SimER: An advanced three-dimensional environmental risk assessment code for contaminated land and radioactive waste disposal applications

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ABSTRACT

SimER (Simulations of Environmental Risks) is a powerful performance assessment code developed to undertake assessments of both contaminated land and radioactive waste disposal. The code can undertake both deterministic and probabilistic calculations, and is fully compatible with all available best practice guidance and regulatory requirements.

SimER represents the first time-dependent performance assessment code capable of providing a detailed representation of system evolution that is designed specifically to address issues found across UK nuclear sites. The code adopts flexible input language with build-in unit checking to model the whole system (i.e. near-field, geosphere and biosphere) in a single code thus avoiding the need for any time consuming data transfer and the often laborious interface between the different codes. This greatly speeds up the assessment process and has major quality assurance advantages. SimER thus provides a cost-effective tool for undertaking projects involving risk assessment from contaminated land assessments through to full post-closure safety cases and other work supporting key site end-point decisions.

A Windows version (v1.0) of the code was first released in June 2004. The code has subsequently been subject to further testing and development. In particular, Viewers have been developed to provide users with visual information to assist the development of SimER models, and output can now be produced in a format that can be used by the FieldView software to view the results and produce animation from the SimER calculations. More recently a Linux version of the code has been produced to extend coverage to the commonly used platform bases and offer an improved operating environment for probabilistic assessments.

Results from the verification of the SimER code for a sample of test cases for both contaminated land and waste disposal applications are presented.

INTRODUCTION

SimER (1, 2) is a powerful Performance Assessment (PA) code developed by Nexia Solutions Ltd, part of the BNFL group, to undertake assessments of both contaminated land and near-surface repositories. SimER represents key processes at a level that is consistent with requirements for regulatory submissions. The code represents a major advance in environmental risk assessment modelling that offers a unique range of functionality that has not been previously available in any single safety assessment tool. SimER represents the first time-dependent performance assessment code capable of providing a detailed representation of system evolution that is designed specifically to address issues such as climate and landscape change found across UK nuclear sites.

The rationale behind the structure and capabilities of the SimER code relates to the assertion that to understand the risks from contaminant leakage from a source requires an understanding of the temporal variations in the patterns of contaminant migration in three dimensions arising from changes to the stresses on the system (groundwater recharge/discharge etc.) and changes to the physical geometry of the subsurface and surface environment over time. The interference between different parts of a dynamic system leads to complex interactions that cannot be readily simulated using idealised one-or two-dimensional models. This is an important concern for all natural systems modelling. SimER adopts a modular approach that uses an Executive to control a number of functional model components. The direct representation of the full three dimensional evolving landscape and engineered features offers a more physical approach and enables easier interpretation of the system dynamics than is possible for some other approaches such as network models.

The extensive capabilities (some unique) of SimER makes it possible, for the first time in a single application, to define a fully probabilistic three dimensional physical representation of an evolving landscape and engineered features, compute water and gas flows, model chemical reactions, calculate contaminant transport and evaluate a wide range of impacts. The capability to represent environmental change explicitly is particularly useful for long-term assessments of impacts to humans and the environment. Its main capabilities can be summarised as follows:

- The source-pathway-receptor analysis for contaminants of interest can be assessed in a single code. This avoids the need for the output from one code to be used as the input to another. This greatly speeds up the assessment process and has major quality assurance advantages.

- Topographical details and geological structures can be represented.

- Groundwater flow and contaminant transport are represented using a 3D 'coarse' continuum approach.

- Ability to represent climate changes, evolving landscape and engineered features.

- Model both radioactive and non-radioactive contaminants.

- Flexible and time dependent inventories component.

- Physical and Chemical Evolution model to represent chemistry and engineered structure degradation.

- Multiple run capability to enable both sensitivity studies and probabilistic assessments.

- Checking that all model parameters have associated units, and that all expressions and algorithms used have consistent units. This checking provides a major contribution to the quality assurance of SimER calculations.

