment of uncertainty | High – stochastic |
| Degree of development and consistency | High – commercially available as computer software |
| Ease of estimating parameters | Medium – application to a new forest landscape would require medium effort, due to re-parameterisation |
| Regulatory acceptance | Low – not used by regulatory agencies |
| Credibility | High – this model is well known and cited examples occur in books and scientific journals |
| Resource efficiency | Medium – it might take moderate effort to apply to a new landscape, although this would be a comparatively simple exercise |
| Use | Multiple tree species and forestry landscapes |
| Applicable to land ERA | Potentially |

**Toxicity extrapolation models**

| | |
|---|---|
| Name/type of model: | HCS[1] |
| Basic principles: | Extrapolates from a sample of LC50s to predict toxicant concentrations in order to protect 50% of most sensitive species |
| Assessment criteria: | |
| Realism | Medium – assumes that all sensitivities follow the same logistic equation, have the same mean and the same variance. The model does not account for links between toxicity and physical factors |
| Relevance | Medium – the model is based on LC50 data and is therefore relevant to ERA, although by aiming to protect the most sensitive species this model may be too precautionary |
| Flexibility | High – provided LC50 data exist, this model can be applied to any system. Number of species in the system can be varied |
| Treatment of uncertainty | Mean – this model takes mean LC50 data, but does not consider the variance about the mean, which will occur due to natural variation and experimental error |
| Degree of development and consistency | Medium – this model has been tested and validated |
| Ease of estimating parameters | Medium – this model uses three parameters (location and dispersion values, and the application factor), all of which can be estimated reasonably easily |
| Regulatory acceptance | Medium – this model has some regulatory use |
| Credibility | High – HCS has been used as the basis for other models |
| Resource efficiency | N/a |
| Use | |
| Applicable to land ERA | Yes, provided terrestrial LC50 data are available |

[1] Hazardous Concentration for the most Sensitive Species

**Toxicity extrapolation models**

| | |
|---|---|
| Name/type of model: | $HC_p$[1] |
| Basic principles: | A modified version of the HCS model, aiming to predict toxicant concentrations that will protect a percentage of species in a community |
| Assessment criteria: | |
| Realism | High – based on the HCS model, but uses NOEC data instead of LC50 data. Assumes that communities will survive minor purturbations |
| Relevance | High – endpoints include growth, survival and reproduction and are, therefore, all important ERA data |
| Flexibility | Medium – originally written for soil invertebrates, but applicable to most systems if sufficient data exist and all assumptions made in the model are valid |
| Treatment of uncertainty | High – although this model takes a mean NOEC, it does account for uncertainty and variance about that mean from multiple experiments |
| Degree of development and consistency | High – these models have been tested many times |
| Ease of estimating parameters | High – parameters are easy to estimate for this model |
| Regulatory acceptance | High – variations of this model have been used for regulatory purposes, particularly in the Netherlands |
| Credibility | High – use of these models has been published in the scientific literature |
| Resource efficiency | N/a |
| Use | |
| Applicable to land ERA | Yes |

[1] Hazardous Concentration for a Population

**Toxicity extrapolation models**

| | |
|---|---|
| Name/type of model: | Acute to Chronic Ratio |
| Basic principles: | Simply an acute toxicity test value (LC50) divided by the maximum allowable toxicant concentration (MATC), allowing estimation of chronic toxicity from acute laboratory tests |
| Assessment criteria: | |
| Realism | Low – simply a ratio drawn from laboratory toxicity data |
| Relevance | Medium – mortality endpoint is relevant to ERA, in the sense that LC50 and MATC are also relevant |
| Flexibility | Medium – can be applied to most systems provided sufficient data are available |
| Treatment of uncertainty | Low – uses point-source LC50 and MATC mean values. Does not account for variability or experimental error |
| Degree of development and consistency | Medium – some validation has been made of this model |
| Ease of estimating parameters | Medium – uses only LC50 and MATC, which can be obtained from the literature, otherwise the model cannot be used |
| Regulatory acceptance | High – used by regulatory agencies in the USA and Canada |
| Credibility | Medium – the application of this model has been validated and published, although the model depends entirely on LC50 and MATC data |
| Resource efficiency | N/a |
| Use | |
| Applicable to land ERA | Yes |

**Toxicity extrapolation models**

| | |
|---|---|
| Name/type of model: | $NOEC_{survival}$ to $NOEC_{endpoint(x)}$ |
| Basic principles: | Predicts NOEC for a specified endpoint using NOEC for survival data |
| Assessment criteria: | |
| Realism | High – design features of this model, where NOECs for each endpoint have been calculated using collated published datasets, are considered realistic |
| Relevance | High – endpoints are significant ecotoxicological data (growth, reproduction, survival etc). Other endpoints are also predicted |
| Flexibility | Medium – designed for fish, but could be used for other systems subject to validation of relationships between NOEC endpoints |
| Treatment of uncertainty | Medium – 95% confidence intervals of $NOEC_{survival}$ are accounted for in the estimation of $NOEC_{growth}$ and an uncertainty factor is applied |
| Degree of development and consistency | Low – these NOEC relationships have not been validated |
| Ease of estimating parameters | High – uses at least three parameters, but all are easy to estimate |
| Regulatory acceptance | Low – not used by regulatory agencies |
| Credibility | Low – very few publications exist, for this unverified model |
| Resource efficiency | N/a |
| Use | |
| Applicable to land ERA | No |

**Toxicity extrapolation models**

| | |
|---|---|
| Name/type of model: | Scaling (birds) |
| Basic principles: | Uses scaling factors based on medial lethal doses (LD50s) to extrapolate toxicity data between bird species. Based on pesticide data |
| Assessment criteria: | |
| Realism | Low – LD50 data used to derive the power curve used in the extrapolation are deliberately screened to remove variation, and include data from artificial dosing experiments |
| Relevance | Medium – LD50 data, the basis of this model, are not particularly useful for ERA purposes |
| Flexibility | High – although based on birds and pesticides, this method could potentially be applied to all species and toxicants |
| Treatment of uncertainty | Low – individual LD50 data are used, with no account for variation, or experimental/statistical error |
| Degree of development and consistency | Low – this model has been validated only once |
| Ease of estimating parameters | High – only requires LD50 data, which are readily available |
| Regulatory acceptance | Medium – has been used, although not officially adopted, by the USEPA |
| Credibility | Medium – some published examples, but since the scaling factor for birds is close to 1.0, this model is not as useful as it might be for other groups |
| Resource efficiency | N/a |
| Use | |
| Applicable to land ERA | Yes |

**Toxicity extrapolation models**

| | |
|---|---|
| Name/type of model: | Allometric scaling (mammals) |
| Basic principles: | Uses a general allometric equation to extrapolate various factors between species of mammal according to their body weight |
| Assessment criteria: | |
| Realism | Low – in terms of extrapolating toxicological effect, this model assumes that toxicity is entirely dependent on metabolic rate, ignoring factors such as diet quality, bioaccumulation etc |
| Relevance | High – can be used to extrapolate useful ERA endpoints between species |
| Flexibility | High – can be used for all mammal species, and a number of different toxicological data points |
| Treatment of uncertainty | Low – does not account for uncertainty |
| Degree of development and consistency | Medium – this model has been used and validated several times |
| Ease of estimating parameters | High – the allometric equations upon which this model is based are generally available for many mammal and bird species |
| Regulatory acceptance | Medium – has been used, although not officially adopted, by the USEPA |
| Credibility | Medium – some published examples of this model's use exist |
| Resource efficiency | N/a |
| Use | |
| Applicable to land ERA | Yes |

**Toxicity extrapolation models**

| | |
|---|---|
| Name/type of model: | Inter-Species Toxicity |
| Basic principles: | Uses polynomial regression lines of LC50 data to extrapolate toxicity values between species |
| Assessment criteria: | |
| Realism | Low – no screening, or careful selection, of LC50 values (the basic data-source for this model) is made |
| Relevance | Medium – uses acute, lethal data (LC50) and the endpoint is also LC50. Although useful at screening level, these are not directly applicable to ERA |
| Flexibility | High – can be used for any species |
| Treatment of uncertainty | Low – makes no account for error, either in collation of LC50 data or experimental error |
| Degree of development and consistency | Low – this model has not been validated |
| Ease of estimating parameters | High – requires only LC50 data, which are widely available in the literature |
| Regulatory acceptance | Low – this model is not used by regulatory agencies |
| Credibility | Medium – some published accounts exist, including critical reviews |
| Resource efficiency | N/a |
| Use | |
| Applicable to land ERA | Screening level only |

**Toxicity extrapolation models**

| | |
|---|---|
| Name/type of model: | AEE[1] |
| Basic principles: | Uses LC50 data for one species to extrapolate toxicity endpoints (LC50, MATC etc) for a similar species |
| Assessment criteria: | |
| Realism | High – extrapolates only to species, and uses simple toxicity data (LC50, MATC) |
| Relevance | High – endpoints (e.g. MATC) are useful ecotoxicological endpoints and applicable to ERA |
| Flexibility | High – potentially applicable to any species |
| Treatment of uncertainty | High – accounts for experimental and extrapolation error |
| Degree of development and consistency | Low – this model has not been validated |
| Ease of estimating parameters | High – LC50 and MATC parameters are obtained easily, and the model allows datasets of different size |
| Regulatory acceptance | Medium – has been used, although not officially adopted, by the USEPA |
| Credibility | High – this model has been reviewed favourably in the literature |
| Resource efficiency | N/a |
| Use | |
| Applicable to land ERA | Yes |

[1] Analysis of extrapolation errors

## 3.1 Bioaccumulation models

The Environment Agency recently commissioned a report assessing the suitability of available bioaccumulation models for use in standard setting (Environment Agency 2007b). The project dealt only with bioaccumulation of organic compounds.

The project presented a brief review of 100 bioaccumulation models (for aquatic, terrestrial and human food chains) and identified the 15 models most suitable for further investigation. Following this further investigation study, six models were put forward for validation and evaluation with ‘real’ data. The two terrestrial models nominated for validation were:

- Arctic terrestrial food-chain bioaccumulation model
- Technical Guidance Document (TGD).

A brief summary of the models considered in Environment Agency (2007) is presented here.

### 3.1.1 Arctic terrestrial food-chain bioaccumulation model

As the name suggests, this model was specifically written for an arctic food chain; specifically comprising lichens, willows, caribou and wolves (Kelly and Gobas 2003). However, it has been identified as one of the very few models that actually considers terrestrial predators (Environment Agency 2007b) and, therefore, potentially useful if the model can be adapted to UK scenarios.

This model assumes that aerial deposition of the chemical is the most likely exposure pathway, and then uses different compartmental models to predict uptake by vegetation and terrestrial mammals (both by predation and passing from mother to foetus). The model incorporates a number of chemical, ecological and physiological parameters for which estimated values have been provided by the model creators (Kelly and Gobas 2003). The ecological and physiological parameters specifically relate to the two terrestrial mammals (i.e. caribou and wolves); the applicability of this model to UK scenarios will depend on a similar food chain being identified and the required parameters being available (either from experimental studies or estimates).

This model has been validated using 25 organochlorine contaminants, using concentrations measured in the environment over 14 years to estimate concentrations in the four receptors (lichens, willow, caribou and wolves). Overall, the model predictions were close to the measured concentrations in all four receptors.

At the moment this model is not suitable for application to UK scenarios because the food chain it models is alien to the UK. However, the basic structure and format of the model could potentially be modified to incorporate UK-significant compartments. At the moment the model exists only in the form of written equations; there is no computer program that incorporates this model, and the equations would need to be entered into a spreadsheet for routine use of the model to prevent time-consuming hand-written calculations (Environment Agency 2007b). Furthermore, the actual modification of the model to fit a suitable UK food web is substantial. However, in theory the model could be modified to include, for example, soil to earthworm to badger (or similar). Given the potential to adapt this model to fit UK scenarios, together with the fact that there are very few models for terrestrial food chains, the benefits probably justify the resources required to modify this model.

### 3.1.2 EU Technical Guidance Document

The Technical Guidance Document (TGD) was devised for the risk assessment of new and existing substances within the European Union (European Commission 2003). The TGD incorporates aquatic, terrestrial and human pathways of exposure; and is available as the EUSES (European Union System for Evaluation of Substances) computer program, which can be downloaded free of charge from the Internet (see Table 3.1). For the purposes of this review, only the terrestrial component of the TGD (an earthworm food chain) will be considered.

The TGD uses concentrations of a chemical in the air, soil, surface waters and marine water (which can be entered as known values or estimated by the model) to predict concentrations at local or regional scales (Environment Agency 2007b). The main route of contamination to soil is via aerial exposure or application of sewage sludge; the model accounts for natural degradation of the substance. Uptake by earthworms is then modelled with a bioconcentration factor, using experimental data if available, or estimated values. Uptake of the contaminant into the worm is from the soil pore-water; it is then assumed that target predators consume the earthworms. When validated against 11 substances, the TGD terrestrial model worked well for uptake of substances from experimental water in isolation, however, the TGD consistently over-estimated the uptake of chemicals from soil pore-water (Environment Agency 2007b).

The table later in this section shows how the model would score according to the criteria highlighted by Pastorok *et al*. (2002).

### 3.1.3 System dynamic model

The system dynamic model is a generalised food-chain model, first described by Carbonell *et al.* (2000), intended to improve regulatory risk assessment protocols, such as the TGD.

The model exists in two versions:

<u>Simple version</u> – this can be used for 'worst case scenario' predictions, and assumes an instantaneous equilibrium exists between the environmental compartments and receptor organisms in the food chain (Environment Agency 2007b). The simple format uses bioconcentration factors (BCFs) and biota–food and biota–sediment accumulation factors.

<u>Complete version</u> – this version considers the uptake rates and depuration rates of substances by the receptor organisms, using kinetic data for the various processes.

The model was initially described for an aquatic food chain (Carbonell *et al.* 2000), but could be applied to other food chains. Indeed, a version of the system dynamic model has now been incorporated into the *Guidance Document for the Risk Assessment of Birds and Wildlife* [Council Directive 91/414/EEC regarding pesticides for plants (European Commission 2002)]. In this version of the model, a number of food chains were considered:

Soil – Soil dwelling invertebrates – Insectivorous birds/mammals – Carnivores Terrestrial top predator, or,

Insects – Insectivorous birds/mammals – Carnivores – Terrestrial top predator, or,

Plants – Herbivorous birds/mammals – Carnivores – Terrestrial top predator.

There is no published validation of this model.

### 3.1.4 Other bioaccumulation models highlighted by Environment Agency (2007b)

Two other models with terrestrial applications were also identified for in-depth review, but on closer inspection considered too complex for general use, needing substantial expertise by the operators (Environment Agency 2007a). Brief descriptions were provided however, which are summarised here.

#### Army Risk Assessment Modelling System (ARAMS)

The United States Department of Defence and Army use ARAMS for performing risk assessments when remediating sites from chemicals used by the military (Environment Agency 2007b). ARAMS is essentially a platform that uses a number of sub-models to estimate the fate and transport of substances, exposure, intake and uptake, and effects of chemicals on wildlife and humans. Sub-models can be used in isolation or in combination with some or all of the other sub-models. In addition, ARAMS is linked to various physico-chemical and biotic information databases providing, for example, BAFs, lipid content of target organisms, environmental effects etc. ARAMS includes a number of pre-programmed habitat types, including desert, coniferous forest, deciduous forest and grassland, among the terrestrial habitats. There is also a facility for other user-defined habitats. Default receptors within the model include mice, rabbits, bats, deer, canine predators, and birds of prey.

#### Total Risk Integrated Methodology (TRIM.FaTE)

TRIM.FaTE was devised by the USEPA for performing ERAs. It is a spatially explicit, mass balance model for predicting the concentrations of pollutants in various environmental media (abiotic and biotic). TRIM.FaTE can also be used for predicting pollutant intake by biota (Environment Agency 2007b). The model allows the input of user-defined food chains, and contains a database of default compartment types to allow the user to construct a model ecosystem. Terrestrial abiotic compartments include surface soil, root zone soil, vadose soil and groundwater; terrestrial biotic compartments include plant components (leaf, stem root), soil detritivores (earthworm, soil arthropods), omnivores (mouse, robin), insectivores (shrew, chickadee), vertebrate herbivores (vole, deer) and predators/scavengers (weasel, hawk).

The model combines any user-defined data with information stored in its data libraries (selected by the user) to construct food chains, either as a static or dynamic system. The model can also perform a sensitivity analysis and Monte Carlo analysis to determine uncertainty in the model outputs (Environment Agency 2007b).

Both ARAMS and TRIM.FaTE are available as computer programs that can be downloaded free of charge from the Internet (see Table 3.1). The relatively extensive databases, compartment libraries, and flexibility to combine whichever components the user defines to form quite specific food chains suggest that both of these models would be suitable for terrestrial ERA, and of course they are. However, the requirement of ‘considerable expert knowledge’ to run these models (Environment Agency 2007b) suggests they are unsuitable for routine use by the Environment Agency.

Further to those models mentioned above, Environment Agency (2007a) also highlighted a number of bioaccumulation models for predicting toxicant uptake by earthworms (e.g. Sample *et al.* 1998; Jager *et al.* 2003; Jager 2004). Although earthworms are likely to be a significant receptor in terrestrial ecosystems, these models are not considered further in this project. The tiered structure of the ERA includes measured tissue-burdens for earthworms, so such models are likely to be redundant in the tiered ERA. They may prove useful if insufficient sampled data are available; in such cases the TGD model could be used as the models described by Jager and co-workers (1998, 2003, 2004, 2005) are incorporated into the TGD.

| | |
|---|---|
| Name/type of model: | Arctic terrestrial food-chain |
| Basic principles: | Mechanistic, mass balance equations relating ambient concentrations in the environment to concentrations in plant, herbivores and mammals |
| Assessment criteria: | |
| Realism | Medium – incorporates a number of physiological data for the predators, providing a realistic assessment of the main factors affecting uptake and bioaccumulation. However, many of these parameters are estimated, not based on experimental data |
| Relevance | Medium – predicts bioaccumulation of organic contaminants along a food chain, and from mother to foetus. Does not relate to how such bioaccumulation might impact on population survival |
| Flexibility | Medium – at present specifically for lichens, willow, caribou and wolves. Structure can be modified to reflect UK scenarios, but modification would be substantial |
| Treatment of uncertainty | Medium – will depend on availability of metabolism data. If enough data are present, Monte Carlo iterations can be used to produce confidence intervals |
| Degree of development and consistency | High – this model has been validated for 25 chemicals and found to predict concentrations in its four receptors with acceptable accuracy |
| Ease of estimating parameters | High – chemistry and ecological data requirements are modest and can be estimated from the literature |
| Regulatory acceptance | Low – this model is not used by regulatory agencies |
| Credibility | Medium – some published accounts exist, including critical reviews |
| Resource efficiency | Low – at present only available as the written equations. Would need to be entered into a spreadsheet for routine use |
| Use | To date, only lichens, willows, caribou and wolves |
| Applicable to land ERA | Potentially high. Very few terrestrial food-chain models exist, and this model could be modified to incorporate food-chain pathways relevant to UK scenarios |

| | |
|---|---|
| Name/type of model: | EU Technical Guidance Document |
| Basic principles: | Bioaccumulation factors applied to target organism |
| Assessment criteria: | |
| Realism | Medium – uses bioconcentration factors to predict uptake by earthworms using either experimental or estimated data. Uptake is only considered via pore-water |
| Relevance | Medium – predicts bioaccumulation of a substance from soil pore-water to give an estimate of earthworm contaminant levels. Does not predict uptake by predators, nor does it consider population survival etc |
| Flexibility | Medium – terrestrial component considers earthworms specifically. Other components of the TGD consider other food chains |
| Treatment of uncertainty | Low - deterministic |
| Degree of development and consistency | Medium – the terrestrial part of the TGD has been validated, although the validation suggests that earthworm bioaccumulation from pore-water is over-estimated |
| Ease of estimating parameters | High – this model uses simple physico-chemical parameters that are readily available. Experimental BCFs can be entered if available |
| Regulatory acceptance | High – this model was specifically designed for risk assessments of new and existing substances within a regulatory context |
| Credibility | Medium – some published accounts exist, including critical reviews |
| Resource efficiency | High – the TGD is available as a computer program (EUSES) |
| Use | Earthworm bioaccumulation; uptake by avian and mammalian predators |
| Applicable to land ERA | Potentially – does not predict risk of extinction directly, but provides estimates of body burden in relation to exposure |

| | |
|---|---|
| Name/type of model: | System dynamic |
| Basic principles: | The simple version uses bioconcentration factors; the complete version uses kinetic data to account for uptake and depuration |
| Assessment criteria: | |
| Realism | Medium – although this depends on which version of the model is used (complete being more realistic than simple). Uses bioconcentration and kinetic relationships |
| Relevance | Medium – predicts concentration of substances present in receptors at each stage of the food chain modelled. Does not consider population survival etc |
| Flexibility | High – although originally described for aquatic food chains, this model can be applied to many food chains |
| Treatment of uncertainty | Medium – Monte Carlo simulation can be used to produce estimates of uncertainty |
| Degree of development and consistency | Medium – this model has not been validated. The model has been developed further for terrestrial food chains |
| Ease of estimating parameters | Low – this model relies on a number of parameters (e.g. bioconcentration factors, assimilation efficiencies and depuration rate constants) for each organism in the food chain selected. Experimental data are unlikely to be available, although some can be estimated (albeit with a degree of uncertainty) |
| Regulatory acceptance | Medium – the initial model has not been used by regulatory agencies. However, a terrestrial version of this model has been proposed for regulatory use in Europe |
| Credibility | Medium – some published accounts exist, including critical reviews |
| Resource efficiency | Low – at present only available as the written equations. Would need to be entered into a spreadsheet for routine use |
| Use | To date, only aquatic (algae, cladoceran, fish) |
| Applicable to land ERA | Potentially – does not predict risk of extinction directly, but provides estimates of body burden in relation to exposure |

## 3.2 Previous Environment Agency reviews of population modelling

In 1998, the Environment Agency (Risk and Forecasting Policy) commissioned WRc to prepare a report reviewing ecological models for potential use in environmental forecasting. Although this report is now more than 7 years old, some of the terrestrial models reviewed may still be of use for ERA for Part 2a, or form the basis of more recent models. The 1998 review specifically looked for models that were available, to some degree, as computer software (which would make them attractive for present-day ERA). A brief summary of the relevant points from the WRc report is presented here.

WRc (1998) presented information on 29 terrestrial models that were of potential use in environmental forecasting (Appendix 3). Of those 29, only 7 were designed specifically to look at the impacts of chemicals or toxicants on the system being modelled:

| | |
|---|---|
| ACAC | a food-web model for assessing uptake of contaminants in foraging species (Freshman and Menzie 1996) |
| CATS | - |
| CemoS | this modelling package has three components: CemoS/Chain, CemoS/Level and CemoS/Plant. CemoS/Chain models chemical degradation and accumulation in producers and consumers; CemoS/Level models the steady state of chemicals in organisms and soil; and CemoS/Plant models contaminant levels in plants. All three components are compartment models |
| CL-CCE | models critical loads of acidity and sulphur in soils |
| PEF | a food-web model for assessing uptake of contaminants in foraging species |
| PLANTX | as its name suggests, this model predicts the accumulation of anthropogenic contaminants in plants (in the roots, stems and leaves) |
| RAMAS® | - |

CATS and RAMAS® are dealt with elsewhere in the present review. As discussed, these models are still used for ERA purposes. ACAC and PEF are both food-web models developed in the USA, but whereas ACAC makes predictions for individuals, PEF assesses effects on populations (WRc 1998). CL-CCE is unlikely to be of use for Tier 2 of the ERA framework, as soil concentrations of contaminants are dealt with at Tier 1 (Environment Agency 2004b). Finally, PLANTX is considered a useful model or assessing accumulation of contaminants in plants at the landscape scale, but is not considered to be of use to Part 2a assessments because receptors at risk will tend to be animals.

Although, therefore, WRc (1998) reviews a number of models that were identified to be of potential use in environmental forecasting and risk assessments, the majority of models identified are not considered suitable for Tier 2. Those models reported in the WRc report (WRc 1998) that are considered to be of use in Tier 2 are reviewed elsewhere in the current document.

