The practical application of the AMBER software tool to support environmental decision making

R. C. Walke[1], J. K. Longworth[2], R. H. Little[1], A. Venter[2]
& B. W. Miller[2]
[1]Quintessa Limited, United Kingdom
[2]Enviros Consulting Limited, United Kingdom

Abstract

This paper presents practical examples of where problem-specific compartment models have been developed and implemented in AMBER to aid environmental decision making.

- An assessment of the disposal of organic pesticides by land spreading to evaluate the protection of surface and groundwater resources. Following a literature review and workshop of experts, a model was developed to provide a scoping assessment and to identify key processes and parameters.
- A contaminated land safety assessment integrating 37 areas of contaminated ground into a 3-D site-wide model that included adjacent farmland and marine environments. The assessment demonstrated the safety of the current management and provided input into remediation decisions.
- The potential for contaminants released as part of routine effluent discharges to be taken up into the foodchain following the use of contaminated sludge from a sewage treatment plant was addressed with a model of the treatment process and subsequent use of the sludge as a soil improver.
- A model of the possible future use of irrigation water potentially contaminated with arsenic, lead and cadmium leached from a proposed hazardous waste disposal facility, and their subsequent uptake in the foodchain was developed as part of the facility's successful submission for regulatory authorisation.

These studies illustrate how, by giving the user the power to create compartment models from basics, AMBER has been successfully applied to a wide range of contaminant modelling situations, from generic, research level studies for regulators to detailed site-wide models for site operators.

Keywords: AMBER, multimedia, contaminant, compartment, modelling, software.

Brownfields: Multimedia Modeling & Assessment, G. Whelan (Editor)
ISBN 1-85312-755-8

1 Introduction

Advances in information technology continue to improve the way in which information is stored, shared and used in modern societies. Few areas of society are unaffected by the ever increasing capacity of computers to manage and process large quantities of data. The field of environmental decision making is no different, with computers providing platforms for the development of assessment tools designed to model complex environmental systems. However, the power provided by modern software tools to manage environmental information and undertake detailed assessments is accompanied by the responsibility to ensure that environmental decision making is supported by appropriate information, understanding and assessments.

AMBER [1] provides users with the complete flexibility to develop transparent models tailored to the specific problem being addressed and includes capabilities that allow the resulting models to interface with other software applications. The flexibility of being able to develop models from basics means that it is essential that AMBER forms an integrated part of a wider, systematic modelling approach in which the models are developed and justified.

This paper provides background information about AMBER and its capabilities along with some illustrations of a range of contaminant modelling assessments undertaken with the software and demonstrates how it has been applied to address problems from research level studies to detailed, 3-D site-specific assessments.

2 Compartment modelling

By necessity, models of complex environmental systems evolving into an uncertain future must adopt a simplified representation of the features, events and processes under consideration in comparison to their true complexity. This simplification is necessary due to limitations of present-day understanding and practical time and resource constraints.

One approach is to discretise the modelled system into compartments and to represent the processes that have the potential to move contaminants around the system as transfers between those compartments. Each compartment represents a discrete component of the environmental system within which it is judged reasonable to assume that contaminants are uniformly distributed, either because the material is physically well mixed, or because the spatially-averaged concentration for that component is sufficient for calculating the endpoints of interest, such as the potential exposure rate to people exposed to that material.

The compartment model approach places two main constraints on the mathematical representation of an environmental system.

The first constraint is that the system has to be discretised into a series of compartments. Using the compartment modelling approach, an environmental system may be represented by breaking it down into compartments that can correspond to the components identified in a conceptual model. It is assumed that, as soon as a contaminant enters a compartment, mixing occurs so that a uniform concentration over the whole compartment can be assumed. Each compartment should be chosen to represent a system component for which this assumption is reasonable.

