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PHE Landfill Modelling System

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PHE Landfill Modelling System

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ABSTRACT

The PHE landfill modelling system (LMS) is a linked suite of models developed for the assessment of doses from the disposal of low level radioactive waste to landfill sites. The system builds on the experience gained in using the individual models incorporated into the system, in assessments of landfill sites in the UK. The component models of the system simulate the key processes in the various media responsible for the transport of radioactivity from a landfill site to the biosphere and the subsequent doses to humans. This report describes each of the component models of the LMS and their verification and validation, discusses their operation together as an integrated system and outlines various options for further developing and improving the system.

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Changes made to this document since first publication are as follows:

July 2014	Title page – Eden Consulting has been amended to Eden Nuclear and Environment
	Table 4 column header has been changed from K_d (m^{-3} kg^{-1}) to K_d (m^3 kg^{-1})
	Figure F2 compartment 3 depth label changed from 5 cm to 4 cm

CONTENTS

1 INTRODUCTION

The PHE landfill modelling system (LMS) has been developed to evaluate doses to humans from a variety of exposure pathways potentially arising from the leaching of radioactive waste from a landfill site and the subsequent movement of the leachate through the geosphere and biosphere. The LMS takes the form of a series of linked models that individually represent generic elements of the loss and migration of radioactivity from a landfill following radioactive waste disposal and provides a flexible approach to the production of indicative estimates of the potential radiological consequences arising from the movement of leachate through the environment. This report describes the component models of the LMS that are used to represent the movement of leachate through the environment that arise from particular combinations of design features. The LMS only considers the migration of leachate from landfill sites; other exposure scenarios which may give rise to radiation doses, such as human intrusion, are discussed in another report (Chen et al, 2007).

Following an overview of the development of the LMS in Section 1.1 there is a brief discussion on landfill design in Section 1.2 and an overview of the verification and validation of the individual models in Section 2. Sections 3 to 7 then describe the main components of the system in more detail, including a description of the verification and validation of each component model and the overall system. Finally, Section 8 discusses limitations and potential future developments of the LMS.

1.1 Background

The full complement of models which constitute the LMS was used for the first time in an assessment of the radiological consequences of disposing of very low level radioactive waste by Chen et al (2007). This assessment used the HYDRUS model (Šimůnek et al, 2005), which can simulate radionuclide transport through the unsaturated zone, for the first time as a component of the system.

The approach originally taken was to run individual models sequentially and manipulate the output of one model to generate the input data needed to run the next model in the sequence. This operation required considerable care, as the outputs and inputs of the component stages were not compatible without the application of several conversion factors. The LMS now streamlines the multistage process to produce a convenient tool for assessing the potential doses from the disposal of waste in landfill sites. The LMS can be run and controlled as a single entity without the need to adjust manually the input and output data transferred between component modules. However, to maintain flexibility the option to run the component models of the LMS separately has also been retained.

1.2 Model representation of landfill types

The EC Landfill Directive (CEC, 1999) classifies a landfill site according to the type of waste that the site can accept. There are three classes of waste: inert, non-hazardous and hazardous. The design specifications and operating practices are different for each landfill class. Figure 1 illustrates schematically the variety of landfill constructions considered by the LMS. Different combinations of the component models of the LMS are used to represent these different types of landfill. The component models used in the modelling of radionuclide migration in the different environments are indicated in Figure 1 and discussed in more detail in Section 1.3. Representative depths for the component regions are shown but these may be replaced by values characteristic of the particular landfill under study when using the LMS.

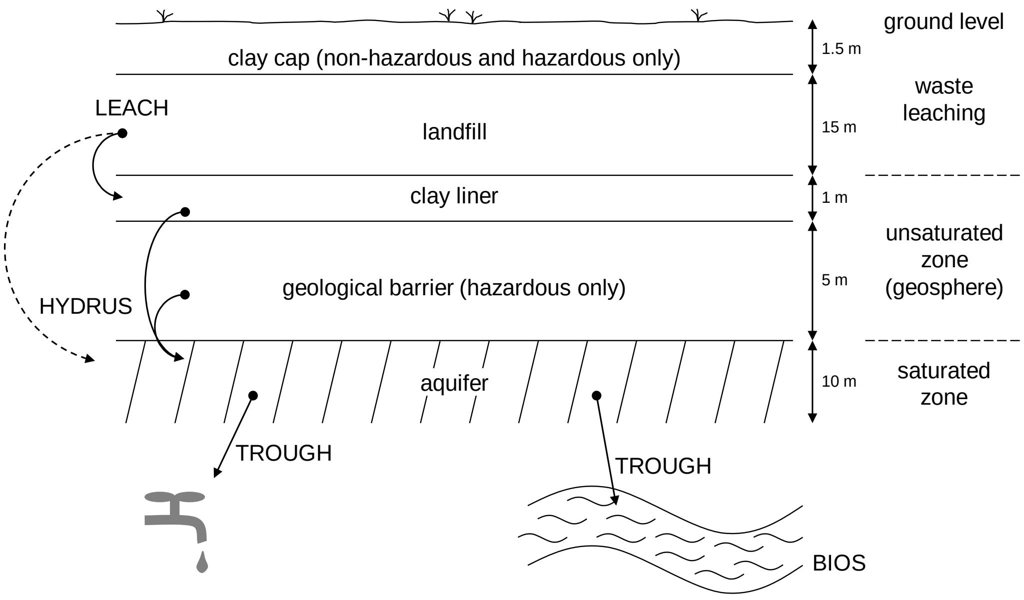

FIGURE 1 Generic environments considered by the LMS including the component models used to represent radionuclide transport through and between these environments

From the perspective of undertaking assessments with the LMS model, the principal differences between the three categories of landfill sites are the barrier requirements designed to impede the flow of water entering or leaving. Schedule 2 of the Landfill (England and Wales) Regulations 2002 (Defra, 2002, 2005) and the Framework for Risk Assessment for Landfill Sites (SEPA, 2002) state that the landfill base and sides shall consist of a mineral layer that protects the soil, groundwater and surface water. Table 1 sets out the barrier requirements for the three different types of landfill sites included in the EC Landfill Directive (CEC, 1999). The mineral layer must be at least equivalent to material with the permeability and thickness combination given in Table 1. The barrier can be less thick than specified in Table 1 if the permeability of the barrier is also less and the result is at least as effective as the combination given in Table 1. The performance of the landfill cap for non-hazardous and hazardous waste sites is not specified numerically by the Landfill Directive but must meet the several requirements specified by the regulatory agencies on, for example, a low permeability layer and surface water drainage (SEPA, 2003).

Radioactive waste is not classified as hazardous waste, but as ‘special waste’, which means that any of the three types of landfill site can be used. The LMS allows these generic types of landfill to be easily customised to meet the requirements of a specific assessment.

Within the broad limitations of the component models of the LMS, a wide variety of landfill designs can be accommodated. Unless an historical site is to be modelled, the design of the landfill site should be selected to be consistent with the requirements of the Landfill Directive and current practice, while site- or design-specific information should be incorporated

TABLE 1 Barrier requirements for the three classes of landfill sites included in the EC Landfill Directive (CEC, 1999)

Property	Inert	Non-hazardous	Hazardous
Mineral layer thickness (m)*	≥ 1	≥ 1	≥ 5
Mineral layer permeability (m s^{-1})*	≤ 1 10^{-7}	≤ 1 10^{-9}	≤ 1 10^{-9}
Cap†	Restoration		
Top soil cover (m)		≥ 1	≥ 1
Drainage layer (m)		≥ 0.5	≥ 0.5
Impermeable mineral layer‡		Yes	Yes
Artificial sealing layer		No	Yes
Gas drainage layer		Yes	No

* Where the geological barrier does not meet these requirements naturally, it may be reinforced by other means providing equivalent protection; in any such case, a geological barrier established by artificial means must be at least 0.5 m thick.

† Inert landfills may only require a cap for restoration purposes but it should be taken into account if they have accepted non-inert waste in the past.

‡ As mineral caps must have some residual permeability, the terminology of the Landfill Directive is less precise for the cap than it is for the liner.

wherever possible. If some of the data required to describe a landfill are unavailable an assessment can nevertheless proceed, using appropriate generic assumptions. Examples of the generic landfill designs included in the LMS are shown in Figure 2, where the non-hazardous and hazardous landfill designs have caps, which inhibit the ingress of rainwater while functional, whereas the inert landfill type is assumed to have no functionally effective barrier preventing rain ingress. The assumption was made that the non-hazardous landfill type has a low-permeability cap, which is assumed to last 50 years, while the cap of the hazardous landfill type is assumed to last 250 years. These estimates of cap lifetimes and other representative properties were agreed with relevant organisations as part of a study sponsored by the Department for Environment, Food and Rural Affairs (Defra) and the Environment Agency (EA) (Chen et al, 2007).

Landfill designs are required to limit the infiltration of rain and surface water using, for example, a low permeability cap (SEPA, 2003). The value of the maximum infiltration rate permitted by the design while the cap is in good repair can be neglected as trivial. Once a cap is no longer functional, some incident rain passes through the cap and the process of leaching radioactivity from the waste starts with leachate containing dissolved radionuclides moving downwards and eventually reaching the top of the clay liner system.

A representative infiltration rate to landfill if no cap is present, or when the cap has fully degraded, can be derived from an examination of UK rainfall data and representative estimates of evapotranspiration and runoff. Although in the absence of site- or assessment-specific information the representative infiltration rate will be uncertain, the LMS assumes that an infiltration rate of 320 mm y^{-1} is appropriate (Chen et al, 2007). It should be noted that this generic infiltration rate is not directly used by the HYDRUS model incorporated within the LMS (see Sections 4.3 and 7.1 and Appendix C).

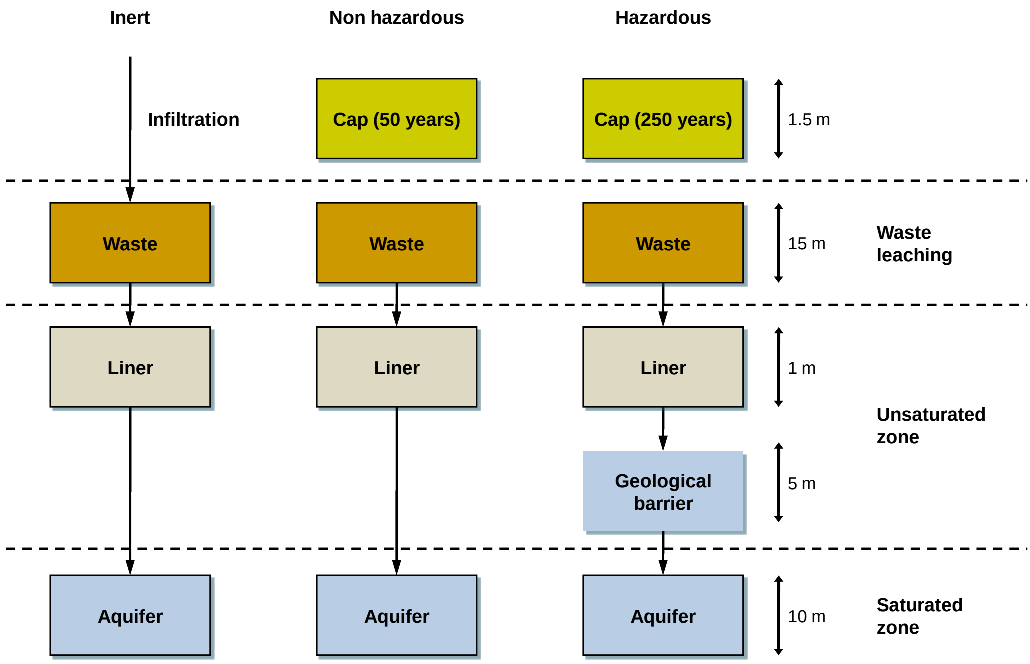

FIGURE 2 Conceptual designs for the three generic landfill classes. These schematic designs are representative of the variety of sites that might be encountered in the UK (Chen et al, 2007)

The clay liner, which is effectively impermeable for a period specific to each landfill type, slows down the rate at which leachate reaches the aquifer (the saturated zone). The generic design of Figure 2 assumes for simplicity that all clay liners are 1 m thick, but they may have different permeabilities. The lifetime of a compacted clay liner depends on maintaining its low hydraulic conductivity, which requires the soil/water mixture of the liner to be kept at, or near, complete saturation (Koerner and Daniel, 1997)*. If the water content is not maintained the effectiveness of a liner is reduced due to the clay shrinking and cracking. The default assumption of the LMS is that the clay liner maintains its effectiveness over the timescale of an assessment.

The hazardous landfill type also has a geological barrier lying under the clay liner. The geological barrier may be a natural feature or an artificial barrier, made of a low permeability mineral layer; an additional 5 m clay liner above the aquifer is specified in a previous assessment (Chen et al, 2007) (see Table 1). The LMS assumes by default that both the clay liner and any subsequent geological barrier are unsaturated and can be modelled as part of a single unsaturated zone, where the clay of the geological barrier is assumed to have the same properties as the clay of the liner†. An alternative perspective, which more naturally accommodates both the need to maintain the effectiveness of the liner and the unsaturated zone between the landfill and the aquifer, is to view the landfill as having a geotechnical membrane over a thin, engineered clay bed which together have an effective permeability equivalent to a 1 m thickness of engineered clay barrier. This description is likely to bear a closer resemblance to the actual barrier employed (eg a clay sandwich sealed between

* The water held in the clay is static and tightly bound to the clay particles.

† In this context, an unsaturated clay liner is a material with limited mobile water and therefore a low hydraulic conductivity although as previously noted it has sufficient tightly bound immobile water to maintain its structural integrity.

two geotechnical membranes), rather than the 1 m thick clay liner assumed in the generic design (US EPA, 2001). Leachate migrates through this thin lens zone and into a vadose zone* of low hydraulic conductivity until eventually reaching the underlying aquifer. Thus, the LMS assumes that the cap fails after a given period which allows water to enter the landfill, whereas the landfill liner, which is not assumed to fail catastrophically, allows water in the landfill to leak continuously into the vadose zone. For simplicity, no modelling distinction is made between the liner and the remainder of the region between the waste and the aquifer. However, if information was available and it was thought appropriate the LMS could be used to model multiple zones with different hydrogeological properties to provide a more complex analysis of the migration of radionuclides from the waste site to the aquifer (see Sections 4 and 8.1). On reaching the aquifer, the radionuclides in the leachate are transported with groundwater until released into the biosphere.

1.3 Component models of the PHE LMS

Figure 3 provides a schematic illustration of how the component models of the LMS link together. A simple leaching model LEACH (see Section 3) provides input to either the unsaturated zone model HYDRUS (Šimůnek et al, 2005) (see Section 4), or directly to the aquifer model TROUGH (Gilby and Hopkirk, 1985) (see Section 5). This latter option allows radioactivity to leach directly from the waste into one or more saturated zones by omitting the

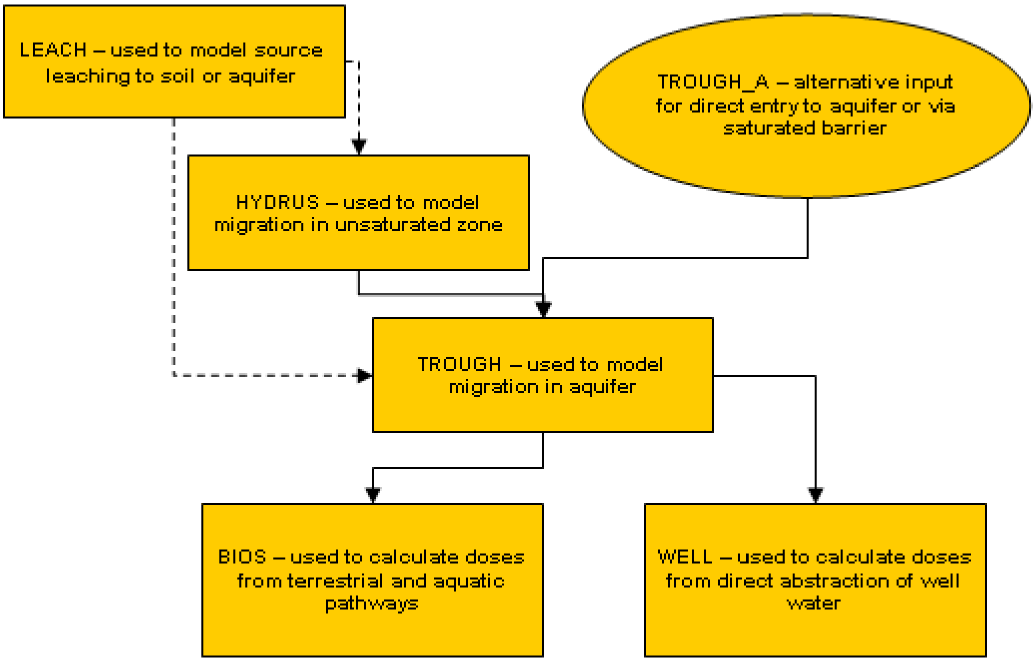

FIGURE 3 Component models of the LMS

* The vadose zone extends from the top of the ground surface to the water table. In fine-grained soils, capillary action can cause the pores of the soil to be fully saturated above the water table at a pressure less than atmospheric. In such soils, therefore, the unsaturated zone is the upper section of the vadose zone and not identical to it. Unless the capillary fringe is specifically discussed, all references in the text to the unsaturated zone refer to the vadose zone.

HYDRUS sub-model of the LMS. This option demonstrates the flexibility of the system, which can be easily modified to represent landfill designs not included in the Landfill Directive, if necessary. On reaching the aquifer, the radioactivity is transported until it can discharge into a river. Doses arising from the potential consumption of plants and animals, are estimated using the model BIOS (see Section 6.1), while those from ingestion of well water are estimated using the WELL model (see Section 6.2).

A list of the default radionuclides considered by the LMS is given in Appendix A. This list can be amended to include additional radionuclides, providing the necessary information can be supplied for the required component models.

2 VERIFICATION AND VALIDATION OF MODELS

To demonstrate the adequacy of the LMS, a process of verification and validation was carried out on both the main component models of the LMS (LEACH, HYDRUS, TROUGH, BIOS and WELL) and the overall system. It was not always possible to apply the validation and verification methods described in the following sections rigorously. However, the best available alternatives were used, such as evidence of verification provided by the software developers, or the validation of parts of a model. Table 2 shows the extent to which verification and validation were carried out and indicates the sections of this report that provide more details.

2.1 Verification

Verification refers to procedures that show that the mathematical model used is, within practical limits, a true representation of the conceptual model of the process being emulated and that the mathematical equations involved are correctly solved. Verification procedures may vary, depending on the particular characteristics of the model and its end use. Typically, verification procedures include:

- **a** Reviewing model structure and basic equations by staff other than those involved in developing the model
- **b** Checking that the model has been correctly implemented
- **c** Comparing computed results with solutions obtained from other models

2.2 Validation

Validation is a technique aimed at demonstrating that a conceptual model, and by implication the numerical representation derived from it, adequately represents the key processes of interest in the real environment. The definition of what constitutes an adequate representation necessarily involves some subjective judgement and may depend on whether the model is intended for general or site-specific applications and how the model results may be used.

Validation is ideally carried out by comparing model calculations with sets of field observations and experimental measurements that are independent of the data used to parameterise the model. In practice, it is not usually possible to validate fully a model representing environmental transfers of radioactivity because of the lack of sufficient independent data to characterise all the radionuclides, timescales and conditions under which the model is likely to be applied. However, if full quantitative validation is not possible, partial validation may be possible or a semi-qualitative approach may be used to check that a conceptual model is likely to be valid. The latter may use data on the behaviour of chemical analogues derived from laboratory experiments and be subject to an external peer review of the assumptions used in developing the model.

TABLE 2 Summary of verification and validation on the PHE LMS

Component	Section	Verification	Validation
LEACH	3.2	By reviewing the model and its implementation	Direct validation is not feasible over the relevant timescales, but the underlying model was qualitatively validated by a literature search
HYDRUS	4.2	Reported intercomparisons with other models	Reported comparisons with experimental results and field data
TROUGH	5.1	By comparison with exact solutions and other models	No validation
BIOS	6.1.1	Through model intercomparison studies	Validation of the full model is not possible over the long timescales involved. However, sub-models have been qualitatively validated and qualitative validation has been carried out on earlier versions of BIOS*
WELL	6.2	By reviewing the model and its implementation including spreadsheet calculations	Validation is not possible
Overall system	7	By comparing LMS results with those of another system	Full validation is not possible but individual components have been validated as above

* The LMS includes version 6B of the BIOS model, referred to as BIOS_6B.