## 3.3 Availability of models

Although a large quantity and range of ecological models exists, not all are easily available. Clearly, some of the simpler models are just mathematical formulae or equations, which can easily be entered into a computer spreadsheet (or even calculated manually). Some of the more complex models, however, may require a great deal of programming. There are two ways in which these more complex models can be used: (i) the various equations can be entered into a software compiler, which translates the input into computer code so that it can be run as a computer program, or (ii) pre-written software may be used. Compilers have the advantage in that only one copy of the compiler is required, and can be used to code any model; their disadvantage is that they require some programming skills by the operator and take time to code and then de-bug. Pre-written software has the advantage that it is ready to use immediately; disadvantages being less flexibility and cost of licensing agreements to use the software. Although many of the software packages now available for ecological modelling are only available commercially, some models are available as 'Freeware' and can be downloaded from the Internet for use without having to pay for either a licence or the software. Table 3.1 gives the Internet addresses for several modelling software sites, including both commercially available software (with licensing/purchasing information) and sites where freeware is available for download.

**Table 3.1 Internet addresses for some modelling software sites**

| Name/description | Freeware | Address |
|---|---|---|
| RAMAS® Modelling Software | No | http://www.ramas.com |
| EcoSim Modelling Software | Yes | http://www.garyentsminger.com/ecosim/index.htm |
| VORTEX Modelling Software | By donation | http://www.vortex9.org/vortex.html |
| Environmental Healthy Safety Homepage | Yes | http://www.ehsfreeware.com/ecoclean.htm |
| Tietjen Web-based Simulations homepage | Yes | http://cas.bellarmine.edu/tietjen/rootweb/simulations.htm |
| Poptools (add-in for Excel) | Yes | |
| EUSES 2.0.3 (European Union System for the Evaluation of Substances) | Yes | http://ecb.jrc.it/existing-chemicals/ |
| ARAMS (Army Risk Assesement Modelling System) | Yes | http://el.erdc.usace.army.mil/arams/ |
| TRIM.FaTE (Total Risk Integrated Methodology) | Yes | http://www.epa.gov/ttn/fera/trim_fate.html |

## 3.4 Model examples

### 3.4.1 Individual-based models

Baveco and DeRoos (1996) described individual-based population models for earthworms. The models are deterministic and based on differential equations that predict equilibrium and dynamic properties of the population. The models examined energetic costs to individual earthworms imposed on vital rates (growth, reproduction etc) due to sublethal exposure to pesticides. Risk is then predicted at the population level by estimating changes in population size, age structure, extinction limits etc. The models can then be used to predict extinction probability and likely recovery times (Baveco and DeRoos 1996; Klok *et al.* 1997). The models have been validated with pesticides, and demonstrated differences in sensitivity of two earthworm species (*Lumbricus rubellus* and *L. terrestris*). The models were concluded to work well, but need further development (e.g. defined relationships between ambient concentration and individual performance) before they could be used productively for ERA.

### 3.4.2 Deterministic age-based models

Several examples using deterministic age- or stage-based models to estimate population level effects of given impacts exist in the literature. Although published examples have tended to be used for aquatic animals, there is no real reason why the same models cannot be applied to terrestrial populations.

Otway *et al.* (2004) used deterministic versions of both age- and stage-based models to estimate the rate of what they called 'quasi' extinction (defined as the time for the population to be reduced to <50 breeding females). The models were run for various scenarios (e.g. worst or best case scenario, inclusion of anthropogenic pressures etc), and produced good results. Although not critically assessed by the authors, the model worked well, and the flexibility of the user-defined parameters allowed a number of scenarios to be modelled.

Wiese *et al.* (2004) used age-based population modelling to determine how two mortality pressures (chronic oil pollution and hunting) affected a species of bird (*Uria lomvia*; the thick-billed murre). In the first instance, potential population growth rate was modelled on the assumption that no mortality was caused by anthropogenic pressure. Wiese *et al.* then ran the model to predict reduced population growth on account of hunting and oil pollution, alone and in combination. The authors concluded that as long as the associated vital rates and numbers killed are known, the models can be used to assess the impacts of any given anthropogenic pressures (Wiese *et al.* 2004).

However, as highlighted in the model description, the deterministic nature of these models means that variability is not considered. So although a number of scenarios can be modelled by simply altering the parameters entered, it is not possible to predict how much variability there might be around any given model output.

### 3.4.3 Deterministic stage-based models

Otway *et al.* (2004) used deterministic versions of both age- and stage-based models to estimate the rate of what they called 'quasi' extinction (defined as the time for the population to be reduced to <50 breeding females). The models were run for various scenarios (e.g. worst or best case scenario, inclusion of anthropogenic pressures etc), and produced good results. Although not critically assessed by the authors, the model worked well, and the flexibility of the user defined parameters allowed a number of scenarios to be modelled.

Chandler *et al.* (2004) combined a full life-cycle laboratory toxicity test with a Leslie matrix stage-based model to predict effects of a pesticide on copepod populations. The toxicity test data were used to predict rate of population growth as well as change in net growth with toxicant concentration and time. The model was used successfully to show depressions in population growth at realistic pesticide concentrations.

### 3.4.4 Stochastic age-based models

Wiese *et al.* (2004) used stochastic versions of their age-based population model to assess the impacts of chronic oil pollution and hunting on populations of *Uria lomvia* (the thick-billed murre). As with their deterministic version of the model (see Deterministic age-based models), potential population growth rate was modelled on the assumption that no mortality was caused by anthropogenic pressure. The stochastic version of the model agreed with predictions of the deterministic version of the model, but had the added advantage of predicting 95% confidence intervals. Having predicted intrinsic growth rate, the model predicted reductions in population growth rate following hunting in isolation, oil pollution in isolation, as well as the combined effects of hunting and oil pollution. As with the deterministic model, the authors concluded that as long as the associated vital rates and numbers killed are known, the models can be used to assess the impacts of any given anthropogenic pressures (Wiese *et al.* 2004).

McGee and Spencer (2001) developed a stochastic stage-based model for predicting effects of sediment toxicity on a marine amphipod. The model predicted trends in growth, survival and fecundity. When tested in the field, predicted values closely matched amphipod numbers (McGee and Spencer 2001). The model was able to identify critical factors controlling the population at different times of the year, and also showed that comparatively small changes in survival had potentially severe consequences on population growth (McGee and Spencer 2001). However, Cooch *et al.* (2003) criticised stochastic matrix modelling on account of seasonal variations in stochastic growth rate due to covariance in matrix parameters. They proposed a modification whereby seasonal matrices are specifically subscripted to a particular year, which removes the artefact variation.

**RAMAS® (Stage)**

Kaye *et al.* (2001) used RAMAS® Stage to model the effects of fire on the population growth and extinction probability of a prairie plant. They constructed stochastic matrix models, selecting each matrix element from a distribution with observed mean and variance (this provided the stochastic element of the model). The model worked well, demonstrating that deliberate burning of the prairie plants was necessary if extinction was to be avoided.

RAMAS® Stage has also been used to predict the risk of extinction of an endangered trout (*Oncorhynchus gilae*) (Brown *et al.* 2001). Variations of several biotic parameters (including population size, fecundity, life-stage structure, number of populations) and anthropogenic or 'event' parameters (regulated fishing, wildfire etc) were used to estimate the likelihood of extinction under various scenarios. In this instance, RAMAS® demonstrated that wildfire was the factor most likely to affect population viability.

Schwartz *et al.* (2000) used RAMAS® Stage to estimate the probability of persistence for a population of coniferous trees in Florida. The tree (*Torreya taxifolia*) is under threat of extinction due to disease and lack of seed production. The model demonstrated that the tree population would survive for the next 50 years.

Risk of extinction was estimated for woodpeckers by Maguire *et al.* (1995) using RAMAS® Stage. A population of red-cockaded woodpeckers (*Picoides borealis*) had been monitored at a wildlife refuge, and so various data existed for the population, including banding (tagging) of the birds. RAMAS® Stage was used to create a stochastic age-based model to estimate population dynamics, and then to see how those dynamics varied according to different parameters being entered into the model. Sensitivity analysis of the model indicated that juvenile survival was the most critical aspect of population viability (Maguire *et al.* 1995).

**Unified Life Model**

Legendre (1999) used the Unified Life Model (ULM) to predict the possibility of extinction of birds due to demographic uncertainties. The ULM software was used to build a two-sex model, in conjunction with a typical life-cycle graph, and Monte Carlo analysis to predict extinction possibilities. The model worked well and predicted that demographic uncertainty causes high extinction risk, particularly for short-lived species.

Ferriere *et al.* (1996) discussed the use of the ULM for performing viability analysis and use in conservation. They used a population of known age structure, reproductive status etc and predicted risk of extinction. The model was used to predict the deterministic growth rate, population structure and reproductive value; stochastic factors influencing risk of extinction (e.g. environmental and demographic variability) were also used in the extinction analysis. The ULM software was reported to be very user-friendly, allowing a number of parameters to be entered to allow the modelling of a number of scenarios. Two case studies (snake and bird of prey) were presented to demonstrate the versatility of the ULM.

### 3.4.5 Metapopulation models

Chaumot *et al.* (2002) highlighted that metapopulation models alone do not work particularly well for risk management due to spatial problems. To counter this, they used dose-response data to populate a multi-region Leslie-matrix model to estimate the responses of brown trout populations to different pollutant release scenarios. The model successfully predicted stable-age structure, asymptotic population growth rate and the reproductive value, and was therefore able to compare different pollutant scenarios.

**RAMAS® (GIS)**

Larson *et al.* (2004) tried to link population viability with habitat suitability using a suite of models, including RAMAS® GIS. They modelled population viability of ovenbirds and linked it to realistic landscape simulations using a Habitat Suitability Index (HSI) model. They then estimated population characteristics for a hardwood forest using the LANDIS model. Applying three scenarios from the HSI model to RAMAS® GIS, Larson *et al.* (2004) linked estimates of habitat suitability to ovenbird population viability by using fecundity and carrying capacity. The authors reported that linking the models together in this way provided extra benefits on population viability modelling.

Schtickzelle *et al.* (2005) transferred data from a healthy Belgian population of butterfly to estimate population viability of an endangered Dutch population using the

RAMAS®/GIS computer-modelling program. The authors needed to use the Belgian data because the high quality data required to run the model did not exist for the endangered population. The model predicted that considerable habitat restoration would be needed to ensure the survival of the Dutch population. The authors concluded that the use of surrogate population data was a suitable way to 'by-pass' lack of (specific) data on the population in question. RAMAS®/GIS worked well in this example.

### 3.4.6 Landscape models

A number of published papers describe the use of the LANDIS landscape model; in fact, the model has been used by boreal ecologists from all over the world for more than 10 years now (e.g. Mladenoff 2004). Most recently, Zollner *et al.* (2005) used LANDIS to investigate different succession scenarios for hardwood species based on the implementation of different management scenarios. Scheller *et al.* (2005) used LANDIS to demonstrate the influence of fire, and absence of fire, on the species composition and landscape structure of a pine forest. Previously, Scheller had modelled the effects of climate change on forest community and landscape structure using LANDIS (Scheller and Mladenoff 2005). In all cases, the model has proved to be a very useful tool in predicting the effects of various forest management strategies on the subsequent community structure of the forest. The model is flexible and under constant modification and improvement (Mladenoff 2004).

### 3.4.7 Model comparisons

Several papers (e.g. Lindenmayer *et al.* 1995; Mills *et al.* 1996; Brook *et al.* 1997) have specifically set out to compare the various population viability analysis (PVA) packages (including RAMAS®, GAPPS, VORTEX).

Brook *et al.* (1997) performed a retrospective analysis of the population dynamics of Lord Howe Island woodhen (*Tricholimnas sylvestris*) using five PVA modelling software packages (including VORTEX, GAPPS, RAMAS®/Stage and RAMAS®/Metapop). Outputs from the various PVA models were compared with each other and, more importantly as a validation exercise, also with real field data. Stochastic, density-independent formulations of all the models gave similar predictions to each other, but none reflected 'real' population dynamics (Brook *et al.* 1997). So, under these conditions the packages were not helpful for predicting realistic outcomes. However, when observed historical population trends data were entered into the models, all of the software packages gave realistic (and similar) estimates. Mills *et al.* (1996) performed a similar comparison of PVA software packages (including GAPPS, VORTEX, RAMAS®/Stage), examining outputs for a single dataset of grizzly bear population dynamics. Although the same dataset was used for each program, small differences in 'input' format required by the various programs necessitated some data manipulation. This initial inconsistency in data input caused small differences in intrinsic growth rate, which in turn caused major differences in risk of extinction and predicted population size. However, environmental and demographic stochasticity caused only small differences in viability between the three programs. However, when density dependence was added to each model the outputs varied widely. The authors attributed this to the way that each model handles density dependence, and recommended that scenarios without density dependence should be modelled unless the data suggest a particular density-dependent model (Mills *et al.* 1996).

In their comparison of available software packages for predicting metapopulation viability, Lindenmayer *et al.* (1995) used ALEX, RAMAS®/Space and VORTEX. However, in contrast to the comparison of model outputs and realistic data described above, Lindenmayer and colleagues assessed the models in terms of their build, assumptions made, and how easy the software is to use. Each software package has, unsurprisingly, a different structure based on the model writer's own perceptions of the parameters that most affect metapopulation viability. Although similar in aim, therefore, the different programs may produce different predictions, even if applied to the same population dataset. As shown by Brook *et al.* (1997), these programs will produce similar results, but small differences may arise due to different weighting of parameters within the program. Although, therefore, any of these models might be suitable for assessing metapopulation viability, care should be taken wherever possible that the strengths, limitations and assumptions made by the chosen model are most appropriate to the dataset being used (Lindenmayer *et al.* 1995). Choice of model may also depend on exactly what output is required from the program.

The results of Brook *et al.* (1997) illustrate that one of the main restricting factors of modelling pollutant effects at the organisation level of population or ecosystem is the availability of suitable data.

## 3.5 Population assessments by other countries

### 3.5.1 Canada

In 2005, the Canadian Council of Ministers of the Environment (CCME) released the first draft of their protocol for deriving environmental and human health soil quality guidelines (CCME 2005). The guidelines have undergone several modifications since the National Contaminated Sites Remediation Program (NCSRP) was established in 1989, and are specifically derived for the assessment of contaminated sites. The CCME has developed a number of tools and combined their use to form a risk assessment framework for the screening and assessment of contaminated sites. This is a tiered framework, which uses generic guidance (Tier 1) and site-specific assessments (Tier 2) to assess the contamination status of a site and identify remediation requirements (CCME 2005). When considering the terrestrial environment, toxicant effects due to exposure from direct contact and ingestion of contaminated soil are considered.

In terms of higher level effects, Tier 2 of the Canadian protocol is where impacts on populations and ecosystems are addressed, being made on a site-specific basis. Accordingly, soil quality guidelines are derived using laboratory and field toxicity data to predict deleterious effects (e.g. factors that affect the survival or reproduction of a species) that impact on the key ecological receptors. Key ecological receptors vary according to the land use type, for example, agricultural and recreational land are afforded more ecological protection than commercial or industrial land (CCME 2005).

In 1988 it was agreed, at an OECD workshop for ecological assessments, that studies to predict species extinction were too difficult and expensive to perform. Although nearly 20 years old now, this argument is maintained by the CCME in its soil quality guidelines (CCME 2005). Consequently, generic soil quality guidelines that are protective of endpoints of higher levels of biological organisation (i.e. species extinction and ecosystem failure) have not been established (CCME 2005). Instead, the Threshold Effects Concentration (for soil dwelling biota) and Daily Threshold Effects Dose (terrestrial fauna) are the endpoints that, if exceeded, are expected to impact on populations (i.e. survival and reproduction). Despite this, only key ecological receptors are used in setting guidelines due to the lack of ecological information on effects on terrestrial animals (CCME 2005).

A number of equations contribute to the overall protocol. For example, the Daily Threshold Effects Dose is estimated by dividing the lowest effect dose (i.e. effect dose of the most sensitive receptor) by an uncertainty factor. The Daily Thresholds Effects Dose can be estimated for primary, secondary consumers etc along a food chain. Bioconcentration factors are used to estimate bioaccumulation along food chains, and ingestion exposure (ingestion rate) is estimated from the rate of dry matter intake and the mean amount of dry matter available.

Population and ecosystem level effects are not specifically considered under the CCME guidelines for soil contamination and remediation. The CCME has agreed that accurate ecological assessment of these higher levels of biological organisation is too expensive and beyond the means of the experimental data currently available. Instead, it assumes that the outputs from equations and models used in the tiered ERA produce guideline values that are sufficiently protective of processes that may impact on populations and ecosystems (e.g. survival and reproduction). The models and equations used by the CCME may therefore be suitably protective of terrestrial fauna exposed to contaminated land in the UK. However, they will only provide guideline values and not give outputs specifically showing that populations are at risk, nor will they provide any information on the remediation that is required to remove that risk.

### 3.5.2 USA

The United States Environmental Protection Agency (USEPA) has recently reviewed ERA principles and practices (Dearfield *et al.* 2005). Of particular relevance to this report was the discussion of individual versus population level effects. Individual level effects have a long history of use in regulation in the USA, and are supported by the courts (USEPA 2004). Similar to the rationale adopted by the Canadian authorities, protection of the individual has been perceived to be protective of the population and community (Dearfield *et al.* 2005, Stahl *et al.* 2005). This is because any pressure on the survival or reproduction of an individual is assumed to impact on its parent population, even if population level effects themselves have not been demonstrated (USEPA 2003, Dearfield *et al.* 2005). However, changes in resource management have meant that population level assessments are now required, and the USEPA has been actively developing population level assessment tools. Consistent with many other international regulatory authorities, the USEPA has recognised that assessment of higher levels of biological organisation necessarily have greatly increased uncertainty due to the lack of suitable ecological information. Generally such assessments are extrapolations of vital rate information (birth rate, death rate etc), accounting for the increased uncertainty.

The USEPA implemented the Federal Insecticide, Fungicide, and Rodenticide Act (FIFRA) to ensure the protection of wildlife and humans from contamination by pesticides, and the ERA for FIFRA has been continually developed since its conception. For example in 1996 a workgroup (ECOFRAM; Ecological Committee on FIFRA Risk Assessment Methods) was established to provide a way forward from deterministic risk assessments, although the specific aim of the group was to develop probabilistic risk assessments for pesticides. Within the ERA developed for FIFRA, there is a terrestrial investigation model, which is a multimedia exposure/effects model that can be used to address acute mortality levels in generic or specific species over a user-defined exposure window. The spatial scale is at the field level, such that the field and surrounding area are assumed to meet habitat requirements for each species. However, although it is recognised that there is a need to consider population level endpoints, the FIFRA risk assessment does not consider population level impacts (relying on the default position that single species endpoints are protective of the whole population).

The USEPA provides ERA guidance[1], which should be followed when assessing risks at USEPA Superfund sites. Each Superfund site is unique in terms of the contaminants present and their potential health effects. Therefore, USEPA conducts risk assessments on a site-by-site basis. The risk assessment estimates the current and possible future risks, if no action were taken to clean up the site. The aim of the Superfund is to ensure that risks are managed to acceptable levels, and that risk managers incorporate risk assessment information with a variety of site factors to select the best clean-up strategies.

There is an eight-step process defined for ERA of Superfund sites, including two screening level assessments (problem formulation and risk calculation), full problem formulation, study design, field sampling plan, site investigation, risk characterisation and risk management. Predictive modelling, using the data from earlier steps, occurs at step 7 (risk characterisation) and will focus on the endpoints defined at the problem formulation stage. Endpoints should include 'ecosystems, communities, and/or species potentially present at the site'. However, at the risk characterisation step, the guidance recommends the use of no observed adverse effects level (NOAEL) and lowest observed adverse effects level (LOAEL) for species and organisms, not populations. As stated earlier, the assessment endpoints used (such as mortality and reproduction) are assumed to include population level effects.

Population modelling is one of the Atlantic Ecology Division's (USEPA) current research themes. The USEPA website has links to a number of population models used for a variety of risk assessment purposes. The website lists current projects under development as well as previous projects. In particular, the models described below may become useful for ERA in the future.

The USEPA has been developing a terrestrial investigation model for assessing the risk of contaminant exposure to birds (Fite *et al.* 2001). The model is designed for risk assessment of exposure to pesticides following crop spraying, but may have some use for risk assessment of contaminated land. The model is based on dose-response data for various avian species, requiring comparatively easily obtained parameter data.

[1] http://www.epa.gov/oswer/riskassessment/risk_superfund.htm

Parameters included in the model are:

- food-habits
- ingestion rate of water
- ingestion rate of food
- frequency of drinking from contaminated site
- frequency of feeding from contaminated site
- distribution of contaminant residues in water
- distribution of contaminant residues in food
- degradation rate of contaminant
- dose response of species.

For each iteration, randomly selected values are entered into the model to estimate the average risk of an individual dying due to contaminant exposure (based ultimately on the dose-response curve for the contaminant and species in question). Many iterations are made via Monte Carlo sampling for a set of individuals, and then for multiple sets to provide a probability density function for per cent mortality. Various case studies applying this model have been conducted, and the model works well.

Given that the USEPA has developed this model, it is likely that the model will be used for regulatory and risk assessment purposes in the USA, and may be adopted by other regulatory agencies. Although designed for exposure to pesticides, this model could potentially be applied to other terrestrial ecosystems with contamination, provided that the required parameters are known (especially those detailing chemical components, particularly distribution).

The US Department of the Interior (including the Bureau of Land Management, Bureau of Reclamation, Fish and Wildlife Service and National Park Service) uses a risk assessment modelling package developed at the Argonne National Laboratory (ANL). The ANL (operated by the US Department of Energy at the University of Chicago) has developed the RESRAD modelling computer package for performing ERAs.

The whole RESRAD package comprises seven models, and most are used for the risk assessment of radionuclides (e.g. RESRAD, RESRAD-BUILD and RESRAD-RECYCLE). However, RESRAD-ECORISK and RESRAD-CHEM are potentially useful for ERA of contaminated land.

RESRAD-ECORISK estimates the movement of contaminants through the terrestrial food webs of wildlife receptors, predicts doses and risks to them, and derives preliminary clean-up goals for site remediation. For terrestrial risk assessments, the RESRAD-ECORISK computer program uses environmental fate and transport models and food-web uptake models. The predicted dose values can then be used to estimate risks to ecological receptors and to calculate possible remediation targets. RESRAD-ECORISK evaluates five wildlife receptors: American robin, mallard, white-tailed deer, eastern cottontail and deer mouse. For each species, it contains data on factors that could affect exposure to, and uptake of, site contaminants; the factors include home range, body weight, food and water ingestion rates, and diet. It allows the user to analyse receptors and exposure routes individually and in combination. The code may be used as a screening tool to determine if site conditions warrant a more detailed baseline risk assessment. It can also be used for detailed risk assessments if site-specific data are available.

The computer program has an interface that lets the user enter site-specific contaminant values and environmental input parameters, identify sensitivity analysis parameters, and graphically view selected input data distributions.

RESRAD-ECORISK has been developed in accordance with current USEPA guidance on, and requirements for, assessing Superfund sites. Various aspects of the RESRAD modelling program have been used in remediation and risk evaluations at more than 300 sites in the USA and around the world.

Lu *et al.* (2003) and Fan *et al.* (2005) describe a computer-based, ERA model (named 'ERA'). The authors, recognising that there were few ecological models suitable for ERA (and that those that were available were often site-specific), developed a model as part of the Department of Defence 'Sustainable Green Manufacturing' initiative (Lu *et al.* 2003). For terrestrial receptors, Lu *et al.* (2003) defined ingestion, inhalation and dermal contact as the main exposure pathways and recognised that potential bioaccumulation was an important aspect of the ingestion pathway in terms of food-web modelling. The ERA package devised by Lu *et al.* (2003) included models for estimating uptake via all three pathways. Equations and parameters used in the models were taken from a number of peer-reviewed publications and databases (e.g. USEPA 1993, 2001). These allow for modelling of a number of receptors, including birds, mammals, reptiles, amphibians, aquatic animals and aquatic plants. The model uses Microsoft Visual Basic 6.0 as a platform (Fan *et al.* 2005), and this is linked to an interactive database management system (DBMS) (Microsoft Access), which acts as a data-storage facility (Lu *et al.* 2003; Fan *et al.* 2005). The DBMS is also linked to external databases such as ECOTOX (USEPA 1993) to allow site-specific modelling.