The second constraint is that processes resulting in the transfer of contaminants from one compartment to another need to expressed as transfer coefficients that represent the fraction of the activity in a particular compartment transferred from that compartment to another one per unit time. The mathematical representation of the inter-compartment transfer processes takes the form of a matrix of transfer coefficients that allow the compartmental amounts to be represented as a set of first order linear differential equations. These equations can be solved through the use of either a Laplace transform solver [2] or a numerical time-step solver [3]. For the i^{th} compartment, the rate at which the inventory of contaminants in a compartment changes with time is given by:

$$\frac{dN_i}{dt} = \left(\sum_{j \neq i} \lambda_{ji} N_j + \lambda_N M_i + S_i(t) \right) - \left(\sum_{j \neq i} \lambda_{ij} N_i + \lambda_N N_i \right) \qquad (1)$$

where *i* and *j* indicate compartments, *N* and *M* are the amounts (mol) of radionuclides *N* and *M* in a compartment (*M* is the precursor of *N* in a degradation chain). *S(t)* is a time dependent external source of contaminant *N* (mol^{-1}). Transfer and loss rates are represented by λ (y^{-1}). λ_N is the degradation constant for radionuclide *N* (y^{-1}) and λ_{ji} and λ_{ij} are transfer coefficients (y^{-1}) representing the gain and loss of contaminant *N* from compartments *i* and *j*. For simplicity, the above equation assumes a single parent and daughter. However,

3 AMBER

AMBER [1] is a flexible Windows-based software tool that allows users to build their own dynamic compartment models to represent the migration, degradation and fate of contaminants in an environmental system. It is used by over 60 organisations in 24 countries. It has been used to model routine, accidental and long-term releases of both radioactive and non-radioactive contaminants in solid, liquid and gaseous phases.

AMBER does not have any in-built mathematical models to represent processes (other than contaminant degradation) and so the user has flexibility to implement their own mathematical models so long as they are consistent with the compartment model approach. AMBER also has the advantage of allowing the entire system's components, migration processes and endpoints of interest to be represented using a single code in a time dependent and probabilistic manner. AMBER allows the representation of multiple parents and daughters.

4 Example applications

4.1 Scoping assessment of landspreading pesticides

One of the potential disposal routes for organic pesticides is to dilute them and spread them onto farmland on the basis that they will degrade in the soil before

Brownfields: Multimedia Modeling & Assessment, G. Whelan (Editor)
© 2004 WIT Press, www.witpress.com, ISBN 1-85312-755-8

reaching surface or groundwater resources. The inclusion of the pesticides as listed substances in United Kingdom groundwater regulations, due to their potential human and environmental toxicity, means that this method of disposal is subject to authorisation. A research-level study was undertaken to establish the level of understanding concerning the degradation and fate of organic pesticides in the environment and to use this knowledge in the development of a simple scoping tool, implemented in AMBER, to investigate sensitivities and key information requirements. The following methodology was adopted:

- a literature review was undertaken to determine the state of knowledge with regards the behaviour of organic pesticides in the environment;
- the literature review formed the input to an expert workshop at which the key processes and parameters that determine the environmental behaviour of organic pesticides were discussed and a conceptual model developed;
- the conceptual model was then developed into a mathematical model and then implemented in AMBER to enable sensitivity calculations to be undertaken.

The literature review highlighted the potential importance of soil type, moisture content, pH, organic matter, pesticide concentration and microbial activity in determining the rate of degradation of organic pesticides in the soil. It also highlighted that organic pesticides can degrade in the soil by both chemical and microbial processes although, in general, there was a general lack of available data regarding the behaviour of specific organic pesticides in soils.

In addition to the soil properties and degradation processes highlighted in the literature review, the workshop identified soil hydrological properties as being important in determining the potential fate of organic pesticides spread onto land. Infiltration and throughflow provide pathways for the advective transport of pesticides with the potential to transfer them to the deeper unsaturated or saturated zone before they have had a chance to degrade. The susceptibility of soils to surface run-off and ‘bypass flow’ through the soil macropores were identified as important considerations that could reduce the interaction of water with the soil during intense rain storms.

Figure 1 shows some screenshots of the scoping model of pesticide application to the soil. The model uses the information gathered during the literature review and expert workshop to include the chemical and physical degradation of organic pesticides in the soil according to the soil pH, clay content, organic matter content and temperature. Water flows through the model either via bypass flow in macropores or via infiltration through micropores. The scoping tool included soil data associated with four different soil types typical of areas of landspreading and allowed the user to vary the meteorological conditions before, during and after the disposal.