- The code uses file-based input and output and enables data libraries to be included in code input.

- Graphical spatial viewers and parameter charter visualisation tools allow model inputs and outputs to be checked visually.

In the following sections the different code components are described. Verification of the code is outlined, and then sample modelled results for contaminated land and near-surface repository applications are presented to demonstrate the capabilities of SimER. As part of an ongoing confidence building process or trialling of the code, some of the more recent testing applied to real site situations are provided.

SIMER CODE

SimER uses an Executive to control the components that comprise the code enabling communication between them. The Executive controls the solvers used by a number of components to advance the solution through time. SimER consists of four types of component, namely:

- the Executive that controls all of the other components;

- the System Evolution components that represent the way the system changes with time;

- Process components that model the various processes that affect the behaviour of contaminants in the environment and potential impacts; and

- Visualisation components that provide the Viewers capability.

A Windows version 1.0 of the code (2) was first released in June 2004. The code has since been subject to further testing, revised with bug fixes, and updated with further enhancements. In version 1.1.1 (1, 3) released in May 2006, Viewers have been developed to provide users with visual information to assist the development of SimER models, and output can now be produced in a format that can be used by the FieldView software (4) to view the results and produce animation from the SimER calculations. The more recent release of the code version 1.1.2 (5) contains enhanced error and warning reporting with the aim of providing more specific details to help the user to identify the cause of errors such as incorrect input syntax more quickly. Version 1.1.2 of the code allows porting to Linux platform (except the Viewers and the graphical front end for the Executive) to extend coverage to the commonly used platform bases and offer an improved operating environment for probabilistic assessments.

SYSTEM EVOLUTION COMPONENTS

External Scenario Description

This component enables the user to describe factors that are external to the system domain being modelled. It includes External Features, Events and Processes, (EFEPs) which can relate to the characteristics and evolution of climate in response to global climate change. Key information that is required includes rainfall, temperature and sea level which can be used throughout the simulation to describe the evolution of the system in response to changing conditions - for example, the type of crops harvested could be dependent on the mean temperature.

In addition to climate information, the user is able to describe various types of event which is defined as a factor that introduces an effectively instantaneous change in some aspect (or several aspects) of the system. The events considered fall into two categories:

- Non-terminal events, which may be naturally-occurring or human-induced. Events of interest may disrupt the system in some way (e.g. an earthquake), or result in some other change considered to be significant to the calculations (e.g. periodic storms).

- Termination events are a special type of disruptive event that result in such substantial disruption to the system that the calculations are terminated. An example of a termination event is glaciation.

Landscape

The Landscape component represents the key features of the system being modelling termed the System Domain, providing a 'satellite view' description. This includes surface features, such as rivers, lakes and land use, and details of the geology in terms of sub-surface strata. The boundaries of these features are specified with a number of vertices.

Topography is defined in terms of elevations above a vertical origin (e.g. the present-day ordnance datum) and allows a three dimensional system to be modelled. A special type of topographical feature is a cliff which was introduced into SimER because a number of UK nuclear sites are situated at coastal locations. SimER can subsequently model a moving cliff that may erode the landscape, resulting in a new topography in the affected area.

Sub-surface structures (strata) are described in a similar manner to the topography. The topographical and subsurface strata data are used to interpolate surfaces for intermediate locations by triangulation from the defined vertices. This provides a three-dimensional representation of the system.

The evolution of the landscape can be described using a series of 'snapshots' of envisaged landscape states at key times during the evolutionary scenario. The Landscape component interpolates the movement of features between these snapshots to provide a continuously evolving landscape. Surface features can also move continuously if the user specifies the location of the points that determine the boundary of the feature to be continuous functions of time. So, for example, the variation in the 'footprint' of a lake as the landscape evolves can be represented either by a series of coordinates for the vertices at specified times, or in terms of algebraic expressions for the locations of these vertices as a function of time.