Lu *et al.* (2003) used the model in a case study looking at metals employed for electroplating purposes (chromium, molybdenum and tantalum) at two Proving Ground sites chosen for their different ecosystems (low-lying marsh, meadow and woodland; and a desert-like system). The case study evaluated risks to a variety of receptors, including birds of prey, duck, deer, beaver, mouse, snake, toad, fern, rush and cactus; using NOAEL as the main endpoint. Where species-specific data did not exist, literature values for similar organisms were used. The model was considered easy to use, flexible, and more detailed than the RESRAD model developed by ANL (see section 3.5.2). The model was further evaluated by the same research team (Fan *et al.* 2005), using the same study sites to assess the risks of depleted uranium, and included Monte Carlo analysis to evaluate uncertainty in the model output. Again, the model was reported to work well, and results were consistent with field measurements (Fan *et al.* 2005).

### 3.5.3 The Netherlands

The National Institute of Public Health and the Environment (RIVM) in the Netherlands has a great deal of experience in the use of models for ERA. RIVM has developed a number of models for ERA purposes and is regarded very highly in this topic throughout the world. Most models devised by RIVM have been employed to set environmental standards in aquatic and terrestrial environments, specifically for standard setting in the Netherlands (e.g. Traas et al 2001). Some of these models may, therefore, have potential use in determining higher level effects of exposure to contaminated land. Furthermore, it is also likely that, being based on ecosystems in the Netherlands, some of the RIVM models will be transferable to UK scenarios. This section describes some of the RIVM models that might be appropriate for assessing risks to populations due to contaminated land.

Models used for setting standards [such as those used by RIVM and those under consideration by the Environment Agency (Environment Agency 2007b)] use a slightly different approach to that required for the assessment of contaminated land. When setting standards for new and existing substances, the intention is to identify a concentration of a substance that is 'safe' for the majority of flora and fauna that might come into contact with it. The definition of 'safe' will, of course, vary, but is likely to be based on a laboratory-derived ecotoxicological test value such as a NOEC (no observed effect concentration) with a 'safety factor' applied (e.g. NOEC × 1000). When assessing the potential risks of contaminated land, however, the substance(s) are already *in situ*, and the problem lies in identifying whether the substance poses a risk to flora and fauna at the concentration found. Although the questions asked are not the same, many of the underlying principles are the same: one wants to know whether a substance (or substances) at a given concentration will be harmful to wildlife. Therefore, the underlying structure of models used for standard setting may be suitable for assessing contaminated land. Unfortunately, many such models do not look at population or ecosystem level effects because of the present inability to accurately model ecological interactions (Mesman and Posthuma 2003).

### Example models derived by RIVM

CATS model

CATS (Contaminants in Aquatic and Terrestrial ecoSystems) is a system of dynamic, multi-compartment models that primarily predict bioaccummulation of toxicants via food chains. CATS models assess the fate of toxicants in both abiotic and biotic components of the ecosystem, and integrate them to assess toxicant load; compartmentalisation of the toxicant within water, sediment and soil; and toxicant uptake by organisms. The models predict the bioavailability using the amount of contamination; the chemical characteristics of the soil, surface water or pore-water (this can be particularly influential); and the characteristics of the organisms being exposed.

An example of the use of the CATS system is that of Traas and Aldenberg (1996), where CATS was used to assess spatial differences in exposure to contaminants in risk assessments. Traas and Aldenberg investigated examples of both aquatic and terrestrial systems (only the terrestrial example is described further here). They modelled cadmium, copper and lead risks for the years 2000 and 2015. Cadmium was predicted to pose no risk in 2000, but target values were exceeded in 2015 (*c.* 0.4–5.4%, depending on soil type). Risk from copper contamination increased between 2000 and 2015, especially for clay soils where risk increased by >40%. The risk from lead doubled between 2000 and 2015, from 12 to 23%. All three metals were predicted to have impacts on wildlife, noticeably cadmium impacts on birds and moles; copper impacts on birds, sheep grazing on sandy soils and earthworms; and lead in earthworms and, subsequently, moles (Traas and Aldenberg 1996). An earlier application of the CATS system also highlighted the risk of cadmium contamination, suggesting that maximum permissible concentrations (MPCs) in soil exceeded all cadmium load reduction scenarios for 2050 (Traas and Aldenberg 1992).

Overall, Traas and Aldenberg (1996) concluded that CATS was useful for comparing regional differences in ecological risk from contaminants. Bioaccumulation predictions were strongly influenced by initial contaminant concentrations, toxicant loading of the system and sorption coefficients. Although CATS allows comparisons between spatially separate ecosystems, the lack of sufficient, suitable assessment data (NOEC etc) for organisms within the same food chain was predicted to make assessment of quality standards for bioaccumulation less reliable.

CATS has also been used in independent studies. For example, Hunter *et al.* (2003) used the CATS model (translated into the MatLab programming software) to predict the transfer of mercury through a lake food web. Hunter *et al.* (2003) reported that, in their programmed version of the model, CATS was robust and flexible.

If enough information and data are available on the ecosystem, dose-response functions and likely significant effects on the population in question, the CATS systems could be tailored to predict population level effects.

<u>Soil Top Predators model</u>

This model extended the model described by Romijn *et al.* (1991) [MPCsoil = NOECsp /BAFsp] by (a) examining major terrestrial food chains, (b) correcting the NOECs to account for field conditions, and (c) introducing stochastic measures for the MPC, NOEC and bioaccumulation (BAF) values (Jongbloed *et al.* 1994, 1996; Traas *et al.* 1996; Luttik and Traas 2001). Top predators for which models were developed were six birds of prey (goshawk, buzzard, kestrel, tawny owl, barn owl, little owl, long-eared owl) and two terrestrial predators (badger and weasel), each being selected for preying on different food items.

The model is based on a simple three-stage food-web, comprising:

Plants and invertebrates – small mammals and birds – top predators

The specific modelling for the eight species described accounts for top predators being exposed to contaminants via more than one food-web link. The food chain:

Soil – worm – bird/mammal

is considered suitable for terrestrial systems, although the chain

Soil – worms and insects – birds – top predators

is more appropriate for highly lipophilic substances.

The model was tested using six contaminants (cadmium, DDT, dieldrin, lindane, methyl mercury and pentachlorophenol) and was concluded to work well. However, data availability inevitably influenced the power of the model. For those contaminants where sufficient NOEC, BAF and BCF data exist, stochastic NOECs can be entered into the model; if insufficient data are present, constant NOECs must be used. Different species were exposed to different risk on account of their main prey type. For example, predators feeding on birds and small carnivorous mammals are exposed to a greater risk than those predators preying on small herbivorous mammals. This model predicts MPCs, and thus is able to highlight the most sensitive food chain for any given contaminant. The model is adaptable, depending on sufficient data being available on the required organism, food chain and ecosystem.

Traas *et al.* (2001, 2002 described a similar probabilistic food-web model for effects of PCBs on otters, combining sediment, food-web and dose-response data via Monte Carlo simulations. Again developed by RIVM, the model is likely to gain regulatory approval, although because of its focus on sediment chemical data it is likely to be of use only in certain scenarios for ERA of land contamination.

**Ecotoxicity of soil mixtures**

In 2003, Mesman and Posthuma (2003) undertook a review of the scientific literature, models and data available for determining environmental quality standards for mixtures in soils. Given that land is unlikely to be contaminated by just one single toxicant, the approaches described by Mesman and Posthuma (2003) are likely to be of use in the ERA of contaminated land. However, the authors acknowledge that our current understanding of ecological interactions is weak (Mesman and Posthuma 2003), so that population and ecosystem level predictions are difficult and likely to have a very high degree of uncertainty. Furthermore, ecotoxicological data are invariably from single species testing, while community level mixture effect data are entirely lacking (Mesman and Posthuma 2003). Regardless, the recommendations made do have use in ERA for contaminated land.

Mesman and Posthuma (2003) report that there are essentially two types of models available for assessing toxicity of mixtures:

(1) Simple similar action – whereby the mixture consists of substances that exert their toxic effects via the same mode of action. In such instances, concentration addition is used to drive the toxicant risk of all the substances in the mixture.

(2) Independent joint action – here, substances in the mixture exert their toxicant effects via completely dissimilar modes of action (but do not interact with each other). For assessing risk of such mixtures, response addition is used. Two approaches may be used here, either each substance that exerts a toxic effect is added to the overall toxicity of the mixture, or only the most toxic substance of the mixture is used.

Outputs from these approaches can then be compared with pre-defined risk limits or species sensitivity distributions etc.

Currently the Dutch government uses both concentration addition and response addition (addition of each toxicant causing a response) for risk assessment of soils (Mesman and Posthuma 2003). Risk limits, site-specific risk assessments and tailored site-specific risk assessments are made using these models. Ecotoxicological standards are based on species sensitivity distributions (SSDs) when sufficient toxicity data exists (Posthuma *et al.* 2002). SSDs (which are typically based on laboratory toxicity tests) have been demonstrated to be predictive of field populations (Hose and van den Brink 2004). Standards are derived on the assumption that a logistic distribution of log(NOEC) data is satisfactory for the calculation of the SSD (Breure and Peijnenburg 2003). Usually, the HC5 (hazardous concentration that is greater than the NOEC for 5% of the exposed species in laboratory tests) is the defined critical point beyond which risk is inferred. This value is called the MTR (maximal tolerable risk level), which is then used to derive the target value in standard setting. The ecotoxicological serious risk concentration (ESRC), the concentration where the soil is considered seriously contaminated, is at the 50th percentile of the SSD curve.

RIVM have developed intervention and target values for more than 125 compounds and compound groups, and detailed the analytical methods used to determine these values (VROM 2000). It is worth noting, however, that in some instances HC5 values derived from static laboratory toxicity tests may not be precautionary enough for predicting community level effects in the field (Schroer *et al.* 2004). Furthermore, measures such as the hazardous concentration do not provide information on levels required to ensure population recovery, and so cannot be used to determine remediation or management measures.

The approach in the Netherlands for site-specific ERA of soil contamination is based on the estimation of effects from the presence of contaminants in soil, and HC5 values (Breure and Peijnenburg 2003). Currently, assessment methods focus on using biological tests, for example bioassays and biological field observations. The TRIAD approach is used to implement this risk assessment framework. The TRIAD is composed of three elements: an assessment of risks from the presence of contaminants in the soil and in biota (substances directed approach), an assessment of risks from the results of bioassays with samples from the site, and biological field observations (Breure and Peijnenburg 2003).

# 3.6 Discussion

This review reports on a variety of ecological models (both individual model types and variations of the same type of model) that could potentially be used for ERA and within Part 2A. Not all of the models will be of use, either because they are too specific for other scenarios (and would therefore require too much re-development and/or re-programming), or because the types of data provided from Tiers 1 and 2 of the developed ERA framework are not suitable. However, some models are of potential use in ERA, and they are listed below (those marked with an asterisk may only have limited use, or should be used with caution):

## 3.6.1 Population models

### Scalar abundance

Scalar abundance models estimate the number of individuals in a population and how that abundance varies with time. These models essentially are used to predict the rate of increase (growth) and/or decrease (decline) of a population. Depending on their complexity, these models can account for various factors that affect population abundance, including density dependence and reproductive recruitment as well as natural variability within the ecological system. Although not all of these models are designed for ERA, by manipulating the parameters entered (e.g. a reduced reproductive output due to toxicant exposure) they can provide useful information for ERA.

- Malthusian population growth
- Logistic population growth
- Deterministic age/stage-based
- Stock-recruitment
- Stochastic differential equations (*)
- Stochastic discrete-time (*)
- Equilibrium exposure (*)

**Life history**

Life-history models specifically predict the structure of age classes within a population (e.g. number of individuals of different age or life stage). They can indicate whether the population has a bias towards a certain age or life stage, and can predict whether various pressures will disrupt the usual distribution of age/life-stage classes within a population. As with the scalar abundance models, even though some of these models are not specifically designed for ERA, the parameters entered can be manipulated such that they reflect toxicant effects and therefore they can be used for ERA.

- Deterministic age/stage-based models
- Stochastic age/stage-based models
- RAMAS® age/stage-based models
- RAMAS® Ecotoxicology
- Unified Life Model (*)
- Ecobeaker (*)
- ECOTOOLS
- GAPPS (*)

### 3.6.2 Metapopulation models

Metapopulation models assess various parameters of different populations of the same species that occur in the same spatial location. They can be used to predict the effects of various interactions between individuals in these populations, as well as how changes in one population will affect the other population(s). Potentially, these models have fewer useful applications for ERA although metapopulation models are included in some modelling software packages (e.g. RAMAS®).

- Incidence function occupancy models (*)
- State transition occupancy models (*)
- RAMAS® Metapop
- RAMAS® GIS
- VORTEX
- ALEX (*)

### 3.6.3 Ecosystem models

**Food-web models**

Transfer of contaminants along a food chain is perhaps one of the main concerns when assessing toxicant impacts on an ecosystem. Depending on the individual biota and toxicants involved, contaminants can be passed from prey to predator in increasing concentrations along the food chain. In addition, populations of prey items exposed to toxicants can decline to such small abundance that they can no longer support the predator population (which may be a protected species). These models, therefore, have a very important role in ERA.

- Population-dynamic food chain
- RAMAS® Ecosystem
- Populus (*)
- ECOTOX

Further to those models listed above, Science Project SC03000197 (Environment Agency 2007a, 2007b) on bioaccumulation identified three models that would progress to the in-depth review stage of the assessment of models for persistence and bioaccumulation of substances in environmental standards:

- System dynamic model (Model Ref. Number 8)
- Arctic terrestrial food-chain bioaccumulation model (Model Ref. Number 29)
- Technical Guidance Document (TGD)/EUSES (Model Ref. Number 60)

**Terrestrial**

A number of large-scale models exist that are highly complex and are able to predict a range of factors affecting whole ecosystems. However, because of their complexity they often require many data parameters to be entered. Furthermore, ecosystem models tend to be highly specific for the ecosystem upon which they are based. Some, however, have some degree of flexibility in terms of parameters entered and may therefore be suitable for ERA and contaminated land. The following models were initially developed for grassland habitats (potentially the closest match to relevant contaminated land sites) and may have some potential use for ERA.

- Short Grass Prairie Model (*)
- SAGE (*)
- SPUR (*)
- SWARD (modified) (*)

### 3.6.4 Landscape models

Landscape models are perhaps the most large-scale ecological models of all, predicting (as their name suggests) impacts, and subsequent changes, on whole landscapes that may cover very large spatial areas. As with ecosystems, these models are usually very complex, and necessarily specific to the type of environment for which they have been written (e.g. forest). Again, a few have some degree of flexibility in the required parameters, allowing for some toxicant impacts to be considered (e.g. toxicant effects in seed production). Three of the landscape models reviewed may be of use in ERA, in terms of their flexibility to incorporate toxicant effects. However, whether these models are suitable for ERA of contaminated land,

and of use to the Environment Agency for Part 2A, is more questionable. Two of the models (STEPPE and LANDIS) are for forest scenarios, and model, for example, succession of trees; there are likely to be few scenarios where forestry models are of use. The Wildlife–Urban model is of potential use, although models only for vegetation and birds (this model may be of use if bird species are identified as receptors). One final consideration in the use of landscape models for ERA and Part 2A is that because they are designed to predict responses to impacts over large scales (both spatially and temporally) they may not have the resolution to detect significant, yet smaller scale, impacts.

- Wildlife–Urban Interface Model (*)
- STEPPE (*)
- LANDIS (*)

### 3.6.5 Toxicity extrapolation models

These models do exactly as their name suggests, and take toxicity data for one biological species or chemical and extrapolate values for other biological species with the same toxicant, or the same biological species with a different toxicant. Although these models do not have any ability to inform assessors of the likely population or ecosystem effects of a toxicant, they are potentially useful to fill in gaps in the database where data for certain species or toxicants are not available. They can, with caution, be used to estimate parameters for some of the more complex models (although assessors must be aware of the extra uncertainty that would be introduced to the final model output). Toxicity extrapolation models, therefore, have a potential use as a screening tool (probably at lower tiers in the ERA), and a limited use for estimating parameters for more complex models.

- HCS
- HCp
- Acute:Chronic ratio
- Scaling for birds
- Allometric scaling
- AAE

## 3.7 Recommendations

As mentioned in the introduction, as one moves from simple population abundance models through to food-chain and ecosystem models, many more input parameters are needed, which may not be available. The choice of model used for ERA may, therefore, be compromised to some extent by availability of data collected within the lower tiers (in that the data may not be available for the most appropriate model, although specific data could be collected for the preferred model). However, the most complicated model is not necessarily required for the ERA; for example, if just one or two protected species are of interest, the simpler population models might be sufficient. The choice of which model(s) to use at Tier 2 is likely, therefore, to depend on both the site under assessment and the data available from that site.

### 3.7.1 Simple population growth models

The simplicity of these models means that they are often included in modelling software packages. Most have some potential use within Tier 2 and can be recommended for use, although it is important that assessors understand the limitations and assumptions of these models. For example, the stochastic age-based models described by McGee and Spencer (2001) and Wiese *et al.* (2004) might be useful for ERA, if adapted with terrestrial parameters. Models based on earthworm populations obviously have a clear link to ERA of contaminated land (e.g. Baveco and DeRoos 1996), because earthworms are used in lower tier testing, and are likely to be a major component of the terrestrial food chain.

### 3.7.2 RAMAS® ecological modelling software

RAMAS® is one of the best-known software applications of ecological modelling, and includes a variety of different models (Age/Stage; Metapop; Ecotoxicology; Ecosystem). RAMAS® is internationally recognised and used by regulatory agencies (e.g. USEPA). Although RAMAS® is a commercial product, and therefore requires a licence agreement, it is recommended that it should be one of the models/packages that are validated in the next phase. RAMAS® Ecotoxicology specifically addresses the effects of toxicants, and RAMAS® Ecosystem specifically examines food-chain linkages – these two components are perhaps of most potential use within Tier 2. RAMAS® is able to predict risk of extinction, a significant endpoint for assessing population and ecosystem level effects of contaminants.

### 3.7.3 VORTEX

This metapopulation model is available as software and is widely used. It is not clear at this stage how useful metapopulation models will be for Tier 2; however, this model is extremely flexible and is potentially useful. Metapopulation models used in isolation are not well suited to risk management, but they can be improved by including dose-response data (Chaumot *et al.* 2002). A metapopulation model is available in RAMAS®, and so VORTEX may not be required if the whole RAMAS® package is used.

### 3.7.4 Unified Life Model

The ULM exists as software and is reportedly flexible and easy to use. Although not the main criteria for assessment of a model's suitability for ERA at Tier 2, these factors are considered important if the models are to be used on a regular basis. The ULM allows a number of parameters to be entered, allowing for different scenarios to be modelled; again this is useful for ERA of contaminated land where a variety of scenarios will need to be modelled. Finally, the ULM can model a number of endpoints, including population growth rate, reproductive rate and risk of extinction; all key endpoints for higher tier ERA. Monte Carlo simulation can be used to measure the variability in the output.

### 3.7.5 Toxicity extrapolation

Many of the toxicity extrapolation models are of potential use for ERA; as their name implies, they extrapolate individual toxicity data to determine population data. The Hazardous Concentration for the most Sensitive Species (HCS) has been used previously by regulatory authorities and forms the basis of a number of other models, but may be too precautionary. The HCS has been further developed into the HCp model (Hazardous Concentration for a Population), which was written specifically for soil invertebrates and is a good candidate for validating with real data. Endpoints of the HCp model are significant for population level ERA (growth, survival and reproduction) and regulatory authorities, particularly in the Netherlands, have used this model. The $NOEC_{survival}$ to $NOEC_{endpoint(x)}$ is another toxicity extrapolation model that may be suitable for validation.

### 3.7.6 Ecosystem models

Currently there are few ecosystem models suitable for ERA of terrestrial systems. SPUR is perhaps the most suitable ecosystem model identified in this review, but does have some disadvantages. SPUR is site-specific and modular in format; thus it requires a lot of data to run, and not all of the required data will be available or estimated easily. However, SPUR is available as a computer package, which does facilitate data entry. Furthermore, the US Department of the Interior developed SPUR and so the model has regulatory recommendation. Although the model does not specifically model for toxicant effects, it can be used for any grassland ecosystem.

### 3.7.7 Bioaccumulation/food-web models

An Environment Agency project is currently assessing the suitability of bioaccumulation models for standard setting. Two models for terrestrial food webs were highlighted for validation: the Arctic terrestrial food-chain model, and the EU Technical Guidance Document (TGD). These two models will be validated under the Bioaccumulation and Standard Setting project. In addition to the recommendations of the bioaccumulation project, the population-dynamic food chain is also recommended for validation in the present project. This model also forms part of RAMAS® Ecosystem, and so could be validated if RAMAS® is validated.

### 3.7.8 Models used by other regulatory agencies

Given the similarities between the terrestrial environments and, in particular, the organisms that make up the terrestrial ecosystems of the UK and the Netherlands, it is recommended that the RIVM Soil Top Predators model be validated for use in ERA at Tier 2. As described, this model assesses terrestrial food chains of significant birds and mammals that are found in the UK, and corrects NOECs to account for field conditions. Having been developed by RIVM it also has good credibility and use by regulatory authorities.

The RESRAD-ECORISK model used by the US Department of the Interior is also potentially useful for terrestrial ERA and, given its regulatory use in the USA, is also recommended for validation in the current project. Although ECORISK uses American bird and mammal species, it may be possible to use similar data for UK/European species. This model exists as a computer program that accepts a variety of user inputs, and can provide environmental risk and remediation evaluations. The program is reported to be 'user-friendly' and could potentially be used by regulators without the requirement for in-depth modelling knowledge.

## 3.8 Conclusions

The following models/model types have been identified as potentially useful at Tier 2 for performing ERA for contaminated land:

- Population growth
- Unified Life Model (ULM)
- RAMAS® Ecotoxicology
- RAMAS® Ecosystem
- VORTEX
- Hazardous Concentration for a Population (HCp)
- SPUR
- Soil Top Predators
- RESRAD-ECORISK

There will necessarily be some flexibility in which models are validated depending on costs of validation supplied by the contractor, models available to the contractor, related Environment Agency projects, and comments from peer reviewers.

# 4 Evaluation of Environment Agency review

## 4.1 Introduction

The Environment Agency review on ecological population models (Chapters 2 and 3) for use in risk assessment was critically assessed. This review drew heavily on recommendations from published reviews, e.g. *Ecological Modelling in Risk Assessment: Chemical Effects on Populations, Ecosystems and Landscapes* (2002) [R.A. Pastorok, S.M. Bartell, S. Ferson and L.R. Ginzburg (eds)].

During the assessment process, the following aspects were considered:

1. The overall approach used by the Environment Agency to develop the review.
2. Gaps in the review (i.e. are there models that would be suitable but which have not been mentioned).
3. An evaluation of the preliminary assessment used by the Environment Agency to identify potential models for use in Tier 2, including an assessment of the suitability of the recommended models to UK scenarios.
4. An assessment of the feasibility of applying the selected modelling approaches to the assessment of contaminated sites in the UK.

During the evaluation, original publications (journal papers, books, Web-based information) describing the different modelling approaches were obtained and used as the basis for the assessments. In the following section, the results of the evaluation are reported.

## 4.2 Purpose

The purpose of the Environment Agency review was to examine the available literature to determine which modelling techniques and specific models may have potential for use at a site-specific level in the proposed ERA framework.