The model was intended as a research-level scoping tool that aimed to make use of the limited data available concerning the environmental behaviour of the pesticides modelled. Error! Reference source not found. illustrates the results of some of the sensitivity calculations that can be undertaken using the model and demonstrates the potential importance of metrological conditions in determining the amount of organic pesticide that is retained and degraded in the soil.

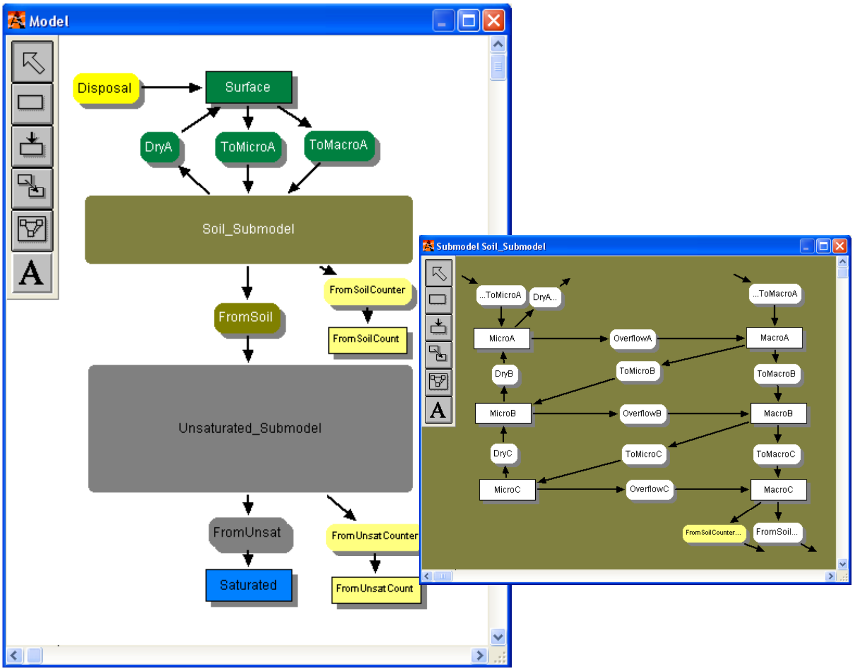

Figure 1: Screenshots of the organic pesticide scoping model.

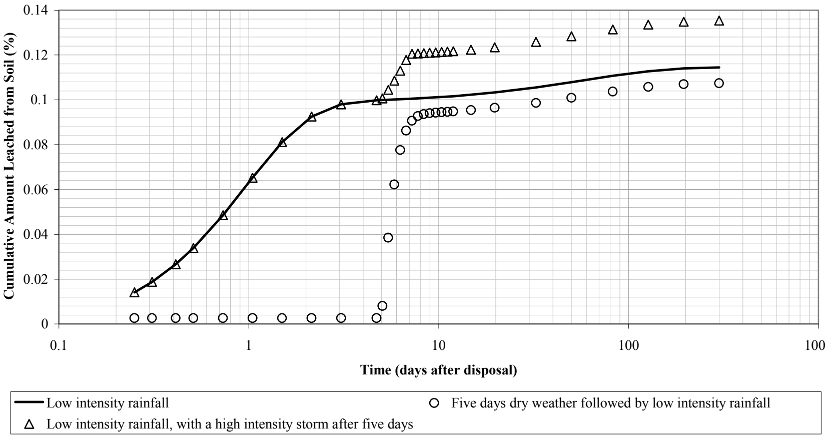

Figure 2: Sensitivity of pesticide leaching to variations in the meteorological conditions after disposal.

4.2 Contaminated land safety assessment

A 3-D site wide model of the United Kingdom Atomic Energy Agency's (UKAEA) site at Dounreay, in the north of Scotland, was developed to provide input to management decisions regarding contaminated land. The assessment approach was firstly to define the assessment context (i.e. what is be assessed and why) and contaminated land source terms, before a conceptual and mathematical model was developed based upon the environment at Dounreay. This model was then implemented in AMBER to enable the calculation of endpoints of interest.