3 LEACH MODEL

The leaching of radioactivity from the waste disposed of in a landfill site once closed is the first of the sequence of processes represented by the LMS. As indicated in Section 1.2, rainwater enters the landfill and dissolves a proportion of the waste material. The leachate then moves downwards through the liner (see Figure 2).

There may be some infiltration during the operational period of the site if the landfill surface is not adequately covered. The amount of radioactivity lost from the waste due to water percolating through the site during this period is difficult to calculate because of the variation of the waste thickness and the unknown amount of infiltration. However, as any effluent produced during this period is likely to be managed according to current regulations it is conservatively assumed that no loss of waste occurs during the operational period of the site.

The concentration of activity released from the waste into the leachate is estimated by the LEACH model, which is discussed briefly in Section 3.1 and in more detail in Appendix B.

3.1 Description of the LEACH model

The LEACH model effectively assumes that the disposed radioactive waste is both homogeneous and distributed uniformly throughout the volume of the landfill, commonly termed the source zone. This implies that the waste is of uniform thickness and, with the additional assumption that the waste site is not on a slope, means that the activity released from the waste is directly determined by the ratio of the infiltration rate of rainwater to the thickness of the waste through which the water percolates. Strictly, within the confines of a one-dimensional representation, the waste does not need to be distributed uniformly or to be homogeneous except in the vertical direction as only the sum of activity in each horizon of the site is considered. Lack of vertical uniformity could affect the rate of leaching over time through the effect of a variable water level within the repository as discussed in Appendix B. However, this is likely to be at least a second-order effect and is therefore not considered further (see Section 4.3).

The dissolution of the waste is represented by a first-order leaching process that matches the amount lost at any time with the amount present while accounting for both decay and sorption. Thus, given a constant infiltration rate, the model of Baes and Sharp (1983) describing the migration of contaminants through soil is applied in LEACH, as shown in Appendix B.

3.2 Verification and validation of LEACH

The LEACH model implemented within the LMS was verified by staff not involved in its development through a process of reviewing the governing equations and their software implementation.

Direct validation of the results from LEACH is not feasible over the timescales relevant to radionuclide migration in the geosphere. However, it is possible to validate qualitatively the underlying Baes and Sharp model with other models through a search of the literature. Atomic Energy of Canada Limited (AECL) and the University of Guelph, Ontario, compared four models assessing the fate of radionuclides in surface soil including the Baes and Sharp leaching model (Sheppard et al, 1997). The comparison used a simple soil model in which the top 15 cm layer is assumed to be instantaneously and homogeneously contaminated. Subsequent downward migration of the contaminant was modelled until the flow conditions reached steady state. The AECL model, SCEMR1, was validated against experimental data and found to behave well numerically. SCEMR1 successfully predicted radionuclide levels over the short term – less than a single growing season – and the migration of lead in soil around churches in Denmark over several hundred years (Hawkins et al, 1995). The Baes and Sharp model was found to compare to within an order of magnitude with SCEMR1. The SCEMR1 model calculates flow based on the soil moisture budget, with daily atmospheric input data including root uptake. The simpler Baes and Sharp approach does not calculate annual water flow or the influence of surface vegetation, but instead uses the net annual ingress of water as input. The Baes and Sharp model has been implemented in modelling software such as GENII, used by the US Environmental Protection Agency (Napier et al, 2005) to perform dose and risk assessments of atmospheric releases of radionuclides and their subsequent deposition.

A validation and verification exercise carried out by McClellan et al (2006) compared three migration models against field data. The models considered were a compartment diffusion model (Landaw and DiStefano, 1984; Kirchner, 1998; Holgye and Maly, 2000), a convection model (Boone et al, 1985; Bunzl et al, 1994) and the leach rate model included in the LMS (Baes and Sharp, 1983; McClellan et al, 1991; Abbott and Rood, 1994). Four experimental sites over which thorium-contaminated sludge was spread and raked into the top soil in 1961 provided the field data for the intercomparison.

Although the study showed that approximately 75% of the radioactivity was retained in the top 15 cm layer at the four sites, the actual movement of thorium and therefore the effective migration rates were significantly higher than the calculated migration rates derived for the compartmental and leach models. However, other factors likely to influence the behaviour of the contaminants were not considered in the study, such as the physical and chemical properties of the thorium sludge or the initial preparation of the site.

The compartmental model and the leach rate model yielded broadly consistent results. However, the migration rate implied by the compartmental model was found to increase with depth, contrary to observations in the measured soil profile. Other studies using the compartmental model have observed the same increase in migration rates with soil depth (Kocher, 1991). McClellan et al (2006) suggest that the assumptions that the diffusion coefficient is independent of soil depth and the time since deposition occurred might be unrealistic and a limitation of the compartmental model. In contrast, the migration rates of the leach model were found to be slightly closer to the measured migration rates, but still lower and therefore very conservative in terms of the amount of radioactivity assumed to remain in the upper soil column. The conclusion reached by comparing the three models to measured field data was to reinforce the importance of using the appropriate physical and chemical properties governing transport processes of water and solutes in soil. In particular, the additional site-specific data used by the leach model, in comparison to the other models, partially compensated for the approximate modelling (see Section 8.1 and the discussion on BIOS in Appendix F).

If required, the LEACH model may be omitted from the LMS and a more detailed analysis of infiltration and loss from the waste site made using the HYDRUS model described in Section 4. However, the added complexity of this would entail is only likely to be justified under particular circumstances, for example, if it is known that the radioactive waste is not distributed uniformly throughout the depth of the repository and that puddling of water may occur to a significant depth. The advantage of including the LEACH model within the LMS is that it provides a simple approach in a zone likely to be poorly characterised. It also enables the LMS to be used without the HYDRUS model, if required, as noted in Section 3.1.

4 HYDRUS MODEL

Within the LMS, the term HYDRUS refers to HYDRUS-1D version 3.0, a program for simulating water flow and the transport of heat or solute in one-dimensional variably saturated media (Šimůnek et al, 2005)*. The representation of variably saturated media requires more data and introduces greater modelling complexity to the analysis of waste transport. However, the greater realism offered by this approach allows more confidence to be placed in the robustness of the modelling. The problem of defining the partially saturated zone and the

* HYDRUS is also available as a licensed product that can model flow in two and three dimensions.

consequences of making different assumptions are discussed in more detail in Appendix C. However, to provide some context Section 4.1 gives a very brief outline of the behaviour of water within the unsaturated zone and the problem of solute transport. Section 4.2 discusses the verification and validation of HYDRUS, while Section 4.3 discusses the use of HYDRUS for modelling the disposal of radioactive waste to landfill.

4.1 Background

The characteristic measure of a partially saturated soil is the water content defined as the volume of water per unit volume of the medium. Within a field environment, the potential energy of soil water has three components: the osmotic, gravity and matric potentials. The first of these potentials is important in semi-arid countries or if the solute concentration is very high but can generally be ignored in the UK. The gravitational potential is simply measured by the height of the water above a chosen reference point, such as the soil surface or the water table. The final component, the matric potential, has the dominant effect on the transport of water and dissolved solutes in a partially saturated soil and arises from surface interactions between soil water and the particles of the medium (Yong, 1999). On a macroscopic scale, the interaction of water in the interstices of the medium with the surrounding particle matrix translates into what is termed the matric potential or matric pressure*. In an unsaturated medium, this pressure is less than atmospheric pressure and therefore normally expressed as a negative value. The greater the matric pressure achieved, the greater the water content, with a maximum value of zero representing a fully saturated system. Similarly, a lower, more negative, pressure implies less water content but the relationship is non-linear and hysteretic and depends strongly on the pore size distribution of the medium (eg whether it is composed of clayey or sandy soil). The relationship between the negative head pressure and the water content is provided by the retention curve. An important related quantity, the hydraulic conductivity, which determines how easily water moves through a medium, also has a sensitive and non-linear dependence on the water content. By extension, the transport of solutes modelled by the LMS and partially dependent on the hydraulic conductivity will have a sensitive and non-linear dependence on the water content in the unsaturated zone.

Figure 4 illustrates the transient condition of water movement in an unsaturated system undergoing recharge. The lower zero flux potential (ZFP) in Figure 4 is the boundary region between water moving to the soil surface to evaporate and moving down to the water table in the summer, while the upper ZFP represents the advance of the wetting front during the autumn when infiltration begins to exceed evaporation. On meeting the lower ZFP, the distinct zones disappear so that during the winter months the soil is at or near complete saturation.

The LMS does not primarily deal with the variation in water content and the movement of water over seasons or years within an unsaturated zone. However, given an appropriate dynamic equilibrium representative of the variation in water content with depth, the LMS is intended to model the transport of solutes within the unsaturated zone. HYDRUS, which is designed to solve the problem of solutes moving through a partially saturated medium, provides the LMS with the required capability.

The creators of HYDRUS, who are principally associated with the Department of Environmental Sciences at the University of California and the US Salinity Laboratory, have

* The matric potential is often measured as a negative head of water or suction pressure.

provided a review of the development history of the software (Šimůnek et al, 2008). HYDRUS was chosen for the LMS because of its history of development and ability to model radioactive decay chains. Within the LMS, HYDRUS is only used to model contaminant transport in the unsaturated zone (the clay liner and geological barriers, see Figure 2) under conditions of dynamic equilibrium, although, as noted in Sections 1.2 and 3.2, this scope could be extended if required. In particular, the LMS does not attempt to determine a suitable equilibrium profile with depth of the water content in the unsaturated zone between the clay barrier of the waste site and the receiving aquifer (see Section 8.1 and Appendix C).

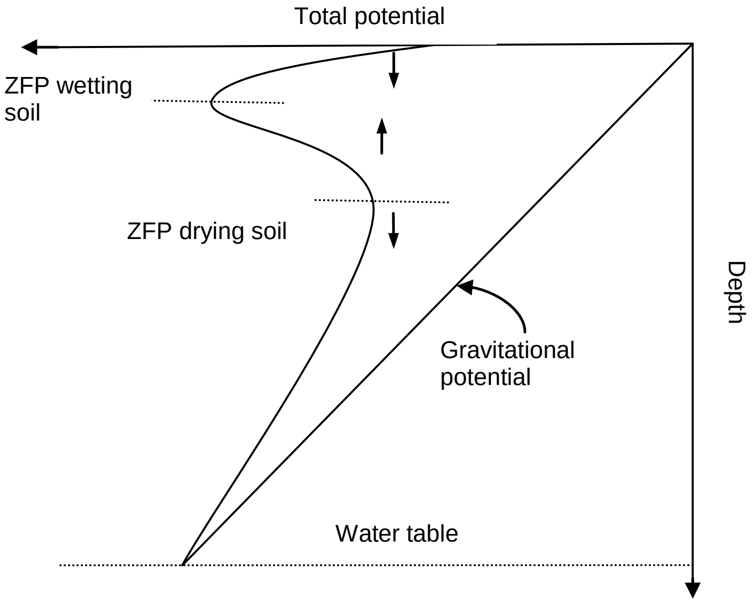

FIGURE 4 Combined matric and gravitational potential (after Wellings and Bell, 1982)

The isolation of waste in landfill sites for non-hazardous and hazardous waste is enhanced by the use of a geological or artificial liner barrier to retard the movement of the contaminant. HYDRUS is used to model the transport of leachate in this unsaturated barrier between the areas of outflow from the waste repository and the reception points for that flow at the receiving aquifer (see Figure 2). The use of HYDRUS to model the retardation of radionuclide flux from the landfill site can provide a more realistic estimate of the concentration of radionuclides entering the aquifer than alternative higher estimates that conservatively assume full saturation. However, the unsaturated zone has a negligible effect on the transport of radionuclides if it is thin and its saturated hydraulic conductivity is high. When this occurs, the leachate flux can be assumed to enter the underlying aquifer directly, with the omission of the retardation effect in the unsaturated zone only introducing a slight increase in the amount entering the aquifer and the conservatism of the results. A fuller description of the model and software is available from the HYDRUS user guide (Šimůnek et al, 2005).

4.2 Verification and validation of HYDRUS

An intercomparison between HYDRUS and four other models was carried out by Chen et al (2002). The other models considered were CHAIN (van Genuchten, 1985), MULTIMED-DP (Liu et al, 1995), FECTUZ (US EPA, 1989, 1995), and CHAIN 2D (Šimůnek and van Genuchten,

1994) and the intercomparison scenario consisted of a hypothetical release of ^{99}Tc at the Las Cruces Trench Site in New Mexico. Sensitivity of three model outputs (peak activity concentrations, time to peak concentrations at the water table and time to exceed the maximum critical level at a representative receptor well) to the input parameters were evaluated and compared among the models for a number of input parameters related to the soil and chemical properties. In general, the five models provided consistent results in water flow simulation and predicted very similar breakthrough curves representing the rate of change in the activity concentration of ^{99}Tc over time at the receptor point. However, slight differences were observed in predicted peak concentrations due to the different mathematical treatments used by the models.

A number of other intercomparisons have been carried out, which have a direct bearing on the application of HYDRUS within the LMS. For example, Perko and Mallants (2007) compared the performance of HYDRUS between its one-, two- and three-dimensional forms with the code PORFLOW. The scenario considered a model representation of a waste container and assumed a fully saturated system. It was found that there was minimal difference in representing the loss of radioactivity from the simple geometry of the waste package in using the one-dimensional HYDRUS model compared to the much more complex three-dimensional version. The HYDRUS and PORFLOW models displayed similar breakthrough curves with comparable peak times and fluxes but the different dimensionalities of the model implementations tended to produce results that were closer to each other than the results of the other model.

Additional performance measures for HYDRUS were provided by Ardois et al (2007), who reported both laboratory work by Mazet (2008) and intercomparisons of HYDRUS predictions with field measurement of water and solute flow of radioactivity released from Chernobyl waste trenches and material analogues composed of sand columns with a radioactive tracer.

Dixon (1999) evaluated the effectiveness of HYDRUS-1D and the SHAW model (Flerchinger and Saxton, 1989) at representing water movement in unsaturated soils in an area of the radioactive waste management site (RWMS) within the Nevada atomic bomb test site. Soil-water and atmospheric data collected from a lysimeter site near the RWMS over a period of approximately five years were used to build the models with initial and boundary conditions representative of the site. The effectiveness of the HYDRUS and SHAW models in predicting unsaturated flow in an arid environment was evaluated by comparing measured storage from the lysimeter with the predicted results from the two calibrated model simulations. Storage results predicted by the HYDRUS and SHAW models were almost identical, and agreed reasonably well with actual lysimeter storage and measured moisture profiles. However, the models were sensitive to the large seasonal fluctuations in meteorological parameters.

In addition, the HYDRUS user manual (Šimůnek et al, 2005) provides further examples of the verification and validation of the model, which are summarised in Appendix C and provide an indication of the scope of the model. However, these additional tests and comparisons are not relevant to the modelling tasks required of HYDRUS within the LMS. Thus, although they confirm the scope and quality of the model in many areas they can only provide background reassurance that the model is robust and likely to provide reasonable results when applied in the context of the LMS.

4.3 Use of HYDRUS as a component of the LMS

The intercomparisons discussed in the previous section and Appendix C illustrate that the HYDRUS model has been applied to the modelling of the migration of radioactive waste from disposal sites or characterising water movement through such sites and has performed well when subject to validation and verification trials. However, it should be remembered that the model is designed for assessments for a particular location specified by the detailed input data required and a particular period during which model parameters either have a known time dependence or can be assumed to be constant. In addition, the HYDRUS user interface only supports input and output times measured in days at its lowest resolution, which is not ideal when considering waste migration from disposal sites over hundreds or thousands of years.

HYDRUS can also be applied to the entire process of leaching and migration from a landfill to an aquifer through an unsaturated zone with eventual abstraction of contaminated drinking water at a well, as shown by Merk (2010). Merk assumed that the leaching of radioactivity from low activity rubble added to a waste site and its migration through a liner and into an unsaturated zone can be modelled by HYDRUS and that a second HYDRUS run can be used to model the lateral flow of the contaminant entering the receiving aquifer. However, although the paper illustrates the potential of this approach only trial parameters were applied in the analysis.

Although HYDRUS generally provides indicative results when used within the LMS, it allows the exploration of potential effects on radionuclide migration of including transport in an unsaturated zone and using different saturation states without precluding more quantitative analysis. For example, HYDRUS could be used to find a matric potential and moisture distribution representative of the unsaturated zone over the long periods of interest in radioactive waste management, which could in turn be applied within other components of the LMS. This additional option is potentially computationally much more intensive than assuming a known saturation state and is discussed in more detail in Appendix C (see also Section 8.1).

5 TROUGH MODEL

The groundwater transport model TROUGH (transport of radionuclide outflows in under-ground hydrology), originally developed by Polydynamics Ltd in the 1980s (Gilby and Hopkirk, 1985), is a one- or two-dimensional transport model that describes the movement of radionuclides and their progeny in multiple geological layers. The model assumes a known steady-state flow rate in each stratum and incorporates geochemical features such as solubility limitation and the effect of equilibrium and non-equilibrium sorption of radionuclides on to solid surfaces in porous media. The one-dimensional version of TROUGH is used within the LMS to model the movement of contaminants in an aquifer (the saturated zone of Figures 1 and 2). The radionuclides entering the saturated zone described by TROUGH are subject to advection, dispersion and sorption as they travel through the geosphere. The model can also represent fracture flow using matrix diffusion in an equivalent porous continuum. The assumption implicit in the use of TROUGH is that any changes in groundwater flow conditions during the modelling period can be neglected. This assumption is appropriate for long-term far-field assessments; however, if the transient behaviour of groundwater flow is likely to be important more detailed modelling would be required. The TROUGH model is described in detail in the TROUGH user guide (Gilby and Hopkirk, 1985).

5.1 Verification and validation of TROUGH

Several verifications of the TROUGH model are discussed in the following sub-sections. Despite a literature search of papers from the validation of geosphere flow and transport models exercise (GEOVAL) (NEA/SKI, 1991, 1995), no evidence of the direct validation of TROUGH was located. Indirect validation can be inferred to some extent from the limited validation of other models that share the same theoretical foundations (OECD/NEA, 1997).

5.1.1 Verification with the INTRACOIN study

The original version of TROUGH was verified in the international nuclide transport code intercomparison (INTRACOIN) Study (Swedish Nuclear Power Inspectorate, 1984, 1986). The INTRACOIN study was divided into three levels:

a Level 1 compared the results of several numerical codes for seven different test cases and, if possible, compared the results to analytical solutions of the transport equations

b Level 2 was principally concerned with the ability of the various computer codes to simulate field experiments involving radioactive tracers

c Level 3 was a limited sensitivity analysis to determine the effects of including or excluding various transport phenomena, such as dispersion, sorption and matrix diffusion, on the results obtained from the various codes

Three of the seven test cases included in level 1 of the INTRACOIN study were amenable to modelling with TROUGH and produced results in good agreement with those of the other codes in the study.

The cases considered in level 2 of INTRACOIN were divided into those dealing with porous media and those dealing with fractured media. The two-dimensional version of the TROUGH code was used for one of the porous media cases. The fractured media cases were not considered by either the one- or two-dimensional version of TROUGH.

The one-dimensional version of TROUGH was used in the level 3 INTRACOIN study to investigate the effect of including different processes in the transport calculation. A central case and 11 variations were considered by five teams using different models. The results from the different models generally differed by less than 10% and demonstrated that the diffusion of radionuclides into the rock matrix was the most important retardation mechanism for the particular scenario analysed.

These studies demonstrated that the TROUGH model provides a representation of the important physical processes associated with the modelling of transport in saturated porous media that is consistent with the results of other models.

5.1.2 Verification with the PSACOIN level E study

A further verification of the one-dimensional version of TROUGH was made by comparing TROUGH as used within the LMS with results of the second NEA probabilistic system assessment code intercomparison exercise (PSACOIN) (OECD/NEA, 1989), known as level E because it provides an exact solution. The existence of an exact solution provided a benchmark against which all the codes participating in PSACOIN could be compared.