Ecological tools in Tier 2 will help a risk assessor to make an assessment of whether the contamination in a system is causing or is likely to cause ‘significant harm’ as defined in the Statutory Guidance for Part 2A Environmental Protection Act 1990 (DETR 2000). The definitions in Table A of the Statutory Guidance legally define significant harm as:

> *harm which results in an irreversible adverse change, or in some other substantial adverse change, in the functioning of the ecological system within any substantial part of that location;*
> or
> *harm which affects any species of special interest within that location and which endangers the long-term maintenance of the population of that species at that location.*

Also included is:

*in the case of a protected location which is a European Site (or a candidate Special Area of Conservation or a potential Special Protection Area), harm which is incompatible with the favourable conservation status of natural habitats at that location or species typically found there.*

*In determining what constitutes such harm, the local authority should have regard to the advice of English Nature[1] [2] and to the requirements of the Conservation Regulations 1994.*

The receptors protected under Part 2A are defined in Table A of the Guidance as 'any ecological system, or living organism forming part of such a system, within a location' and specific locations are listed. These are locations with conservation protection status, for example Sites of Special Scientific Interest.

There are opportunities to leave the framework at screening tiers if the evidence suggests that no significant pollutant linkage exists between the source–pathway–receptor or where the contamination levels are not likely to cause harm.

All information (Table 4.1) collected in any ERA can be used in decision-making. For example, the concentration of contaminants at a site may be used in Tier 1 for comparison with soil screening values. The same data may be used again in any modelling efforts undertaken in Tier 2.

By reviewing the modelling approaches and some specific models using predefined criteria it is possible to target, from the plethora of available options, the most promising for further investigation.

**Table 4.1 Data that are likely to be available for a contaminated site**

| Data type | |
|---|---|
| Site characteristics | Ecotoxicity to plants |
| Contaminant concentrations | Ecotoxicity to soil microbes |
| Physico-chemical properties of soil | Soil functional measurements |
| Ecotoxicity to invertebrates | Field surveys |
| Body burdens | Species of interest |

# 4.3 Approach used in Environment Agency report

A sensible approach was taken in the review. Specific criteria were laid out in advance and judicious examination of previous reviews of ecological modelling were undertaken, including those in previous Environment Agency projects (Environment Agency 2003, 2007a). A recent Environment Agency report (Environment Agency 2007b) on bioaccumulation models was also considered. The latest models were taken from the literature following searches on the Web of Knowledge. The use of multiple previous reviews and the extensive publications database alongside more general Internet searches ensured a wide-ranging investigation, reducing the likelihood of missing any key models or techniques. The use of specific criteria is the key to success in this kind of review, as without a specific focus when approaching

[1] These definitions are taken from the regulations for England. The corresponding conservation agencies are statutory consultees in any ecological risk assessment in other parts of the UK
[2] English Nature now forms part of Natural England

each model it is very easy to get bogged down in the complex minutiae of methods, notation and mathematics.

## 4.4 Evaluation of conclusions

In order to evaluate the conclusions made in the report as to the suitability of individual models and modelling approaches, we initially identified a number of model requirements that we believe are essential for contaminated land assessment at Tier 2. These were:

1. The model or model approach should be applicable (or has the flexibility to be made applicable) to terrestrial systems (individuals, populations, communities, ecosystems).
2. The model or model approach should allow the effects of a contaminant stressor on terrestrial systems (individuals, populations, communities, ecosystems) to be established.
3. The model or model approach should be applicable (or has the flexibility to be made applicable) to species in the UK.
4. The output of the model should determine an impact on individuals, populations, communities or ecosystems or determine trophic transfer of a contaminant.

While it would be beneficial for a model to be already in use by regulators elsewhere (thus demonstrating the utility of the model) and to be user-friendly and cheap, these characteristics were not considered essential at this research stage.

These model requirements were then applied to each of the models reviewed in the Environment Agency report and other models identified by the project team [e.g. The EU Risk Assessment Scheme for Terrestrial Vertebrates: Risk Assessment for Birds and Mammals (RASTV)](Tables 4.2 and 4.3).

Using these model requirements, the following models and modelling approaches were identified as potentially suitable for contaminated land assessment in the UK context:

**Models**

- Population Growth
- Unified Life Model (ULM)
- RAMAS® Ecotoxicology
- RAMAS® Ecosystem
- VORTEX
- Hazardous Concentration for a Population ($HC_p$)
- SPUR
- Soil Top Predators
- RESRAD-ECORISK
- SAGE
- ECOTOX
- CATS
- Risk Assessment Scheme for Terrestrial Vertebrates (RASTV)

**Modelling approaches**

Population Growth Models can be split into six basic types:

- Malthusian population growth models
- Logistic population growth models
- Stock-recruitment population growth models
- Stochastic differential equation models
- Stochastic discrete-time models
- Equilibrium exposure models

This is in general agreement with the recommendations in the Environment Agency review earlier in this report.

**Table 4.2 Applicability of generic modelling approaches to Tier 2 assessment of contaminated land**

| Model type | Terrestrial application | Contaminant application | Species flexibility | Model availability | Population | Community | Ecosystem | Trophic transfer |
|---|---|---|---|---|---|---|---|---|
| Individual-based models | Yes | ? | Yes | Yes | No | No | No | No |
| Deterministic age-based models | Yes | Yes | Yes | Yes | Yes | No | No | No |
| Deterministic stage-based models | Yes | Yes | Yes | Yes | Yes | No | No | No |
| Stochastic age-based models | Yes | Yes | Yes | Yes | Yes | No | No | No |
| Stochastic stage-based models | Yes | Yes | Yes | Yes | Yes | No | No | No |
| Metapopulation modelling | Yes | Yes | Yes | Yes | Yes | No | No | No |
| Population viability analysis | Yes | Yes | Yes | Yes | Yes | No | Yes | No |

? = Possible contaminant application depending on model to be used.

**Table 4.3 Suitability of named modelling approaches to Tier 2 assessment of contaminated land**

| Model | Terrestrial application | Contaminant application | Species application | Model availability | Population | Community | Ecosystem | Trophic transfer |
|---|---|---|---|---|---|---|---|---|
| RAMAS®-Stage | Yes | No | Yes | Yes | Yes | No | No | No |
| RAMAS®-Ecotoxicology | Yes | Yes | Yes | Yes | Yes | No | No | No |
| RAMAS®-Metapop | Yes | ? | Yes | Yes | Yes | No | No | No |
| RAMAS®-GIS | Yes | No | Yes | Yes | Yes | No | No | No |
| RAMAS®-Ecosystem | Yes | Yes | Yes | Yes | Yes | Yes | Yes | Yes |
| RAMAS®-Landscape | Yes | No | Yes | Yes | Yes | No | No | No |
| ULM | Yes | No | Yes | Yes | Yes | No | No | No |
| SIMPDEL | Yes | No | Yes | ? | Yes | No | No | No |
| SIMSAR | Yes | No | No | ? | Yes | No | No | No |
| Ecobeaker | Yes | ? | Yes | Yes | Yes | Yes | No | Yes |
| ECOTOOLS | Yes | No | Yes | Yes | Yes | No | No | No |
| GAPPS | Yes | No | Yes | No | Yes | No | No | No |
| Occupancy models | Yes | No | Yes | No | No | No | No | No |
| VORTEX | Yes | ? | Yes | Yes | Yes | No | No | No |
| ALEX | Yes | No | Yes | Yes | Yes | No | No | No |
| Populus | Yes | ? | Yes | No | Yes | Yes | No | No |

**continued on next page**

? = Possible contaminant application depending on model to be used, or unable to determine model availability.

**Table 4.3 Suitability of named modelling approaches to Tier 2 assessment of contaminated land (continued)**

| Model | Terrestrial application | Contaminant application | Species application | Model availability | Population | Community | Ecosystem | Trophic transfer |
|---|---|---|---|---|---|---|---|---|
| ECOTOX | Yes | Yes | Yes | Yes | Yes | No | Yes | Yes |
| Short Grass Prairie Model | Yes | No | No | Yes | Yes | No | No | Yes |
| SAGE | Yes | Yes | Yes | No | Yes | Yes | No | Yes |
| SPUR | Yes | No | Yes | Yes | Yes | Yes | No | Yes |
| Modified SWARD | Yes | No | No | No | No | Yes | No | No |
| Wildlife–Urban Interface Model | Yes | No | Yes | Yes | Yes | No | No | No |
| STEPPE | Yes | No | Yes | ? | No | Yes | No | No |
| LANDIS | Yes | No | No | Yes | No | Yes | Yes | No |
| HCS | Yes | Yes | Yes | Yes | No | No | No | No |
| $HC_P$ | Yes | Yes | Yes | Yes | Yes | No | No | No |
| Acute to Chronic Ratio | Yes | Yes | Yes | Yes | No | No | No | No |
| $NOEC_{survival}$ to $NOEC_{endpoint(x)}$ | Yes | Yes | Yes | Yes | Yes | No | No | No |
| Scaling (birds) | Yes | Yes | Yes | Yes | No | No | No | No |
| Allometric scaling (mammals) | Yes | Yes | Yes | Yes | No | No | No | No |
| Interspecies toxicity | No | Yes | Yes | Yes | Yes | No | No | No |
| AEE | Yes | Yes | Yes | Yes | No | No | No | No |
| Arctic terrestrial food-chain | Yes | Yes | No | Yes | No | No | No | Yes |
| EU Technical Guidance Document | Yes | Yes | No | Yes | No | No | No | Yes |
| System dynamic model | Yes | Yes | Yes | No | No | No | No | Yes |
| RASTV | Yes | Yes | Yes | Yes | No | No | No | Yes |

? = Possible contaminant application depending on model to be used, or unable to determine model availability.

## 4.5 Feasibility of applying identified modelling approaches

### 4.5.1 Data input requirements and outputs

While the Environment Agency report recommended models and modelling approaches for use at Tier 2, no consideration was given to the feasibility of applying the models. The models selected by the Environment Agency and the additional models identified in this study were therefore examined in detail to determine which data would be required to run the models and to determine the form of the output. A consideration of how the models could be used in contaminated land assessment was also made. The results of this evaluation for each model are provided in Appendix 4.

### 4.5.2 Availability of input data

An assessment of the likely availability of model input data was performed to determine whether it is feasible to use a named model for contaminated land assessment in the UK. The assessment considered the following:

1. Whether an input variable would be available from the site characterisation and assessments made in previous tiers.
2. If not, whether the input data could potentially be estimated, obtained from the literature or derived experimentally.
3. Whether it was not possible to obtain a critical input parameter.

The results of the assessment are summarised in Table 4.4. The results illustrate that in order to run any of the models, additional data would be required over and above those generated in previous tiers of an ERA.

The assessment also demonstrates that at least one key input parameter would be absent (from any of the possible information sources) for almost all of the models. These missing data, which currently are not available, include ecological baseline conditions (i.e. when the contaminant is absent) for a site as well as information on carrying capacity, density dependence, noise, reproduction and growth rates and trophic interactiions. Without suitable ecological data for an uncontaminated (‘control’) condition, we believe it is not possible to predict site-specific impacts. It is likely that the models are also unsuitable for assessing impacts of remediation as remediation effects may lead to unexpected ecological effects, particularly if the method of remediation affects the habitat in a significant way.

**Table 4.4 Likely data availability to run recommended models**

| Model type/name | No. of data requirements | No. of data requirements fulfilled in Tiers 1 and 2 | No. of data requirements potentially fulfilled or potentially estimated | No. of data requirements unfulfilled |
|---|---|---|---|---|
| Generic population growth models | 2–4 | 1 | 1 | 2 |
| ULM | 5 | 1 | 2 | 2 |
| RAMAS® Ecotoxicology | 7 | 1 | 3 | 3 |
| RAMAS® Ecosystem | 12 | 2 | 4 | 6 |
| VORTEX | 16 | 4 | 5 | 7 |
| $HC_p$ | 4 | 0 | 4 | 0 |
| SPUR | 16 | 9 | 4 | 3 |
| Soil Top Predators | 9 | 3 | 4 | 2 |
| RESRAD-ECORISK | 11 | 4 | 3 | 4 |
| SAGE | 18 | 11 | 2 | 5 |
| ECOTOX | ? | ? | ? | ? |
| CATS | 28 | 15 | 1 | 12 |
| RASTV | 12 | 8 | 4 | 0 |

? = Data requirements unavailable

### 4.5.3 Use of ecological modelling in risk assessment

**Requirements for ecological modelling at Tier 2**

The requirement at Tier 2 in the proposed ERA is for a modelling approach to be used to supply enough information to the user to either provide an 'exit' from the ERA framework or to lead to a requirement for remediation or management of the site. Chapter 1 of this report summarises the requirement thus:

> *In summary, in addition to assessing biological effects, Tier 2 will use modelling techniques to determine the effects of exposure to contamination on biota (receptors) at population, community and ecosystem levels, and to predict how different approaches to remediation might affect an ecosystem. If significant effects of contamination are predicted from Tier 2 modelling, environmental management will be required (e.g. remediation of the site).*

In order for the modelling tools used within Tier 2 to have value for widespread use, they need to be generic. They should be readily usable by competent risk assessors, who can decide upon the most appropriate modelling approach to use, and are able to enter their data and understand the output in a straightforward manner.

Most importantly, there must be a high degree of confidence that the final output on whether the contamination on the site is causing a risk to certain species is accurate (i.e. the assessment should be shown to be accurate in a series of validation cases undertaken prior to its general use). These decisions can have serious ramifications for the site owner (e.g. financial cost of remediation is potentially considerable) and/or the site itself (remediation itself is likely to have considerable effects on the ecosystem). The system must seek to avoid both false positives (leading to unnecessary remediation) and false negatives (leaving the indicator species under threat). It is recognised that no modelling system will be foolproof; however, it is important that the system minimises the likelihood of inaccurate results.

There is a reasonable possibility that these decisions could end up being reviewed in a court of law, where any potential for inaccurate advice would be very carefully investigated. Thus, any approach undertaken in Tier 2 must be both transparent and accurate. If the approaches used do not give consistently accurate advice then the users will no longer trust the system and its output will be consistently challenged by those involved.

Modelling the effects of exposure to contamination on biota (receptors) at population, community and ecosystem levels in any single system is complex and challenging and requires detailed information on, for example, food webs, population dynamics of multiple species, lethal and sub-lethal effects of the contaminants and the uptake of particular contaminants by organisms along the food chain.

**Data requirements of complex models capable of modelling at the population, community and ecosystem level**

The complex models that have been highlighted as having the potential for use in Tier 2 require a wide range of data inputs. This is not surprising as the models are attempting to approximate very complex ecological/biological systems. Table 4.4 has shown that under some circumstances some of the required data will not be available for use in these systems. The general trend is that the greater the complexity of the system that is being modelled, the greater the number of data requirements and the greater the number of interactions between these data. Although it is possible to estimate some of the required data, there are still a number of issues that relate to the need for demonstrable accuracy as has been discussed above. Table 4.4 also highlights that there are some data requirements that cannot be reliably estimated and would require the inclusion of values that are potentially highly inaccurate.

Much of the data collected from the contaminated site(s) will be biological data, which by its very nature contains a certain amount of *variability*. It is also likely that the data will actually be from a small sub-set of the available data and will thus provide information on the variability in the sample rather than the variability in the population. Many modelling systems are able to work with this variability and take it into account in the output produced.

If a dataset is not available from the site under investigation it is possible that it can be estimated (e.g. via expert judgement, use of surrogate data etc). The use of estimated data introduces *uncertainty* into the approach and this is more difficult to deal with, not least because in some cases we will also be trying to estimate the variability of a dataset as well as mean values.

For example, if one of the data requirements is the fecundity of an organism, yet it has not been possible to obtain this datum, it could be estimated by suggesting a likely mean number of offspring with an estimated variability parameter [e.g. Standard Deviation (SD)]. Table 4.5 shows three examples that illustrate how similar estimates can lead to large differences.

If we look at Estimates 1 and 2, we can see that for Estimate 1 the average number of offspring is 6 and the variability around the mean has been measured as a SD of 1. This implies that 68% of the population have 5, 6 or 7 offspring and 95% have between 4 and 8 offspring (this example is making another assumption – that the data is normally distributed, which may not be the case). However, the estimate is likely to be inaccurate, to some degree at least. If however the actual population mean was slightly higher and a bit more variable (as in Estimate 2), say 6.5 and 1.5 for the mean and SD respectively, we go from 2.5% of the population with more than 8 offspring to 16% with more than 8 offspring.

**Table 4.5 Example estimate fecundity parameters and effects on potential output**

| | Mean | SD | % where offspring > 8 | % where offspring <4 |
|---|---|---|---|---|
| Estimate 1 | 6 | 1 | 2.5 | 2.5 |
| Estimate 2 | 6.5 | 1.5 | 16 | 5 |
| Estimate 3 | 6.5 | 0.5 | 0.13 | 0.00003 |

Clearly, models run with these parameters have the potential to provide different final outputs; therefore systems that do not attempt to explicitly deal with the uncertainty associated with parameter values run the risk of seriously diverging from the actual situation. The problem of uncertainty in models is considerable, particularly as the amount of uncertainty in complex models with many parameters can be compounded through the simulation to a greater extent than in the models with fewer parameters (Regan *et al*. 2003).

The following example provides an illustration of how the use of several estimated parameters in a couple of simple models could lead to a serious divergence from the actual situation.

Given a modelling scenario where there are six parameters (A–F, Figure 4.1) that have to be estimated, the potential for inaccuracy in the model is considerable. This diagram illustrates several things:

- Estimates are always likely to differ from the real values.
- Using expert judgement on uncertainty, the 'real value' is likely to fall within the range.
- Where expert judgement is difficult (i.e. where parameters cannot be estimated) the 'real value' could well be outside the estimated range (e.g. parameter E).

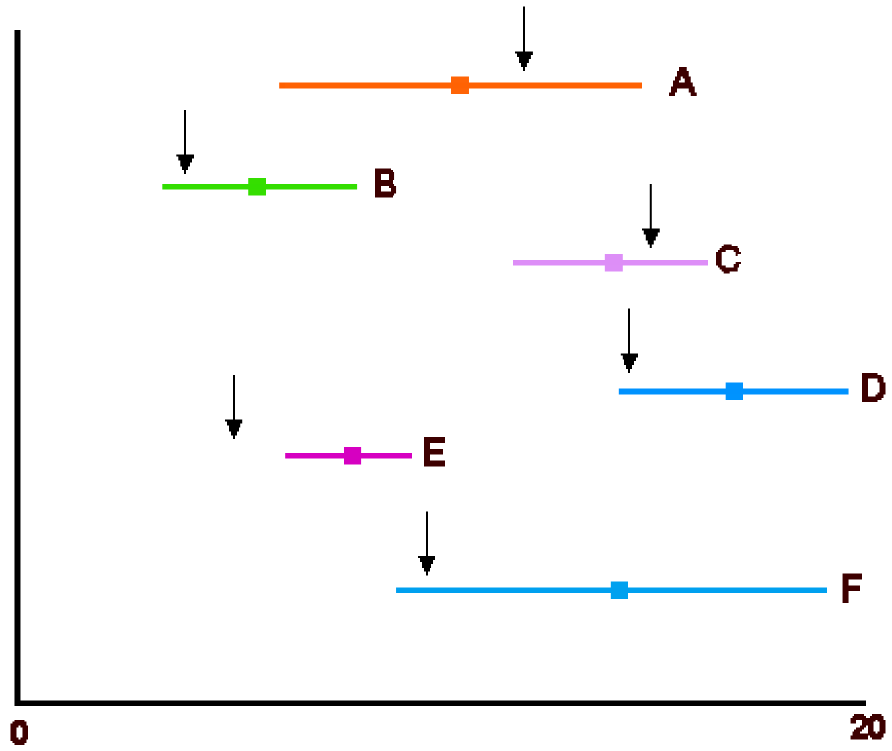


**Figure 4.1 Example of parameter uncertainty. Square is estimated value, line indicates estimated uncertainty around that mean, arrow indicates 'real value'. Letters represent different parameters**

Note that the line covers the range of possible parameter values in the judgement of the person estimating the value and not the variation around a mean. This implies that the variability around the mean value needs to be superimposed onto these values, and will also need to be estimated.

If we consider the parameter values from Figure 4.1 in two simple models, we can see that the output can vary considerably from the real value (Table 4.6):

**Table 4.6 Example estimate fecundity parameters and effects on potential output**

| Model | Estimate | Real | % increase in model output |
|---|---|---|---|
| A+B+C+D+E+F | 68 | 60.5 | 12.4 |
| A+B+C+D+E+F | 68 | 60.5 | 12.4 |
| A*B*C*D*E*F | 1332500 | 522000 | 155 |

The examples shown here illustrate that using a modelling system to make unequivocal decisions can be problematic, and that this becomes a greater issue as the modelling system increases in complexity.

There are methods of explicitly investigating the uncertainty and using the results of these investigations to put the model output into context or to target those parameters which contribute most to the uncertainty in the system and attempt to gain better data for them (Regan *et al.* 2002). These approaches include Monte Carlo techniques and the use of probability bounds analysis (Regan *et al.* 2002) and are used in some of the modelling systems under review (e.g. RAMAS® Ecotoxicology). Although the use of these methods does not remove the uncertainty, at least it makes some of it explicit and provides the results in terms of probability of events. However, greater interpretation of the outcome is required and it is possible that the results are still divergent from the actual situation.

As these complex modelling systems require many parameters that will have to be estimated, it is not possible to be confident enough that they will be able to be used consistently, across a range of species and ecological systems, to provide the requirements of Tier 2.

### A simpler modelling approach?

If it is accepted that these complex ecological models cannot be consistently accurate enough, across a range of situations, to provide a methodology that users and site owners can be confident in using, is there a simpler method that has fewer data requirements yet is still able to make a prediction about the ramifications of the site contamination on the indicator species? Of the models identified and detailed in Table 4.4, the only simple approach (i.e. few data requirements; less complex modelling approach) is the use of population models. All other options take a more complex modelling approach or require a large number of variables (and indeed will probably include population models within them).

The population models suffer from a similar drawback to the complex systems in that they also have parameter requirements that the user will almost certainly be unable to fulfil without using estimates. Table 4.4 shows that the likelihood is that none of the data requirements are met for this type of model.

As already stated, there must be a generic approach at Tier 2 to enable users to undertake the modelling without a requirement for strong modelling or programming skills. This essentially requires that the modelling can be done via an interface (PC or Web-based) that gives them the opportunity to enter their data and any assumptions, has a transparent methodology and provides the output in an interpretable manner.

The reliance of the population models on estimated parameters coupled with the fact that there is no generic software for the development of the models (most population models are developed under specific research projects and are generally based on equations without any specific software) suggests that the simpler approach is not really suitable for Tier 2.

### Control data

A further complication is the fact that we are looking at contaminated sites, so some of the data on the species collected from the site may already include the effects of that contamination. However, many sites will be very large in area, with only specific areas that are contaminated, possibly providing the opportunity of unimpacted, control data.

### Conclusion on the use of ecological modelling in environmental risk assessment

Although the use of ecological models within ERA is desirable, there are currently too many inherent problems for the available systems to meet the criteria for the models as described in Tier 2. Ecosystems are such complex phenomena that modelling the interactions of the organisms within them and the effects on those organisms of contaminants and attempts to remediate the contamination is likely to be too challenging to undertake in a manner that is applicable to the various situations that may be encountered by the ERA framework.

Where data are available for a range of species, species sensitivity distributions can be generated and hazardous concentrations (HC) affecting a certain proportion of the community derived. However, we believe that this approach is probably more suited to application at lower tiers in the assessment process.

A modified version of the RASTV (illustrated in Figure 5.1 and described in detail in European Commission 2002) approach may, however, provide valuable information for Tier 2 assessment. The RASTV approach is already used in the regulatory assessment of pesticides and determines the risk of a contaminant to a species of interest. These data could also be used to evaluate the implications of contaminated sites on ecosystems. The RASTV approach and its application to three hypothetical land contamination scenarios are therefore described in the following chapter.

# 5 Proposed approach for Tier 2 assessment

A potential scheme, based on the RASTV approach (Figure 5.1), for the assessment of contaminated land at Tier 2 is described in the following sections. The approach is then illustrated using information for three hypothetical scenarios. A full description of the approach and all the underlying assumptions can be found in European Commission (2002).