Engineering

This component is concerned with the engineered parts of the system. These 'man made' regions can provide the source of the contaminants under consideration, although a range of alternative source representations can also be used. A number of different types of engineered feature can be represented: for example for a waste disposal site, drains (effectively one-dimensional), walls (effectively two-dimensional) and vaults (three-dimensional). Properties associated with the engineering features such as degradation of cut off walls and vertical drains, and conceptualised water flows can be allowed to vary in time within the Engineering component.

PROCESS COMPONENTS

Inventories

This component enables the user to specify the initial inventory of contaminants in the engineered part of the system. For a waste disposal facility, the contaminants may be encapsulated and packaged. For applications to

contaminated land, the initial distribution of contaminants in the engineering domain can be estimated from a series of site measurements. For waste disposal sites in particular, the time series behaviour or history of the disposals can be modelled in SimER for various waste streams and waste treatment processes.

System Disaggregation

This component uses information from the Landscape and Engineering components to produce a Process Grid. This grid is then available for use by all of the other process components. The Process Grid consists of a number of prisms (grid cells) that fill the region under consideration. The top and bottom faces of the prisms are triangular and planar (although not necessarily horizontal) and the sides are vertical. Thus, when viewed from above, the grid is seen as a set of triangles.

Water Flow

This component has a mathematical flow solver that enables calculations of groundwater flows in the System Domain to be undertaken using input information on boundary conditions and material properties within the Process Grid. The solver calculates an initial condition that is consistent with the imposed boundary conditions and then steps the solution through time to the defined assessment endpoint. The calculated degree of saturation of the Process Grid cells enables the position of the water table to be inferred. Water flows through engineered features (including drains) may change as they degrade.

The degree of discretisation for a typical Process Grid (up to about one or two thousand cells) means that the calculated water flows will provide a fairly coarse representation of water movement, which is appropriate for a PA-level model. More detailed modelling of the hydrogeology of the system can be undertaken using supporting-level codes such as MODFLOW (6), and information from such calculations can be fed back into the Water Flow modelling in SimER.

Transport

The Transport component is the most complex component. It calculates the evolution of both contaminants and other substances relevant to the chemical evolution of the system (collectively referred to as 'monitorables') within the System Domain and within any extensions to it defined by the user. Extensions in this context can refer to additional spatially based compartments that can be linked to regions in the Process Grid. This enables additional compartments representing local (e.g. surface water features) and more distant (e.g. nearby sea) regions of the Biosphere to interface with a Process Grid representation of the Geosphere.

There are three types of compartment:

- Feature Compartments that inherit the material of a specified feature in the Landscape. Such compartments directly represent the feature in question.

- Adjunct Compartments that follow the position of a feature but do not inherit its properties.

- Free Compartments that are not associated with any specific Landscape feature.

An example of a Feature Compartment might be a lake that is included in the description of the Landscape. Associated with this lake might be bed sediments, and these could be represented as an Adjunct Compartment. The lake might be drained by a river to the sea, and a region of the sea could be represented as a Free Compartment.

Transport has two service components: Physical and Chemical Evolution (PCE) and Gas Flow. The PCE component provides information on biogeochemical reactions that affect contaminant transport properties (for example, sorption). At any given time each Process Grid cell is taken to be in one of a few specified chemical 'regimes' (for example, 'reducing and acidic'). The PCE component also provides information on the generation of bulk gas (for example, from the corrosion of metals or methanogenesis). The Gas Flow component can then calculates the pathways taken by this gas to the surface, and the time taken for the transport involved. Some contaminants can be in gaseous form and the Transport component calculates the transport of these contaminants with the bulk gas.

The Transport component facilitates the representation of a wide range of processes that affect the evolution of monitorable concentrations. Two types of process are considered: built-in and user-defined. Most of the processes involve the transfer of a monitorable from one cell to another (neighbouring) cell, but there are also 'local' processes such as gas generation.