Although the TROUGH model was included in the original PSACOIN exercise, it was considered appropriate to verify that in the process of modifying the pre-processor of TROUGH to adapt it for use as part of the LMS no substantial changes had occurred. Therefore, TROUGH, with the revised pre-processor used in the LMS, was retested against the PSACOIN level E study and the results of the comparison results are reported in detail in Appendix D. The level E specification of a deep geological disposal facility was necessarily limited by the requirement to be amenable to an analytical solution (Robinson and Hodgkinson, 1987). Thus, the repository was represented very simply without any complexities of physical structure or chemical composition. After a delay representing failure of the primary containment, the release of radionuclides to the geosphere depends only on the leach rate and the inventory, modified by radioactive decay. The released radionuclides were then transported by groundwater through two geosphere layers with different hydrogeological properties. The radionuclides leaving the geosphere were assumed to enter a simple biosphere – a dilution model of drinking water – from which doses were estimated.

Four radionuclides were considered for each of the three test cases of the PSACOIN level E study: ^{129}I and ^{237}Np with its progeny ^{233}U and ^{229}Th. The source term was always assumed to leach at a constant rate following the failure of the initial containment. The quantities compared with the exact solutions were the peak flux and the time of occurrence at the end of the first layer and the peak dose at peak time from ingestion of drinking water abstracted from a river at the end of the second layer

The maximum discrepancy between the LMS results from TROUGH and the exact solution for any of the radionuclides and test cases was found to be 1.4% for the flux at the end of the first layer and 3.2% for the peak dose.

Appendix D also compares the flux calculated using TROUGH to the results of the analytical model CHAIN (van Genuchten, 1985) for ^{129}I and ^{239}Pu and some of its progeny. In the case of ^{129}I a further comparison was performed between the flux calculated by TROUGH in two-layer mode and those obtained by running TROUGH sequentially as two consecutive single layers. This intercomparison showed that the results produced by TROUGH are in good agreement with those obtained using an independent analytical model.

6 BIOS AND WELL MODELS

Two exposure pathways are normally considered for the radionuclides released into the biosphere following their transport from the waste site by groundwater. The first is the consumption of the groundwater extracted directly by a well sunk into the transporting aquifer. The second is the consumption of food that is either irrigated with water abstracted from a river or lake receiving groundwater, fish from the river or lake, or food grown or reared on soil that takes up groundwater released from an underlying aquifer. In the LMS doses from the consumption of food are modelled using the compartmental model BIOS, which simulates the movement of radioactivity through the biosphere, while doses from the ingestion of drinking water abstracted from the transporting aquifer, are estimated using the simple model WELL. BIOS also provides estimates of the possible dose from drinking contaminated water. However, the WELL model provides a higher estimate than BIOS by modelling the direct abstraction of water from the aquifer, before any dilution with uncontaminated water in the river or lake receiving the aquifer discharge occurs.

6.1 BIOS model

The BIOS model divides the terrestrial and aquatic biosphere into a number of idealised compartments. BIOS assumes that the contents of any compartment are instantaneously well mixed and that the rate of transfer between compartments can be approximated using equilibrium rate constants representative of the different processes operating between the compartments. The conceptual model can be represented by a set of linear first-order differential equations with constant coefficients governing the rate of movement of radionuclides between compartments and can be solved using standard numerical methods.

This model is simpler than the approach employed by HYDRUS (see Section 4) with no consideration given to variations in the water content of the soil and the transport of radioactivity in an unsaturated zone subject to the varying effects of rainfall and evapotranspiration from the covering vegetation. The use of a simpler model, such as BIOS, reflects the greater uncertainty in the competing processes involved at future times, more distant locations and greater spatial extents affected by the discharging aquifer. The BIOS model is also considerably broader in scope than HYDRUS, providing dose estimates for intakes of a wide range of foods as well as from inhalation and external exposure. The idealised compartments of the BIOS model represent elements of the environment such as soil layers or parts of plants and animals that enable estimates to be made of the activity concentrations in each compartment as a function of time. Particular combinations of compartments are often described as models for particular foods or environmental materials and Appendix F describes briefly the models used to represent the transfer of radioactivity between soil, plant and animal for some of the foods considered by BIOS.

6.1.1 Verification and validation of BIOS

The version of BIOS implemented in the LMS is BIOS_6B. Each version of BIOS was benchmarked against previous versions to ensure that improvements to particular parts of the model did not adversely affect other parts. Different versions of BIOS have been validated through model-model intercomparison studies: BIOS_3A (Martin et al, 1991) through the biosphere model validation study (BIOMOVS) (SSI, 1993), and BIOS_5C through the biosphere models for safety assessment of radioactive waste disposal (BIOMOSA) study (Pröehl et al, 2005). BIOS_3A was also subjected to detailed peer review as a result of its use in the Nirex research programme (Baker et al, 1995). A simplified version of BIOS, called MiniBIOS, was verified by means of detailed benchmarking against BIOS_3A for the PACOMA study (CEC, 1991) and through model-model comparisons within an NEA probabilistic system assessment code (PSAC) user group and BIOMOVS II (SSI, 1996).

It is not possible to validate BIOS quantitatively because of the long-term nature of the predictions for which it is most commonly used. In addition, available data have often been used to parameterise the component models. However, most of the component models of BIOS and MiniBIOS are based on models that have been qualitatively validated to some extent, even if only for a few radionuclides and for short-term predictions.

The validations of BIOS_3A and MiniBIOS carried out within the BIOMOVS programmes were qualitative. BIOMOVS was an international cooperative study to test models designed to quantify the transfer and bioaccumulation of radionuclides and other trace substances in the environment using measurements of radioactive fallout from the Chernobyl nuclear plant accident in 1986. The first phase of BIOMOVS (BIOMOVS I) was completed in 1990 (SSI, 1993) while the second phase, BIOMOVS II, ran from 1991 to 1996 (SSI, 1996). Similarly, the IAEA programme on the validation of model predictions (VAMP) (IAEA and CEC, 1993) was followed in 1996 by the IAEA programme on biosphere modelling and assessment (BIOMASS) (Linsley and Torres, 2004). The BIOMASS programme followed the same approaches used in VAMP and BIOMOVS for the testing of models and continued the work started in BIOMOVS II to define a reference biosphere for use in assessments of the long-term safety of underground radioactive waste repositories. BIOS_3A was not considered in the BIOMASS programme, which ended in 2001. However, there then followed the biosphere models for safety assessment of radioactive waste disposal (BIOMOSA) study (Pröehl et al, 2005) which used the reference biosphere methodology specified within BIOMASS to develop a generic biosphere tool based on BIOS_5C, to compare five site-specific biosphere models for five typical locations in Europe. In general, there was an acceptable agreement between the results of the generic biosphere tool, for both the deterministic and stochastic calculations, with the results from the site-specific models.

In addition to the intercomparison studies discussed above, and to demonstrate the consistency of BIOS results over time and developing technology, Appendix F compares results obtained with earlier versions of BIOS with those from the version used within the LMS (BIOS_6B).

6.2 WELL model

Well water may be used to irrigate crops or to provide drinking water for livestock. However, these exposure pathways are usually radiologically less important than the use of well water for human consumption and are not considered by the simple well water model, WELL, included in the LMS. The model is described in detail in Appendix E but, essentially, it applies a correction factor to the activity concentration predicted at the sampling location in the aquifer by TROUGH to account for the filtering of the water to remove suspended sediment and then calculates the dose to individuals consuming the filtered water.

The results of the WELL model used in the LMS can be reproduced by a spreadsheet calculation that implements the essential elements of the methodology discussed in Appendix E. However, the spreadsheet calculation only verifies that the equations are correctly implemented in the LMS; a lack of suitable information prevented validation of the model.

7 VERIFICATION AND VALIDATION OF THE OVERALL LMS

The previous sections have illustrated the verification and validation of the individual models contributing to the LMS. This section details the verification of the system as a whole by comparing the results of LMS calculations using different combinations of these models with each other and with an independent landfill assessment. A comparison with earlier assessments using an alternative geosphere model (GEOS) is also reported in Appendix F. A full quantitative validation of the overall system is not possible due to the long timescales involved.

7.1 Verification of the LMS

The verification exercise undertaken was divided in two parts: a comparison between two different combinations of the component models of the LMS and a comparison with the results of the case study for the Sniffer consortium undertaken by Galson Ltd (Reedha and Wilmot, 2005), hereafter referred to as the Sniffer study. The two LMS model combinations that were compared use, respectively, the component models LEACH, TROUGH and WELL or LEACH, HYDRUS, TROUGH and WELL. For convenience, these combinations are referred to as the TROUGH (T) and HYDRUS and TROUGH (HT) options, respectively. The first option (T) assumes that there is a fully saturated zone below the landfill. For this option the radionuclides leached from the landfill site enters a two layer saturated region of barrier and aquifer modelled by TROUGH. In the second option (HT) the barrier is modelled by HYDRUS and the aquifer by TROUGH. This option allows a range of saturation states to be represented, including fully saturated, for the zone between the landfill and the aquifer. The HT option was evaluated under both saturated and unsaturated conditions to give three sets of results together with an independent set of results for the same scenario*.

The model used in the Sniffer study implements a framework developed by the Environment Agency (EA) to assess sites for special precaution burial disposals with input data derived for a generic landfill site subject to a particular migration scenario. The model assumes a fully saturated zone below the landfill site. The generic landfill site described in the EA framework and the associated data were used in the intercomparison between the LMS and the Sniffer study. The parameter values in each LMS combination were either set to their default value or to a value from the scenario adopted in the Sniffer study (Reedha and Wilmot, 2005). The parameters of the landfill site are given in Table 3, while K_d values of the radionuclides considered in the intercomparison are shown in Table 4. The outputs calculated for the intercomparison exercise were the peak annual effective doses from the consumption of well water by a person representative of a group of people with very high intake rates of drinking water arising from the disposal of 1 MBq of activity for each radionuclide and the time the peak effective dose occurs for each of the disposed radionuclides. The peak times were not presented in the report of the Sniffer study.

* The only difference between saturated and unsaturated when applied to the use of HDRUS in this context is that the former assumes a matric pressure of zero.

TABLE 3 Parameter values of the landfill site adopted in the Sniffer model (Reedha and Wilmot, 2005)

Parameter	Value
Surface area (m^2)	$42.39\ 10^{4}$
Volume (m^3)	$4.0\ 10^{6}$
Distance to water abstraction point (m)	$2.5\ 10^{2}$
Drinking water consumption rate ($m^3\ y^{-1}$)	$7.3\ 10^{-1}$
Net water infiltration rate after cap failure ($m\ y^{-1}$)	$1.55\ 10^{-1}$
Time of cap failure (y)	$1.0\ 10^{2}$
Thickness of effective geological barrier (m)	$1.0\ 10^{0}$
Thickness of unsaturated zone (m)	$2.0\ 10^{0}$
Total barrier thickness for modelling as a single zone (m)	$3.0\ 10^{0}$
Hydraulic conductivity of barrier ($m\ s^{-1}$)	$1.0\ 10^{-9}$
Bulk density of barrier ($kg\ m^{-3}$)	$2.0\ 10^{3}$
Porosity of barrier	$5.0\ 10^{-1}$
Thickness of groundwater zone (m)	$3.0\ 10^{1}$
Hydraulic gradient	$5.0\ 10^{-2}$
Hydraulic conductivity of groundwater bearing rock ($m\ s^{-1}$)	$1.0\ 10^{-5}$
Bulk density of groundwater bearing rock ($kg\ m^{-3}$)	$2.3\ 10^{3}$
Porosity	$4.0\ 10^{-1}$

TABLE 4 K_d and decay constants of the radionuclides considered in the intercomparison between the LMS and the Sniffer model (Reedha and Wilmot, 2005)

Radionuclide*		K_d ($m^3\ kg^{-1}$)			
Parent	Progeny	Waste	Barrier	Aquifer	Decay constant (y^{-1})
^{3}H		0.0	0.0	$1.0\ 10^{-6}$	$5.63\ 10^{-2}$
^{14}C		0.0	$1.0\ 10^{-3}$	$1.0\ 10^{-6}$	$1.21\ 10^{-4}$
^{36}Cl		0.0	$1.5\ 10^{-2}$	$1.0\ 10^{-6}$	$2.30\ 10^{-6}$
^{99}Tc		0.0	$1.0\ 10^{-3}$	$1.9\ 10^{-1}$	$3.25\ 10^{-6}$
^{129}I		0.0	$1.0\ 10^{-3}$	$1.0\ 10^{-6}$	$4.41\ 10^{-8}$
^{232}Th		0.0	6.0	$5.0\ 10^{-1}$	$4.95\ 10^{-11}$
	^{228}Ra	0.0	9.0	$1.0\ 10^{-3}$	$1.21\ 10^{-1}$
	^{228}Th	0.0	6.0	$5.0\ 10^{-1}$	$3.63\ 10^{-1}$
^{238}U		0.0	$4.6\ 10^{-2}$	$1.0\ 10^{-2}$	$1.55\ 10^{-10}$
	^{234}U	0.0	$4.6\ 10^{-2}$	$1.0\ 10^{-2}$	$2.84\ 10^{-6}$
	^{230}Th	0.0	6.0	$5.0\ 10^{-1}$	$9.00\ 10^{-6}$
^{239}Pu		0.0	7.6	$1.0\ 10^{-1}$	$2.88\ 10^{-5}$
	^{235}U	0.0	$4.6\ 10^{-2}$	$1.0\ 10^{-2}$	$9.84\ 10^{-10}$

* Only the parent radionuclides were assumed to be present initially in the waste disposed of.

7.1.1 Results of the intercomparison of the LMS with the Sniffer study

The results of the intercomparison between the LMS and the Sniffer study are shown in Table 5. The table reports results for three variants of the LMS: option T, option HT with a fully saturated barrier (matric suction of 0 m) and HT with the default matric suction assumed by Chen et al (2007) of –1 m. The results presented in Table 5 show that for many radionuclides there is broad agreement between the peak dose estimated by the LMS for both the T and HT options under fully saturated conditions. The largest difference is for ^{3}H for which the peak dose calculated by the LMS under saturated conditions for option T differs from the peak dose calculated for option HT by a factor of 10. This difference in the estimated dose is consistent with the difference in the estimated time of the peak dose and peak flux of the breakthrough curve predicted by the T or HT options, as shown in Figure 5.

As noted in Section 4.3, the use of HYDRUS within the LMS enables the system to take account of the effect of transporting radionuclides through partially saturated soils. It is important to note that one consequence of the implementation of HYDRUS within the LMS is that calculations with a fully saturated barrier for options T and HT are not equivalent and therefore the results cannot be expected to agree. The calculation for option HT does not consider the effect of water puddling within the waste site and does not require the Darcy flux* below the liner to match the average rate of rainwater ingress. This difference does not affect the doses for longer-lived radionuclides, estimated under saturated conditions by the LMS, which are in good agreement when calculated using the T and HT options. Figure 5 and Table 5 demonstrate that the two options available in the LMS to describe radionuclide transport under saturated conditions produce broadly similar doses, provided the half-lives of the radionuclides are long in comparison to the travel times considered (see also Section C5).

Figure 5 demonstrates that the most important difference between the results for options T and HT under saturated conditions is a delay in the peak time due to the difference in water velocity assumed by the two approaches. The results of Table 5 contrasting the HT option applied under fully and partially saturated conditions demonstrates the effect that the reduced water content of partial saturation may have on the expected doses. In addition, the water velocity effect observed between the T and HT options under saturated conditions shown in Figure 5 will also apply under partially saturated conditions and lead to an underestimate of the flux as the effect of partial saturation on the hydraulic conductivity is overestimated. As discussed in Section 4.1, the matric potential and saturation state of the soil are likely to vary with depth and interact in a complex way with the head of water expected in the landfill.

The peak dose for ^{239}Pu calculated by any of the LMS options considered differs markedly from the much larger peak doses calculated in the Sniffer study. This result may reflect the cautious nature of the Sniffer calculations but no specific information is supplied by the case study that would indicate a difference in the treatment of ^{239}Pu migration via groundwater in comparison to other radionuclides (see Section D2). The reverse effect occurs for ^{232}Th when the calculation by the LMS is compared with the Sniffer result. The migration of ^{232}Th is difficult to model due to the very long breakthrough time and this difficulty may be exacerbated in the simple Sniffer approach and lead to the less conservative Sniffer result. However, as no information on the timing of the peak dose is reported in the Sniffer study a definitive conclusion cannot be drawn.

* The Darcy flux or specific discharge is the average flux crossing a surface large enough to be viewed as a homogeneous material with a given porosity. It must match the net rainfall infiltration rate entering the volume if there is no swelling or shrinkage of the medium (see Appendix B).

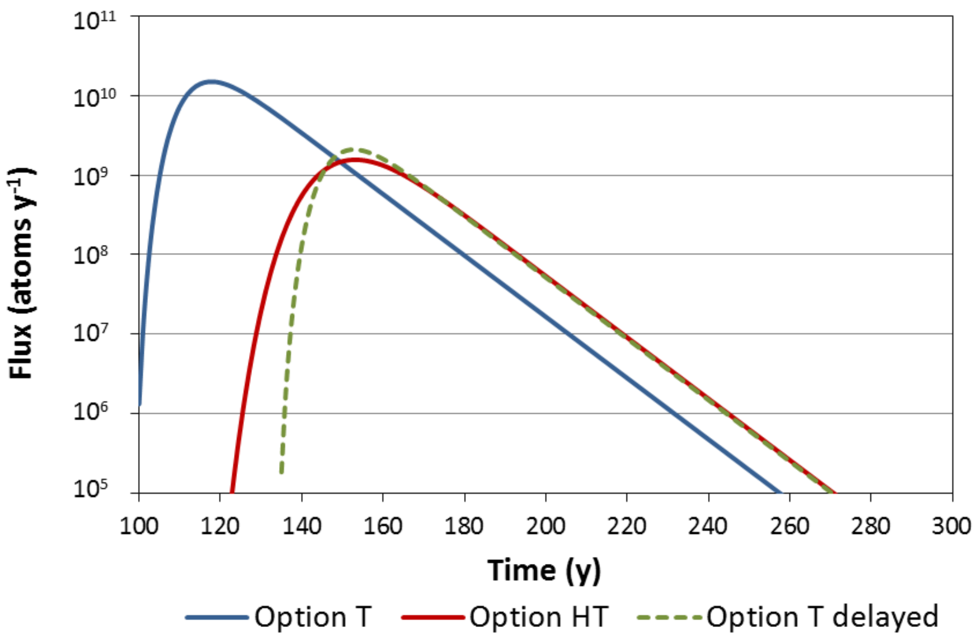

FIGURE 5 ^{3}H breakthrough curve for the Sniffer scenario calculated under saturated conditions using the LMS options T or HT. The broken line represents the results for option T delayed by 35 years, the approximate difference in the peak times between the two options

TABLE 5 Results of intercomparison between the Sniffer study and the LMS

	LMS excluding HYDRUS (option T)		LMS including HYDRUS (option HT) Fully saturated barrier		LMS including HYDRUS (option HT) Unsaturated barrier		Sniffer case study
Radionuclide	Peak dose (Sv y^{-1})	Peak time (y)	Peak dose (Sv y^{-1})	Peak time (y)	Peak dose (Sv y^{-1})	Peak time (y)	Peak dose (Sv y^{-1})
^{3}H	2.3 10^{-15}	1.18 10^{2}	2.4 10^{-16}	1.53 10^{2}	1.5 10^{-20}	2.14 10^{2}	2.8 10^{-14}
^{14}C	3.5 10^{-11}	1.64 10^{2}	2.1 10^{-11}	3.51 10^{2}	3.0 10^{-13}	2.33 10^{3}	2.6 10^{-11}
^{36}Cl	8.1 10^{-12}	5.93 10^{2}	3.3 10^{-12}	2.82 10^{3}	6.5 10^{-19}	3.33 10^{3}	6.6 10^{-12}
^{99}Tc	6.4 10^{-13}	4.51 10^{3}	4.8 10^{-13}	5.45 10^{3}	2.6 10^{-13}	9.97 10^{3}	4.4 10^{-14}
^{129}I	6.9 10^{-9}	1.64 10^{2}	4.2 10^{-9}	3.52 10^{2}	7.7 10^{-11}	2.66 10^{3}	3.2 10^{-9}
^{232}Th	6.5 10^{-9}	1.87 10^{5}	5.4 10^{-9}	1.07 10^{6}	7.9 10^{-11}	1.17 10^{7}	3.0 10^{-17}
^{238}U	1.3 10^{-10}	1.81 10^{3}	5.6 10^{-11}	8.64 10^{3}	1.0 10^{-12}	9.28 10^{4}	3.0 10^{-11}
^{239}Pu	2.1 10^{-16}	4.31 10^{3}	1.9 10^{-16}	1.12 10^{4}	2.6 10^{-17}	1.36 10^{5}	1.8 10^{-13}

The effect of partial saturation on the results is strongly influenced by the time required with respect to the half-life of the radionuclide to pass from the low saturation regime into the aquifer. Highly mobile long-lived radionuclides are least affected by partial saturation, while short-lived less mobile radionuclides may decay completely before they can cross a partially saturated zone. In distinction to the Sniffer model, the LMS version that includes HYDRUS allows the potential effect of an unsaturated zone between the waste and the aquifer to be considered.