## 5.1 Risk Assessment Scheme for Terrestrial Vertebrates

The RASTV (Figure 5.1) was developed for use with pesticides in the framework of Directive 91/414/EEC (Pesticides Directive) and is described in detail in a European Commission report (2002). The approach estimates the risks to wildlife arising from the consumption of contaminated food and prey items. While the scheme was developed specifically for birds and mammals and for use on plant protection products, if the necessary data are available the approach can also be applied to other organisms. The approach is also suitable for assessing the risks of non-pesticide contaminants.

The initial risk characterisation is done by means of toxicity exposure ratios (TERs) based on either acute LD50 values, acute LC50 values, acute no observed effect levels (NOELs), or chronic NOELs. The TERs are compared with assessment factors of 10 for the acute and short-term scale and 5 for the long-term tests.

For assessment of contaminated sites, a five-step process is proposed (Figure 5.2) – this is described below.

It is recommended that the risk assessment be performed in two phases. The first phase uses default values for the exposure estimate in Step 3 and can be performed with low effort. This will provide a conservative estimate of risk. If a potential risk is indicated then a number of refinements can be made to the exposure estimate (using site-specific data on accumulation, feeding behaviour and on-site investigations etc) at phase 2 to refine the assessment.

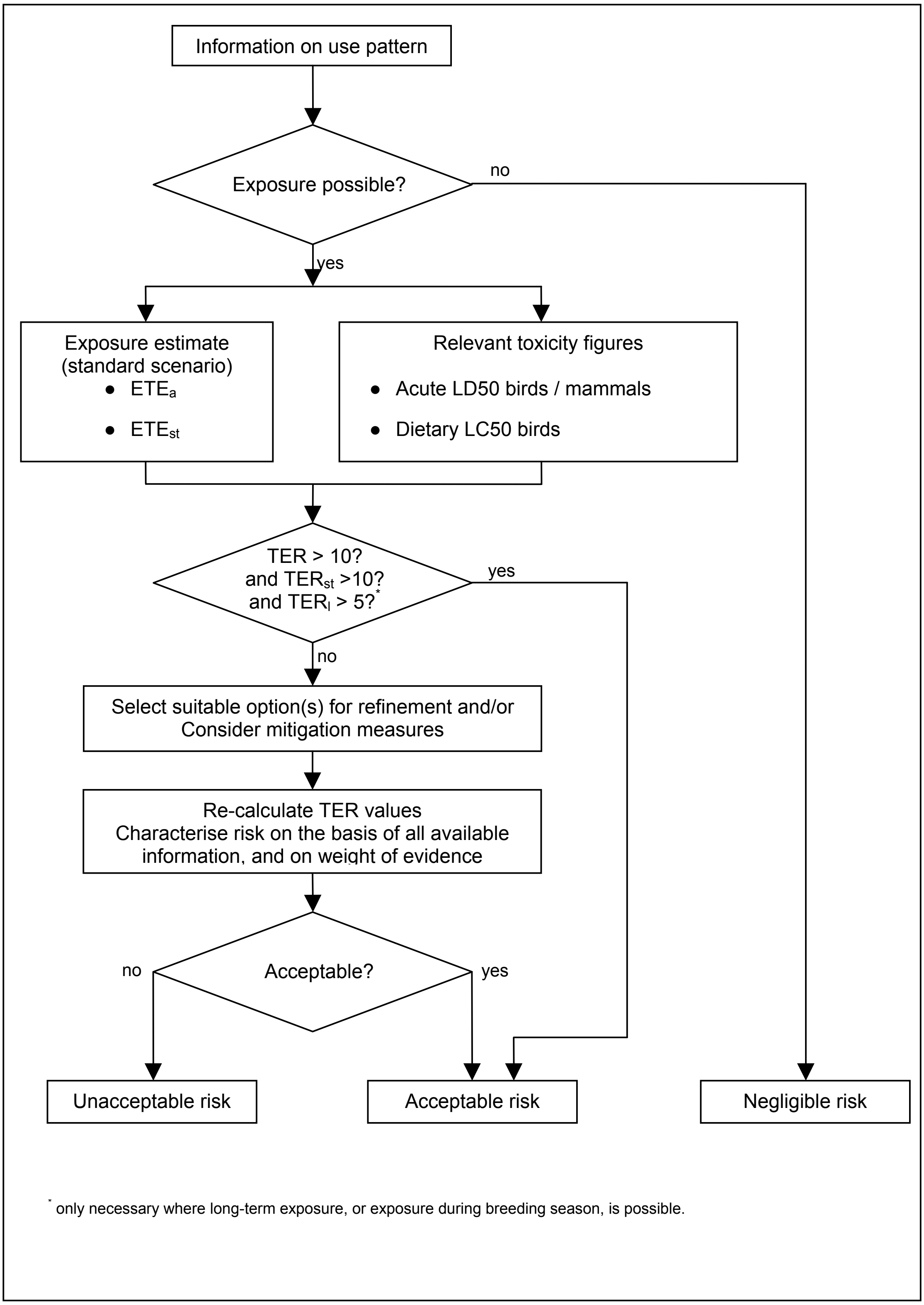


**Figure 5.1 The Risk Assessment Scheme for Terrestrial Vertebrates. TER – toxicity exposure ratio; ETE – estimated theoretical exposure, in this document defined as dose (mg/kg bw) or daily dose (mg/kg bw/d); acute TER for birds and mammals ($TER_a$) based on LD50; short-term TER for birds ($TER_{st}$) based on LC50; short-term TER for mammals ($TER_{st}$) based on NOEL; long-term TER for birds and mammals ($TER_{lt}$) based on NOEL**

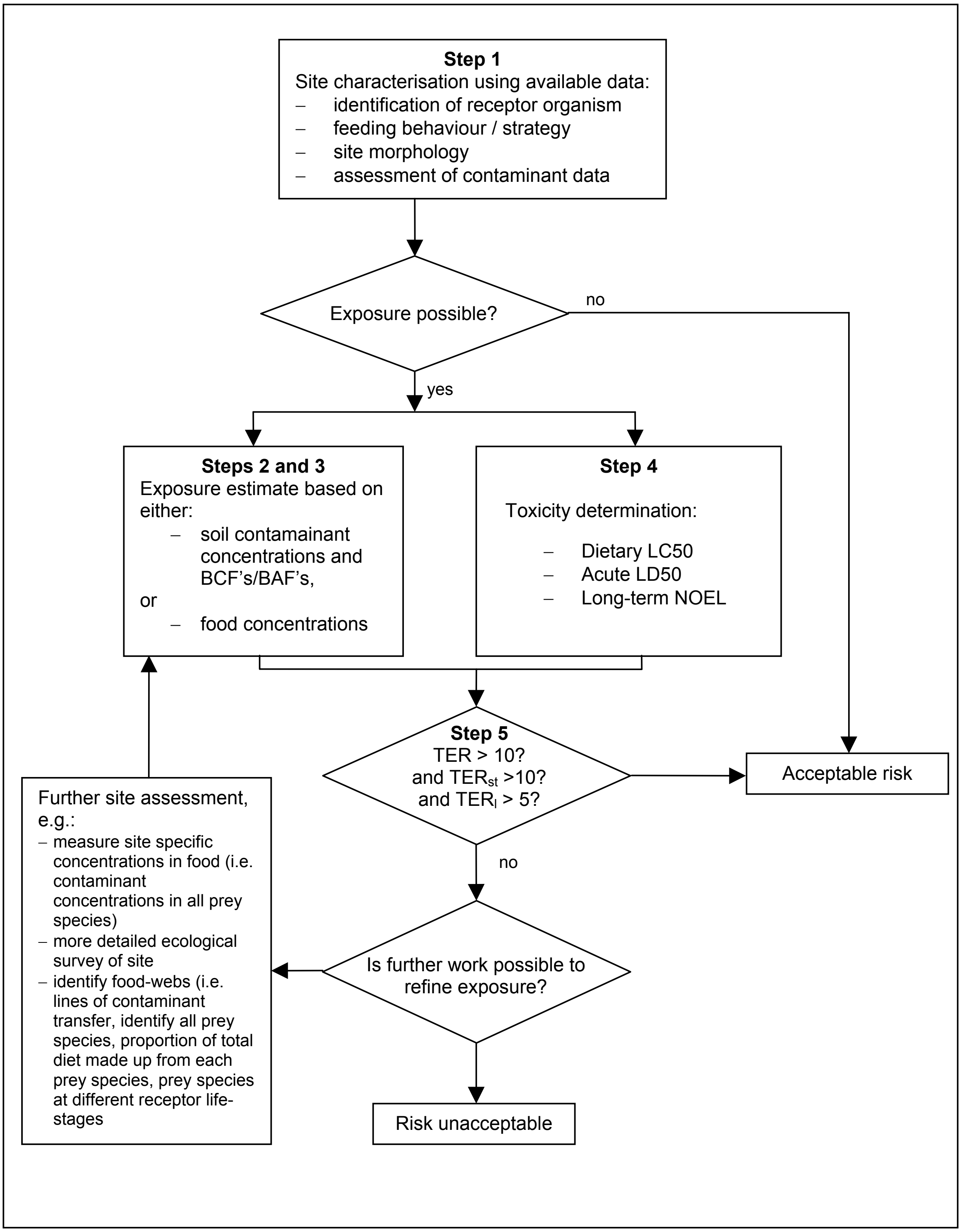


**Figure 5.2 Risk Assessment Scheme adapted for use in ecological risk assessment of contaminated land**

## 5.2 Data collation

In order to perform the assessment using this approach, information is required on contaminant bioavailability and toxicity as well as the ecological characteristics (feeding behaviour, mobility, life cycle) of species of concern. In many instances, this information can be obtained from the published literature or online databases. Potential sources include numerous commercial databases covering chemistry, the environment, medicine and toxicology, agriculture, and the life sciences. As well as commercial host publications, extensive use can also be made of Web-based sources, including the USEPA ECOTOX database and the SRC (Syracuse Research Corporation) environmental fate databases. Databases identified in this study that contain information for potential use at Tier 2 are summarised in Table 5.1.

**Table 5.1 Web-based data sources used for identification of bioconcentration/accumulation factors and toxicity data in the three scenarios**

| Website name | Web address | Data description |
|---|---|---|
| USEPA ECOTOX database | http://cfpub.epa.gov/ecotox/ | Provides single chemical toxicity information for aquatic and terrestrial life.<br>Peer-reviewed literature is the primary source of information encoded in the database. Pertinent information on the species, chemical, test methods, and results presented by the author(s) are abstracted and entered into the database. Another source of test results is independently compiled data files provided by various US and international government agencies. |
| PAN Pesticides database | http://www.pesticideinfo.org/ | Current toxicity and regulatory information for pesticides.<br>The aquatic ecotoxicity database provides summaries of aquatic ecotoxicity studies by organism group, species, chemical or effect. The complete dataset includes over 223,000 results extracted from the scientific literature by USEPA through the AQUIRE program. Summary ecotoxicity information is also presented on each chemical detail page, which can be accessed from the chemical search page. |
| United Nations Environment Programme: Chemicals | http://www.chem.unep.ch/ | Provides information on persistent organic pollutants including: CAS chemical name and no., properties and acute toxicity data for a number of species groups. |
| Canadian Wildlife Service RATL: a database of reptile and | http://www.cws-scf.ec.gc.ca/publications/AbstractTemplate.cfm?lang=e&id=321#abstr | Contains data extracted from the primary literature for amphibian and reptile ecotoxicology studies published up to and including 1997 plus some data from 1998 and 1999. Includes laboratory studies, field studies, |

| | | |
|---|---|---|
| amphibian toxicology literature | act | tissue residue studies, acute toxicity studies, studies examining the effects of pH changes, frog embryo teratogenicity assay – xenopus studies, contaminant review papers and general publications dealing with amphibian and reptile population declines. |
| IPCS INCHEM Environmental Health Criteria Monographs | http://www.inchem.org/pages/ehc.html | A means of rapid access to internationally peer-reviewed information on chemicals commonly used throughout the world, which may also occur as contaminants in the environment and food. It consolidates information from a number of intergovernmental organisations whose goal it is to assist in the sound management of chemicals.<br>Provides toxicity data for animal and plant groups collected from the primary literature. |
| EXTOXNET – The EXtension TOXicology NETwork | http://extoxnet.orst.edu/ghindex.html | Provides pesticide information profiles (PIPs) that give general information on individual pesticides including trade names, regulatory status, chemical class, formulation, toxicological effects (acute toxicity, chronic toxicity, reproductive effects, teratogenic effects, mutagenic effects, carcinogenic effects and organ toxicity), ecological effects and environmental fate. |
| Oak Ridge National Laboratory's Environmental Science Division Ecological Risk Analysis: Guidance, Tools and Applications | http://www.esd.ornl.gov/programs/ecorisk/contaminated_sites.html | This page contains guidance and screening benchmark documents for evaluating ERA data, as well as complete text copies of ERA reports for selected Department of Energy sites.<br>Some documents on this page contain toxicity data for avian and mammalian wildlife. |
| SRC environmental fate database | http://www.syrres.com/esc/efdb.htm | Bibliographic and experimental values data files on environmental fate and physical/chemical properties. |

### 5.2.1 Step 1 – Characterisation of source–receptor pathways

In the first instance it is necessary to identify the species of interest (receptor) and the main potential pathways of exposure. These exposure pathways could include:

1. Consumption of prey items at a contaminated site; or
2. Consumption of other food material from a contaminated site.

At this stage, a detailed review of the ecology of the species of interest should be performed to determine data relating to the feeding behaviour of the receptor species, including the major food sources for the organisms at different times of the year and at different life stages, and time spent eating and proportion eaten, both on and off of the contaminated site. Information should also be obtained on the behaviour and size distribution of the organism.

Also important at this stage is an assessment of the contaminant data collected in previous tiers: the contaminants of concern should be identified in terms of their bioaccumulation potential as well as whether any of the contaminants exceeds soil screening values (SSVs). Inherent in this assessment is a morphological study of the site. Details of contaminant pathways need to be identified in order to highlight the major areas of concern in terms of exposure to contamination of both receptor and prey species.

### 5.2.2 Step 2 – Prediction of concentration of contaminant in food

Data on the concentrations of individual contaminants in the soil at the site are then used along with soil bioconcentration factors (BCFs) or bioaccumulation factors (BAFs) to estimate the likely concentrations of each individual contaminant in the main sources of food material ($C_{food}$) identified at Step 1 (Equation 5.1).

$$C_{food} = \text{BCF or BAF} \times C_{soil} \qquad \text{Equation 5.1}$$

where:

$C_{food}$ = likely concentrations of each individual contaminant in the main sources of food material;

BCF = bioconcentration factor; ratio of concentration in body or organs related to concentration in media (e.g. soil, water);

BAF = bioaccumulation factor; generally used for net accumulation from all exposure routes; in this document: ratio of concentration in body or organs related to concentration in food;

$C_{soil}$ = concentration of each contaminant in soil.

If site-specific data are available on the concentrations of contaminants in food material then this should be used in preference to estimates of $C_{food}$.

### 5.2.3 Step 3 – Estimating exposure

Exposure assessment for terrestrial vertebrates is a complex matter that not only encompasses concentrations in various environmental media but also behavioural parameters (time spent on site, time spent feeding etc) and information on feeding ecology (% of contaminated food source consumed as part of the total diet, proportions of total diet made up from each food source, feeding rate, changes in food source over time etc). For the majority of situations, the principal risk is considered to arise through ingestion, and it is rarely necessary to consider other exposure routes in detail. However, identification of the most important route of exposure can only be made on a case-by-case basis, taking into account the mode of contaminant deposition, transport, site-specific environmental and ecological conditions and the environmental properties of the contaminant in question (EPPO

1994). But it is important to remember that in the context of contaminated land assessment, exposure to volatile substances may occur and inhalation would be an important exposure route.

Using information from Step 2, the exposure (which should be expressed as a daily dose) can then be calculated, for species eating one food type, using Equation 5.2.

$$ETE = (FIR/bw) \times C_{food} \times AV \times PT \times PD \qquad \text{Equation 5.2}$$

For a scenario with a mixed diet it is necessary to calculate partial ETE values for each food type and sum them up to derive the overall ETE (Equation 5.3).

$$ETE = \sum_{1}^{type} ((FIR/bw) \times C_{food} \times AV \times PT \times PD) \qquad \text{Equation 5.3}$$

where:

ETE = estimated theoretical exposure (mg/kg bw/d);

FIR = overall food intake rate for all food sources (g fw/d);

bw = body weight;

$C_{food}$ = concentration of individual compound in major food items (mg/kg);

AV = avoidance factor (1 = no avoidance, 0 = complete avoidance);

PT = fraction of diet obtained from the contaminated area; dimensionless (between 0 and 1);

PD = fraction of food type(s) under consideration in diet.

In some instances, toxicity data may be expressed in mg/g diet/d. In these cases exposure can be estimated using Equation 5.4 (definitions as for Equations 5.2 and 5.3):

$$ETE = C_{food} \times AV \times PT \times PD \qquad \text{Equation 5.4}$$

Or where a number of food types are consumed:

$$ETE = \sum_{1}^{type} (C_{food} \times AV \times PT \times PD) \qquad \text{Equation 5.5}$$

In the first instance, when performing these calculations, it is assumed that there is no avoidance, that all food is obtained from the contaminated area and that animals feed on a single food type. However, through detailed ecological surveys of a site, it should be possible to characterise the feeding behaviour of a species to allow a refinement of the exposure estimate.

### 5.2.4 Step 4 – Assessment of toxicity

Data are then collated on the toxicity of the contaminants to the species of interest. Where this data is not available then it may be appropriate to use data for closely related species. The following types of toxicity data are appropriate:

Acute: Birds: LD50 from acute oral test

Mammals: LD50 from acute oral test

Short-term: Birds: LC50 from 5-day dietary test

Mammals: (this assessment is covered by acute and long-term assessment)

Long-term: Birds: NOEL from avian reproduction study

Mammals: based on most sensitive endpoint of relevance for survival rate, reproduction rate and development of individuals, for example results from multi-generation studies or teratology studies on mammals.

### 5.2.5 Step 5 – Risk characterisation

In the final step, exposure concentrations are compared with toxicity data (TV) for the species of interest (or if this is not available a closely related species) to characterise the risk (Equation 5.6). If the trigger values proposed for pesticides are used, if the TER is greater than 5 when based on long-term toxicity data, or greater than 10 when based on short-term data, this would indicate that the risk of the contaminant is acceptable.

$$TER = TV/ETE \qquad \text{Equation 5.6}$$

where:

TER = toxicity exposure ratio;

TV = toxicity value

ETE = estimated theoretical exposure (mg/kg bw/d).

In the following sections we use the pesticide trigger values to illustrate the approach. However, if this system is to be advocated at Tier 2, we would recommend that these trigger values be further evaluated and discussed in terms of their suitability for contaminated land assessment.

## 5.3 The potential for more sophisticated modelling

The ERA approach described in section 5.1 generally uses a worst-case scenario using a limited amount of data with a number of assumptions about those data. This provides a daily dose of the contaminant for comparison with toxicity data gained from the literature. What it does not provide is the ability to swiftly get an understanding of the range of scenarios based on the available data, nor does it allow the user to undertake more complex modelling if more extensive datasets are available. It is important within the context of this report to consider both these situations in greater detail, and examine what needs to be done to enable these elements to be incorporated into the final tier of the ERA.

### 5.3.1 2D Monte Carlo modelling of the proposed approach

The approach has been to take a specific scenario (e.g. worst case) at the time of year when the organisms of interest are most likely to be at risk of ingesting high levels of contaminant. Assumptions have been made that the food items with the greatest chance of contamination should make up 100% of the study organisms' diet and that the study organisms spend 100% of their time foraging in the most contaminated area. In reality, the organisms will most likely have other food items in their diet and forage in a wider area.

The data used in the equations are:

- BCF/BAF of the prey item;
- $C_{soil}$ = concentration of contaminant in soil;
- ETE = estimated theoretical exposure (mg/kg bw/d);
- FIR = food intake rate (g fw/d);
- bw = body weight of the study organism;
- $C_{food}$ = concentration of compound in fresh diet (mg/kg);
- AV = avoidance factor (1 = no avoidance, 0 = complete avoidance);
- PT = fraction of diet obtained in contaminated area;
- PD = fraction of food type in diet.

The approach has been to take the worst case (or median/best case) data points from all of these. However, it is likely that for any case study there will be several data points for each of these parameters.

In order to gather more information from the proposed modelling approach, a bespoke system could be developed that allows the use of more than one data point from each dataset. By considering the full datasets, we can use a Monte Carlo approach to generate a range of model outputs. Monte Carlo models are run for many iterations and within each, the data values in the model are chosen from the data distributions using random number generation. Depending upon the level of sophistication required the outputs of the model could provide:

- the range of daily doses;
- the percentage of model runs where the daily dose was greater than the LD50;
- correlations between the inputs and the model output (sensitivity analysis provides information on which of the inputs has greatest influence on the output);
- pointers to where further data could be gathered to increase certainty in input parameters and hence the output.

A system like this could be set up as, for example, an Internet-based system or PC-based software and allows the data to be input by the site assessors.

An illustration of how this could be set up is given below (distributions mentioned refer to how the model will select values in each iteration). Please note that this is an illustration only; the development of Monte Carlo approaches requires careful consideration of uncertainty and variability and the selection of the most appropriate distributions. See USEPA (1997) for further guidelines.

1. Enter data relating to the model (i.e. that differentiates it from previous model runs). Includes site, organism of interest, notes.
2. Enter the soil contamination data (initial assumption that data is normally distributed; however, other distributions could be incorporated if required, e.g. Log Normal).
3. Enter proportion of time spent feeding in the contaminated area. This is probably expert judgement and could be entered as three values: minimum, best estimate and maximum (e.g. triangular distribution).
4. Enter data on body weight of study organisms (e.g. normal distribution).
5. Enter data on weight of food intake of study organisms (e.g. normal distribution).
6. Enter the number of food items to be considered.
7. Enter data on the proportion of each food item in the diet. This is probably expert judgement and could be entered as three values: minimum, best estimate and maximum (e.g. triangular distribution).
8. For each prey item enter either the actual contamination data collected at the site or BCF data (initial assumption that data is normally distributed; however; other distributions could be incorporated if required, e.g. Log Normal).
9. Enter LD50 or other measure of interest for comparison with model output.

Once all these data have been entered, the model could be run for a predefined number of iterations (e.g. 1000 – needs to be tested in advance and should be sufficient for the convergence of key outputs) and the output from each stored in the database. These could include:

- tables of percentile values;
- frequency histograms;
- correlation graphs and coefficients between inputs and outputs.

This modelling approach will provide users with information to allow them to consider whether they should take some extra data (e.g. on feeding habits) or decide whether they have satisfied the criteria that allows them to state that there either is or is not a contamination problem on the site. It may be that the output is still inconclusive, and in some sites may lead to a requirement for more extensive data collection.

## 5.4 Application of approach to hypothetical contaminated sites

The RASTV risk-based approach was applied to three hypothetical contaminated land scenarios in order to show its application in ERA.

Data on the ecology and contamination at the hypothetical sites were provided by the Environment Agency. Where necessary, additional information (e.g. physico-chemical properties and persistence, ecotoxicity and ecological inputs) was obtained from the published literature or online databases. Contaminants are considered individually but it is important to recognise that if the approach is applied to a 'real world' situation, then the potential for interactive effects of contaminant mixtures should also be considered.

### 5.4.1 Scenario 1

This fictional scenario uses real contaminant information collected in a previous research project by the Environment Agency (2004). The scenario is a disused cadmium, lead and zinc smelter and the area covered by its plume. This is up to 3.2 km (sampling location 3) in length and approximately 1 km in width (i.e. about 3 $km^2$).

Adjacent to the eastern boundary of the site, at sampling location 3, is pastoral grassland, bounded by scrub and hedging, adjoining ancient oak woodland to the east. The woodland is a protected local habitat (e.g. Biological Heritage Site). The farmland and woodland in this location is the primary nesting and feeding habitat of song thrushes (*Turdus philomelos*) (Cramp 1988).

#### Contamination

High levels of metals occur in soils along the length of the plume (Table 5.2). Sampling location 4 is closest to the smelter (1.5 km), then sampling location 3 (3.2 km) and finally sampling location 1 (8.1 km). Associated soil properties are given in Table 5.3.