The built-in processes include radioactive decay, water-borne processes (advection, dispersion and diffusion) sorption and solubility limitation. User-defined processes can extend this set of processes in a flexible way, providing prescriptions for how to calculate the rates of transfer across each relevant interface. These rates can be calculated using various defined quantities, including the various concentrations from partitioning, and the interface area. An example of a user-defined process might be bioturbation in the soil above the water table.

Human Activities

The Human Activities component enables the user to specify the way in which humans inhabit, use and affect the system under consideration. In particular, it enables the user to specify the Potentially Exposed Groups (PEGs) and their habits associated with occupancy, inhalation of dust, and ingestion of foodstuffs. Interpolation can take place in relation to the envisaged landscapes such as occupancy of the PEGs as defined for each landscape state.

Impacts

This component calculates the impacts of interest relating to exposure pathways associated with the PEGs and doses associated with these pathways. These impacts are based on the time-dependent calculated concentrations, amounts or fluxes of contaminants in the system.

VISUALISATION COMPONENTS

There are two types of Visualisation components: the Spatial Viewers and the Parameter Charter.

The Spatial Viewers provide two- and three- dimensional views of: the landscape and engineering features, the Process Grid, properties (such as Darcy velocities, water heads) of the groundwater flow system, and time dependent contaminant concentrations from the Transport module. They are useful in confirming that the system has been set up correctly from the input data provided and in part that the groundwater flows have been calibrated appropriately from measured data. Also, that the transport of contaminants is as expected in time from the shape of the plumes shown and profiles of the distributions of the magnitudes of the concentrations within the plumes.

The Parameter Charter enables the user to plot values of parameters as a function of time which can be used to check that input data is being correctly processed such as the desired interpolation between a number of set points. Also key output parameters such as a PEG dose can be plotted as a function of time.

Another useful utility application is the SimER Viewer Launcher that makes it possible to store results from a Viewer and reload them later to replay the results without the need to rerun SimER. Plots of graphs created with the Parameter Charter can also be reloaded without the need to rerun SimER.

CODE TESTING: VERIFICATION AND VALIDATION

Verification and validation needs to be undertaken for any code development. Generally code verification is concerned with ensuring that the code correctly carries out the calculations it is designed to undertake, whilst validation relates to the accuracy or adequacy of the mathematical modelling that can be achieved using the code particularly with respect to model results compared to observed measurements.

The approach to software verification undertaken by Nexia Solutions (7) includes the adoption of a formal modelling protocol and is broadly in line with the approaches described in references (8, 9). Three types of testing have been used for the verification of the SimER code:

- Component testing – These tests check that individual SimER components function according to their specified design.

- Coverage testing – This is source-code level testing to ensure that readily accessible lines of code in a component have been executed and are functioning correctly.

- Integration testing – This ensures that all of the components interact correctly and that the SimER code as a whole functions as designed.

Two example test cases designed to utilize all the SimER component models have been devised for the integrated testing, one test case for contaminated land and the other for a waste disposal facility (3). Although hypothetical,

these test cases were nevertheless designed to be realistic and representative of the types of environmental systems likely to be considered by the nuclear industry.

As part of the confidence building or the trialling of SimER, the code has been used to replicate previous modelling assessments of contaminated land and a shallow waste disposal site at two coastal site locations within the United Kingdom. For the former, SimER has produced for contamination entering the aquifer, favourable comparisons of time dependent radionuclide fluxes at the geosphere-biosphere interface zone with previous model results. SimER has also been able to replicate successfully the temporal behaviour of the radionuclides and magnitudes of the fluxes particularly at peak levels. For this comparison, a conceptualisation of the contaminated land and underlying groundwater flow system and associated geological structures had to be provided in three dimensions for SimER and geared towards the 'cruder' one dimensional pipe system approach as adopted by the previous models.