8 DISCUSSION

The LMS estimates the amount of radioactive waste material leaching from a landfill site, models the subsequent movement of the released solutes through the geosphere and biosphere, and calculates the resulting doses to humans from the associated exposure pathways. This system is applicable to landfill sites that operate in Europe and is designed to support simple assessments and to provide indicative results through the simple representation of key processes. A simple one-dimensional model of a landfill requires the net flow of water entering the landfill to match the amount of water assumed to enter the aquifer from the waste site. However, the LMS, when used with HYDRUS, is not yet designed to conserve automatically the net amount of water traversing the system and transporting the radioactivity held in the waste site to the aquifer. The LMS in this configuration therefore tends to overestimate the time of peak breakthrough and due to radioactive decay and dispersion potentially underestimate the peak and total amount of activity reaching the aquifer.

The verification and validation of the component models described in this report demonstrate the robustness of the individual components of the LMS. A partial verification of the entire system was undertaken through the comparison of the LMS with the Sniffer model. A more detailed intercomparison, with Sniffer and if possible other models, would provide additional insights into the capabilities and limitations of the LMS and the robustness of the results it produces.

A novel feature of the LMS is the ability to use HYDRUS to model the unsaturated zone between the radioactive waste and the aquifer. The use of HYDRUS within the LMS provides an indication of the potential significance of an unsaturated zone on the timing and magnitude of doses. However, the disadvantage of using HYDRUS within the LMS is that the results produced are likely to underestimate the potential doses because of the way HYDRUS has been incorporated into the LMS. Fortunately, the LMS allows a conservative (dose maximising) calculation to be undertaken that omits the use of HYDRUS and in most circumstances results in estimated doses well below regulatory concern. It is therefore only for a limited number of scenarios when an alternative implementation of the HYDRUS model within the LMS, producing a smaller and more realistic overestimate, is required to provide additional reassurance on the low level of predicted doses. The resolution of this problem would allow the LMS to provide more realistic estimates of releases to the biosphere when HYDRUS is included, rather than indicative results. Potential solutions to this problem are considered in Section 8.1.

The LMS is a flexible combination of models that can be used in many ways. However, great care should be exercised when setting up a calculation, as the input files for one model often require that the information supplied by other models is reformulated. The LMS does not check that repeated data are used consistently or even that the same number of progeny are used by different models.

In summary, the LMS can be used for quantitative but cautious assessments by omitting the HYDRUS option. It is recommended that the LEACH option to allow direct input to TROUGH by bypassing HYDRUS is also omitted as LEACH was designed to supply the leachate flux from the parent in the landfill to HYDRUS while omitting any contribution from ingrown progeny. The TROUGH program has a built in pre-processor program that provides more functionality than available with LEACH such as a leachate flux for the ingrown progeny.

Therefore, for the purposes of the type of assessment likely to be carried out by PHE the default mode of the LMS is to include only the TROUGH, BIOS and WELL models, while the other components (LEACH and HYDRUS) are used only for research and development.

8.1 Future developments

A number of improvements could be made to the design of the LMS as outlined below. For example, it would be useful to identify the characteristic parameter combinations when saturation is not expected to occur. If a less cautious and more realistic calculation is required under such circumstances then generic pressure profiles could be developed that would complement the generic waste site designs and parameterisation and allow HYDRUS as currently implemented to be used in a semi-quantitative way. The development of such a profile would allow, as far as possible, the net infiltration of rainfall assumed for the waste site and the flow into the aquifer to match and thus provide a consistent steady-state representation*. This approach would enable semi-quantitative results to be produced within the existing framework (Kao et al, 2001). As discussed in Appendix C data are available on the hydrological parameters of the soils near landfill sites throughout the UK.

In a further refinement, HYDRUS may be run in an iterative mode to determine the equilibrium water flow, matric potential and hydraulic conductivity. This option can be computationally expensive but may be required under certain circumstances to achieve a dynamic water balance. The approach should allow more realistic results to be produced than those obtained by omitting the unsaturated zone, while remaining cautious when calculating doses. Changes in the way HYDRUS is run would allow bathtubbing events, when leachate from the waste site overflows, to be linked to particular rain sequences either when particular scenarios are investigated or as part of an uncertainty analysis.

The capabilities provided by HYDRUS can also be used to review and refine the assumptions surrounding the way radioactivity initially enters and then moves through the biosphere from the transporting aquifer. The soil included in BIOS is assumed to be fully saturated and therefore does not consider the modelling features for unsaturated soil included in the HYDRUS model; however, the advection–diffusion modelling of HYDRUS together with the information on soils in the UK (see Appendix C, Section C2.1) can improve the representation and calibration of the BIOS soil model.

A number of assumptions made in the current version of BIOS that stem from earlier versions of the model (Martin et al, 1991), such as those used to calculate doses arising from releases of ^{3}H and ^{14}C into the biosphere via an aquifer, would benefit from a review.

Consideration could be given to linking the component models in a more seamless and effective way, which would have the advantage of removing some of the limitations of the current system. For example, in some circumstances it would be advantageous to start the LMS with HYDRUS rather than the LEACH model. The HYDRUS model can cope with a larger number of input and output fluxes as well as sources within the modelled volume so that HYDRUS, in addition to modelling the unsaturated zone below the waste site, could be applied to the variably saturated zone above the waste liner. This more comprehensive

* It may be difficult to achieve an exact match when the water flow solution is applied in the LMS if alternative software, grid sizes or even boundary conditions are used to solve the water flow problem from those used to solve the solute transport problem using HYDRUS.

approach to the representation of a waste site would remove many of the limitations of the current system. However, such complexity will not always be required and it is important that the LMS retain the potential to provide simple and flexible results.

Structurally, the LMS could also be simplified by uniting the various models into a single code. This simplification would require the replacement of the HYDRUS executable file with the available source code from the original HYDRUS unsaturated model. These changes would require considerable effort but have the added advantage of removing any perceived requirement to use a time step of a day as currently implemented within the LMS. In any case, even if no major software redevelopment of the system is carried out, the operation of the LMS should be further refined and streamlined to increase the overall convenience of the tool.

In the longer term, the scope of the LMS may be extended in other ways by considering, for example, the more detailed representation required of a two- or three-dimensional representation or the modelling of additional phenomena affecting the transport of radionuclides and other pollutants.

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APPENDIX A Default Radionuclides

The default set of radionuclides for which data are available in the landfill modelling system (LMS) is given in Table A1. The radionuclides were selected because of their potential contribution to doses to workers and the public from the migration of activity to the biosphere and for consistency with other work carried out over the years on inadvertent intrusion and exposure to the releases of gas from a landfill site. Additional radionuclides can be added to the system by supplying the required data.

The LEACH model only calculates the loss of the parent radionuclide from a landfill site but the LMS supports the ingrowth of a single progeny in the first and again in the second generation from the parent radionuclide within either the HYDRUS or TROUGH models. If the TROUGH model is used without LEACH, additional progeny can be included in the calculations if required. To limit the maximum time that BIOS requires to complete a run the LMS default option is to consider just the first two generations of the radionuclide at the head of the decay chain that are not in secular equilibrium. However, if LEACH and HYDRUS are omitted this restriction is not enforced and a longer decay chain can be included explicitly. Thus, for example, calculations of doses for ^{238}U in natural uranium generally include the contributions from its progeny ^{234}U, ^{230}Th, ^{226}Ra, ^{210}Pb and ^{210}Po in secular equilibrium, while for a pure ^{238}U source the contributions from the progeny in its decay chain would be taken into account through ingrowth*. Where required, dose coefficients of a radionuclide take account of progeny in secular equilibrium.

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* Previous reports using the GEOS or TROUGH models have used the notation U+238 as a shorthand reference to the use of an extended decay chain.

TABLE A1 Default radionuclides included in the LMS

Radionuclide	Half-life (y)	Progeny*	Data source
^{3}H	1.23 10^{1}		Barnard, 1993; King, 2002; Reedha and Wilmot, 2005
^{14}C	5.73 10^{3}		Barnard, 1993; CEC, 1988; King, 2002; Reedha and Wilmot, 2005; US DoE, 1996
^{36}Cl	3.01 10^{5}		Barnard, 1993; Egan, 2006; King, 2002; Reedha and Wilmot, 2005; US DoE, 1996
^{41}Ca†	1.40 10^{5}		Egan, 2006
^{55}Fe	2.70 10^{0}		Reedha and Wilmot, 2005
^{60}Co	5.27 10^{0}		Reedha and Wilmot, 2005; US DoE, 1996
^{59}Ni	7.50 10^{7}		Barnard, 1993; US DoE, 1996
^{63}Ni	9.60 10^{1}		US DoE, 1996
^{79}Se	6.50 10^{4}		Barnard, 1993; King, 2002; US DoE, 1996
^{90}Sr	2.91 10^{1}		Egan, 2006; King, 2002; Reedha and Wilmot, 2005
^{94}Nb	2.00 10^{4}		US DoE, 1996
^{93}Zr	1.53 10^{6}	^{93m}Nb	CEC, 1988
^{99}Tc	2.13 10^{5}		Barnard, 1993; Egan, 2006; King, 2002; Reedha and Wilmot, 2005; US DoE, 1996
^{106}Ru	1.01 10^{0}		Reedha and Wilmot, 2005
^{107}Pd	6.50 10^{6}		CEC, 1988
^{108m}Ag	1.27 10^{2}		Reedha and Wilmot, 2005
^{126}Sn	1.00 10^{5}		Barnard, 1993; Egan, 2006; King, 2002; Reedha and Wilmot, 2005
^{129}I	1.57 10^{7}		Barnard, 1993; Egan, 2006; King, 2002; Reedha and Wilmot, 2005; US DoE, 1996
^{135}Cs	2.30 10^{6}		Barnard, 1993; King, 2002
^{137}Cs	3.00 10^{1}		US DoE, 1996; King, 2002; Reedha and Wilmot, 2005
^{152}Eu	1.33 10^{1}		US DoE, 1996
^{154}Eu	8.80 10^{0}		US DoE, 1996
^{210}Pb	2.23 10^{1}	^{210}Po	CEC, 1988
^{226}Ra	1.6 10^{3}	^{210}Pb, ^{210}Po	Egan, 2006; King, 2002; Reedha and Wilmot, 2005; US DoE, 1996
^{228}Ra	5.76 10^{0}	^{228}Th	US DoE, 1996
^{227}Ac	2.17 10^{1}		Barnard, 1993; Egan, 2006; US DoE, 1996
^{231}Pa	3.28 10^{4}	^{227}Ac	Barnard, 1993; US DoE, 1996
^{229}Th	7.34 10^{4}		Egan, 2006
^{230}Th	7.54 10^{4}	^{226}Ra, ^{210}Pb	Barnard, 1993; Egan, 2006; King, 2002; US DoE, 1996
^{232}Th	1.41 10^{10}	^{228}Ra, ^{228}Th	Reedha and Wilmot, 2005; US DoE, 1996
^{233}U	1.59 10^{5}	^{229}Th	Egan, 2006; King, 2002; US DoE, 1996
^{234}U	2.45 10^{5}	^{230}Th, ^{226}Ra	Barnard, 1993; Egan, 2006; US DoE, 1996
^{235}U	7.04 10^{8}	^{231}Pa, ^{227}Ac	Barnard, 1993; US DoE, 1996
^{238}U	4.47 10^{9}	^{234}U, ^{230}Th	Egan, 2006; King, 2002; Reedha and Wilmot, 2005; US DoE, 1996
^{237}Np	2.14 10^{6}	^{233}U, ^{229}Th	Barnard, 1993; Egan, 2006; King, 2002; US DoE, 1996

Radionuclide	Half-life (y)	Progeny*	Data source
^{238}Pu	$8.77\ 10^{1}$	^{234}U, ^{230}Th	Barnard, 1993; US DoE, 1996
^{239}Pu	$2.41\ 10^{4}$	^{235}U, ^{231}Pa	Barnard, 1993; Reedha and Wilmot, 2005; US DoE, 1996
^{240}Pu	$6.54\ 10^{3}$	^{236}U, ^{232}Th	US DoE, 1996
^{241}Pu	$1.44\ 10^{1}$	^{241}Am,^{237}Np	King, 2002; US DoE, 1996
^{242}Pu	$3.76\ 10^{5}$	^{238}U, ^{234}U	US DoE, 1996
^{241}Am	$4.32\ 10^{2}$	^{237}Np	Barnard, 1993; King, 2002; Reedha and Wilmot, 2005; US DoE, 1996
^{242m}Am	$1.52\ 10^{2}$	^{234}U, ^{230}Th	CEC, 1988
^{243}Am	$7.38\ 10^{3}$	^{239}Pu, ^{235}U	CEC, 1988
^{244}Cm	$1.81\ 10^{1}$	^{240}Pu, ^{236}U	King, 2002; US DoE, 1996

* Explicitly considered progeny included in calculations.

† A full plant model for ^{41}Ca cannot yet be implemented within BIOS due to the lack of FARMLAND data (Brown and Simmonds, 1995). It may be necessary to carry out a separate BIOS run, using a soil to plant transfer factor rather than run the full plant compartmental for this nuclide. Alternatively, an analogue nuclide may be run instead of ^{41}Ca.

APPENDIX B LEACH Model

The LEACH model provides a simple estimate of the activity concentration of contaminated effluent in a landfill site commonly termed, in this context, the source zone, subject to water ingress from infiltrating rainfall. The waste buried at the site is assumed to be uniform, homogeneously distributed throughout the landfill site and of constant depth. On this basis the release of activity from the waste can be simply determined by the ratio of the infiltration rate of rainwater to the uniform thickness of the waste through which the infiltrating water must percolate. A second inherent assumption is that the waste is subject to a broadly uniform microporous flow of water throughout its entire extent. The uniform flow is likely to maximise the amount of radioactive waste leached from the landfill site as the whole volume is equally affected. In reality, there may be preferential flow channels in the waste which allow water to reach the liner rapidly, but may cause particular volumes of the waste to remain relatively dry for extended periods and therefore not subject to the same degree of leaching.

In LEACH the dissolution of the waste is represented by a first-order leaching process that matches the amount lost at any time with the amount present while accounting for both decay and sorption. The model of Baes and Sharp (1983) for the migration of contaminants through soil assuming a constant infiltration rate is used in the model to determine the activity concentration in the leachate. The leach rate constant λ_L (y^{-1}) is given by:

$$\lambda_L = \frac{P_{inf}}{V_{landfill} R_f \theta} \tag{B1}$$

where P_{inf} is the volumetric percolation rate (m^3 y^{-1}), $V_{landfill}$ the volume of the landfill holding the waste (m^3), R_f is the retardation factor of radionuclides in the waste volume and θ is the effective porosity of the waste if it is fully saturated, or the volumetric moisture content of the waste if unsaturated (R_f and θ are dimensionless). P_{inf} and $V_{landfill}$ are given by:

$$P_{inf} = A_{landfill} I_{inf} \tag{B2}$$

$$V_{landfill} = A_{landfill} H_{landfill} \tag{B3}$$

where $A_{landfill}$ is the surface area of the landfill site (m^2), I_{inf} is the net water infiltration rate or Darcy flux (m y^{-1}) and $H_{landfill}$ (m) is the depth of the waste in the landfill site.

The retardation factor R_f is given by:

$$R_f = 1 + \frac{K_d \rho_{waste}}{\theta} \tag{B4}$$

where K_d is the distribution coefficient of the radionuclide in the waste (m^3 kg^{-1}) (see Table B1, which gives K_d values for several media) and ρ_{waste} is the bulk density of the waste (kg m^{-3}).

Substituting equations (B3) and (B4) in equation (B1) gives:

$$\lambda_L = \frac{P_{inf}}{V_{landfill} R_f \theta} = \frac{A_{landfill} I_{inf}}{A_{landfill} H_{landfill} \theta \left(1 + \frac{K_d \rho_h}{\theta}\right)} = \frac{I_{inf}}{H_{landfill} \left(\theta + K_d \rho_{waste}\right)} \tag{B5}$$

The distribution coefficient K_d plays an important role in the rate at which the contaminant is leached out: a lower value of K_d means a lower retardation factor and the lower the retardation factor, the higher the release rate and leachate concentration. This simple model ignores chemical kinetics and therefore does not take account of changes in the rate of dissolution that might occur because of temperature changes or solubility thresholds.

The model also assumes that the waste has a constant saturation state, whereas in reality the saturation state may change with depth, as water can accumulate at the bottom of the waste site until the rate of loss matches the rate of ingress. The fully saturated fraction of the total depth of the waste at the site may then change cyclically with the seasons. Temporal changes in the horizon that is saturated could interact with any inhomogeneous distribution of activity within the wastes vertical distribution. However, this issue is not likely to be significant in terms of the timing or amount leached from the waste, as the amount lost will be bounded by the results obtained assuming either complete saturation with minimal void spaces (see Appendix C, Section C2) or alternatively that no puddles form and the site only maintains residual water content. The more complex view of the landfill site, namely a perched water table providing a head of water above an unsaturated zone that leads to an aquifer is discussed further in Appendix C. The LEACH model only simulates the migration of a single radionuclide from a waste site, although multiple progeny may leach from the site at distinct rates over a considerable length of time.

If no other loss mechanisms are considered, the activity remaining in the waste at time t, I(t) (Bq), is given by:

$$I(t) = I(0)e^{-(\lambda + \lambda_L)t} \qquad \text{(B6)}$$

where I(0) is the initial activity in the source (Bq) and λ is the radioactive decay rate constant (y^{-1}).

TABLE B1 Default distribution coefficients K_d for several geological media (Chen et al, 2007)

	K_d ($m^3\ kg^{-1}$)			
Radionuclide	**Waste**	**Clay**	**Unsaturated**	**Aquifer**
^{3}H	0	0	0	0
^{14}C	0	0	0	0
^{36}Cl	0	0	0	0
^{60}Co	0	$1.0\ 10^{0}$	$1.0\ 10^{-1}$	$1.0\ 10^{-1}$
^{90}Sr*	$1.0\ 10^{-2}$	$1.0\ 10^{-1}$	$1.0\ 10^{-2}$	$1.0\ 10^{-2}$
^{129}I	0	$1.0\ 10^{-3}$	$1.0\ 10^{-3}$	$1.0\ 10^{-6}$
^{137}Cs*	$1.0\ 10^{-1}$	$1.8\ 10^{0}$	$2.0\ 10^{-1}$	$2.0\ 10^{-1}$
^{226}Ra*	$5.0\ 10^{-1}$	$1.0\ 10^{0}$	$5.0\ 10^{-1}$	$5.0\ 10^{-1}$
^{232}Th	$5.0\ 10^{-1}$	$5.4\ 10^{0}$	$1.0\ 10^{0}$	$1.0\ 10^{0}$
^{238}U*	$1.0\ 10^{-1}$	$1.5\ 10^{0}$	$1.0\ 10^{-2}$	$1.0\ 10^{-2}$
^{239}Pu	$2.0\ 10^{-1}$	$4.9\ 10^{0}$	$6.0\ 10^{-1}$	$6.0\ 10^{-1}$
^{241}Am	$1.0\ 10^{-1}$	$8.1\ 10^{0}$	$7.0\ 10^{-1}$	$7.0\ 10^{-1}$

* Progeny in secular equilibrium are included.