#### Source–pathway–receptor linkage

The song thrush is resident in Britain all year round. It mainly feeds on garden snails but also eats worms, insects and berries. Earthworms form a large component of thrush diets in summer (Appendix 5).

Favoured habitats of the song thrush are grassland field boundaries (hedgerows), deciduous woodland, grassland, scrub and gardens. Studies comparing thrush populations across different farmland habitats have shown that usage is higher in grassland and woodland habitats and that habitat selection does not change through the breeding season. Information on the British Trust for Ornithology (BTO) website suggests thrushes live on average for 3 years. Breeding pairs produce 3–6 eggs, incubation is 12–13 days and young fledge at 14 days. Successful pairs can produce 2–3 broods per year. Nests are lined with mud and are located in trees and shrubs. There are estimated to be 1.1 million breeding pairs in the UK (2001 survey). A 1980 census of thrushes in Sussex estimated an average of 9 breeding pairs per square kilometre in the county.

The main source to exposure pathway considered here is soil – earthworm – thrush.

**Table 5.2 Concentrations of contaminants at sites (mg/kg)**

| | Hg | | Cd | | As | | Cu | | Zn | | Pb | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | Mean | ±SE | Mean | ±SE | Mean | ±SE | Mean | ±SE | Mean | ±SE | Mean | ±SE |
| Sampling location 1 | 0.12 | 0.02 | 5.6 | 0 | 12.5 | 1.3 | 27.1 | 1.1 | 752 | 59 | 106 | 2 |
| Sampling location 3 | 0.16 | 0.07 | 24.2 | 2.8 | 13.5 | 2 | 44.6 | 5.3 | 212 | 229 | 514 | 53 |
| Sampling location 4 | 0.15 | 0.06 | 29.9 | 4.7 | 12.0 | 2.6 | 38.1 | 9.7 | 3280 | 435 | 309 | 77 |

**Table 5.3 Soil properties**

| | pH | | % loss on ignition |
|---|---|---|---|
| | Mean | Range | Mean |
| Sampling location 1 | 5.30 | 5.17–5.54 | 6.25 |
| Sampling location 3 | 6.55 | 6.31–6.73 | 2.68 |
| Sampling location 4 | 6.50 | 6.09–6.58 | 4.53 |

### Concentration of contaminant in food items

Data on the concentrations of the metal contaminants (As, Cd, Cu, Pb and Zn) in earthworms are presented in Table 5.4 (Environment Agency 2004a). These were used as the basis for the exposure estimations.

**Table 5.4 Metal concentrations in earthworms in g/g (dry weight)**

| | As | Cd | Cu | Pb | Zn |
|---|---|---|---|---|---|
| | Mean | Mean | Mean | Mean | Mean |
| Sampling location 1 | 6.31 | 0.50 | 177.83 | 3.55 | 3.16 |
| Sampling location 3 | 22.39 | 0.89 | 562.34 | 31.62 | 6.31 |
| Sampling location 4 | 39.81 | 0.63 | 1000.00 | 39.81 | 6.31 |

Measured data were not available for mercury, but there is a reported BCF value for mercury in soils of 0.64 (Fischer and Koszorus 1992). Using this BCF and measured soil mercury concentrations, the maximum concentration of mercury in earthworms would be 0.1024 mg/kg.

Measured data for contaminant concentrations in other prey species were not available, but there are BAF values for snail and slug species (Haque *et al*. 1988; Graff *et al*. 1997; Scheifler *et al*. 2002).

### Exposure concentrations

Dietary toxicity data were available for avian species so the concentrations of contaminants in food items were therefore used as the basis for the exposure estimate. Data were not available on the fresh weight concentrations in the worms so dry weight concentrations of contaminants were used.

### Risk characterisation

Data were not available on the toxicity of the individual metal contaminants to thrush so data for other avian species were obtained (Hill *et al.* 1975; Hill and Soares 1984; Hill and Camardese 1986; Crocker *et al*. 2002; http://pmep.cce.cornell.edu/). In instances where a number of toxicity values were available for different avian species, the lowest LC50 value was selected. Using these values, with the exception of copper (calculation illustrated below), TERs for all metal contaminants were significantly greater than 10, indicating that these contaminants pose an acceptable risk to the song thrush (Table 5.5). The copper concentration (TER 0.6) may however pose an unacceptable risk to the song thrush. Different food consumption scenarios were also investigated (Tables 5.6 and 5.7) and these indicated that birds would have to obtain 95% of their food off-site before the risks become acceptable (Table 5.6)

### Worked example for copper

The TER for copper contamination of the song thrush is calculated as the toxicity value divided by the exposure concentration, which in this case is the LC50 value for copper in avian species (mg/kg) divided by the metal concentration in the prey species (mg/kg) (Tables 5.5 and 5.6).

TER = LC50/exposure concentration

= 600/1000

= 0.6

**Table 5.5 TER determination for Scenario 1**

| | Exposure concentration (mg/kg) | Test species | Toxicity value (mg/kg) | TER |
|---|---|---|---|---|
| Based on diet of 100% earthworm | | | | |
| Hg | 0.1024 | Japanese quail | 36 | 351 |
| As | 39.8 | Japanese quail | 5000 | 126 |
| Cd | 0.89 | Pheasant | 651 | 731 |
| Cu | 1000 | Duck | 600 | 0.6 |
| Pb | 39.8 | Japanese quail | 5000 | 126 |
| Zn | 6.3 | No data | No data | No data |
| Based on diet of 100% snail | | | | |
| Cd | 82.04 | Pheasant | 651 | 7.94 |
| Based on diet of 100% slug | | | | |
| Cd | 24.2 | Pheasant | 651 | 26.9 |
| Pb | 514 | Japanese quail | 5000 | 9.73 |

**Table 5.6 TER determinations for Scenario 1 based on hypothetical scenarios for the percentage of food taken from the contaminated site**

| | % eaten on contaminated site | | | | | | |
|---|---|---|---|---|---|---|---|
| | 100 | 75 | 50 | 25 | 10 | 5 | 1 |
| | Based on diet of 100% earthworm | | | | | | |
| Hg TER | 351 | 469 | 703 | 1406 | 3516 | 7031 | 35156 |
| As TER | 126 | 168 | 251 | 503 | 1256 | 2513 | 12563 |
| Cd TER | 731 | 975 | 1463 | 2926 | 7315 | 14629 | 73146 |
| Cu TER | 0.6 | 0.8 | 1.2 | 2.4 | 6 | 12 | 60 |
| Pb TER | 126 | 168 | 251 | 503 | 1256 | 2516 | 12563 |
| | Based on diet of 100% snail | | | | | | |
| Cd TER | 7.94 | 10.58 | 15.87 | 31.74 | 79.35 | 158.7 | 793.5 |
| | Based on diet of 100% slug | | | | | | |
| Cd TER | 26.9 | 35.87 | 53.8 | 107.6 | 269 | 538 | 2690 |
| Pb TER | 9.73 | 12.97 | 19.46 | 38.9 | 97.28 | 194.6 | 972.8 |

**Table 5.7 TER determinations for Scenario 1 based on varying hypothetical proportions of different prey items consumed**

| Proportion of prey item consumed (cadmium toxicity) | | | | | | | |
|---|---|---|---|---|---|---|---|
| Worm:Slug | TER | Worm:Snail | TER | Slug: Snail | TER | Worm:Slug :Snail | TER |
| 100 | 731 | 100 | 731 | 100 | 27 | 80:10:10 | 57 |
| 90:10 | 202 | 90:10 | 72 | 90:10 | 22 | 70:20:10 | 48 |
| 80:20 | 117 | 80:20 | 38 | 80:20 | 18 | 70:10:20 | 33 |
| 70:30 | 83 | 70:30 | 26 | 70:30 | 16 | 50:30:20 | 27 |
| 60:40 | 64 | 60:40 | 20 | 60:40 | 14 | 50:20:30 | 22 |
| 50:50 | 52 | 50:50 | 16 | 50:50 | 12 | 30:20:50 | 14 |
| 40:60 | 44 | 40:60 | 13 | 40:60 | 11 | 30:50:20 | 23 |
| 30:70 | 38 | 30:70 | 11 | 30:70 | 10 | 20:30:50 | 13 |
| 20:80 | 33 | 20:80 | 10 | 20:80 | 9.2 | 20:50:30 | 18 |
| 10:90 | 30 | 10:90 | 8.8 | 10:90 | 8.5 | 10:10:80 | 10 |
| 100 | 27 | 100 | 7.9 | 100 | 7.9 | 10:80:10 | 24 |

**Recommendation**

The toxicity value for copper based on a diet of 100% earthworms is lower than the exposure concentration, indicating that the site may pose an unacceptable risk. This is also the case for cadmium (based on a diet of 100% snails) and lead (based on a diet of 100% slugs). Heikens *et al*. (2001) found that there were significant differences in accumulation levels of a factor of 2–12 between taxonomic groups. They discovered that metal concentrations were high in Isopoda and low in Coleoptera with Annelida (Lumbricidae) somewhere in between. The differences in accumulation level between taxonomic groups show the relevance of including a detailed feeding behaviour in risk assessment for invertebrate feeding animals (Heikens *et al*. 2001). By observing the feeding behaviour of the song thrush to determine the proportion of its diet that is obtained from the site and off the site as well as the make up of its diet, it should be possible to further refine the risk assessment. It is likely that data of this type will increase the TER.

It may also be appropriate to use distributions of concentrations of copper in worms, cadmium in snails and lead in slugs across the site rather than the maximum mean concentrations that have been used here. It is recommended that statistical advice is obtained before performing such adaptations.

## 5.4.2 Scenario 2

This fictitious site covers 180 hectares. It is located 1 km south-east of the confluence of a river and a canal, both of which are used for industrial transportation. The northern boundary of the site lies between 0.1 and 1.0 km from the river. The western boundary is 250 m from the canal. Much of the land to the north, east and south is designated as green belt and there are several farms in the vicinity.

The site is currently an operational chemical manufacturing facility. When the site was constructed, the land was levelled with sand, gravel and shingle (up to 2m in places). When old facilities were demolished everything was removed, apart from small pieces of concrete which were left and add to the shingle covering. These areas are populated with plovers (*Charadrius* sp.) during the breeding season (Crampe 1983).

Following a pollution incident some 30 years ago, the local canal was dredged and sludge spread to land adjacent to ponds linked to the canal. Wildfowl are regularly seen feeding in this area, particularly around the ponds.

### Contaminants

Recent soil sampling along the riverbank shows that contamination from the sludge-spreading activity is still present. The sludge contained various contaminants, such as polychlorinated biphenyls (PCBs), telodrin, dieldrin, and chlorobenzenes – these contaminants are now found in the soil. Two locations from this area were sampled.

Soil samples were taken from two sample areas (1 and 2), and analysed for general physico-chemical characteristics (clay content, pH, percentage organic carbon content, moisture; Table 5.8) as well as for organic contaminants (Table 5.9).

**Table 5.8 Soil characteristics from study site**

| Characteristic | Sampling location 1 | Sampling location 2 |
|---|---|---|
| Clay content; ≤ 2 μm (%) | No data | 24.3 |
| pH | 7.7 | 7.5 |
| Organic C content (%) | 0.066 | 0.085 |
| WHC50 (g water/$g_{dwt}$ soil) | 0.50 | 0.53 |

**Table 5.9 Soil contaminant concentrations**

| Contaminants | log $K_{ow}$ | Sampling location 1 (μg/kg dry soil) | Sampling location 2 (μg/kg dry soil) |
|---|---|---|---|
| HCB | 5.73 | 360 | 32 |
| Telodrin | 5.20 | 4100 | 64 |
| Dieldrin | 5.40 | 38000 | 550 |
| 2,3,3',4',6-pentachlorobiphenyl | 6.84 | 53 | 58 |
| 2,2',3,4',5',6-hexachlorobiphenyl | 7.30 | 120 | 110 |
| 2.2',4,4',5,5'-hexachlorobiphenyl | 7.53 | 54 | 64 |
| 2,2',3,4,4',5'-hexachlorobiphenyl | 7.68 | 89 | 92 |
| 2.2',3,3',5,6,6'-heptachlorobiphenyl | 7.45 | 14 | 15 |
| 2.2',3'4,4',5,5'-heptachlorobiphenyl | 8.06 | 71 | 64 |

### Receptor

The only significant ecological receptor(s) that could be affected by contaminants in the soil and/or groundwater at the site are several pairs of ringed plovers (*Charadrius hiaticula*) and little ringed plovers (*Charadrius dubius*) which regularly nest in the area adjacent to the land-spreading activities. Both species are protected by law.

The ringed plover is mainly sedentary in Britain. Its habitat is primarily coastal (shores and estuaries), but in recent years it has spread inland to breed as the number of remote coastal habitats has declined as a result of pressure from humans. In 2000, there were an estimated 8500 breeding pairs in Britain (Mead 2000).

The little ringed plover is a migratory visitor to Britain from March to October. Its favourite nesting sites are gravel pits and shingle banks along rivers. In 2000, there were an estimated 950 breeding pairs in Britain (Mead 2000).

It is not unusual to find either species on derelict industrial sites where there is standing water.

The territory of a nesting pair of plovers is in the region of 0.5–1.0 hectares. They are usually solitary, but colonial nesting (approximately 9 m apart) does occur. The breeding season runs from mid-March to mid-August. Ringed plovers produce 3–4 eggs per pair, incubation time is 22–28 days and young fledge at 24–27 days. Little ringed plovers produce 4 eggs with incubation taking 3–4 weeks and chicks then grow to young fledging after about 4 weeks.

They feed primarily on insects (flies, beetles and other adult and larval insects), crustaceans, snails, spiders and also mud-dwelling invertebrates in shallow water (Appendix 5). Given the nature of the nesting site, suitable food may be scarce and it is likely that the plovers spend a significant portion of their time away from the nesting area. However, the young of both species will feed themselves from a very young age, well before fledging, and will, therefore, gain the majority of their food from the nesting site.

While it is recognised that worms are unlikely to be a major food source, for the purposes of this study, the surrogate source–receptor pathway was selected to be soil–earthworm–plover. The reason for this is that site-specific body burden data were available for contaminants in worms. A more detailed ecological investigation on feeding behaviour at the site would identify the major prey species, and chemical analyses of these would provide a more relevant risk assessment.

### Concentrations of contaminants in food

Two species of earthworm (*Eisenia andrei* and *Aporrectodea caliginosa*) were collected from the site and analysed. Earthworm body contents were analysed by gas chromatography mass spectrophotometry (GC-MS). Body burdens of *E. andrei* were analysed for worms from area 2 only (Table 5.10); body burdens of *A. caliginosa* were measured for worms from both areas (Table 5.11). Bioaccumulation factors of HCB for the slug *Deroceras reticulatum* were found in the literature (0.4–0.6) and multiplied by the soil concentration to produce a body burden (Haque and Ebing 1983). These concentrations were used to estimate the potential exposure of the plovers.

**Table 5.10 Contaminant body burdens for *E. andrei* (mean from at least three samples, ± SE)**

| Contaminants | log $K_{ow}$ | Concentration (µg/mg fresh worm) | | | |
|---|---|---|---|---|---|
| | | Sampling location 1 | | Sampling location 2 | |
| | | Mean | SE | Mean | SE |
| HCB | 5.73 | No data | - | 0.0044 | 0.0003 |
| Telodrin | 5.20 | No data | - | 0.0729 | 0.0044 |
| Dieldrin | 5.40 | No data | - | 0.3015 | 0.0180 |
| 2,3,3',4',6-pentachlorobiphenyl | 6.84 | No data | - | 0.0164 | 0.0011 |
| 2,2',3,4',5',6-hexachlorobiphenyl | 7.30 | No data | - | 0.0578 | 0.0050 |
| 2.2',4,4',5,5'-hexachlorobiphenyl | 7.53 | No data | - | 0.0221 | 0.0020 |
| 2,2',3,4,4',5'-hexachlorobiphenyl | 7.68 | No data | - | 0.0245 | 0.0023 |
| 2.2',3,3',5,6,6'-heptachlorobiphenyl | 7.45 | No data | - | 0.0047 | 0.0004 |
| 2.2',3'4,4',5,5'-heptachlorobiphenyl | 8.06 | No data | - | 0.0221 | 0.0027 |

**Table 5.11 Contaminant body burdens for *A. caliginosa* (mean from at least three samples, ± SE)**

| Contaminants | log $K_{ow}$ | Concentration (µg/mg fresh worm) | | | |
|---|---|---|---|---|---|
| | | Sampling location 1 | | Sampling location 2 | |
| | | Mean | SE | Mean | SE |
| HCB | 5.73 | 0.1005 | 0.0255 | 0.0031 | 0.0005 |
| Telodrin | 5.20 | 2.2800 | 0.3300 | 0.0360 | 0.0030 |
| Dieldrin | 5.40 | 6.6900 | 0.8250 | 0.1986 | 0.0146 |
| 2,3,3',4',6-pentachlorobiphenyl | 6.84 | 0.0076 | 0.0014 | 0.0115 | 0.0010 |
| 2,2',3,4',5',6-hexachlorobiphenyl | 7.30 | 0.0380 | 0.0084 | 0.0599 | 0.0074 |
| 2.2',4,4',5,5'-hexachlorobiphenyl | 7.53 | 0.0099 | 0.0020 | 0.0200 | 0.0035 |
| 2,2',3,4,4',5'-hexachlorobiphenyl | 7.68 | 0.0096 | 0.0021 | 0.0179 | 0.0039 |
| 2.2',3,3',5,6,6'-heptachlorobiphenyl | 7.45 | 0.0026 | 0.0008 | 0.0025 | 0.0003 |
| 2.2',3'4,4',5,5'-heptachlorobiphenyl | 8.06 | 0.0125 | 0.0027 | 0.0236 | 0.0056 |

**Exposure concentrations**

Dietary toxicity data were available for avian species so the concentrations of contaminants in food items were therefore used as the basis for the exposure estimate.

## *Risk characterisation*

Data were not available on the toxicity of the individual contaminants to plovers so data for other avian species were obtained (Hill *et al*. 1975; http://extoxnet.orst.edu;

http://www.chem.unep.ch; Sample *et al.* 1996). In instances where a number of toxicity values were available for different avian species, the lowest LC50 value was selected. Only data for HCB, dieldrin and general PCBs were available. As toxicity data for specific PCBs were unavailable, the minimum and maximum toxicity values for general PCBs were used in calculating TERs to reflect the differing toxicities of different groups of PCB. The TERs for HCB and PCBs based on a diet of 100% earthworms were greater than 10 (Table 5.12) and indicated that these substances would pose an acceptable risk to the plover. However, the exposure concentrations for dieldrin and HCB based on a diet of 100% earthworms and 100% slugs respectively, were more than two orders of magnitude higher than the LC50 values indicating an unacceptable risk. No toxicity data were available for telodrin so it was not possible to characterise the risk posed by this contaminant.

**Table 5.12 TER determination for site contaminants**

| | Exposure concentration (mg/kg) | Toxicity test | LC50 (mg/kg/d) | TER |
|---|---|---|---|---|
| Based on diet of 100% earthworms | | | | |
| HCB | 100.5 | Japanese quail | 568 | 5.7 |
| Telodrin | 2280 | No data | No data | No data |
| Dieldrin | 6690 | Pheasant | 30 | 0.004 |
| 2,3,3’,4’,6-pentachlorobiphenyl | 16.4 | Quail | 747–>6000 | 45.5–>366 |
| 2,2’,3,4’,5’,6-hexachlorobiphenyl | 59.9 | Quail | 747–>6000 | 12.5–>100 |
| 2.2’,4,4’,5,5’-hexachlorobiphenyl | 22.1 | Quail | 747–>6000 | 33.8–>271 |
| 2,2’,3,4,4’,5’-hexachlorobiphenyl | 24.5 | Quail | 747–>6000 | 30.5->245 |
| 2.2’,3,3’,5,6,6’-heptachlorobiphenyl | 4.7 | Quail | 747->6000 | 159–>1277 |
| 2.2’,3’4,4’,5,5’-heptachlorobiphenyl | 23.6 | Quail | 747–>6000 | 31.7–>254 |
| Based on diet of 100% slugs | | | | |
| HCB | 216000 | Japanese quail | 568 | 0.003 |

**Recommendation**

By observing the feeding behaviour of the plover to determine the proportion of its diet that is obtained from the site and off the site as well as the make up of its diet, it should be possible to further refine the risk assessment. It is likely that data of this type will increase the TER although the birds would need to source more than 99.9% of their diet offsite in order to reduce the risk to an acceptable level. No toxicological data were available for telodrin so experimental toxicity studies on this compound may be required.

### 5.4.3 Scenario 3

A former gasworks site is vacant and all former above-ground structures have been demolished to foundation level. Land around the site is largely agricultural with a nature reserve on the northern boundary.

The ground-cover in the former process areas is predominantly concrete and tarmac (approximately 70%). The majority of the rest of the gasworks is covered with demolition waste and reworked soils. The foundations of the structures are often visible. Much of the site has been colonised by mixed vegetation.

**Contaminant**

A mixture of contaminants, typical of gasworks, has been identified at surface level from previous site investigations. A number of these exceeded the soil screening values (Table 5.13)

**Table 5.13 Concentrations of contaminants in Scenario 3**

| Contaminant | Maximum measured concentration (mg/kg) |
|---|---|
| Naphthalene | 8.1 |
| Anthracene | 89.9 |
| Benzo(a)pyrene | 24.5 |
| Arsenic | 38.3 |
| Copper | 233 |
| Nickel | 51.2 |
| Lead | 128 |
| Mercury | 0.2 |
| Zinc | 179 |

**Receptor**

A mixture of habitats at different stages of succession is present including areas of hard standing where above-ground structures have been demolished but foundations are left intact. One such foundation is home to great-crested newts (*Triturus cristatus*) (Beebee and Griffiths 2000). Another population of newts is concentrated in a separate area of the site. Newts feed on a wide range of prey species (Appendix 5) depending on the season and the life stage. In this scenario, the pathway soil – earthworm – newt was considered.

**Concentrations of contaminants in food**

No data were available on the concentrations of the contaminants in earthworms so these were estimated based on BCFs obtained from the literature (Morgan and Morgan 1988; Corp and Morgan 1991; Fischer and Koszorus 1992; Van Gestel *et al*. 1993; Gibb *et al*. 1997)(Table 5.14). BCFs were unavailable for the PAHs or nickel.

**Table 5.14 Estimated concentrations of contaminants in earthworms**

| | Maximum BCF | Soil concentration (mg/kg) | Earthworm concentration (mg/kg) |
|---|---|---|---|
| Lead | 1 | 128 | 128 |
| Zinc | 72 | 179 | 12888 |
| Mercury | 0.64 | 0.2 | 0.13 |
| Arsenic | 18.1 | 38.3 | 693 |
| Copper | 4.2 | 233 | 979 |

### Exposure concentrations

Toxicity data were available as LD50s so it was necessary to estimate daily exposure concentrations using Equation 5.1. The mean maximum weight of a great crested newt is 10.6 g. It was assumed that a newt will typically eat its own body weight in worms in 1 day (Piran White, University of York, personal communication) and that all the contaminant was bioaccessible. Daily doses for the newts are provided in Table 5.15.

**Table 5.15 Estimated daily doses of the contaminants**

| | Daily dose (mg/kg/d) |
|---|---|
| Lead | 128 |
| Zinc | 12888 |
| Mercury | 0.13 |
| Arsenic | 693 |
| Copper | 979 |

### Risk characterisation

Toxicity data were unavailable for the newt. Data were available for other amphibians but these were generated using aquatic exposures so were not comparable. It was therefore not possible to characterise the risk to the newts from soil contamination or soil organisms.

### Recommendations

In order to assess the risks of this site to the newts it will be necessary to obtain information on the dietary toxicity of the contaminants to amphibians. It would also be worthwhile to generate information on actual concentrations of the contaminants in the prey items. As with the previous site assessments, an assessment of the feeding behaviour of newts on the site will allow the assessment to be further refined.