The Dounreay site stretches for approximately 1.5 km along the coastline and inland for approximately 500 m. This area was separated into 18 regions within the assessment model, each of which was discretised in the vertical plane into surface soil, unsaturated fill, saturated rock and deep saturated rock. In addition to these site compartments, the surrounding farmland, foreshore and marine environments were also included in the compartment model. 37 discrete areas of surface and subsurface contamination were then included within this overall model structure, with their characteristics being derived from UKAEA's Information Management and Geographical Evaluation System (IMAGES) geographical information system (GIS).

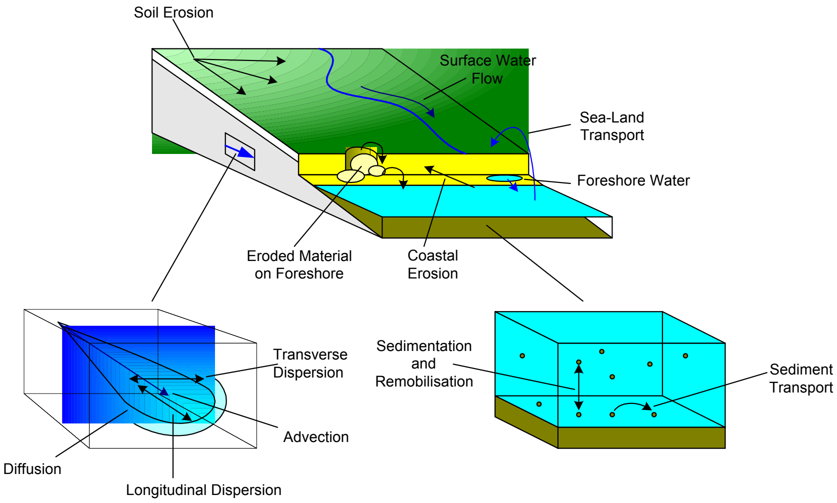

Figure 3: Transport processes considered in the contaminated land safety assessment.

Figure 3 illustrates some of the transport processes considered in the safety assessment model. The resulting model included 30 contaminants, including decay chains, 194 compartments and over 700 transfers. Endpoints of interest included environmental concentrations, fluxes of radionuclides around the system, potential dose rates to surveyors monitoring the areas of contamination, along with potential dose rates that may arise to members of the public due to the potential migration of contaminants from the site.

The calculations extended to 360 years into the future, the period of decommissioning and institutional control that is assumed in the current Dounreay Site Restoration Plan (DSRP) [5]. The model results demonstrated the safety of the current management strategy for contaminated land at Dounreay. The calculated dose rates remain below a level that may give rise to concern (see figure 4). The results indicated that potential dose rates are dominated by a relatively small number of sources terms, which provides input to future remediation decisions.

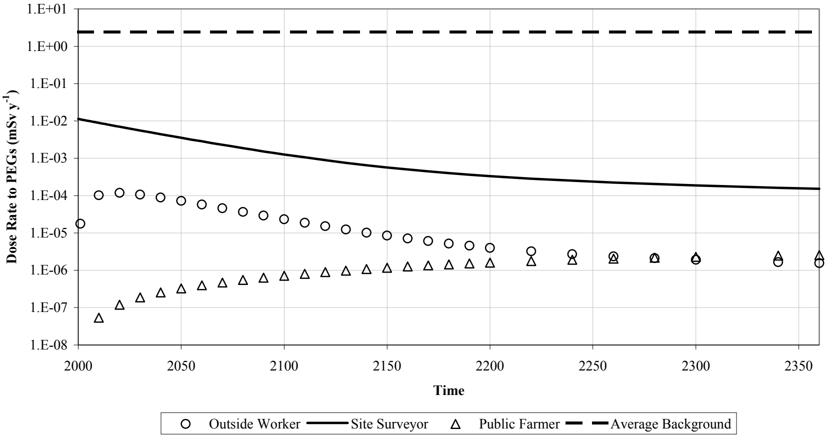

Figure 4: Potential dose rates calculated with the contaminated land safety assessment model.

4.3 Sewage sludge model

The Cardiff Laboratories of Amersham plc., formerly Nycomed Amersham International, were established in 1979 for the production of compounds containing radionuclides for use in health care and other industries. The original regulatory authorisation for the discharge of aqueous waste effluent from the laboratories approved the discharge into a main piped sewer, which subsequently discharged into the Severn Estuary. With subsequent plans to upgrade the waste collection system, it was proposed that effluent should be re-directed to a new wastewater treatment works being constructed by the local water utility and that the sewage sludge, arising from the sewage treatment process, be applied as a soil-improver on agricultural land.