The instantaneous contaminant flux, F_{out} (Bq y^{-1}), released from the waste at time t is proportional to the instantaneous activity in the waste, where the constant of proportionality is the leach rate λ_L. Thus:

$$F_{out}(t) = \lambda_L I(t) \tag{B7}$$

Substituting I(t) from equation (B6) gives:

$$F_{out}(t) = \lambda_L I(0) e^{-(\lambda + \lambda_L)t} \tag{B8}$$

The activity concentration in the leachate at time t, $C_{leachate}(t)$ (Bq m^{-3}), is given by:

$$C_{leachate}(t) = \frac{F_{out}(t)}{P_{inf}} \tag{B9}$$

The total activity of a particular radionuclide that leaches from a landfill in a given time t, $Q_{out}(t)$ (Bq), is calculated by integrating the flux released, as given by Equation (B8), over the release period:

$$Q_{out}(t) = \int_0^t C_{leachate}(t')dt' = \frac{\lambda_L I(0)\left(1 - e^{-(\lambda + \lambda_L)t}\right)}{\lambda_L + \lambda} \tag{B10}$$

Taking into account the containment period T (y) during which no leaching occurs, which in this case is assumed to be the lifetime of the cap (see Section 1.2), the activity concentration in the leachate at time t > T (OECD/NEA, 1989) is:

$$C_{leachate}(t) = \frac{\lambda_L I(0) e^{-\lambda T} e^{-(\lambda + \lambda_L)(t - T)}}{P_{inf}} \tag{B11}$$

For some radionuclides, the leachate concentration in the pore fluid (ie the fluid occupying the pore spaces in the rock or soil) is limited by its solubility. The landfill modelling system (LMS) does not currently support limits on solubility. However, this feature could be added by adjusting the mass balance of the contaminant in the waste using the equation (Rood, 1999):

$$I(t) = I(0)e^{-\lambda t} - R_s \frac{\left(1 - e^{-\lambda t}\right)}{\lambda} \tag{B12}$$

where R_s (Bq y^{-1}) is the solubility limited release rate during the period of interest. R_s depends on the solubility of the radionuclide and the amount of water available and can be evaluated using the following equation:

$$R_s = C_s P_{inf} \tag{B13}$$

where C_s is the solubility of the radionuclide in water (Bq m^{-3}).

If the activity concentration in the leachate of equations (B9) or (B11) exceeds the solubility limit, leaching is limited by the solubility of the radionuclide. After a period of infiltration, the radionuclide inventory is depleted sufficiently for the leachate not to exceed the solubility limit and equations (B6), (B8), (B9), (B10) and (B11) will then apply with the leach rate then being limited by the distribution coefficient K_d.

It is beyond the scope of the LEACH model to consider phenomena that are more complex. For example, uranium or plutonium may form complexes with organic ligands in the waste or surrounding soil. The leaching of any metal organic complexes formed depends on their solubility, which differ from that of free metals.

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APPENDIX C HYDRUS Model

C1 Introduction

HYDRUS is an advanced tool for modelling the migration of water, contaminants gas flow and heat in the partially saturated zone above the water table (Šimůnek et al, 2005). The software is well suited to the needs of the landfill modelling system (LMS) with the caveat that it is designed for the detailed modelling of flows over short periods and, therefore, offers time steps of a day or less and expects any potentially time dependent input to be supplied for times characteristic of this time step.

Section C2 provides a brief discussion on the problem of defining the partially saturated zone and the consequences of making different assumptions with subsequent sections elaborating on how HYDRUS can be used within the LMS. In particular, Section C5 discusses the problem of producing a representative result from HYDRUS, which uses data and reports results in much more detail than is required by the LMS.

C2 Flow in unsaturated media

Section 4.1 briefly introduced concepts important in the description of a partially saturated soil where the dominant effect on the transport of water generally arises from surface interactions between water, held in the pores and interstices of the soil, and the surrounding soil. These microscopic interactions translate into the macroscopic matric pressure that in a partially saturated soil is at less than atmospheric pressure and is therefore normally expressed as a negative value with respect to atmospheric pressure. Thus, the greater the matric pressure the greater the water content until at zero matric pressure (atmospheric pressure) the soil is completely saturated.

The flow of water in such an unsaturated system is derived from solving Richards' equation (Richards, 1931), which combines Darcy's law with the continuity equation for water and requires that two properties of the medium are known, the unsaturated hydraulic conductivity K_h (m s^{-1}) and the differential water capacity. Both of these quantities can be calculated from the water retention curve, which gives the relationship between water content and the matric suction or potential. This approach is analogous to the formulation under saturated flow where the advective flux density of water* is the product of the saturated hydraulic conductivity and the gradient of the hydrostatic head (ie the head drop per unit distance in the flow direction). The advective flow in unsaturated sediments is the product of the unsaturated conductivity, which varies spatially, and the total potential composed of the gravitational potential and the matric potential (or suction) which also varies spatially. The suction gradient defines the direction of flow from areas of low to high suction (high to low potential). As a soil is progressively desaturated, increasing suction is required to remove the remaining water. The hydraulic conductivity reflects the ease with which water flows through the media and decreases with decreasing moisture saturation (ie there is greater resistance to flow when there is a lower water content). In addition, hydraulic conductivity is also highly dependent on soil texture. Nielsen et al (1986) noted that in unsaturated soils, in addition to water held within

* The advective flux density simply depends on the flow velocity of the water through a cross-sectional area per unit time.

aggregates, immobile water, which also occurs in saturated systems, may exist in thin liquid films around soil particles, in dead-end pores, or as relatively isolated regions, associated with unsaturated flow. Thus, as the pathway for water flow becomes more tortuous, more of the water held in films and small pores becomes disconnected from the flow network.

In addition to the effects on flow of water becoming disconnected within a fixed soil matrix, the soil can also shrink and the pore space reconfigure as moisture is lost, which, for example, may lead to cracking and the loss of integrity of clay barriers. However, for simplicity, if the problems of cracking and compaction are ignored, a schematic representation of a typical water retention curve for a rigid and homogeneous soil is of the form shown in Figure C1. By definition, the volumetric water content, θ, is equal to the saturated water content, θ_s, when the soil matric potential also termed the head, h_m, is equal to zero. However, only under specific circumstances is the saturated water content equal to the porosity, φ, as entrapped air generally prevents the water content being greater than $\theta_s \approx 0.85\ \varphi$ to $0.9\ \varphi$ (Kosugi, et al, 2002).

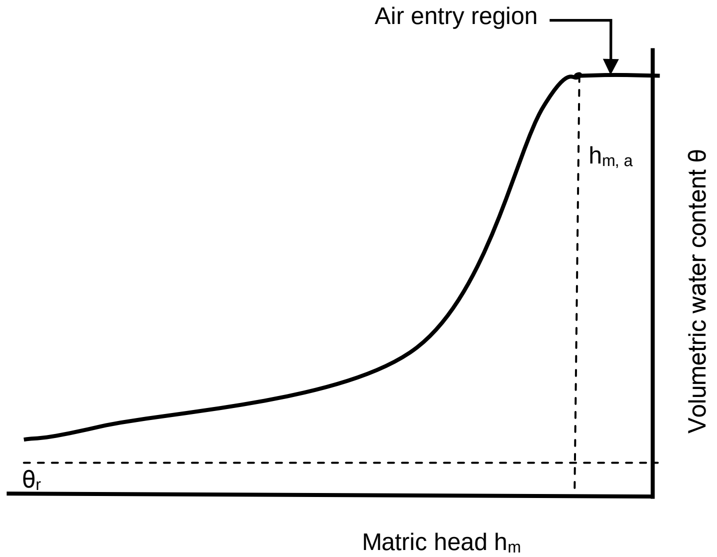

FIGURE C1 Water retention curve of a typical soil with definitions of parameters (after Kosugi et al, 2002)

For many soils, the value of θ remains at θ_s for values of h_m slightly less than zero. The value of h_m at which the soil starts to desaturate is defined as the air-entry value, $h_{m,a}$. It is assumed inversely proportional to the maximum pore size forming a continuous network of flow paths within the soil. As h_m decreases below $h_{m,a}$, θ usually decreases according to a S-shaped curve with an inflection point. As h_m decreases further, θ decreases seemingly asymptotically towards a soil-specific minimum water content known as the residual water content, θ_r. The finite value of θ_r is an historical artefact of water content measurements being made in moist soils, from which soil water retention models assumed an asymptotic form for the retention curve at low levels of water content. As a result, most retention models only describe retention curves in the range of $\theta_r \leq \theta \leq \theta_s$ and it is therefore often convenient to define an effective saturation, which varies between zero and one – see equation (C3).

Relationships between the hydraulic conductivity, matric potential and water content are well established (Jury et al, 1991; Hillel, 1998). However, as noted above, the nature of θ_r is still controversial since the water content theoretically goes to zero as h_m becomes infinitely negative. In practice, θ_r is treated as a fitting parameter that improves the match between model and observation in relatively wet soils. However, because the water content theoretically goes to zero as the matric head becomes infinitely negative, retention models that contain θ_r as a fitting parameter disagree with measured data in the low matric head range ($h_m < -10$ m). Fayer and Simmons (1995) proposed modified parametric soil water retention functions that adequately represent retention across the whole soil water matric head range of 0 to -10^5 m, while combinations of power functions and logarithmic functions were used by Rossi and Nimmo (1994) to characterise soil water retention from saturation to oven-dryness. When retention and conductivity functions are coupled through mutual parameters, the shape of the retention function has a large influence on the prediction of the unsaturated hydraulic conductivity, especially near saturation. For example, a bimodal soil water retention function, allowing the formulation of a secondary macroporous pore system, may improve the predicted value of the unsaturated hydraulic conductivity in structured soils near saturation. Finally, it should be noted that extrapolating model values outside the range of input data for the water content and pressure head, with a negative head representing the matric suction and a positive value a simple hydrostatic head, should only be done with caution.

In addition to the four parameters $h_{m,a}$, $h_{m,}$, θ_s, and θ_r, most retention models include a dimensionless parameter, which characterises the width of the soil pore size distribution. Many functions have been proposed to relate the matric head to the volumetric water content; although most of these functional relationships are empirical, some include parameters that have a physical basis. These parameters are discussed further in the context of the parameterisation used by HYDRUS in Section C3.

HYDRUS assumes that the upper surface has an atmospheric boundary condition. This implies that HYDRUS should be used to model either water flow from the upper surface of the liner including any potential puddling or from the surface of the waste site in an approach analogous to that proposed by Merk (2010). The difference assumed in the two descriptions of the waste is that the former is consistent with a loose packed aggregate while the latter assumes that the waste can be characterised as a pseudo-soil without rapid finger or crack flow (Chen et al, 2002; van Dam et al, 2004).

C2.1 Soil data

Table C1 provides an example of the data available for England and Wales at a resolution of 1 : 250,000 from the National Soil Resources Institute (NSRI) at Cranfield University. This includes soil densities and textures, hydraulic parameters and the permanent wilting point θ_{pwp}, which is the value of volumetric water content at which plants can no longer recover turgidity even when placed in a saturated environment (Hillel, 1982) and characterises the critical point at which all models shut down evaporation. The permanent wilting point is related to the energy involved in transporting water up to the root zone and corresponds to a very large value of the matric potential. A value of 153 m (15 bar) is widely accepted as the characteristic value of the matric potential at the permanent wilting point for most soils (Viterbo, 2002). Based on Cosby et al (1984), it is possible to obtain the matric potential at the permanent wilting point for each soil type of the classification by the US Department of Agriculture (see Section C3) using the critical review by Patterson (1990) of the experimental estimates.

TABLE C1 Example of soil data available for England and Wales*

Property	Example data	Description
Land use	PG	Land use group: AR (Arable), PG (Permanent Grass), LE (Ley Grassland) or OT (Other)
UPPER_DEPTH	20	Horizon upper depth in cm
LOWER_DEPTH	35	Horizon lower depth in cm
BULK_DENSITY	1.28	Bulk density (g cm^{-3}) observed
PARTICLE_DENSITY	2.63	Calculated particle density (g cm^{-3})
φ	51.2	Total pore space (%) volume
θ_{V5}	16	Volumetric water content (%) at 5 kPa tension (field capacity)
θ_{V10}	11.5	Volumetric water content (%) at 10 kPa suction (equated with field capacity in sandy soils
θ_{V40}	6.1	Volumetric water content (%) at 40 kPa suction
θ_{V200}	3.2	Volumetric water content (%) at 200 kPa suction
θ_{pwp}	1.8	Volumetric water content (%) at the wilting point (1500 kPa suction)
K_s_SV	804.1	Saturated hydraulic conductivity (sub-vertical)
K_S_LAT	859.7	Saturated hydraulic conductivity (lateral)
θ_s	0.3401	Water content at quasi-saturation
θ_r	0.0085	Residual water content
α	0.1325	van Genuchten's parameter (m^{-1})
n	1.5373	van Genuchten's parameter
m	0.3495	van Genuchten's parameter

* http://www.landis.org.uk/data/horhydraulics.cfm

C3 HYDRUS representation and solution approach

The HYDRUS program solves Richards' equation for both saturated and unsaturated water flow and Fickian-based advection dispersion equations for heat and solute transport using linear finite element schemes (Šimůnek et al, 2005)*. The program may be used to analyse water and solute movement where the unsaturated soil hydraulic properties, such as the unsaturated hydraulic conductivity, can be described using Brooks and Corey (1964), van Genuchten (1980) and modified van Genuchten type analytical functions with the last form introduced to improve the description of hydraulic properties near saturation (see Section C2). The one-dimensional transport of water and solute can be extended in any direction with the water flow satisfying constant or time-varying head and flux boundaries controlled, for example, by the atmospheric conditions while solute transport supports both constant concentration and concentration flux boundary conditions. Table C2 illustrates the default data held by HYDRUS on the 12 soil types classified by the US Department of Agriculture (US DA) and the experimental support base for the values, as reported by the US EPA (US EPA, 1997).

* The dispersion coefficient for solute transport includes terms that reflect the effects of molecular diffusion and tortuosity.

TABLE C2 Mean values of the van Genuchten soil water retention parameters for the 12 soil types of the US Department of Agriculture (US EPA, 1997)

Soil texture (US DA)	Saturated water content, θ_s	Residual water content, θ_r	van Genuchten parameters			Saturated conductivity, K_s ($m\ d^{-1}$)
			α (m^{-1})	n	m	
Clayey soil*	0.38	0.068	0.8	1.09	0.083	$4.80\ 10^{-2}$
Clay loam	0.41	0.095	1.9	1.31	0.237	$6.24\ 10^{-2}$
Loam	0.43	0.078	3.6	1.56	0.359	$2.50\ 10^{-1}$
Loamy sand	0.41	0.057	12.4	2.28	0.561	3.50
Silt	0.46	0.034	1.6	1.37	0.270	$6.00\ 10^{-2}$
Silt loam	0.45	0.067	2.0	1.41	0.291	$1.08\ 10^{-1}$
Silty clay	0.36	0.070	0.5	1.09	0.083	$4.80\ 10^{-3}$
Silty clay loam	0.43	0.089	1.0	1.23	0.187	$1.68\ 10^{-2}$
Sand	0.43	0.045	14.5	2.68	0.627	7.13
Sandy clay	0.38	0.100	2.7	1.23	0.187	$2.88\ 10^{-2}$
Sandy clay loam	0.39	0.100	5.9	1.48	0.324	$3.14\ 10^{-1}$
Sandy loam	0.41	0.065	7.5	1.89	0.471	1.06

* Clayey soil refers to agricultural soil with less than 60% clay.

C4 Verification and validation of HYDRUS

The user manual for version 3.0 of HYDRUS-1D (Šimůnek et al, 2005) provides evidence of verification and validation of the code through a series of examples. Not all the examples are directly related to the unsaturated zone represented in Figure 2; however, the examples briefly described below are included to demonstrate the robustness of the model.

Example 1 simulated a one-dimensional laboratory infiltration experiment used as a test problem for the UNSAT2 code (Neuman, 1972) and thus provides comparisons of the water flow part of the HYDRUS code with results from the UNSAT2 code. The simulation was carried out for 90 minutes, corresponding to the total time duration of the comparison. The calculated instantaneous and cumulative infiltration rates simulated with HYDRUS agree closely with those obtained using the UNSAT2 code.

Example 2 considered one-dimensional water flow in a field profile of the Hupselse Beck watershed in the Netherlands. The calculations were performed for the period from 1 April to 30 September 1982, a relatively dry year. Simulation results from HYDRUS were compared with those from the SWATRE code of Belmans et al (1983). Calculated values of cumulative transpiration and cumulative bottom leaching were nearly identical for the HYDRUS and SWATRE codes. The mean pressure head of the root zone simulated by HYDRUS was very similar to that simulated by the SWATRE code, as was the level of the groundwater table simulated over time.

Example 3 was used to verify solute transport within HYDRUS by comparing numerical results for a problem with three solutes (NH_4^+, NO_2^- and NO_3^-) involved in a sequential first-order decay reaction against results obtained with an analytical solution during one-dimensional steady-state water flow (van Genuchten, 1985). The analytical solution holds for solute transport in a homogenous, isotropic porous medium during steady-state unidirectional groundwater flow. Concentration profiles for the three solutes at times of 50, 100 and 200 hours were the same for the numerical (HYDRUS) and analytical results.

Example 4 considered one-dimensional transport through Abist loam of a solute undergoing non-linear cation adsorption. The breakthrough curve for magnesium produced using version 6.0 of the HYDRUS software was compared with version 5.0 of the code, numerical solutions obtained with the MONOC code (Selim et al, 1987) and experimental data. The HYDRUS 6.0 and MONOC results were very close, showing close correspondence with the HYDRUS 5.0 results (within around 10–15%), and a reasonable prediction of the experimental results (the difference was between 5 and 25%). Breakthrough curves for calcium from HYDRUS and MONOC were also in good agreement with measured data (differences were about 10%).

Example 5 considered the movement of H_3BO_4 through clay loam. HYDRUS numerical results for non-equilibrium adsorption were compared with experimental data and previous numerical predictions assuming physical non-equilibrium and non-linear adsorption (van Genuchten, 1981), with good agreement between the three sets of results (differences were between 5 and 25%).

Example 6 (inverse analysis of outflow experiment) recorded cumulative outflow with time from a core sample. Three hydraulic parameters were estimated by numerical inversion of the data and from this calculation the optimised HYDRUS results for cumulative outflow against time gave a very close match with measured results. There was very good agreement between predicted and measured values of retention and diffusivity.

Example 7 dealt with an outflow experiment in which the pressure head in the soil sample was measured along with the cumulative outflow while the pneumatic pressure was increased in several small steps. Inverse analysis was used again to produce numerical results. Excellent agreement was obtained between measured and optimised cumulative outflows and pressure heads.

Example 8 involved an experiment in which evaporation from a core sample was measured over time. The laboratory experiment was analysed using a revised version of Wind’s evaporation method (Wendroth et al,1993) and soil hydraulic parameters were obtained using the RETC code (van Genuchten et al, 1991). A close match was obtained between analysed laboratory data and results from parameter optimisation for water retention and hydraulic conductivity.

In addition, to ensure that the software to be used for the LMS was working correctly the output from two of the test cases supplied with the software were compared with the outputs given in the HYDRUS user manual (Šimůnek et al, 2005). Inspection of the results showed matches for the relevant outputs (soil water retention and hydraulic conductivity for one test case, and for the unsaturated hydraulic properties and pressure head at the soil surface in the other case).

C5 Use of HYDRUS for disposal to landfill

The previous section illustrated that the HYDRUS model has performed well when subject to validation and verification trials. However, HYDRUS is not designed for the modelling of waste migration from disposal sites over hundreds or thousands of years. One of the principal requirements of HYDRUS is information on the rainfall on a daily basis and of the initial matric potential*. For example, Scanlon et al (2002) compared the performance of HYDRUS and other models in an exercise which simulated water balance in warm and cold semi-arid regions to avoid the complexity of modelling vegetative cover and, in particular, evapotranspiration. HYDRUS performed well in this test, which is consistent with the general approach adopted for the LMS where HYDRUS is not used to model vegetated soils. Figure C2 provides examples of the initial matric potentials measured at the two trial sites. Although a waste repository in the UK will not fit these semi-arid profiles the results provide an example of the wide range of matric profiles that may occur†.