As it is not possible to report in detail on the results of the replication of previous assessments involving SimER and the models used for these two UK sites, an example application of using SimER to undertake the integrated test case for the hypothetical waste disposal site is presented below as a first sample test case, followed by the application of SimER to simulate a real situation on the remediation of contaminated land at the Y12 site in the US.

SAMPLE TEST CASE 1 – HYPOTHETICAL WASTE DISPOSAL SITE AT COASTAL LOCATION

The waste disposal system considered in this illustrative example comprises a concrete vault for Low Level Waste (LLW) and adjacent trench for soil and decommissioning wastes. Both are located in the unsaturated zone, lying between 9 and 14 m above Ordnance Datum (OD), several hundred metres from the coast.

Given the modular nature of the SimER code, the specification of the problem is presented on a module basis. Details are outlined below to demonstrate the level of detail expected to be representative of applications of SimER. Further details are given in the verification report (3) and the User Guide (1).

Geosphere

Fine to medium grained sandstone forms the bedrock under the site with a zone of weathered material on the upper surface. The rock head is located at a depth of about 20 - 30 m beneath the surface of the site and dips gradually to the south. The sandstone is overlain by a patchy layer of clay of varying thicknesses. This is overlain by two quaternary drift formations with different hydrogeological properties. The water table is generally located within these drift layers.

Groundwater flow is sub-horizontal, from the inland hills to the coast. At the northern edge of the region of interest, the groundwater table is 5 m beneath the surface. At the surface, recharge occurs through the drift. Terrestrial groundwater discharges under the seabed, due to density driven flow at the saline interface which is assumed to be located 100 m offshore. Surface runoff and some groundwater enters a river flowing from the hills to the coast. The water table meets the surface at this river.

Biosphere

The region of interest is located on a coastal plain from which mountains rise to the north-east. A river drains the coastal plain and enters the sea. The coastline is characterised by a beach and inter-tidal zone and low cliffs inland. Most of the coastal plain consists of grassy fields with a small area of woodland and land used for the growing of crops. Roads and minor tracks allow access to the coastal plain and to settlements that are located there.

The region of interest extends from about 1 km inland to the sea, and covers a total area of about 1.5 km x 1 km. The site slopes gently, falling from about 40 m above sea level at the northern boundary of the site to only a few metres above sea level at the southern boundary (marked by low cliffs). A river runs into the sea. The sea is generally shallow, typically between 20 m and 40 m deep.

The present day climate is cool temperate with prevailing winds from a westerly direction. The mean annual temperature is about 10˚C, and average annual precipitation has been recorded at about 1000 mm.

The vegetation characteristics are dominated by a variety of agricultural land uses. Most farms can provide a large part of their own fodder for their cows and sheep. The good quality soil surrounding the site is divided into four nominal regions, north, south, east and west of the site itself. In addition, a region of poorer quality soil is present