A study was therefore required to assess the radiological impact on the food-chain and annual individual dose to a representative member of the public arising from the presence of carbon-14 and tritium in sewage sludge applied as a fertiliser [6].

Radionuclides in the sludge applied as fertiliser to agricultural land would only become available for uptake by plants once the sludge had decomposed. Decomposition of sludge in soil is a microbial process. In aerobic agriculturally productive soils, the carbon-14 in the sludge is converted to carbon dioxide and released from the soil-sludge matrix by degassing to the near ground and the crop canopy atmosphere before being taken up again by crops or lost to the wider atmosphere. Root uptake of carbon-14 was also modelled as well as the release of carbon dioxide from crops to the canopy atmosphere during aerobic respiration (and subsequent re-uptake by crops during photosynthesis). During sludge decomposition, tritium was assumed to be released as tritiated-water into the soil matrix, where it became part of the pore water. Uptake of tritiated-water from soil into the plant was modelled, as well as the release of tritiated-water into the canopy atmosphere (by evaporation and evapotranspiration from the crops). These processes were each modelled dynamically and further processes explicitly included rather than simply assessed as occurring in equilibrium (an approach commonly adopted in other assessments).

It was assumed that accumulation of activity would occur in the soil due to repeated annual applications of sludge. Losses from the system were assumed to occur through annual cropping, soil erosion and leaching to deeper soil layers (with infiltrating rainwater).

The uptake and distribution of carbon-14 and tritium by animals were also modelled dynamically. This part of the model was largely based on the UK Food Standard Agency's models for Short-Term Atmospheric Release (STAR) that allow for an assessment of both a fast and slow turnover of the radionuclides in animal tissues. Direct ingestion of sludge by grazing animals, as well as inhalation of tritium and carbon-14 from the canopy atmosphere, were also included in the assessment. Figure 5 shows an AMBER screenshot of the resulting model.

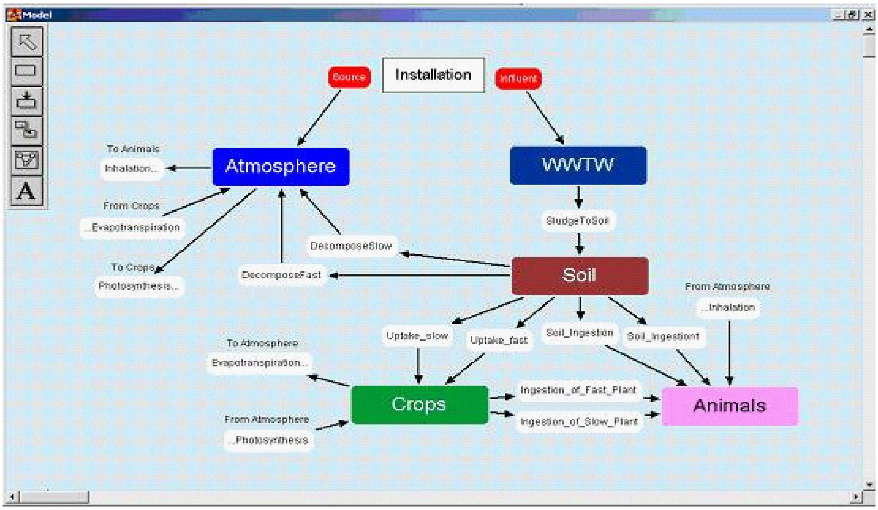

Figure 5: AMBER screenshot of the carbon-14 and tritium sewage sludge model.

The uptake of carbon-14 and tritium by members of the local population was defined as occurring via the ingestion of vegetables, fruit, and animal produce, including milk and eggs. Based on these assumptions, the assessed dose rates to various defined members of the local population were found to be below regulatory limits. Authorisation to discharge via the waste water treatment works was granted and all planned aqueous discharges were successfully re-routed in April 2001.