# 6 Discussion and conclusions

A tiered approach utilising chemical, biological and ecological data is promoted for use within the ERA framework for contaminated land. The ERA framework is performed in tiers. At Tier 2, a risk assessor will need to interpret toxicity data in meaningful terms at population, community, or ecosystem levels. The Environment Agency therefore performed a review to identify suitable modelling approaches for assisting with assessments at Tier 2.

In the current study, the Environment Agency review was critically evaluated to determine whether it had adequately covered the available approaches and whether the conclusions were justifiable. The Environment Agency review has been performed in a logical and stepwise manner. With a few exceptions, all the major models or modelling approaches that might be applicable to assessment of contaminated land have been considered in the review. In the current study a set of criteria for model selection have been developed and applied to the different models and approaches. Original articles (papers, books etc) describing individual models and approaches were examined to determine whether the models met these criteria. There is close agreement between the models selected using our criteria and those selected by the Environment Agency.

The Environment Agency review did not consider the feasibility of applying the models to contaminated land – even though a model is suitable, the absence of data may mean that it will not be feasible to run it. A detailed assessment of the shortlisted models was therefore performed to identify the input requirements for each model. A comparison of these requirements with information on the data that are likely to be available for a particular site or could be predicted or obtained from the literature indicates that key input data will be lacking for the majority of the models.

Two approaches may be able to be run, namely the HC approach and the EU method for predicting risk to birds and mammals (RASTV). While it is possible to run the HC approach, we believe that it is more likely to be applied at lower tiers in the assessment approach. However, the RASTV method could provide a useful tool for Tier 2 assessments.

An illustration of how the RASTV approach could be extended to incorporate a greater level of variability and uncertainty has been discussed, and may provide a more appropriate range of values for the ERA.

The RASTV approach has been applied to three hypothetical scenarios. Data on the characteristics of the sites (contaminant concentrations, flora and fauna) were provided by the Environment Agency. A literature review was performed to obtain information on toxicity and bioaccumulation of the different contaminants that is necessary to use the approach. Using the approach it was possible to characterise the risks posed by the majority of contaminants found at the smelter site. However, a lack of data on toxicity of contaminants meant that it was not possible to characterise the impacts of contaminants at the other two hypothetical sites. Through a series of targeted toxicity studies and more detailed site surveys it would be possible to address these data gaps in the future.

# 7 Recommendations

The literature review of ecological models for terrestrial ecosystems (Chapter 3) is comprehensive and provides a valuable critique from which risk assessors can identify potentially useful models. The review has deliberately focused on terrestrial ecosystems to meet the requirements of an ERA framework for soil. Considerable literature exists for modelling toxicity and ecological information for aquatic systems but similar data and uncertainty challenges exist such that when considering both environmental compartments the conclusions would be similar.

The applied part of the review has demonstrated that at present a large number of ecological models have been developed, but few are considered suitable for direct application at a site-specific level across the UK. Reasons include no control data, too many datasets missing, too much uncertainty, and specificity.

The Risk Assessment Scheme for Terrestrial Vertebrates (RASTV; an EC developed scheme for assessing secondary poisoning by pesticides) can be adapted for use in the risk assessment of contaminated land. Model output remains the same (i.e. the risk of an animal being exposed to contaminants via its food), but the use of the scheme is not restricted to pesticides. The example scenarios presented in this report describe a range of potential contaminants and receptors. Each ERA will vary depending on the contaminants present, the receptor species and the food chain that presents the pathway of the contaminant to receptor. This report does not represent guidance, but instead demonstrates how the RASTV model can be applied to a land contamination scenario.

This section presents some general considerations for using ecological models and specific recommendations for the use of the RASTV and other potential modelling methods, at a site-specific level of ERA (Tier 2).

## 7.1 General considerations

The ERA framework encourages the consideration of different types of data – contaminant, toxicity and ecological. Outputs from Tier 2 are not expected to demonstrate unequivocally that an organism is, or is not, at risk of significant harm from land contamination. However, outputs are expected to provide evidence to make defensible decisions against the legal tests in the Government's Statutory Guidance.

Tier 2 is about gathering and assessing evidence for adverse effects at a species, population and community level (also, 'favourable conservation status' at sites with European conservation status). In previous screening tiers of the framework evidence is gathered to identify potential pollutant linkages, develop conceptual site models, agree problem formulation and compare contaminant concentrations against screening values. Detailed investigations at Tier 2 may involve extrapolating information based on surrogate organisms or limited information on the receptor of concern to judge contaminant impacts at population or community levels. In this sense, as demonstrated by this review, Tier 2 assessments may be limited by the information available to populate detailed ecological assessment models or methods to address site-specific concerns.

However, there are certain cost/effort/outcome considerations that should be considered alongside the use of ecological modelling. For example sometimes a small amount of extra ecological monitoring (e.g. measuring the frequency of feeding from a certain location) might allow substantially more specific ecological modelling and reduce the number of assumptions or uncertainty when making decisions about the potential for adverse effects. A little more investigation might avoid extensive remediation effort.

As with all ecological modelling, there is inevitable variation and uncertainty in model outputs. Variation is a part of all living systems and some models demonstrate an estimated range of values given that each individual may respond differently to a contaminant. Uncertainty can be more problematic, as shown by the example in Chapter 4 (Figure 4.1), because it represents how sure (or unsure) we are that the model accurately reflects what is occurring in the real world. Therefore, high uncertainty demonstrates that we are very unsure as to the accuracy of the model, which can obviously weaken legal argument when decision-making. Uncertainty is not restricted to Tier 2 of the ERA Framework, but applies to some degree at all stages. It must be considered to be an explicit part of ERA although the level of confidence is a matter for policy makers and statutory consultees. Agreeing what these confidence limits should be is currently work in progress and when agreed will be described in guidance supporting the ERA framework.

## 7.2 Recommendations

We concur with the Central Science Laboratory’s conclusions to recommend the RASTV model as a tool that is immediately ready for use in the ERA framework.

The Environment Agency and national conservation authorities are currently developing guidance to support the ecological assessment aspects of the framework. The ERA framework is not designed to be an expert system; however, reliable ecological assessments do require expert ecologists to gather, model and interpret information.

As much detailed information about the receptor should be collected as possible. Most organisms feed and drink from a variety of sources, some of which might not be on the site. Since the RASTV approach is based on food-chain poisoning, the more information that one can have about the amount of contaminated food being eaten by the receptor, the more accurate the output will be. As shown in example scenario 1, percentage time spent feeding on contaminated food can be considered in the model (see section 5.4.1). Indeed the legal tests in Part 2A require assessors to establish the boundary of contamination and verify the pollutant linkage.

Most models that predict the passage of contaminants along food chains (including RASTV) use bioaccumulation factors etc that have been measured in the laboratory for a limited number of species. These typical laboratory species (including worms for invertebrates; rats, mice and rabbits for mammals; and quail and ducks for birds) are therefore used as surrogates for the species in the risk assessment. For example, a bioaccumulation factor for a mouse might be used as a surrogate for a field vole; or, as shown in example scenarios 1 and 3, a quail might be used as a surrogate for a thrush or a plover. The use of surrogate species is an accepted paradigm in regulatory risk assessment but clearly it is important to consider which species are used as surrogates, and how closely their feeding behaviour, ecology, physiology, body size etc resemble the real species believed to be at risk in the investigation.

Furthermore, different taxonomic groups can show markedly different rates of bioaccumulation. It is therefore important to consider the mode of action of a contaminant and the ecology of the target species carefully to assess how closely the surrogate(s) matches it.

Consideration should be made as to the benefits of performing additional ecological surveys. Again, additional information can improve output accuracy and/or reduce uncertainty associated with the use of 'assumed' or surrogate data.

Furthermore, while this report has highlighted that certain parameters are likely to be missing for most of the models identified, the challenge of acquiring those missing data will vary from model to model and from site to site. Data may be required to parameterise the model's initial set-up as well as to run it for site-specific assessments. For example, if the contaminant is the same in both the prey and predator, a bioaccumulation coefficient can be determined many times across a range of situations or sites to provide a parameter (with associated error terms). To apply the model to a site-specific assessment it may then need site-specific data, for example, estimates of relative composition of prey in the predator's diet at that particular site if that is known to be variable between sites.

While it is impractical to develop new models each time for every ERA it might be relatively easy to collect extra data to fill those missing parameters and so allow some of the other models to be run, adding confidence to the output of Tier 2. In particular, this might apply if additional monitoring might add confidence to concluding no requirement for remediation if the cost of collecting extra data is less than remediation costs.

In many cases, this project has rejected models due to lack of 'control' data. But this need not necessarily exclude the use of such models in all instances if good reference information exists (e.g. species, habitats, mode of action of contaminants) or it is possible to use good surrogates (i.e. similar site conditions but without the contamination). For example, if the initial receptor is a common invertebrate species (e.g. a woodlouse or a snail) found at many other sites (more, less or not contaminated) it might be possible to build a dataset of estimates of the range of parameter values at all types of site. These estimates could then be combined with life-history data from the literature, which might allow other population models (e.g. the Unified Life Model, ULM) to be run for these sites and allow interpretation of population level effects. Depending on the species in question and available datasets, the costs of such a process need not be excessive.

We believe that the Central Science Laboratory's review overstates the problem of lack of 'control' data, particularly because the whole site will not necessarily be contaminated. The methodology described above might be a suitable approach where sufficient control data are lacking.

The ERA framework and recommended tools should not be 'set in stone' but should strive for improvement as ERAs are reported and lessons learned. This also encourages the sharing of information on methods and data within the contaminated land community in the UK and internationally, both at the time of reporting and during 'live' investigations (e.g. Web-based discussion groups).

The RASTV approach can only be used for modelling food-chain effects (i.e. where the pathway from source to receptor is via consumption of contaminated food). This approach is not suitable for other pathways (e.g. inhalation or dermal absorption).

Although initially designed for assessing risk of secondary poisoning to vertebrates, the approach described in this review can be applied equally well to invertebrates if data are available. In many cases, however, there is likely to be considerably less supporting data (e.g. LD50s from acute oral tests) available to support modelling of invertebrates. If the target species of the risk assessment is an invertebrate, and bioaccumulation data (or surrogates) are not available, it will be necessary to collect other supporting data to allow a different model to be used. This supporting data can then be stored and contribute to an ever-growing database of comparative values for future assessments, as described earlier.

For organic contaminants, Environment Agency (2007b) should also be consulted, which considers the use of two models for standard setting in terrestrial environments. The models are the arctic terrestrial food-chain model (Kelly and Gobas 2003) and the earthworm bioaccumulation model described in the EU's Technical Guidance Document (TGD) (European Commission 2003).

Outputs from the RASTV should not be considered in isolation. They help provide evidence as to whether a species is, or is likely to be, subject to adverse effects from contaminants, but are unlikely to prove so beyond doubt. For example, in example scenario 2, exposure concentrations of HCB and PCBs were lower than the toxicity values so it might be assumed that the site does not pose a risk to plovers feeding only on earthworms due to these substances (see section 5.4.2). Alternatively, if the output shows that the exposure concentration is higher than the toxicity value, it indicates that the site may pose a risk (e.g. copper concentrations on example scenario 1; HCB concentrations on example scenario 2 for plovers feeding only on slugs) (sections 5.4.1 and 5.4.2).

Clearly, if the exposure concentration is significantly more than the toxicity value (i.e. TER >1), the site must be considered to pose a risk.

Only if the exposure concentration is significantly less than the toxicity value might one assume that the site does not pose a risk. However, this decision should be made in combination with outputs from lower tiers. Becaues of the nature of the ERA framework, information from lower tiers must have shown that there was a potential risk.

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# List of abbreviations

| | |
|---|---|
| ANL | Argonne National Laboratory |
| ATLSS | Across Trophic Level System Simulation |
| BAF | Bioaccumulation factor |
| BCF | Bioconcentration factor |
| CCME | Canadian Council of Ministers of the Environment |
| CSL | Central Science Laboratory |
| $C_{food}$ | Concentration in food |
| $C_{soil}$ | Concentration in soil |
| DBMS | Database management system |
| DDT | Dichloro-diphenyl-trichloroethane |
| DETR | Department of the Environment, Transport and the Regions (UK) |
| ECOFRAM | Ecological Committee on FIFRA Risk Assessment Methods |
| ERA | Ecological risk assessment |
| ESRC | Ecotoxicological serious risk concentration (50th percentile of SSD) |
| ETE | Estimated theoretical exposure (daily exposure estimate via food) |
| FIFRA | Federal Insecticide, Fungicide, and Rodenticide Act |
| FIR | Overall food intake rate from all sources |
| HC | Hazardous concentration |
| HC5 | Hazardous concentration (that is greater than the NOEC for 5% of lab-tested species) |
| HCB | Hexachlorobenzene |
| HSI | Habitat Suitability Index |
| IIASA | Institute for Applied System Analyses |
| $K_{ow}$ | Octanol–water partition coefficient |
| LC50 | Median lethal concentration |
| LD50 | Median lethal dose |
| LOAEL | Lowest observed adverse effects level |
| LOEC | Lowest observed effect concentration |
| MATC | Maximum allowable toxicant concentration |
| MPC | Maximum permissible concentration |
| MTR | Maximal tolerable risk |
| NCSRP | National Contaminated Sites Remediation Program |

| | |
|---|---|
| NOAEL | No observed adverse effects level |
| NOEC | No observed effect concentration |
| NOEL | No observed effect level |
| OECD | Organisation for Economic Co-operation and Development |
| PAH | polycyclic aromatic hydrocarbon |
| PCB | Polychlorinated biphenyl |
| PD | Fraction of food type in diet |
| PT | Fraction of diet obtained from contaminated area |
| PVA | Population viability analysis |
| RASTV | Risk Assessment Scheme for Terrestrial Vertebrates |
| RIVM | National Institute of Public Health and the Environment (the Netherlands) |
| SSD | Species sensitivity distribution |
| SSV | Soil screening value |
| TER | Toxicity exposure ratio |
| TV | Toxicity value |
| UFIS | Environmental Research Information System |
| USEPA | United States Environmental Protection Agency |
| WHC | Water holding capacity |

# Appendices

# Appendix 1: Some terminology, and definitions, used commonly in ecological modelling

| Term | Meaning |
|---|---|
| Deterministic | Precise values are calculated for the predicted output. There are no random elements in the model |
| Stochastic | Predicted values are calculated as a range, allowing for 'natural' variability within the system. At least one random component is included in the model |
| Reductionist | The model includes as many details specifically relevant to the system as possible |
| Holistic | The model uses general ecological principles |
| Static | Predicted values are not dependent on time |
| Dynamic | Time is a defining function for variables entered into the model. The model can therefore describe temporal changes in the system |
| Autonomous | Derivatives are not explicitly dependent upon time |
| Non-autonomous | Derivatives are explicitly dependent upon time |
| Distributed | Parameters of the model are dealt with as functions of time and space |
| Lumped | Parameters are dealt with where space and time are predefined constants |
| Causal | All aspects of the model are inter-related by causal relationships |
| 'Black-box' | In 'black-box' models no causality is required by the model's components |
| Explicit modelling[1] | Where a model is made more complex to determine functional relationships of toxicity, and run for one scenario |
| Implicit modelling[1] | Where a model is used without increasing its complexity, but run several times for different scenarios so as to encompass likely predicted effects |
| Monte Carlo simulation | A method of taking randomly sampled values from probability distributions to predict likely scenarios |

[1] Pastorok *et al.* (2002)

# Appendix 2: Model acronyms

| | |
|---|---|
| AEE | Analysis of extrapolation errors |
| ALEX | None |
| ARAMS | Army Risk Assessment Modelling System |
| ATLSS | Across Trophic Level System Simulation |
| CATS | Contaminants in Aquatic and Terrestrial ecoSystems |
| ECOTOOLS | None |
| ECOTOX | None |
| EUSES | European Union System for Evaluation of Substances |
| GAPPS | None |
| $HC_p$ | Hazardous Concentration for a Population |
| HCS | Hazardous Concentration for the most Sensitive Species |
| LANDIS | None |
| RAMAS | None |
| RESRAD | RESidual RADioactive |
| SAGE | None |
| SPUR | Simulating Production and Utilization of Range Land |
| STEPPE | None |
| SWARD | None |
| TGD | Technical Guidance Document |
| TRIM.FaTE | Total Risk Integrated Methodology |
| ULM | Unified Life Model |
| VORTEX | None |

# Appendix 3: Summary information on models of interest relating to terrestrial ecosystems (from WRc 1998)

| Model name | Country of origin | Model type | Biota modelled | Modes of impact addressed | Status | Area/habitat covered and spatial scale | Ease of application in E&W | Reference |
|---|---|---|---|---|---|---|---|---|
| ACAC | USA | Simple | Foraging animal species | Uptake of hazardous chemicals through foodweb | Operational | Single contaminated sites | Unknown | Freshman and Menzie 1996 |
| BIOME-BGC | USA | Compartment model | Forests | Effects of climate change | Operational | Forests | Generic | UFIS database[1] Hunt *et al.* 1996 |
| CARBON | Netherlands | Compartment model (ordinary differential equations) | Woody and herbaceous vegetation (6 types) | General carbon cycle model | Operational | Global/regional | Generic | UFIS database |
| CARDYN | Belgium | Compartment model | Forest stands | Impact of climate change on carbon fluxes | Operational | Forests | Generic | UFIS database Veroustraete 1994 |
| CATS | Netherlands | Compartment model | Bioaccumulation within different compartments of the food web | Exposure to chemicals | Presumed still under development | Covers habitats such as grassland, scrub, forest and aquatic habitats | Generic | Traas and Aldenberg 1992 |
| CemoS/Chain | Germany | Compartment model | Chemical degradation and accumulation in consumers/producers | Exposure to environmental chemicals | Operational | Non-spatial | Generic | UFIS database |

[1] Environmental Research Information System (developed by Forschungszentrum für Umwelt und Gesundheit, Germany*)*

| Model name | Country of origin | Model type | Biota modelled | Modes of impact addressed | Status | Area/habitat covered and spatial scale | Ease of application in E&W | Reference |
|---|---|---|---|---|---|---|---|---|
| CemoS/Level1 | Germany | Compartment model | Steady state distribution of chemicals in plants, fish, soil etc | Exposure concentration estimates of environmentally hazardous chemicals | Operational | Ecosystems | Generic | UFIS database |
| CemoS/Plant | Germany | Compartment model | Plants | Exposure concentration estimates of environmentally hazardous chemicals | Operational | Organism | Generic | UFIS database |
| CENTURY | USA | Compartment model (ordinary differential equations) | Grasslands and agro-ecosystems | Impact of regional climate change on a variety of important grassland ecosystems | Operational | Regional | Generic | UFIS database Parton *et al.* 1993 |
| CL-CCE | Netherlands | Expert system | Forest soils and surface waters | Model calculates critical loads of acidity and sulphur | Operational | Ecosystems – areas of variable size | Generic | UFIS database |
| ECOCRAFT | UK and eight collaborating countries | Process-based, deterministic | European trees | Impacts of rising $CO_2$ and temperature on forest stands | Under development | Forest stands | Applicable (UK lead project) | EC CORDIS homepage |
| EXPECT | Netherlands | Modelling system comprising dynamic and empirical models | Forests and heathlands | Effect of environmental policy scenarios on acidification, growth and overfertilisation | Operational but extension work halted | Regional (districts) | Developed for the Netherlands | Bakema *et al.* 1994 |

| Model name | Country of origin | Model type | Biota modelled | Modes of impact addressed | Status | Area/habitat covered and spatial scale | Ease of application in E&W | Reference |
|---|---|---|---|---|---|---|---|---|
| FBM (Frankfurt Biosphere Model) | Germany | Compartment model | 32 vegetation types | Seasonal and long-term carbon dynamics (exchange between terrestrial ecosystems and atmosphere) | Operational | Global/regional | Generic | Jørgensen *et al.* 1996<br>Ludeke 1997 |
| GVM | USA | Static model | Biomes | Impact of climate change on geographic extent of biomes | Operational | Coarse scale ($0.5^{deg}$ X $0.5^{deg}$) | Requires IIASA global climate database as input[1] | UFIS database |
| HRBM | Germany | Dynamic | Terrestrial vegetation | Carbon cycling through terrestrial vegetation in response to climate and $CO_2$ forcing | Operational | Regional to global scale | Generic | Jørgensen *et al.* 1996 |
| HYBRID | UK | General global ecosystem model | Generalised plant types (grass, broadleaf and coniferous trees) | Effect of environmental factors on carbon, nitrogen and water cycle | Operational | Global ecosystem | Applicable | UFIS database |
| IMAGE | Netherlands | Unknown | Vegetation | Climate and land use change | Unknown | Global | Unknown | Pers comm J Wiertz, RIVM |
| MEDRUSH | UK | Dynamic GIS-based distributed process model | Vegetation (growth and distribution) | Effects of seasonal/annual and long-term climate and land use variations on vegetation growth and distribution | Under development | Areas up to 5000 $km^2$ | Applicable | UFIS database |
| NELUP | UK | Biological component is empirical | Species and species assemblages | Land use change | Operational | 1 km grid suitable for regional/national scale | High | O'Callaghan 1996 |

[1] Institute for Applied System Analyses (IIASA; Laxenburg, Austria)

| Model name | Country of origin | Model type | Biota modelled | Modes of impact addressed | Status | Area/habitat covered and spatial scale | Ease of application in E&W | Reference |
|---|---|---|---|---|---|---|---|---|
| PEF | USA | Simple | Foraging animal species | Uptake of hazardous chemicals through food web | Operational | Individual contaminated sites | Unknown | Freshman and Menzie 1996 |
| PLANTX | Germany | Compartment model | Plants | Accumulation of anthropogenic chemicals in roots, stem and leaves | Operational | Landscapes | Generic | UFIS database |
| RAMAS® | USA | Not specified | Wildlife populations | Human impact on wildlife populations | Operational | Landscape | Generic | UFIS database Kingston 1995 |
| SAEM | Not specified | Empirical (2D stepwise regression model) | Forests (predicts number of species) | Impact of environmental characteristics on biodiversity (e.g. annual rainfall, human population density) | Operational | Regional landscapes | Generic (relatively little information provided) | UFIS database |
| SWIM | Germany / USA | Dynamic, distributed model | Vegetation (growth) | Effects of climate change and land use change on hydrology and water quality (and subsequently plant growth) | Operational | Watersheds (100 to 20,000 $km^2$) | Generic | UFIS database |
| TEMFES | USA | Process-oriented model | Forests | Transient response of unmanaged forest systems to long-term changes in climate and atmospheric $CO_2$ concentration | Should be completed | Forests | Generic | Jørgensen *et al.* 1996 |

| Model name | Country of origin | Model type | Biota modelled | Modes of impact addressed | Status | Area/habitat covered and spatial scale | Ease of application in E&W | Reference |
|---|---|---|---|---|---|---|---|---|
| TREGRO | USA | Dynamic process model | Most tree species | Response (growth and patterns of carbon allocation) to levels of ozone, nutrient stress and water availability | Operational | Individual trees | Generic | UFIS database Weinstein and Yanai 1994 |
| European terrestrial modelling activity | Sweden / UK / Italy / Germany / France | Modular modelling framework | Vegetation | Human impact and natural disturbance – ecosystem-planetary boundary layer interactions, $CO_2$ and $H_2O$ fluxes | Under development | Simulation of ecosystem at 'patch' scale (<0.1 km) or regional scale (10–100 km) | Applicable | EC CORDIS homepage |
| Integrated vegetation and economic model | UK | Empirical | Upland plant communities | Costs of achieving a given area of desired vegetation | Operational | Upland area of River Tyne catchment | Applicable | Moxey *et al.* 1995 |
| Model of woody riparian vegetation | UK/France | Dynamic, GIS-based model | Woody riparian vegetation species | Germination and establishment in relation to hydrological and ecological determinants | Operational | Floodplains | Applicable | EC CORDIS homepage |

# Appendix 4: Model summaries

Blue text = data requirements fulfilled through completion of Tiers 1 and 2.

Green text = data requirements potentially fulfilled through estimation or further experimentation.

Red text = data requirements unfulfilled.

* = May not be available for all species (especially protected species, substitute data from similar species may need to be used in these cases).