close to the sea and a forest is present to the east of the river. A beach, about 50 m wide, is present between the base of the cliffs and the sea. Figure 1 shows the main surface features at several periods.
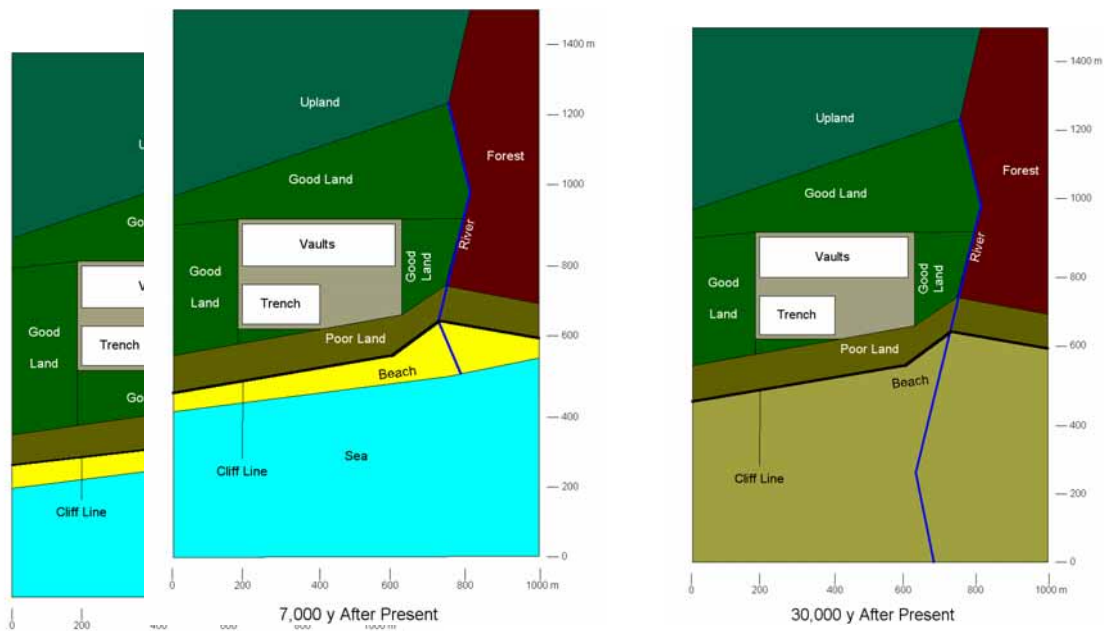

Fig. 1 Evolution of the main Landscape Features at Present Day (left); and 7,000 y (middle) and 30,000 y after present (right).

Waste Disposal

The vault has a capacity for 200 000 m^3 of wastes and is divided into two rows of four cells, each 50 m x 100 m. The cells have concrete floors and walls 0.3 m thick. There is a 0.5 m thick low permeability cut-off wall upstream of the facility, and a 5 m thick cap constructed of various layers including anti-intrusion layers, low permeability layers, and drainage layers. This cap is predicted to have a lifetime of 2000 years (90% effective after 500 years and 30% effective after 1000 years). At closure, the vault will be backfilled with cementitious grout. Estimates of the performance of the engineered materials suggest that their degradation will be controlled by the volume of water that has flowed through the pores in the material divided by the volume of the pores. Concrete is assumed to degrade at a rate of 10^{-3} y^{-1} per turnover of the pore water volume, whilst cement is assumed to degrade at a rate of 6 10^{-4} y^{-1} per turnover of the pore water volume.

The trench has a total capacity of about 10 000 m^3. It is excavated directly into the subsurface sediments and rock, with the only engineered features being 0.3 m clay lining in the base and a 2 m earth cap. This simple cap is predicated to have a lifetime of 2000 years (90% effective after 300 years and 20% effective after 500 years).

The engineering properties (i.e. hydraulic conductivity, density, porosity, degradation factor) of the various materials that comprise the facilities need to be specified. The `Degradation Factor' is the factor by which the hydraulic conductivity increases by when the feature is fully degraded.

Most of the wastes disposed of to the vault are contained in 20 m^3 steel containers, into which either raw wastes or compressed drums are grouted. In addition, some large items of decommissioning waste are grouted into the vault directly. Four main types of waste streams (i.e. general trash, concreted sludges activated metals and bulky redundant items) are disposed to the vault in sequences over time. All but the redundant items are disposed of in steel containers.

The trench contains contaminated soil and rubble, which is disposed of without packaging. 70 000 m^3 of rubble is disposed of to the trench at a uniform rate between 20 and 40 years. A further 29 000 m^3 of contaminated soil is disposed of at a uniform rate between 35 and 45 years. The average concentrations of contaminants and other monitorables of interest in the wastes are specified by the users.