4.4 Hazardous waste assessment

In 2002, the Minosus proposal to site an underground hazardous waste disposal facility within Winsford Rock Salt Mine, Cheshire, required a quantitative assessment of long-term safety in answer to the articles of Annex II of the EU Directive 1999/31/EC on the landfill of waste and several requirements of the Environment Agency of England and Wales's Integrated Pollution Prevention and Control (IPCC) application process. A key objective of the assessment was to provide confidence that the proposed actions to manage the wastes would not present an inappropriate hazard to human health or the environment [7].

Two conservative scenarios were assessed based on a possible pessimistic evolution of the proposed facility and its environment. Both scenarios envisaged a breakdown of engineered seals with flooding of the proposed disposal zones and a return of arsenic, lead and cadmium-contaminated groundwater into the biosphere after 500 years of closure. However, one scenario considered the use of contaminated groundwater to irrigate agricultural soil, whilst the other scenario considered the discharge of contaminated groundwater to a surface water course, which is subsequently used to supplying drinking water.

Both cases were assessed for two distinct post-closure periods: 500 to 5000 years and 5000 to 50 000 years. During these periods, the conceptual model defined the exposure pathways as including: irrigation of agricultural soils with contaminated water, uptake by grain and pasture on which cows and sheep are fed and subsequent uptake by humans via ingestion of animal produce, vegetables and contaminated drinking water and inhalation of contaminated soil particles by both humans and animals.

Concentrations of contaminants in soil, vegetables, animals and drinking water were calculated from mathematical models implemented in AMBER. These concentrations were compared with statutory limits set by various regulatory agencies. Endpoint results were calculated as the annual intake by a representative member of a potentially exposed group living within the local area (hypothesised as a self-sufficient local farmer).

Whilst a deterministic approach was used throughout the assessment, the study concluded with an examination of the effect of varying certain parameters values to enable an understanding of which processes, contaminants and exposure pathways dominated the resulting dose.

The results from this study strongly indicated that even if a pessimistic evolution of the proposed system was to be considered possible, long-term safety was assured. Following completion of the assessment, and having undergone a lengthy planning application process, the scheme was approved in January 2004.

Brownfields: Multimedia Modeling & Assessment, G. Whelan (Editor)
© 2004 WIT Press, www.witpress.com, ISBN 1-85312-755-8

5 Discussion

The example applications of AMBER described in this paper illustrate how, by giving the user the power to create compartment models from basics, the software can be applied to a wide range of contaminant modelling situations.

Whilst AMBER provides the user with a powerful tool with which to undertake contaminant modelling assessments, it must be recognised that the tools can only be as good as the underlying conceptual models, data and assumptions that they are used to represent. Therefore, it is important to ensure that an appropriate amount of effort is applied to all aspects of the assessment and that the focus is not dominated by software implementation.

References

[1] AMBER Contaminant Modelling Software. www.enviros.com/amber.

[2] Robinson P. C. and Maul P. R., Some Experience with the Numerical Inversion of Laplace Transforms. *Mathematical Engineering in Industry*, **3(2)**, pp. 111-131, 1991.

[3] Robinson P. C., *DYLAN Time-stepping Algorithms: The Approach Used in the DYLAN Solver*, Quintessa, Henley-on-Thames, UK, 2001.

[4] Wham! *Web-Hosted AMBER Model*, www.quintessa-online.com.

[5] UKAEA, *Dounreay Site Restoration Plan*, UKAEA Report DSRP(00)P001, Issue 01, 2000, http://www.ukaea.org.uk/dounreay/rplan.htm.

[6] Venter A, Smith G and Walden-Bevan R., *Modelling the Radiological Impact of C-14 and Tritium in Sewage Sludge from Cardiff Waste Water Treatment Works: Assessment of Exposure via the Food Chain.* Enviros Report for Amersham plc. Enviros Consulting, Culham, Oxon, UK, 2001.

[7] Robinson C and Hooker P., *Quantitative Long-term Safety Assessment of the Minosus Proposal for an Underground Hazardous Waste Disposal Facility.* Enviros Report for Minosus Ltd. Enviros Consulting, Abingdon, Oxon, UK, October 2002.

Brownfields: Multimedia Modeling & Assessment, G. Whelan (Editor)