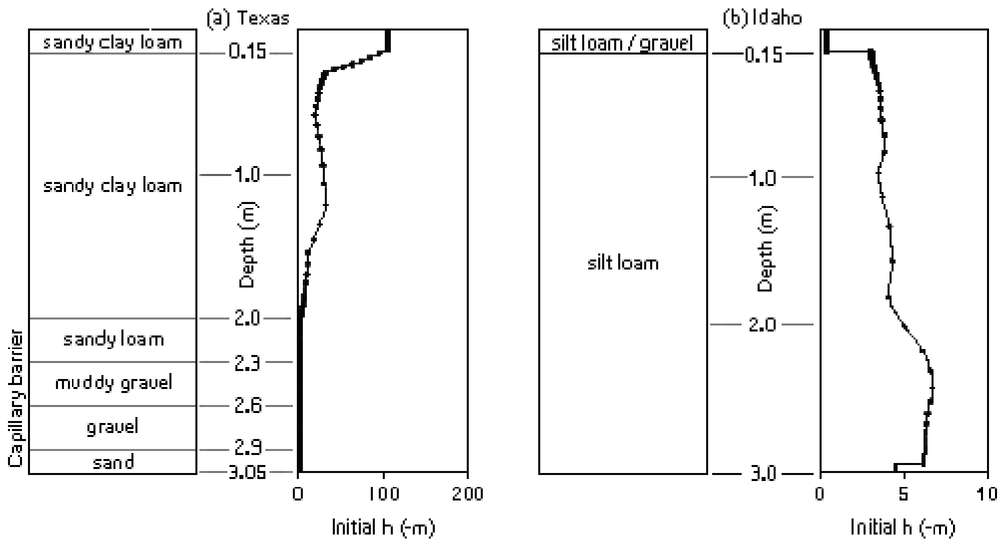

FIGURE C2 Texture profiles and initial matric potentials for the two sites considered in the trial of HYDRUS and other models by Scanlon et al (2002) (copyright 2002 the American Geophysical Union, reproduced by permission of the American Geophysical Union)

The difficulties of not having detailed data of the history of water ingress and movement at a site is specifically discussed by Chen et al (2002) who state that despite the above difficulties, initial flow distributions must be specified. A common approach is to assume a constant, steady flow through the domain. By removing the effect of a drying and wetting cycle hysteretic effects are eliminated, as well as time-varying infiltration rates at the soil surface. Miyazaki et al (1993) assert that steady state water flow represents water moving continuously without storage or consumption in the soil. They further state that saturated flows in groundwater and unsaturated flows in the vadose zone, when suction is less than the air entry value and therefore the gas phase is solely composed of entrapped air, can be considered steady flow if the flow boundary conditions do not fluctuate‡. In the field, downward vertical

* The HYDRUS interface accepts information on rainfall on a minute-by-minute or hourly resolution but no coarser than per day.

† Until the cap and liner fail, the unsaturated zone only receives water through lateral ingress from the surrounding area. As a one-dimensional model, this type of flow is not modelled by the LMS.

‡ If the volume of entrapped air is negligible then the soil is saturated.

water flows under ponded water at the soil surface and lateral flows of groundwater are typical steady flows. However, a completely steady flow in unsaturated soil can only be generated in the laboratory where flow boundary conditions can be fixed. Flows of water in unsaturated soils are usually in unsteady states due to changes in the flow boundary conditions eg variable precipitation and evaporation rates, changes in water storage in soil pores, impacts of soil hysteresis and the consumption of soil water by plant roots. This problem is circumvented within the LMS as HYDRUS is applied to the stage following leaching of the waste from the packaging and its subsequent passage through the site liner into the soil below. Thus, for example the liner may buffer the flow to smooth out the effects of rainfall variation. However, to use HYDRUS as part of the LMS requires either an assumption for the initial matric potential or the calculation of the matric potential assuming known rates of ingress. In the LMS the default assumption in lieu of more specific information is to assume a constant value with depth (Chen et al, 2007). As discussed in Section 7, the particular value chosen can have a significant effect on any results produced.

From the above discussion, HYDRUS can be used in two ways to support LMS calculations. Primarily, conventional LMS calculations of the solute flux can be carried out for a known or assumed description of the matric potential for a particular soil profile. Additionally, a preliminary calculation using the assumed water ingress into the soil can be used by HYDRUS to calculate iteratively the equilibrium matric potential for a given soil profile. The latter option can be generalised to accommodate time varying rates of ingress. The known short-term seasonal variation in soil conditions and rainfall would be too detailed, in most cases, for the broad perspective and timescales of interest to the LMS. Such a generalisation would therefore only be relevant if modelling the effects of changes in the average rainfall in a region over an extended period due, for example, to the effect of global warming or if looking at the likelihood and consequences of bathtubbing events when a waste site floods and contamination is spread over the surrounding land.

Assuming that explicit experimental information is lacking, the primary modelling of solute transport through the unsaturated zone by the LMS can be considered in three ways. The first option is to adopt the simpler of two assumed descriptions of the matric potential, ie a constant negative matric potential that applies at all depths below the waste liner but above the aquifer. At the aquifer, the carrying medium is saturated and transport calculations are taken over by the TROUGH model as discussed in Section 5. This approach neglects any capillary rise from the aquifer that affects the degree of saturation in the soil close to the aquifer and leaves open the appropriate choice of matric head at the top of the unsaturated zone immediately below the landfill liner. Previous calculations using the components of the LMS separately have used a uniform pressure head with a matric potential of –1 m (Chen et al, 2007). The second option is to assume that the matric potential varies uniformly with depth so that on reaching the aquifer the soil is saturated. The assumed linear variation of the pressure head with depth from zero pressure at the aquifer to the liner is a less severe environment for the migration of solute, although the specification of the matric head remains to be settled and the boundary conditions introduce other complexities (see Figure 4 and Figure C3). The third option is to consider some approximate modelling of the water flow in the unsaturated zone, which translates the problem from an unknown matric head to the requirement to know or assume particular details of soil structure below the liner. This approach would also allow the waste liner to be represented as a lens material supporting a saturated zone above the unsaturated soil below. This latter option, discussed in Section 8.1, would allow the soil saturation to be consistent with the amount of ingress into the site and thus enable quantitative results to be produced. An additional advantage of the more comprehensive approach would be the direct link to bathtubbing events following particular rainfall conditions that would then be possible.

The LMS assumes that the hydraulic properties in the unsaturated zone can be represented by the van Genuchten equation relating water content to matric head (van Genuchten, 1980):

$$h_m = \frac{1}{\alpha}\left(\Theta^{-\frac{1}{m}} - 1\right)^{\frac{1}{n}} \tag{C1}$$

where Θ is the dimensionless effective saturation of the soil, and α (m^{-1}), n and m are fitting parameters. Parameters n and m are linked by the equation:

$$m = 1 - \frac{1}{n} \tag{C2}$$

The effective saturation of the soil, Θ, is given by:

$$\Theta = \frac{\theta - \theta_r}{\theta_s - \theta_r} \tag{C3}$$

where θ_s is the saturated water content and θ_r is the residual water content.

Applying the default LMS parameterisation to the above equation gives the retention curve shown in Figure C3 and labelled LMS default. Figure C3 also shows example curves derived from the data of Table C2.

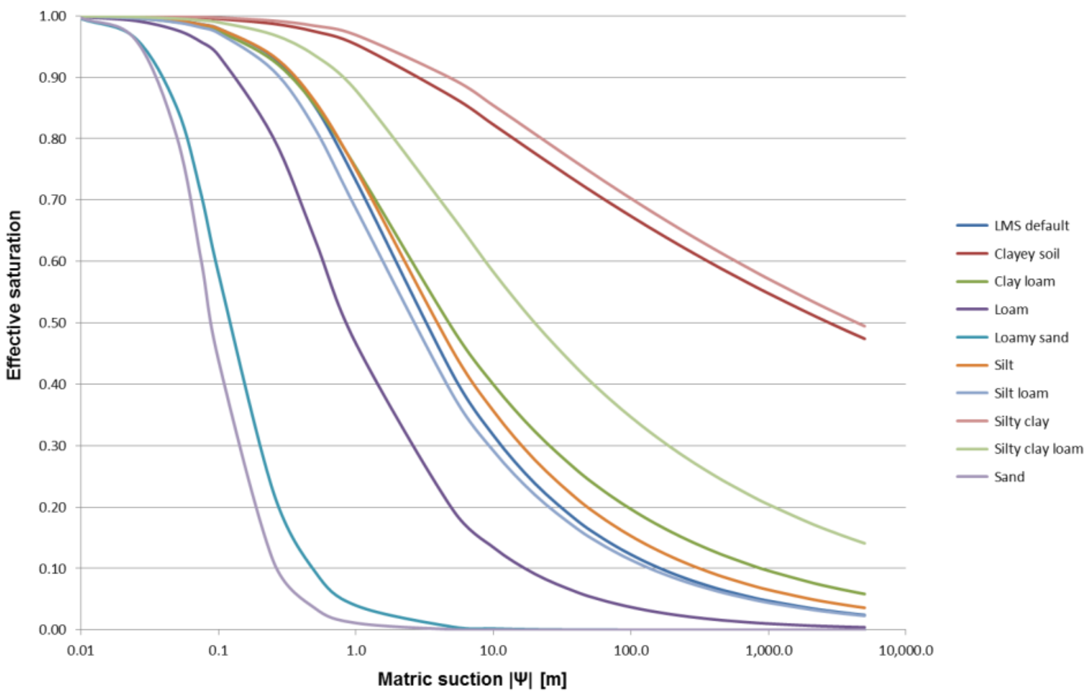

FIGURE C3 Effective saturation as a function of pressure head, shown for the default LMS van Genuchten parameter values and those of a selection of standard soils from Table C2

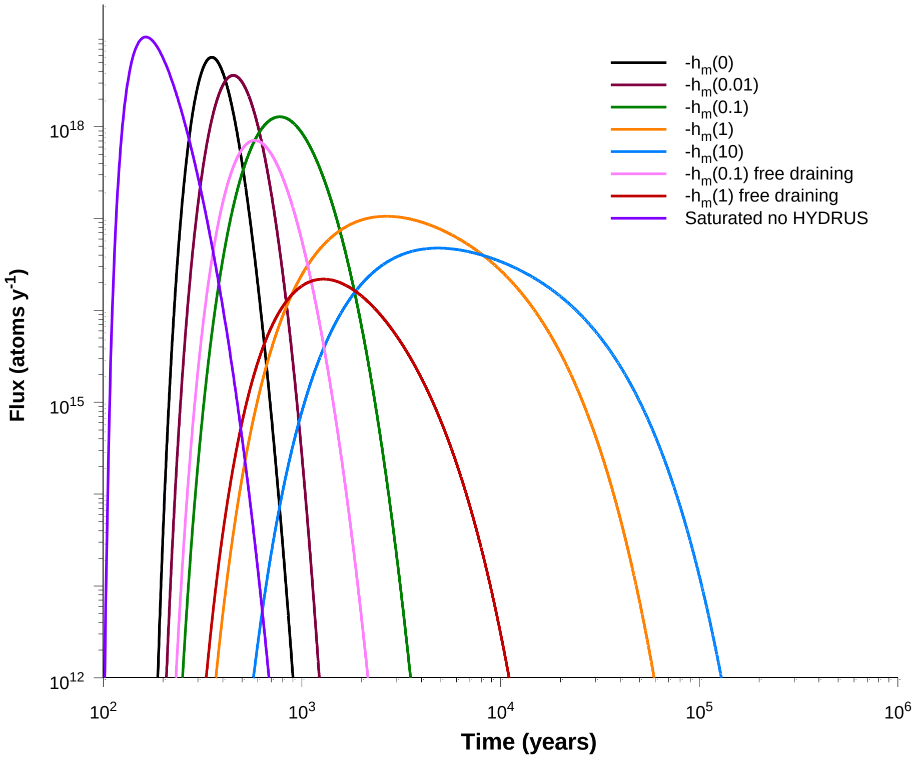

FIGURE C4 Variation in timing and magnitude of the predicted ^{129}I flux released from a waste site matching the Sniffer defaults for a variety of initial matric head suctions and lower boundary conditions. The matric head h_m (m) is either constant with depth or increases uniformly with increasing depth until matching the zero matric head of the aquifer at the depth of the aquifer, as indicated by the free draining label

The variation in pressure head with depth translates into a variation in the water content and hydraulic conductivity. Figure C4 shows the effect on the final flux of ^{129}I estimated by the LMS to leave the aquifer when emulating the Sniffer scenario discussed in Section 7.1 under conditions of either constant matric pressure or a pressure head that varies linearly between the liner and the aquifer.

Figure C4 displays the expected trend with greater saturation, indicated by a less negative pressure head, resulting in a larger peak flux occurring earlier. A similar, but less dramatic effect occurs if the matric potential between the waste site and the aquifer is assumed to vary linearly from a negative value at the base of the waste liner to a fully saturated zero pressure head at the top of the aquifer as indicated by the free draining label in Figure C4. Linearly varying the matric potential with depth from the initial value to zero lowers the peak flux, when compared to maintaining a constant initial matric potential throughout the unsaturated zone, but advances it in time. This reflects the shorter travel time required because of the increase in water content with depth, while the increase in spatial dispersion with depth results in the lower peak flux. A uniform reduction in the level of saturation slows down the flux allowing temporal dispersion to reduce and broaden the peak. The very long half-life of ^{129}I ($1.57\ 10^7$ y) combined with the radionuclide's high mobility means that radioactive decay plays very little part in diminishing the peak flux. A low saturation environment has a much greater effect on radionuclides that are less mobile and have shorter half-lives. Errors in the estimation of the level of soil saturation could have a very large impact on the predicted flux.

Figure C4 also shows how the flux is estimated to vary if the HYDRUS component of the LMS calculation is replaced by a saturated layer modelled using TROUGH. The difference between this result and the calculation made for a fully saturated system using HYDRUS is a measure of the likely discrepancy between the results with and without water balance in the implementation of HYDRUS within the LMS.

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APPENDIX D Comparison of the TROUGH Model with Analytical Results

The performance of the geosphere model TROUGH, a key component of the landfill modelling system (LMS), was directly assessed by comparing results from TROUGH with the corresponding results calculated using an exact analytical model. In the first instance the three deterministic examples of the PSACOIN level E study, prepared by the PSAC User Group (OECD/NEA, 1989), were compared with the predictions of TROUGH. This simple comparison was then extended by using the analytical model CHAIN (van Genuchten, 1985) to provide a more comprehensive test of the adequacy of TROUGH.

D1 Comparison of TROUGH with the analytical solution of PSACOIN level E

The scenarios of the PSACOIN level E study (OECD/NEA, 1989) simulate deep geological disposal within the limits imposed by the analytical solution of Robinson and Hodgkinson (1987). This simple screening model, which includes the most important aspects of radionuclide migration, contains components representing the source term and geosphere transport for both single radionuclides and, under limited circumstances, radionuclides that are part of a decay chain. The analytical solution assumes that after a delay the primary containment fails and allows the radionuclides to leach from the waste following the ingress of water. The released radionuclides are then transported through a two-layer geosphere by groundwater, with the geological layers defined by their hydrogeological properties (eg path length, flow velocity, sorption and dispersivity). Finally, the radioactivity is released into a simple biosphere consisting of a dilution model of drinking water and doses from the ingestion of drinking water are calculated. Two radionuclides were considered: ^{129}I and ^{237}Np with progeny ^{233}U and ^{229}Th. The parameter values required to represent the three cases in the PSACOIN level E study, including a description of the two layers, called layer A and layer B, are given in Table D1. The flux at the inlet boundary is considered to be a purely advective flux with no diffusive flux and the size of the spatial grid used in TROUGH is set to be half of the dispersive length of the layer.

TROUGH and the analytical model have identical initial fluxes entering the first layer of the geosphere (layer A) for each radionuclide and case considered. However, on traversing the first geological layer the peak flux and the time at which the peak occurs no longer match for any of the cases and radionuclides, although the differences between the results are small. Estimates of peak flux and peak time at the end of the first layer of TROUGH and the exact results of the analytical formulation are shown in Table D2. The comparison shows the original values calculated by TROUGH in the PSACOIN level E study and the values derived using the TROUGH component model of the LMS. The differences between the original and LMS results are predominately the result of changes in the step size used, which allow the peak flux and time to be more accurately determined.

Table D2 illustrates that in all cases, the error in the peak flux calculated by the TROUGH component of the LMS at the end of layer A of the geosphere is less than 1.5% and the error in the timing of the peak flux is less than 2.3%. In addition, there are no marked differences in performance between the three scenarios. Differences between TROUGH results for the original PSACOIN level E intercomparison and analytical results are generally higher but are still considered to be acceptable for the LMS. The maximum errors are 23% and 44%,

TABLE D1 Parameter values used for TROUGH calculations of PSACOIN level E cases (OECD/NEA, 1989)

Parameter			Case 1	Case 2	Case 3
Delay before leaching starts (y)			1 10^{2}	3 10^{2}	1 10^{3}
Release rate (y^{-1})		^{129}I	1 10^{-2}	3 10^{-3}	1 10^{-3}
		^{237}Np	1 10^{-5}	3 10^{-6}	1 10^{-6}
		^{233}U	1 10^{-5}	3 10^{-6}	1 10^{-6}
		^{229}Th	1 10^{-5}	3 10^{-6}	1 10^{-6}
Source term (mol)		^{129}I	1 10^{2}	1 10^{2}	1 10^{2}
		^{237}Np	1 10^{3}	1 10^{3}	1 10^{3}
		^{233}U	1 10^{2}	1 10^{2}	1 10^{2}
		^{229}Th	1 10^{3}	1 10^{3}	1 10^{3}
Groundwater velocity (m y^{-1})		Layer A	1 10^{-1}	5 10^{-2}	3 10^{-2}
		Layer B	1 10^{-1}	3 10^{-2}	1 10^{-2}
Dispersion length (m)		Layer A	1 10^{1}	1 10^{1}	1 10^{1}
		Layer B	5 10^{0}	5 10^{0}	5 10^{0}
Geosphere path length (m)		Layer A	1 10^{2}	2 10^{2}	5 10^{2}
		Layer B	5 10^{1}	1 10^{2}	2 10^{2}
Retardation factor (–)	Layer A	^{129}I	1 10^{0}	3 10^{0}	3 10^{0}
		^{237}Np	3 10^{2}	5 10^{2}	8 10^{2}
		^{233}U	3 10^{1}	5 10^{1}	8 10^{1}
		^{229}Th	3 10^{2}	5 10^{2}	8 10^{2}
	Layer B	^{129}I	1 10^{0}	3 10^{0}	3 10^{0}
		^{237}Np	3 10^{2}	1 10^{3}	8 10^{2}
		^{233}U	3 10^{1}	1 10^{2}	8 10^{1}
		^{229}Th	3 10^{2}	1 10^{3}	8 10^{2}
Receiving stream flow (m^{3} y^{-1})			3 10^{5}	1 10^{6}	3 10^{6}

respectively, which reflect the use of a more refined time step in the LMS calculations. Two other minor factors that may have slightly affected the results are that the LMS version of the pre-processor used by TROUGH calculates the rate of progeny ingrowth more accurately and that the mechanism for handling the terminal boundary condition is slightly different*.

Table D3 shows the predicted peak doses received from drinking water abstracted from the aquifer at the end of layer B of the geosphere and the timing of the doses as estimated by TROUGH and the corresponding values determined by the analytical solution. As might be expected, after allowing for the effect of the additional distance through which radionuclides are transported the error in the doses estimated for the LMS calculations are generally slightly

* The numerical precision of the calculation of ingrowth of progeny was increased to improve the estimates of the initial progeny fluxes. Instead of applying a particular TROUGH boundary condition option an extra-long terminal layer is added with properties that match those of the actual end layer to avoid any anomalous boundary effects in the estimated end layer flux.