Within the wastes, iron corrodes and cellulose degradation can take place. The characteristics of these reactions are assumed to be dependent on the degree of saturation only and it should be noted that this simple set of reactions have been chosen to be purely illustrative. For example, reactions considered include 1 mole of cellulose degrades to 1 mole of glucose in saturated conditions; or 1 mole of cellulose degrades to 6 moles of carbon dioxide in unsaturated conditions..etc. Cellulose degradation and iron corrosion are assumed to be dynamic reactions, whilst others listed above are assumed to occur effectively instantaneously. In practice the conceptual chemical reactions implemented in the SimER model need to be underpinned using more detailed chemical models.

Evolution of the System

Climate Change

An assessment of potential future climate change has developed two snapshots of the potential landscape, at 7000 and 30 000 years in the future (Figure 1). In the first period, coastal erosion results in northern movement of the cliff line, as illustrated in Figure 1. This shows the maximum expected inland extent of erosion. This is anticipated to be followed by a period of global cooling in which the sea level falls progressively, revealing the seabed which can develop into soil. Between about 20 000 and 25 000 years a lake is expected to be present in the former seabed. Landscape changes further at 30 000 years as glaciers are assumed to encroach on the site at this time.

Values for temperature, precipitation and sea-level change are input over a number of time periods for this climate scenario. Periodic major storms can also be specified to affect the site.

Human Activities

Six hypothetical human exposure groups are considered: a farmer, a fisherman, a resident of the site, a worker in an office on the site, a construction worker (building houses etc) and a surveyor/geoscientist (involved in site investigation works) These humans are assumed to use the landscape in a variety of ways, including: arable farming, livestock farming, rough grazing, recreation, forestry, residential use, business use, roads and fishing. The occupancy of the farmer and fisherman is dependent on the climate, with varying time spent outdoors. The use of the land also varies with the climate, and can be specified by user.

Modelled Results

The results of the integration test for the waste disposal (3) are presented to demonstrate that all of the individual SimER components function correctly as an integrated whole, and that the code calculates results that are consistent with the input specification. The results are demonstrated using screenshots of the SimER Spatial Viewer and Parameter Charter.

The operation of the Transport component is examined by considering the calculated concentrations (and other derived results, calculated with the Impacts component). Because of the complexity of the model, it is not feasible to undertake detailed verification calculations. Therefore, the checks are largely semi-quantitative (e.g. does the relative concentrations of a contaminant in the waste and the environment seem reasonable) and qualitative in nature (e.g. is the plume of contaminants downstream travel in a sensible direction).