**Population Growth Models – Scalar Abundance**

| | |
|---|---|
| Name/type of model | Malthusian population growth |
| Input data | Population abundance<br>Reproductive rate |
| Model output | Population abundance at specified future time<br>Possible effects of chemicals on population size |
| Recommendation | May be of use in initial comparative screening-level assessments for ERA |

| | |
|---|---|
| Name/type of model | Logistic population growth |
| Input data | Population abundance<br>Reproductive rate<br>Carrying capacity |
| Model output | Population abundance at specified future time<br>Time to carrying capacity<br>Possible effects of chemicals on population size |
| Recommendation | May be of use in initial comparative screening-level assessments for ERA |

| | |
|---|---|
| Name/type of model | Stock-recruitment population models |
| Input data | Population abundance<br>Recruitment<br>Population growth rate<br>Strength of density dependence |
| Model output | Population abundance at specified future time<br>Time to carrying capacity<br>Multiple stable states<br>Population decline or extinction<br>Possible effects of chemicals on population size |
| Recommendation | May be of use in initial comparative screening-level assessments for ERA |

| | |
|---|---|
| Name/type of model | Stochastic differential equation models |
| Input data | Population abundance<br>Reproductive rate<br>Magnitude of environmental stochasticity<br>White noise for environmental and demographic stochasticity |
| Model output | Population abundance at specified future time<br>Possible effects of chemicals on population size<br>Risk of population decline or extinction<br>Estimates of mean time to extinction |
| Recommendation | May be of use in initial comparative screening-level assessments for ERA; however, study of differential equations of population growth is very difficult and nonlinearity to model density dependence usually renders problem analytically intractable.<br>Requirement of programming effort involving advanced numerical techniques may not be economically viable or practical |

| | |
|---|---|
| Name/type of model | Stochastic discrete-time models |
| Input data | Annual population abundance<br>Intrinsic rate of population increase<br>Carrying capacity<br>Gaussian white noise |
| Model output | Population abundance at specified future time<br>Possible effects of chemicals on population size<br>Probability of decline or extinction<br>Chance of recovery<br>Mean time to decline or recovery |
| Recommendation | Should be further developed for use in screening-level ERA<br>Can be used to estimate population level risks, yet are simple to understand and easy to parameterise<br>May be used as part of a fully probabilistic framework |
| References | Fagan *et al.* (1999)<br>Ferson (1999) |

| | |
|---|---|
| Name/type of model | Equilibrium exposure model |
| Input data | Population abundance<br>Carrying capacity<br>Population biomass<br>Concentration of toxicant in an organism over time<br>Concentration of toxicant in the environment over time<br>Mortality or reproduction rate |
| Model output | Birth and death rate over time<br>Time to decline of a population<br>Time to extinction of a population |
| Recommendation | Could be used for screening assessments that forecast qualitative population level effects and for planning bioremediation strategies. Would be especially useful if it were generalised to include stochasticity |
| References | Hallam *et al*. (1983a, 1983b) |

**Population models – life history**

| | |
|---|---|
| Name/type of model | Unified Life Model (ULM) |
| Input data | Survival rate of all age classes<br>Fecundity of all age classes<br>Population size and structure including sex<br>Number of matings<br>Primary sex ratio<br>Optional:<br>Density dependence<br>Environmental stochasticity<br>Demographic stochasticity<br>Inter- or intra-specific competition<br>Parasitism<br>Metapopulations |
| Model output | Population trajectories<br>Population distributions<br>Population growth rate<br>Population stage or age structure<br>Generation times<br>Sensitivities to changes in parameters<br>Probability of extinction<br>Extinction time |
| Recommendation | |

| | |
|---|---|
| Name/type of model | RAMAS® Ecotoxicology |
| Input data | Bioassay data*<br>Population size<br>Population age or stage structure and size (defined by age or weight or size etc)<br>Fecundity<br>Survivorship<br>Reproduction rate<br>Density dependence |
| Model output | Effects of toxic chemicals<br>Expected population size<br>Abundance of individual age or stage classes<br>Asymptotic population growth rate or related parameters (e.g. sensitivity, elasticity) |
| Recommendation | See VORTEX |

**Ecosystem models – food web**

| | |
|---|---|
| Name/type of model | RAMAS® Ecosystem |
| Input data | Initial toxic chemical concentration in environment (bioavailable)<br>Toxic chemical loss rate<br>Toxic chemical uptake rate by organisms<br>Organism elimination rate<br>Dose-response curve specifying mortality over range of toxic chemical doses<br>Bioassay data*<br>Population size/biomass of each species<br>Population age or stage structure of each species<br>Predator–prey interactions<br>Trophic interactions<br>Carrying capacity<br>Abundance of food |
| Model output | Abundances of component species in the food web<br>Biomass of component species<br>Species richness (i.e. number of species)<br>Trophic structure (e.g. food-chain length, dominance)<br>Risk of decline<br>Risk of extinction<br>Expected crossing time |
| Recommendation | See VORTEX |
| References | Spencer *et al.* (1999) |

**Population models – metapopulations**

| | |
|---|---|
| Name/type of model | VORTEX |
| Input data | Areas and locations of suitable habitat patches<br>Presence/absence data for the species from two or more yearly inventories<br>Carrying capacity<br>Survival<br>Fecundity<br>Dispersal rates<br>Parameters for describing catastrophes<br>Time series of habitat maps<br>Habitat-specific information (vegetation type etc)<br>Age<br>Size<br>Sex<br>Physiological stage<br>Social status<br>Genetics<br>Social structure<br>Mating systems<br>Catastrophe data |
| Model output | Metapopulation persistence<br>Metapopulation occupancy, local occupancy duration<br>Deterministic rate of growth<br>Stable age distribution<br>Observed rate of growth<br>Mean population size<br>Expected abundance, expected variation in abundance<br>Movement rates, occupancy rates<br>Spatial patterns of occupancy<br>Transitions in the status of patches (vacant to occupied, occupied to extinct)<br>Risk of extinction<br>Risk of decline<br>Time to extinction for the metapopulation and for each sub-population<br>Number of founder alleles remaining<br>Where appropriate standard deviations and standard errors are given for each variable |
| Recommendation | The use of several PVA packages is recommended so that results can be compared; also it is not possible to input the same data into different packages which will lead to differences in the projected results, both in terms of projected population growth and predicted extinction possibility. Divergences are likely to become increasingly pronounced in more complex situations, as additional factors |

| | |
|---|---|
| | are considered (Mills *et al.* 1996; Brook *et al.* 1997).<br>It is essential that PVA software packages be tested against data from real and experimental populations (Mills *et al.* 1996; Brook *et al.* 1997) to gain a clearer picture of the usefulness of PVA packages |
| References | |

**Toxicity extrapolation models**

| | |
|---|---|
| Name/type of model | $HC_p$ |
| Input data | Laboratory bioassay*<br>NOEC<br>LC50<br>EC50 |
| Model output | Growth<br>Survival<br>Reproduction |
| Recommendation | May be appropriate for use in assessment of contaminated sites |
| References | Aldenberg and Slob (1993)<br>Aldenberg and Jaworska (2000)<br>Wheeler *et al.* (2002) |

**Ecosystem models – terrestrial**

| | |
|---|---|
| Name/type of model | SPUR |
| Input data | Daily minimum and maximum temperatures of air and soil<br>Precipitation<br>Soil water potential<br>Daily solar radiation<br>Accumulated wind run<br>Soil bulk density<br>Plant biomass<br>Nitrogen and carbon content of various environmental components<br>Standing green vegetation<br>Live roots<br>Propagules<br>Standing dead vegetation<br>Litter<br>Dead roots<br>Soil organic matter<br>Soil inorganic nitrogen |
| Model output | Abundance of individuals within species or trophic guilds<br>Biomass<br>Productivity<br>Food-web endpoints (species richness, trophic structure)<br>Carbon/nitrogen available in forage to grazing ungulates on an areal basis<br>Grassland productivity |
| Recommendation | Substantial modifications would be required to incorporate toxic chemical effects |
| References | |

| | |
|---|---|
| Name/type of model | Soil Top Predators |
| Input data | Laboratory bioassay data of all species to be modelled* (NOEC)<br>Toxic chemical concentration in soil<br>Weight of food items<br>Population sizes<br>Bioaccumulation factors for all species to be modelled<br>Metabolic rate<br>Calorific content of food<br>Food assimilation efficiency |
| Model output | Abundance of component species in the food web<br>Biomass of component species<br>Species richness<br>Trophic structure |
| Recommendation | The derivation of maximum permissable concentrations for top predators will probably be hampered seriously by a lack of bioaccumulation data for invertebrate and vertebrate species |
| References | Jongbloed *et al*. (1996) |

**Ecological risk assessment models**

| | |
|---|---|
| Name/type of model | RESRAD-ECORISK |
| Input data | Home range of all species to be modelled<br>Body weight<br>Food and water ingestion rates<br>Diet composition<br>Trophic structure<br>Contaminant concentrations in soil, air and water<br>Bioassay data*<br>Site-specific data<br>Environmental data<br>Physiological data<br>Ecotoxicological data |
| Model output | Dose of contaminant to receptors<br>Movement of contaminant through food chain<br>Risk of population decline<br>Risk of extinction<br>Preliminary clean-up goals<br>Growth<br>Biomass production<br>Food consumption rates<br>Egestion rates<br>Excretion rate<br>Respiration rate<br>Contaminant effects on growth and production |
| Recommendation | Is restricted to five terrestrial receptors and for site-specific cases, the user cannot modify the code to address other receptors (Lu *et al.* 2003).<br>The model is limited by its contaminant database and only includes those which can be weighed in the model (Lu *et al.* 2003) |
| References | Lu *et al.* (2003) |

| | |
|---|---|
| Name/type of model | SAGE |
| Input data | Solar radiation<br>Air temperature<br>Precipitation<br>Relative humidity<br>Wind speed<br>Cloud cover<br>Carbon, nitrogen and sulphur concentrations in plant and soil<br>Biomass of plants in terms of young, actively growing tissue, non-growing but photosynthetically active mature tissue and root crowns/rhizomes<br>Soil temperature<br>Soil moisture<br>Nutrient availability<br>Plant age structure<br>Litter fall<br>Soil profile description<br>Population life-cycle dynamics<br>Food consumption (ruminant)<br>Metabolic energy requirements (ruminant)<br>Nitrogen and sulphur requirements for growth and maintenance (ruminant) |
| Model output | Primary production<br>Ruminant production<br>System sensitivity to secondary perturbations<br>Availability of nutrients<br>Soil nutrient transformations<br>Litter composition<br>Microbial processes<br>Fractionation of soil organic matter<br>Transport of nutrients between soil layers<br>Photosynthetic rate<br>Plant ageing<br>Plant ion uptake<br>Plant nutrient allocation<br>Plant growth translocations<br>Respiration<br>Senescence<br>Litter fall<br>Risk of plant death<br>Risk of plant decline |
| Recommendation | The system level models require large amounts of data to use, yet these data are often unavailable and parameters are hard to establish |
| References | Hanson *et al.* (1985) |

| | |
|---|---|
| Name/type of model | ECOTOX |
| Input data | ? |
| Model output | ? |
| Recommendation | ? |
| References | ? |

? = Data not available

| | |
|---|---|
| Name/type of model | CATS |
| Input data | Soil litter content<br>Soil water content<br>Soil depth<br>% organic matter<br>% clay<br>Soil density<br>Soil pH<br>Porosity<br>Precipitation<br>Leaching<br>Residence time (water/contaminant)<br>Food-web structure: functional groups, trophic interactions<br>Initial biomass<br>Physiology: growth and reproduction, respiration, mortality<br>Nutrients: trophic state of ecosystem, trophic state of population<br>Toxicant properties: load (scenario), initial concentration, abiotic behaviour (sorption, degradation, volatilisation)<br>Biotic behaviour (assimilation, degradation, metabolism, excretion)<br>NOECs*<br>Dose-response functions |
| Model output | Predicted number of offspring<br>Bioaccumulation risks<br>Distributions of soil toxicant content<br>Toxicant concentrations in food<br>Exceedance of quality objectives for food webs<br>Fate of toxicant |
| Recommendation | Large amounts of data are required to use this model; however, much of this data is unavailable and estimation leads to very large uncertainties in model predictions |
| References | Traas and Aldenberg (1992) |

**Trophic transfer model**

| | |
|---|---|
| Name/type of model | Risk Assessment Scheme for Terrestrial Vertebrates: Risk Assessment for Birds and Mammals Under Council Directive 91/414/EEC |
| Input data | LD50<br>LC50<br>NOEL<br>Route of exposure<br>Mode of toxicant application<br>Crop-specific conditions<br>Environmental properties of active substance<br>Intake via contaminated feed<br>Food intake rate of indicator species<br>Body weight<br>Concentration of compound in fresh diet<br>Fraction of diet obtained in polluted area |
| Model output | Potential risk based on the responses of individual organisms observed in controlled laboratory experiments |
| Recommendation | May be appropriate for use in assessment of contaminated sites |
| References | European Commission (2002) |

# Appendix 5: Feeding characteristics of study species

| | Spring (March – May) | Summer (June – August) | Autumn (September – November) | Winter (December – February) |
|---|---|---|---|---|
| Great crested newt, *Triturus cristatus* – adult, aquatic | Tadpoles – frog, toad and other newt spp. Water fleas – *Daphnia*, *Chydoridae*. Midge – *Chironomus* spp. Water lice – *Asellus* spp. Water shrimp – *Gammarus* spp. Small water snails – *Lymnaea* and *Plunorbidae* spp. Water boatman – *Corixa* spp. Fly larvae – *Diptera* spp. | Tadpoles – frog, toad and other newt spp. Water fleas – *Daphnia*, *Chydoridae*. Midge – *Chironomus* spp. Water lice – *Asellus* spp. Water shrimp – *Gammarus* spp. Small water snails – *Lymnaea* and *Plunorbidae* spp. Water boatman – *Corixa* spp. Fly larvae – *Diptera* spp. | Water fleas – *Daphnia*, *Chydoridae*. Midge – *Chironomus* spp. Water lice – *Asellus* spp. Water shrimp – *Gammarus* spp. Small water snails – *Lymnaea* and *Plunorbidae* spp. Water boatman – *Corixa* spp. Fly larvae – *Diptera* spp. | |
| Great crested newt – adult, terrestrial | Earthworms – *Eisenia* and *Lumbricus* spp. Slugs – *Limax* spp. Beetles – Coleoptera Woodlice – *Oniscus* spp., *Philoscia* spp., *Porcellio* spp., *Trichoniscus* spp. Spiders – *Araneae* spp. | Earthworms – *Eisenia* and *Lumbricus* spp. Slugs – *Limax* spp. Beetles – *Coleoptera* spp. Woodlice – *Oniscus* spp., *Philoscia* spp., *Porcellio* spp., *Trichoniscus* spp. Spiders – *Araneae* spp. | Earthworms – *Eisenia* and *Lumbricus* spp. Slugs – *Limax* spp. Beetles – *Coleoptera* spp. Woodlice – *Oniscus* spp., *Philoscia* spp., *Porcellio* spp., *Trichoniscus* spp. Spiders – *Araneae* spp. | Earthworms – *Eisenia* and *Lumbricus* spp. Slugs – *Limax* spp. Beetles – *Coleoptera* spp. Woodlice – *Oniscus* spp., *Philoscia* spp., *Porcellio* spp., *Trichoniscus* spp. Spiders – *Araneae* spp. |
| Great crested newt – larvae | Phytoplankton. Water fleas – *Daphnia* spp., *Chydoridae* spp. Midge larvae – *Chironomus* spp. Fly larvae – *Diptera* spp. Mayfly nymphs – *Centroptilum* spp. Water lice – *Asellus* spp. Water shrimp – *Gammarus* spp. | Phytoplankton. Water fleas – *Daphnia* spp., *Chydoridae* spp. Midge larvae – *Chironomus* spp. Fly larvae – *Diptera* spp. Mayfly nymphs – *Centroptilum* spp. Water lice – *Asellus* spp. Water shrimp – *Gammarus* spp. Small tadpoles | Phytoplankton. Water fleas – *Daphnia* spp., *Chydoridae* spp. Midge larvae – *Chironomus* spp. Fly larvae – *Diptera* spp. Mayfly nymphs – *Centroptilum* spp. Water lice – *Asellus* spp. Water shrimp – *Gammarus* spp. | Water fleas – *Daphnia* spp., *Chydoridae* spp. Midge larvae – *Chironomus* spp. Fly larvae – *Diptera* spp. Mayfly nymphs – *Centroptilum* spp. Water lice – *Asellus* spp. Water shrimp – *Gammarus* spp. |
| Ringed plover, *Charadrius hiaticula* – adult, breeding grounds | Larval and adult flies – *Diptera* spp. Beetles – *Coleoptera* spp. Periwinkles – *Littorina* spp. Polychaete worms. Amphipods. Molluscs. *Talitrus*. *Mysidacea*. Oligochaetes. Larval and adult insects. Spiders – *Araneae* spp. Freshwater invertebrates. Sticklebacks – *Gasterosteus* | Larval and adult flies – *Diptera* spp. Beetles – *Coleoptera* spp. Periwinkles – *Littorina* spp. Polychaete worms. Amphipods. Molluscs. *Talitrus*. *Mysidacea*. Oligochaetes. Larval and adult insects. Spiders – *Araneae* spp. Freshwater invertebrates. Sticklebacks – *Gasterosteus* | | |
| Ringed plover – adult, away from breeding grounds | Polychaete worms. Crustaceans. Amphipods. Molluscs. Oligochaetes. Larval and adult insects. Spiders – *Araneae* spp. Freshwater invertebrates. Sticklebacks – *Gasterosteus* | Sand hopper – *talitrus saltator*. Polychaete worms. Crustaceans. Amphipods. Molluscs. Oligochaetes. Larval and adult insects. Spiders – *Araneae* spp. Freshwater invertebrates. Sticklebacks – *Gasterosteus* | Sand hopper – *talitrus saltator*. Polychaete worms. Crustaceans. Amphipods. Molluscs. Oligochaetes. Larval and adult insects. Spiders – *Araneae* spp. Freshwater invertebrates. Sticklebacks – *Gasterosteus*. | Polychaete worms. Crustaceans. Amphipods. Molluscs. Oligochaetes. Larval and adult insects. Spiders – *Araneae* spp. Freshwater invertebrates. Sticklebacks – *Gasterosteus*. |
| Ringed | Self-feeding. Larval | Larval and adult flies – | | |

| | | | | |
|---|---|---|---|---|
| plover – chick | and adult flies – *Diptera* spp. Beetles – *Coleoptera* spp. Periwinkles – *Littorina* spp. Polychaete worms. Amphipods. Molluscs. *Talitrus*. *Mysidacea*. Oligochaetes. Larval and adult insects. Spiders – *Araneae* spp. Freshwater invertebrates | *Diptera* spp. Beetles – *Coleoptera* spp. Periwinkles – *Littorina* spp. Polychaete worms. Amphipods. Molluscs. *Talitrus*. *Mysidacea*. Oligochaetes. Larval and adult insects. Spiders – *Araneae* spp. Freshwater invertebrates | | |
| Little ringed plover, *Charadrius dubius* – adult, breeding grounds | Beetles – *Coleoptera* spp. Flies – *Diptera* spp. Ants – *Hymenoptera* spp. Moth and butterfly larvae – *Lepidoptera* spp. Bugs – *Hemiptera* spp. Spiders – *Araneae* spp. Freshwater shrimps – *Gammarus* spp. Mussels. Any moving invertebrate small enough to eat | Beetles – *Coleoptera* spp. Flies – *Diptera* spp. Ants – *Hymenoptera* spp. Moth and butterfly larvae – *Lepidoptera* spp. Bugs – *Hemiptera* spp. Spiders – *Araneae* spp. Freshwater shrimps – *Gammarus* spp. Mussels. Any moving invertebrate small enough to eat | | |
| Little ringed plover – adult, away from breeding grounds | Shrimp – *Gammarus* spp. Oligochaete worms – *Tubificidae* spp. Midge larvae – *Chironomidae* spp. Leeches – *Hirudinea* spp. Seeds – grasses (*Graminae*), sedges (*Carex*). Mayfly larvae – *Ephemeroptera*. Dragonfly larvae – *Odonata*. Bugs – *Hemiptera* spp. Flies – *Diptera* spp. Ants – *Hymenoptera* spp. Caddisflies. Crickets. Butterfly and moth larvae. Earwigs. Spiders. Worms – *Enchytraeidae*, *Tubfex* spp. Molluscs. Beetles. | Shrimp – *Gammarus* spp. Oligochaete worms – *Tubificidae* spp. Midge larvae – *Chironomidae* spp. Leeches – *Hirudinea* spp. Seeds – grasses (*Graminae*), sedges (*Carex*). Mayfly larvae – *Ephemeroptera*. Dragonfly larvae – *Odonata*. Bugs – *Hemiptera* spp. Flies – *Diptera* spp. Ants – *Hymenoptera* spp. Caddisflies. Crickets. Butterfly and moth larvae. Earwigs. Spiders. Worms – *Enchytraeidae*, *Tubfex* spp. Molluscs. Beetles. | Shrimp – *Gammarus* spp. Oligochaete worms – *Tubificidae* spp. Leeches – *Hirudinea* spp. Seeds – grasses (*Graminae*), sedges (*Carex*). Mayfly larvae – *Ephemeroptera*. Dragonfly larvae – *Odonata*. Bugs – *Hemiptera* spp. Flies – *Diptera* spp. Ants – *Hymenoptera* spp. Caddisflies Crickets. Earwigs. Spiders. Worms – *Enchytraeidae*, *Tubfex* spp. Molluscs. Beetles. | Shrimp – *Gammarus* spp. Oligochaete worms – *Tubificidae* spp. Leeches – *Hirudinea* spp. Seeds – grasses (*G*raminae), sedges (Carex). Dragonfly larvae – *Odonata*. Bugs – *Hemiptera* spp. Flies – *Diptera* spp. Ants – *Hymenoptera* spp. Caddisflies. Crickets. Earwigs. Spiders. Worms – *Enchytraeidae*, *Tubfex* spp. Molluscs. Beetles. |
| Little ringed plover – chick | Any moving invertebrate small enough to eat from 2 hours old (self-feeding), some evidence of parental feeding | Any moving invertebrate small enough to eat from 2 hours old, some evidence of parental feeding | | |
| Song thrush, *Turdus philomelos* – adult | Earthworms – *Oligochaeta* spp. Snails – *Gastropoda* spp. Slugs – *Pulmonata* spp. Bugs – *Hermiptera* spp. Ants - *Hymenoptera* spp. Adult and larval beetles – *Coleoptera* spp. Any other terrestrial invertebrates | Fruits and seeds. Earthworms – *Oligochaeta* spp. Snails – *Gastropoda* spp. Slugs – *Pulmonata* spp. Bugs – *Hermiptera* spp. Adult and larval lacewings – *Neuroptera* spp. Adult and larval butterflies and moths – *Lepidoptera* spp. *Hymenoptera* spp. Adult and larval beetles – *Coleoptera* spp. Any other terrestrial invertebrates | Fruits and seeds. Earthworms – *Oligochaeta* spp. Snails – *Gastropoda* spp. Slugs – *Pulmonata* spp. Bugs – *Hermiptera* spp. Adult and larval lacewings – *Neuroptera* spp. Adult and larval butterflies and moths – *Lepidoptera* spp. *Hymenoptera* spp. Adult and larval beetles – *Coleoptera* spp. Any other terrestrial invertebrates | Earthworms – *Oligochaeta* spp. Snails – *Gastropoda* spp. Slugs – *Pulmonata* spp. Bugs – *Hermiptera* spp. *Hymenoptera* spp. Adult and larval beetles – *Coleoptera* spp. Any other terrestrial invertebrates |
| Song | | Earthworms – | | |

| | | | | |
|---|---|---|---|---|
| thrush – chick | | *Oligochaeta* spp. Snails – *Gastropoda* spp. Slugs – *Pulmonata* spp. Larval butterflies and moths – *Lepidoptera* spp. Fly larvae – *Diptera* spp. Beetle larvae – *Coleoptera* spp. Spiders – *Araneae* spp. | | |

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