TABLE D2 Comparison of peak times and peak fluxes on leaving layer A calculated by TROUGH with analytical results

	Analytical results		TROUGH estimates				Error with analytical result (%)*			
			Peak time (y)		Peak flux (mols y^{-1})		Peak time		Peak flux	
Radionuclide	Peak time (y)	Peak flux (mol y^{-1})	LMS	PSACOIN	LMS	PSACOIN	LMS	PSACOIN	LMS	PSACOIN
Case 1										
^{129}I	$9.55\ 10^{2}$	$1.06\ 10^{-1}$	$9.71\ 10^{2}$	$9.75\ 10^{2}$	$1.06\ 10^{-1}$	$1.00\ 10^{-1}$	–1.62	–2.09	0.30	5.66
^{237}Np	$3.07\ 10^{5}$	$2.52\ 10^{-3}$	$3.06\ 10^{5}$	$3.11\ 10^{5}$	$2.55\ 10^{-3}$	$2.46\ 10^{-3}$	0.26	–1.30	–1.42	2.38
^{233}U	$5.24\ 10^{4}$	$6.95\ 10^{-4}$	$5.16\ 10^{4}$	$7.51\ 10^{4}$	$7.01\ 10^{-4}$	$6.93\ 10^{-4}$	1.50	–43.32	–0.86	0.29
^{229Th}	$6.63\ 10^{4}$	$3.12\ 10^{-6}$	$6.53\ 10^{4}$	$8.42\ 10^{4}$	$3.15\ 10^{-6}$	$3.10\ 10^{-6}$	1.45	–27.00	–0.91	0.64
Case 2										
^{129}I	$1.10\ 10^{4}$	$1.16\ 10^{-2}$	$1.08\ 10^{4}$	$1.10\ 10^{4}$	$1.17\ 10^{-2}$	$1.13\ 10^{-2}$	1.40	0.00	–0.74	2.59
^{237}Np	$1.92\ 10^{6}$	$3.22\ 10^{-4}$	$1.90\ 10^{6}$	$1.99\ 10^{6}$	$3.21\ 10^{-4}$	$2.84\ 10^{-4}$	0.99	–3.65	0.14	11.80
^{233}U	$1.12\ 10^{6}$	$1.48\ 10^{-4}$	$1.11\ 10^{6}$	$1.10\ 10^{6}$	$1.50\ 10^{-4}$	$1.45\ 10^{-4}$	0.99	1.79	–1.44	2.03
^{229}Th	$1.12\ 10^{6}$	$6.86\ 10^{-7}$	$1.10\ 10^{6}$	$1.17\ 10^{6}$	$6.96\ 10^{-7}$	$6.75\ 10^{-7}$	1.88	–4.46	–1.43	1.60
Case 3										
^{129}I	$4.91\ 10^{4}$	$4.14\ 10^{-3}$	$4.87\ 10^{4}$	$4.\ 88\ 10^{4}$	$4.16\ 10^{-3}$	$3.98\ 10^{-3}$	0.87	0.61	–0.44	3.86
^{237}Np	$1.17\ 10^{7}$	$2.53\ 10^{-6}$	$1.14\ 10^{7}$	$1.29\ 10^{7}$	$2.53\ 10^{-6}$	$1.95\ 10^{-6}$	2.26	–10.26	–0.15	22.92
^{233}U	$9.17\ 10^{6}$	$3.14\ 10^{-6}$	$8.97\ 10^{6}$	$9.64\ 10^{6}$	$3.18\ 10^{-6}$	$3.00\ 10^{-6}$	2.19	–5.13	–1.24	4.46
^{229}Th	$9.17\ 10^{6}$	$1.46\ 10^{-8}$	$8.98\ 10^{6}$	$9.64\ 10^{6}$	$1.48\ 10^{-8}$	$1.39\ 10^{-8}$	2.08	–5.13	–1.25	4.79

* Error = (Analytical result – TROUGH result) / Analytical result.

TABLE D3 Comparison of peak times and peak doses from drinking water abstracted from the aquifer at the end of layer B calculated by TROUGH with analytical results

Radionuclide	Analytical results: Peak time (y)	Analytical results: Peak dose (Sv y^{-1})	TROUGH estimates: Peak time (y)		TROUGH estimates: Peak dose (Sv y^{-1})		Error with analytical result (%)*: Peak time		Error with analytical result (%)*: Peak dose	
			LMS	PSACOIN	LMS	PSACOIN	LMS	PSACOIN	LMS	PSACOIN
Case 1										
^{129}I	$1.47\ 10^{3}$	$1.22\ 10^{-5}$	$1.48\ 10^{3}$	$1.45\ 10^{3}$	$1.22\ 10^{-5}$	$1.18\ 10^{-5}$	–0.61	1.36	0.02	3.28
^{237}Np	$4.62\ 10^{5}$	$3.54\ 10^{-5}$	$4.58\ 10^{5}$	$4.35\ 10^{5}$	$3.59\ 10^{-5}$	$3.53\ 10^{-5}$	0.78	5.84	–1.60	0.28
^{233}U	$6.95\ 10^{4}$	$9.21\ 10^{-6}$	$6.84\ 10^{4}$	7.5110^{4}	$9.28\ 10^{-6}$	$8.82\ 10^{-6}$	1.58	–8.06	–0.81	4.23
^{229}Th	$8.33\ 10^{4}$	$1.27\ 10^{-5}$	$8.14\ 10^{4}$	$8.42\ 10^{4}$	$1.28\ 10^{-5}$	$1.26\ 10^{-5}$	2.31	–1.08	–0.81	0.79
Case 2										
^{129}I	$2.10\ 10^{4}$	$3.49\ 10^{-7}$	$2.07\ 10^{4}$	$2.05\ 10^{4}$	$3.48\ 10^{-7}$	$3.46\ 10^{-7}$	1.42	2.38	0.05	0.86
^{237}Np	$4.86\ 10^{6}$	$3.22\ 10^{-7}$	$4.78\ 10^{6}$	$4.75\ 10^{6}$	$3.20\ 10^{-7}$	$3.16\ 10^{-7}$	1.61	2.26	0.47	1.86
^{233}U	$3.43\ 10^{6}$	$2.07\ 10^{-7}$	$3.35\ 10^{6}$	$3.30\ 10^{6}$	$2.10\ 10^{-7}$	$2.05\ 10^{-7}$	2.44	3.79	–1.43	0.97
^{229}Th	$3.43\ 10^{6}$	$2.94\ 10^{-7}$	$3.36\ 10^{6}$	$3.30\ 10^{6}$	$2.98\ 10^{-7}$	$2.90\ 10^{-7}$	2.15	3.79	–1.41	1.36
Case 3										
^{129}I	$1.08\ 10^{5}$	$3.23\ 10^{-8}$	$1.07\ 10^{5}$	$1.06\ 10^{5}$	$3.34\ 10^{-8}$	$3.28\ 10^{-8}$	0.74	1.85	–3.26	–1.55
^{237}Np	$2.45\ 10^{7}$	$2.59\ 10^{-11}$	$2.41\ 10^{7}$	$2.45\ 10^{7}$	$2.60\ 10^{-11}$	$2.39\ 10^{-11}$	1.81	0.00	–0.44	7.72
^{233}U	$2.12\ 10^{7}$	$3.60\ 10^{-11}$	$2.07\ 10^{7}$	$2.07\ 10^{7}$	$3.64\ 10^{-11}$	$3.54\ 10^{-11}$	2.31	2.36	–1.30	1.67
^{229}Th	$2.12\ 10^{7}$	$5.10\ 10^{-11}$	$2.07\ 10^{7}$	$2.09\ 10^{7}$	$5.16\ 10^{-11}$	$5.02\ 10^{-11}$	2.31	1.42	–1.32	1.57

* Error = (Analytical result – TROUGH result) / Analytical result.

greater than the corresponding flux error at the end of layer A, although differences are marginal. The dose contribution calculated for each radionuclide at the end of layer B is a direct proxy for the flux at the interception point and the differences between the original PSACOIN level E study and new LMS results are likely to be predominately due to changes in the step size used in the TROUGH calculations of the flux.

D2 Comparison of TROUGH with the model CHAIN

An analytical solution for a single layer system supporting a decay chain of up to four radionuclides has been published by van Genuchten (1985). A software program, called CHAIN, produced by van Genuchten evaluates the solution for various parameter and radionuclide combinations and allows a detail comparison to be made with results produced by TROUGH.

Figure D1 summarises the results of a test carried out using the case 1 scenario of the PSACOIN level E exercise for ^{129}I. It shows that there is a close match between the results produced by CHAIN and TROUGH. A test was also conducted to compare the sequential use of TROUGH with the use of TROUGH in two-layer mode under conditions when little difference is expected between the sequential and two-layer approaches. Figure D1 illustrates, for the particular boundary conditions chosen, the excellent agreement between TROUGH run separately as two consecutive layers with the output of the first (layer A) supplying the second (layer B) and the TROUGH results from a single two-layer calculation. The results for layer A are also in good agreement with the results from the analytical model CHAIN. Table D3 shows that the result of the analytical model CHAIN agree with those from layer B of TROUGH.

Fluxes calculated using TROUGH with a single layer geosphere for ^{239}Pu and three radionuclides in its decay chain (^{235}U, ^{231}Pa and ^{227}Ac) were also compared with those calculated by the CHAIN model for the same general PSACOIN scenario. The results, shown in Figure D2, illustrate that TROUGH can successfully reproduce the flux of the analytical model over the majority of the temporal extent of the breakthrough curve for each of the four radionuclides considered in the ^{239}Pu chain, although TROUGH allows a small amount of flux to traverse the barrier more quickly than predicted by the analytical result.

The outcome of the intercomparison exercise with the model CHAIN demonstrates that TROUGH can produce results that are in very good agreement with independent analytical formulations.

D3 References

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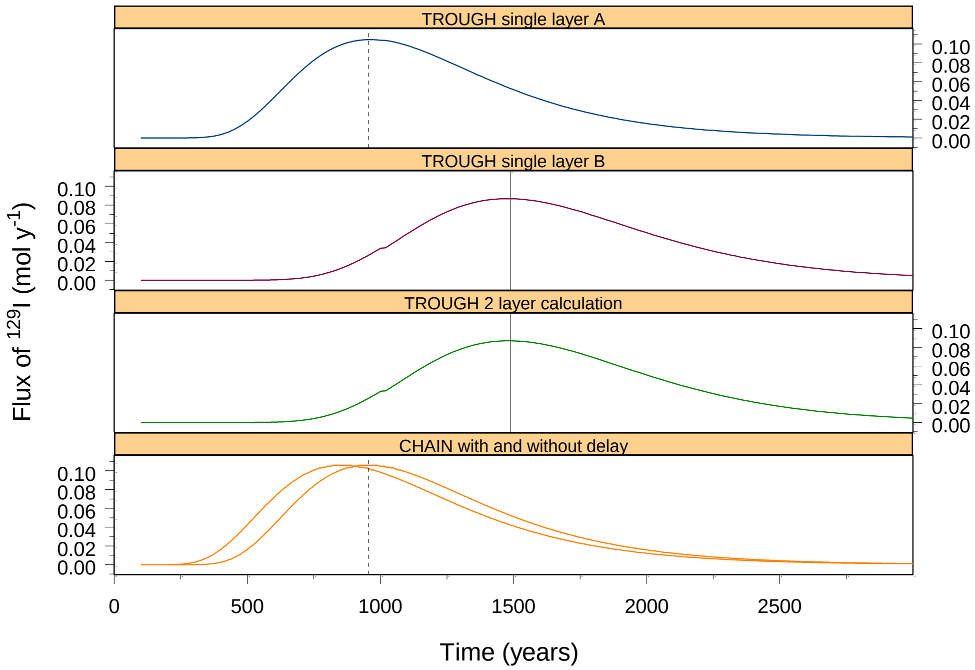

FIGURE D1 Comparison of fluxes of ^{129}I calculated by TROUGH for case 1 of the PSACOIN study with the results of the analytical model CHAIN

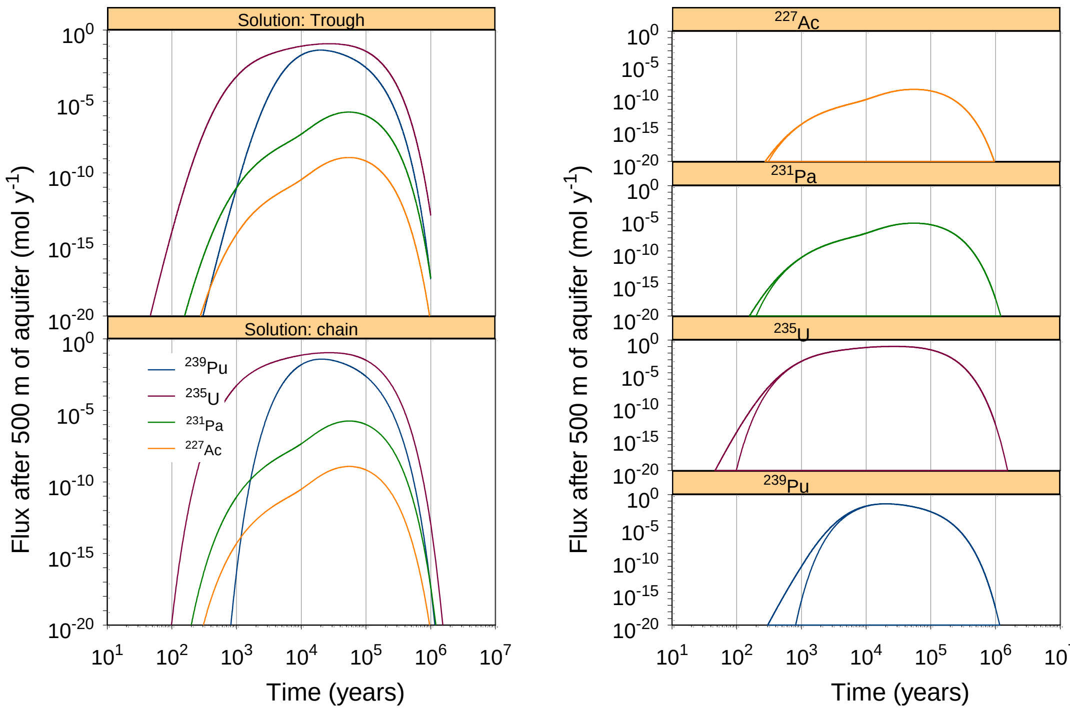

Figure D2 Comparison of the flux of ^{239}Pu and three radionuclides in its decay chain (^{235}U, ^{231}Pa and ^{227}Ac) calculated by TROUGH with a single layer geosphere for case 1 of the PSACOIN study with the results of the analytical model CHAIN

APPENDIX E WELL Model

The landfill modelling system (LMS) includes a simple model to calculate the peak annual dose from drinking water abstracted from a well using a variant of a similar BIOS calculation developed to assess the dose from drinking river water (see Section F2). This dose is proportional to the activity concentration in the water, assumed uniform across the aquifer, at a particular downstream location at a time when it leads to the highest annual dose. The peak committed effective dose rate from drinking filtered well water, D_{water} (Sv y^{-1}), is given by:

$$D_{water} = C_{water} R_{fil} I_{water} DC_{ing} \qquad (E1)$$

where C_{water} is the peak activity concentration in aquifer water (Bq m^{-3}) averaged over a year, I_{water} is the ingestion rate of water (m^3 y^{-1}) (Smith and Jones, 2003), DC_{Ing} is the ingestion dose coefficient (Sv Bq^{-1}) (ICRP, 1996) and by extension of the approach used in BIOS for river modelling (see Section F2) R_{fil} is the fraction in filtered well water given by:

$$R_{fil} = \frac{1}{(1 + K_d SSL)} \qquad (E2)$$

where SSL is the suspended sediment load in well water (10^{-2} kg m^{-3}) and K_d is the sediment partition coefficient (m^3 kg^{-1}). C_{water} is given by:

$$C_{water} = \frac{F_{TROUGH} T_{1/2} W_{landfill} L_{landfill}}{A_{aquifer} W_{aquifer} H_{aquifer} v \theta} \qquad (E3)$$

where F_{TROUGH} is the peak radionuclide flux from the aquifer into a well over a period of a year (atoms y^{-1}), $T_{1/2}$ is the radioactive half-life (y^{-1}), $W_{landfill}$ (m) and $L_{landfill}$ (m) are the width and the length of the landfill, respectively. $A_{aquifer}$ is the area of the aquifer (assumed to be 1 m^2), and $W_{aquifer}$ (m) and $H_{aquifer}$ (m) are the effective width and the thickness of the aquifer, respectively, while v is the flow rate of the pore water in the aquifer (m y^{-1}) and θ is the dimensionless effective porosity of the aquifer.

The mixing zone of the leachate in the aquifer, within a 250 m travel distance of the source, is limited to the top part of the aquifer; a transverse dispersivity of 1% of the travel length is assumed, giving a mixing zone of around 2.5 m (Ingebritsen et al, 2006). However, when the groundwater is abstracted, it is assumed that the radioactivity in the water abstracted at the well is mixed with water abstracted over the entire thickness of the aquifer. This has the effect of diluting the activity by the volumetric flow over the effective width of the aquifer.

E1 References

ICRP (1996). Age Dependent Doses to Members of the Public from Intakes of Radionuclides: Part 5 Compilation of Ingestion and Inhalation Dose Coefficients, ICRP Publication 72. Ann ICRP, **26**(1).

Ingebritsen SE Sanford WE and Neuzil CE (2006). Groundwater in Geologic Processes, 2nd Edition. Cambridge University Press.

Smith KR and Jones AL (2003). Generalised Habit Data for Radiological Assessments. Chilton, NRPB-W41.

APPENDIX F Comparison of LMS with an Unpublished Assessment

To support the verification of the landfill modelling system (LMS) a comparison was made with selected results previously calculated in an unpublished assessment of the radiological impact of disposal to landfill of small quantities of solid radioactive waste (Cabianca et al, to be published). The unpublished assessment used an alternative geosphere model GEOS (Hill, 1989) instead of TROUGH and version 4A of the BIOS model, which is an earlier but essentially equivalent version of the BIOS_4B model implemented in the LMS (see Section F2). The unpublished assessment considered ranges of values for the release coefficient and other key variables in an uncertainty analysis as well as using best estimate parameter values. However, only some of the best estimate results from the previous unpublished assessment are compared with the corresponding LMS predictions in this appendix.

F1 Comparison of the GEOS model with TROUGH

The GEOS model (Hill, 1989)*, developed by the then National Radiological Protection Board†, is similar to TROUGH in its representation of migration through a one-dimensional geosphere with multiple layers. The model predicts the transport of radionuclides with pore water in rocks and includes the processes of advection, dispersion, radioactive decay and absorption on to rocks. The model assumes that radionuclides are released into the saturated zone or aquifer at a fixed rate that is dependent on an element-specific release coefficient and the quantity of water flowing through the landfill.

The intercomparisons are based on the generic waste site representative of a site for hazardous waste described, in the unpublished assessment of the radiological impact of disposal to landfill of small quantities of solid radioactive waste, as type C. Modelling of the unsaturated zone was omitted. The site has the general structure shown in Figure 2 with the parameters characterising the cap barriers and waste, including element-dependent parameters, given in Tables F1 and F2.

Table F2 provides the distribution coefficient values used by the unpublished assessment for deterministic calculations. The K_d values in Table F2 can be assumed to be the same as the best estimate values of a probability distribution, if the deterministic value is greater than zero. Deterministic values represent the most likely values and are generally the distribution-weighted mean of the appropriate ranges. In the unpublished assessment, if the deterministic K_d value was zero (ie if it the radionuclide was not sorbed on to sediments) the probability distribution used in the uncertainty analysis was assumed to be a beta distribution with a range between zero and ten‡.

* This GEOS model should not be confused with the model of the same name developed by Ferry (1996).

† In 2005 the NRPB was incorporated into the Health Protection Agency (HPA). On 1 April 2013 the HPA was abolished and its staff and functions transferred to Public Health England.

‡ No information is given in the unpublished assessment on the value of the two parameters used to specify the particular form of the beta distribution used, which can vary in shape from forms similar to right and left skewed lognormals to straight lines. However, it may be assumed that the form selected would confine the extent of significant probability to a small region near the origin with a residual asymptotic tail.

TABLE F1 Characteristics of type C (hazardous) landfill site used in the intercomparison between GEOS and TROUGH

Parameter	Value
Volume (m^3)	2 10^6
Area (ha)	2 10^1
Average depth (m)	1 10^1
Waste density (t m^{-3})	7.5 10^{-1}
Total activity disposed (Bq)	1 10^{10}
Lifetime (y)	1.5 10^1
Rain ingress (m y^{-1})	3 10^{-1}
Volumetric flow rate of the aquifer (m^3 y^{-1})	1 10^6
Layer 1 Clayey subsoil (m)	5 10^0
Layer 2 Sandy aquifer (m)	5 10^2

TABLE F2 Release, distribution and retardation coefficients in clay and a sand aquifer used in the intercomparison between GEOS and TROUGH

	Distribution coefficient, K_d (m^3 t^{-1})		Retardation coefficient*		
Element	Clay	Sand aquifer	Clay	Sand aquifer	Release coefficient
C	0	0	1 10^0	1 10^0	9 10^{-2}
Cl	0	0	1 10^0	1 10^0	3 10^{-1}
Pb	6 10^3	2 10^2	4 10^4	1 10^3	2 10^{-3}
Ra	7 10^1	5 10^2	5 10^2	3 10^3	2 10^{-3}
Ac	3 10^3	6 10^2	2 10^4	3 10^3	2 10^{-3}
Th	1 10^4	2 10^3	7 10^4	1 10^4	4 10^{-4}
Pa	6 10^2	5 10^2	4 10^3	3 10^3	3 10^{-3}
U	4 10^2	5 10^1	2 10^3	3 10^2	1 10^{-3}
Pu	4 10^3	6 10^2	3 10^4	3 10^3	3 10^{-4}
Am	3 10^3	7 10^2	2 10^4	4 10^3	3 10^{-3}

* The retardation coefficient was calculated assuming a bulk density of 2.0 t m^{-3} and a porosity of 0.3 in clay and 0.35 in sand.

The unpublished assessment of the radiological impact of disposal to landfill of small quantities of solid radioactive waste does not provide best estimate values derived from a probability distribution for the K_d values assumed to be zero in Table F2. Calculations by the LMS using the parameter values of Table F2 were therefore unable to reproduce accurately the best estimate results of the unpublished assessment as the K_d values used in the GEOS calculations were not reported if the corresponding deterministic value in Table F2 was zero.

F1.1 Comparison of doses from ingestion of well water

The use of well water from an aquifer close to a landfill is likely to be a significant exposure pathway. Although the well may not directly disrupt the waste, it is likely to shorten the migration path for radionuclides in groundwater, potentially leading to higher activity concentrations in drinking water and hence higher doses. The unpublished assessment assumed that individuals obtain all their drinking water from the well and that the water is of sufficient quality not to need filtering. Although the LMS assumes by default that well water is filtered, this assumption was not used in the comparison. The total activity released to the aquifer each year, $A_{aquifer}$, was calculated for a number of radionuclides typically disposed of to landfill using the TROUGH model and the resultant ingestion doses were compared with the calculations carried out using GEOS. The comparison was based on the estimated peak dose, calculated using a combined activity released to the aquifer of all the progenies in the decay chain, suitably weighted to take account of the contribution to the dose from ingestion of the progeny.

The doses from ingestion of drinking water were calculated using the equation:

$$D_{water} = \frac{R_{aquifer}\, I_{water}}{V_{aquifer}} \qquad \text{(F1)}$$

where $R_{aquifer}$ is the radiologically weighted release (Sv y^{-1}), I_{water} is the quantity of water ingested in a year (0.6 m^3 y^{-1} for adults) (Smith and Jones, 2003) and $V_{aquifer}$ is the volumetric flow rate in the aquifer (m^3 y^{-1}).

The radiologically weighted release $R_{aquifer}$ is given by:

$$R_{aquifer} = \sum_i DC_{ing,i}\, A_{aquifer,i} \qquad \text{(F2)}$$

where $A_{aquifer}$ is the activity released to the aquifer (Bq y^{-1}) of the ith radionuclide in the decay chain and $DC_{ing,i}$ is the dose coefficient of the same radionuclide (Sv Bq^{-1}) (ICRP, 2001).

Doses from ingestion of drinking water from a well provided in the report of the unpublished assessment cannot be compared directly with those calculated by the LMS as they are based on the estimated maximum flux of a radionuclide into the underlying aquifer, while the appropriate deterministic parameters to reproduce the calculation are not reported. However, by applying the same methodology the best estimate activity concentrations from the GEOS calculations can be used to generate a set of doses that can be compared to those produced by the LMS using the deterministic parameters provided, as shown in Table F3. The lower peak doses at longer times for the GEOS estimates for ^{14}C and ^{36}Cl in comparison to those of the LMS are a consequence of using non-zero distribution coefficient values in the best estimate calculation (see Table F2). These particular calculations are therefore not directly comparable, although the lower dose predicted by the GEOS estimates is an expected consequence of partial sorption. The remaining calculations are in good agreement with the worst differing by approximately a factor of two.

F2 BIOS model

BIOS is a compartmental model, used to simulate the dispersion of radioactivity in the biosphere. The main compartments represent deep and surface soils, rivers and seas (Martin et al, 1991). BIOS calculates activity concentrations in environmental media and the doses

TABLE F3 Comparison of the deterministic and best estimate doses from ingestion of drinking water calculated by the LMS and GEOS

	GEOS		LMS	
Radionuclide	Peak time (y)	Dose (Sv y^{-1})	Peak time (y)	Dose (Sv y^{-1})
^{14}C	1.40 10^{2}	9.0 10^{-10}	1.22 10^{2}	7.5 10^{-9}
^{36}Cl	1.13 10^{2}	4.6 10^{-9}	9.83 10^{1}	3.1 10^{-8}
^{226}Ra	1.42 10^{4}	1.2 10^{-11}	1.59 10^{4}	1.8 10^{-11}
^{232}Th	2.45 10^{6}	5.2 10^{-9}	2.24 10^{6}	5.5 10^{-9}
^{235}U	2.13 10^{5}	1.4 10^{-8}	1.48 10^{5}	3.2 10^{-8}
^{238}U	4.35 10^{5}	7.1 10^{-9}	2.14 10^{5}	9.6 10^{-9}
^{239}Pu	2.44 10^{5}	4.7 10^{-13}	2.03 10^{5}	7.5 10^{-13}

likely to result following discharges into rivers or deep soil from an aquifer. The soil components represent farmland near to a river or lake that may be contaminated by irrigation or by a direct upwelling of radionuclides into the soil on which animals are raised and crops are grown. In BIOS a coupled set of linear first-order differential equations represent the transfer of radioactivity between various model compartments. Transfer rates represent the various processes described by the model, such as the uptake of radionuclides from soils and grasses and are calculated from available equilibrium data as described in Martin et al (1991) and Smith and Simmonds (2009). Element-dependent equilibrium transfer factors are also used to predict the concentrations of radionuclides in freshwater fish.

Figures F1 to F4 show different components of the BIOS model. Figure F1 shows the terrestrial biosphere model that includes a river and a lake, and the interactions with the associated arable and pasture compartments. The size of the lake, the number of river segments and branches can be specified to transform the generic model to fit a particular assessment. Figure F2 shows the BIOS soil model for both arable and pasture land, while Figure F3 shows a typical plant model for green vegetables including transfer processes representing uptake via irrigation and root uptake from arable soil. Finally, Figure F4 shows the BIOS pasture model linking into the pasture soil model. When appropriate, slight modifications are introduced to these models to account for the fixation of caesium.

F2.1 Comparison of doses calculated by BIOS_4A and BIOS_6B

The BIOS model has evolved over a number of years and a number of different versions have been produced. Each new version has been compared with the previous version and other independent models (see Section 6.1.1). However, to provide additional credibility to the intercomparison between the LMS and calculations using a combination of the GEOS and BIOS_4A models, a direct comparison between BIOS_4A and BIOS_6B is provided in Table F4 for a continuous release of 1 MBq y^{-1}.

As shown in Table F4 the doses calculated by BIOS_4A are generally in very good agreement with those calculated for ^{99}Tc and ^{235}U by BIOS_6B the version included in the LMS. This level of agreement between the latest and earlier versions of the BIOS model indicates that, although BIOS_6B is implemented using different solution methods and software, the underlying conceptual models have been consistently interpreted.

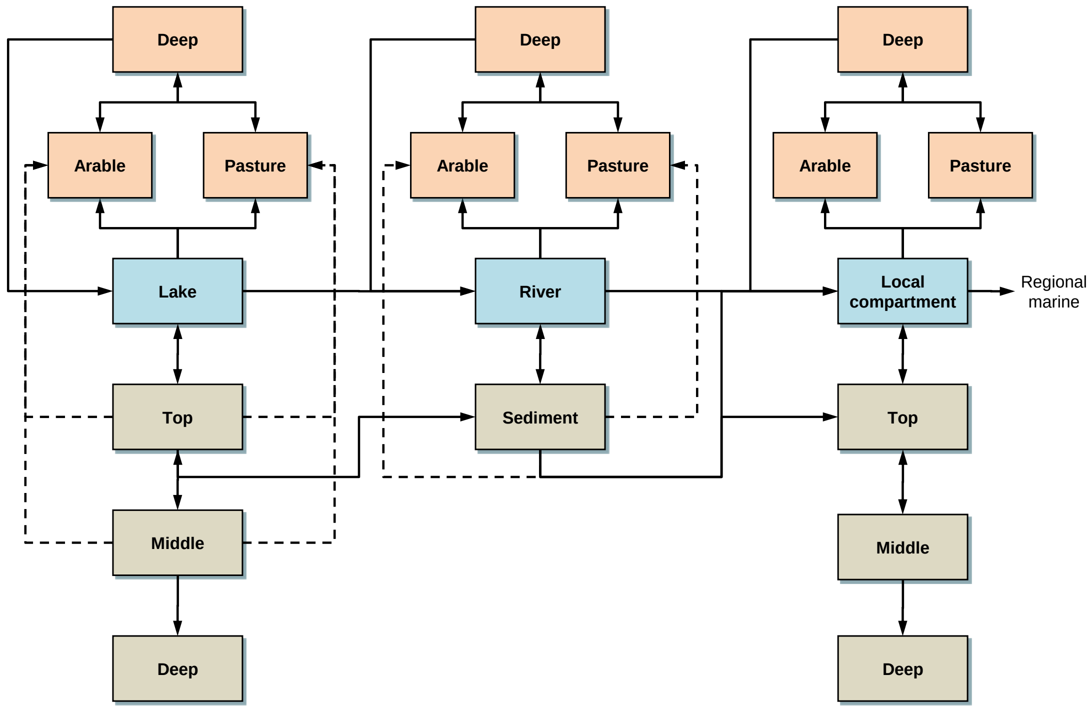

FIGURE F1 Generic terrestrial and aquatic biosphere model, transfers between the compartments are indicated by arrows

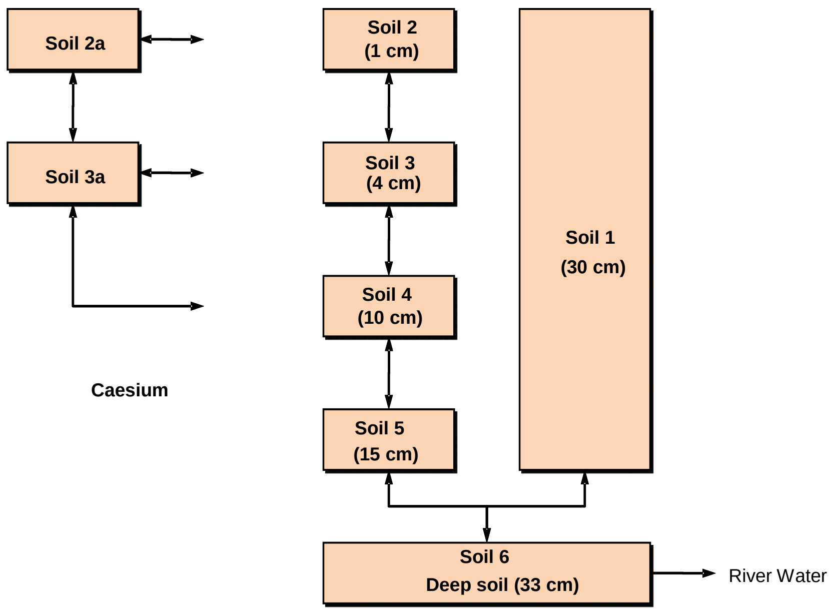

FIGURE F2 Pasture and arable soil model (arable soil single compartment linking to deep soil and caesium recycling optional pasture model extension), transfers between the compartments are indicated by arrows

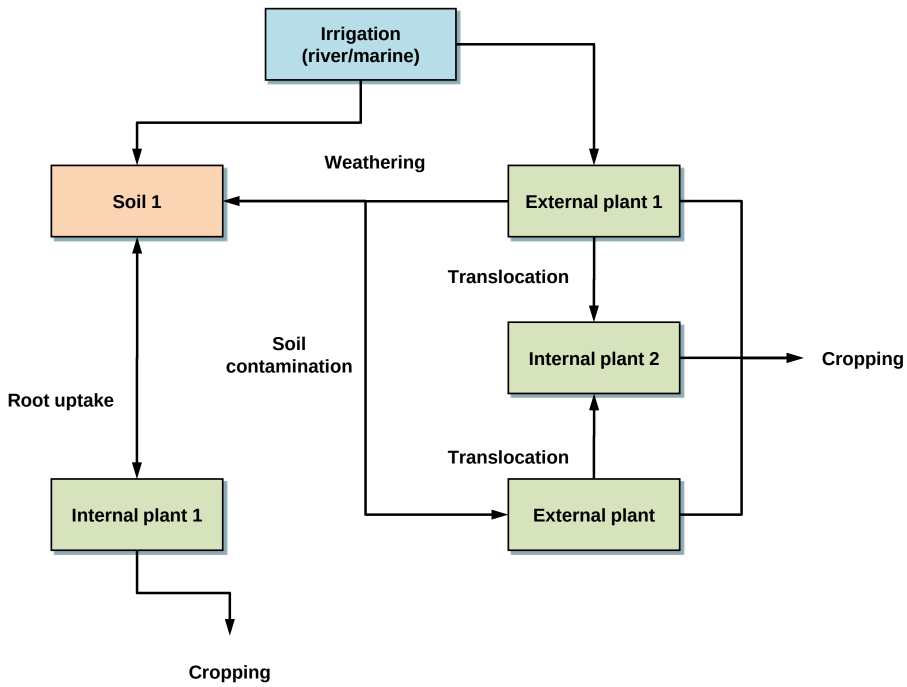

FIGURE F3 Green vegetable model, transfers between the compartments are indicated by arrows

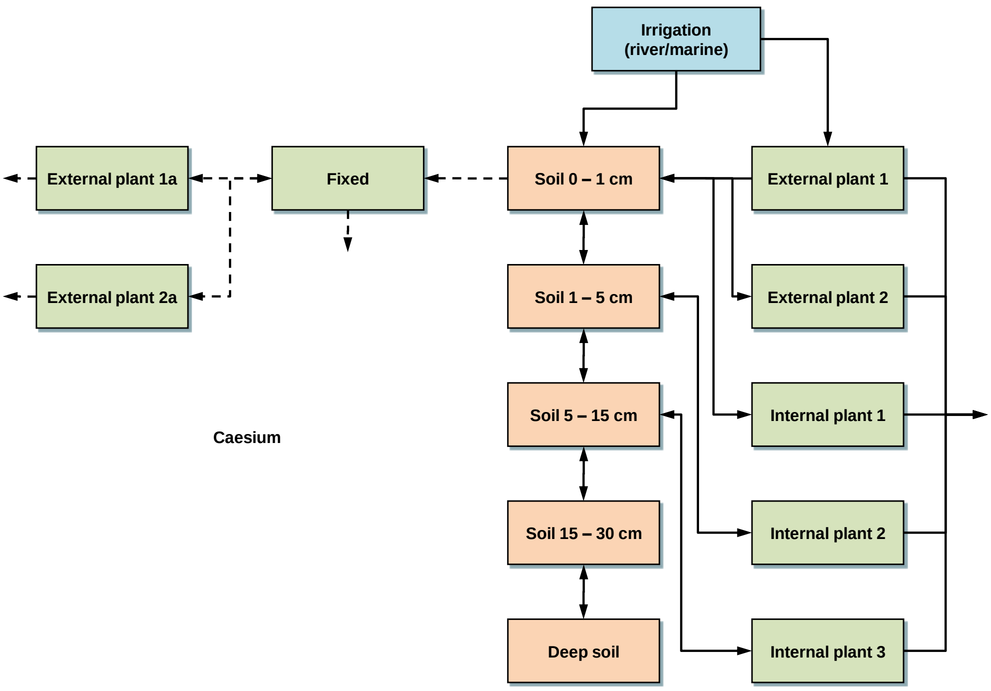

FIGURE F4 Pasture model including additional compartments for caesium, transfers between the compartments are indicated by arrows

TABLE F4 Comparison of individual doses calculated by BIOS_4A and BIOS_6B for a continuous release of 1 MBq y^{-1}

	Dose (Sv y^{-1})			
	^{99}Tc (release period 10^4 years)		^{235}U* (release period 10^5 years)	
Exposure pathway	**BIOS_4A**	**BIOS_6B**	**BIOS_4A**	**BIOS_6B**
Ingestion				
Drinking water	$5.8\ 10^{-13}$	$5.8\ 10^{-13}$	$3.6\ 10^{-11}$	$4.4\ 10^{-11}$
Freshwater fish	$2.9\ 10^{-13}$	$2.9\ 10^{-13}$	$1.2\ 10^{-11}$	$1.5\ 10^{-11}$
Beef	$8.3\ 10^{-14}$	$7.8\ 10^{-14}$	$3.3\ 10^{-11}$	$1.1\ 10^{-10}$
Cow liver	$7.4\ 10^{-14}$	$6.9\ 10^{-14}$	$2.8\ 10^{-11}$	$9.8\ 10^{-11}$
Milk	$5.6\ 10^{-13}$	$5.3\ 10^{-13}$	$2.7\ 10^{-12}$	$6.5\ 10^{-12}$
Mutton	$7.0\ 10^{-14}$	$6.5\ 10^{-14}$	$2.6\ 10^{-11}$	$9.1\ 10^{-11}$
Sheep liver	$8.3\ 10^{-14}$	$7.8\ 10^{-14}$	$1.1\ 10^{-10}$	$4.0\ 10^{-10}$
Chicken	$6.0\ 10^{-14}$	$5.3\ 10^{-14}$	$3.9\ 10^{-12}$	$8.1\ 10^{-12}$
Eggs	$5.0\ 10^{-14}$	$4.4\ 10^{-14}$	$3.9\ 10^{-12}$	$8.6\ 10^{-12}$
Green vegetables	$4.4\ 10^{-12}$	$4.2\ 10^{-12}$	$2.6\ 10^{-10}$	$9.5\ 10^{-10}$
Grain	$9.9\ 10^{-12}$	$9.3\ 10^{-12}$	$5.8\ 10^{-10}$	$2.1\ 10^{-9}$
Root vegetables	$1.2\ 10^{-11}$	$1.1\ 10^{-11}$	$7.0\ 10^{-10}$	$2.5\ 10^{-9}$
Inhalation of resuspended material				
Farmer ploughing	$1.9\ 10^{-16}$	$2.0\ 10^{-16}$	$2.4\ 10^{-10}$	$4.8\ 10^{-10}$
Arable	$1.1\ 10^{-15}$	$1.2\ 10^{-15}$	$1.4\ 10^{-9}$	$2.8\ 10^{-9}$
Pasture	$3.3\ 10^{-18}$	$3.0\ 10^{-18}$	$8.1\ 10^{-10}$	$1.6\ 10^{-9}$
External exposure				
On arable soil	0.0	–	$2.6\ 10^{-10}$	$1.4\ 10^{-9}$
On pasture	0.0	–	$9.0\ 10^{-11}$	$5.5\ 10^{-10}$

* Doses for ^{235}U include contribution from in-growth of progeny ^{231}Pa and ^{227}Ac (see Table A1).

F3 References

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