Once released to the Upper Drift, contaminants migrate by advection and dispersion in groundwater. The Darcy velocities determining the rate of transport are obtained on a cell-by-cell basis from the Water Flow component, and are time-dependent. Figure 2 shows the changes in distribution of one of the radionuclide contaminants (Nb-94) over time. The plot at 50 years illustrates the disposals of Nb-94 to the vault and trench. After 500 years the niobium has begun to disperse to the cells around the facilities and then into the associated compartments. By 5000 y, a plume is evident in the direction of groundwater flow (left to right in the figures), although the plume does not penetrate significantly through the clay to the low-flowing sandstone strata at the base of the model.
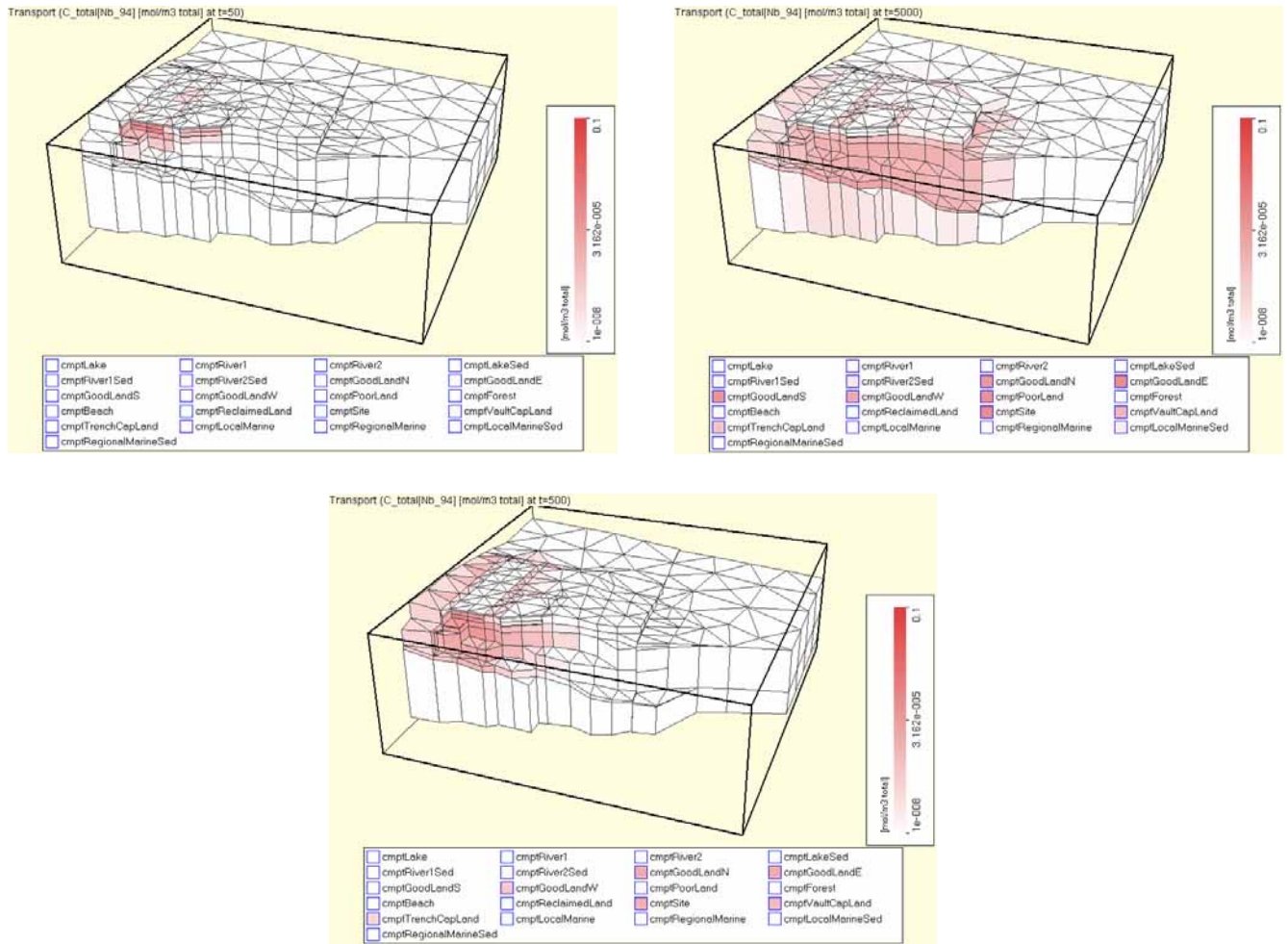
Fig. 2 Example output from the Spatial Viewer showing concentration of Nb-94 (mol m^{-3}) at: 50 y (top left), 500 y (bottom) and 5000 y (top left).

The variation of the average concentrations of selected contaminants with different behaviours in these layers can be seen in Figure 3. Tritium, which is unsorbed, is rapidly dispersed to essentially equal concentrations in the Upper and Lower Drift strata, with average concentrations in the Sandstone about a factor of two lower. It then decays rapidly. Of the longer lived radionuclides considered, U-234 migrates more rapidly but at lower concentrations than Nb-94. In both cases, it can be seen that there is relatively rapid dispersion in the drift layers (concentrations are similar), but the groundwater flows mean that the concentrations in the Sandstone remain lower, and peak later, than the concentrations in the drift.
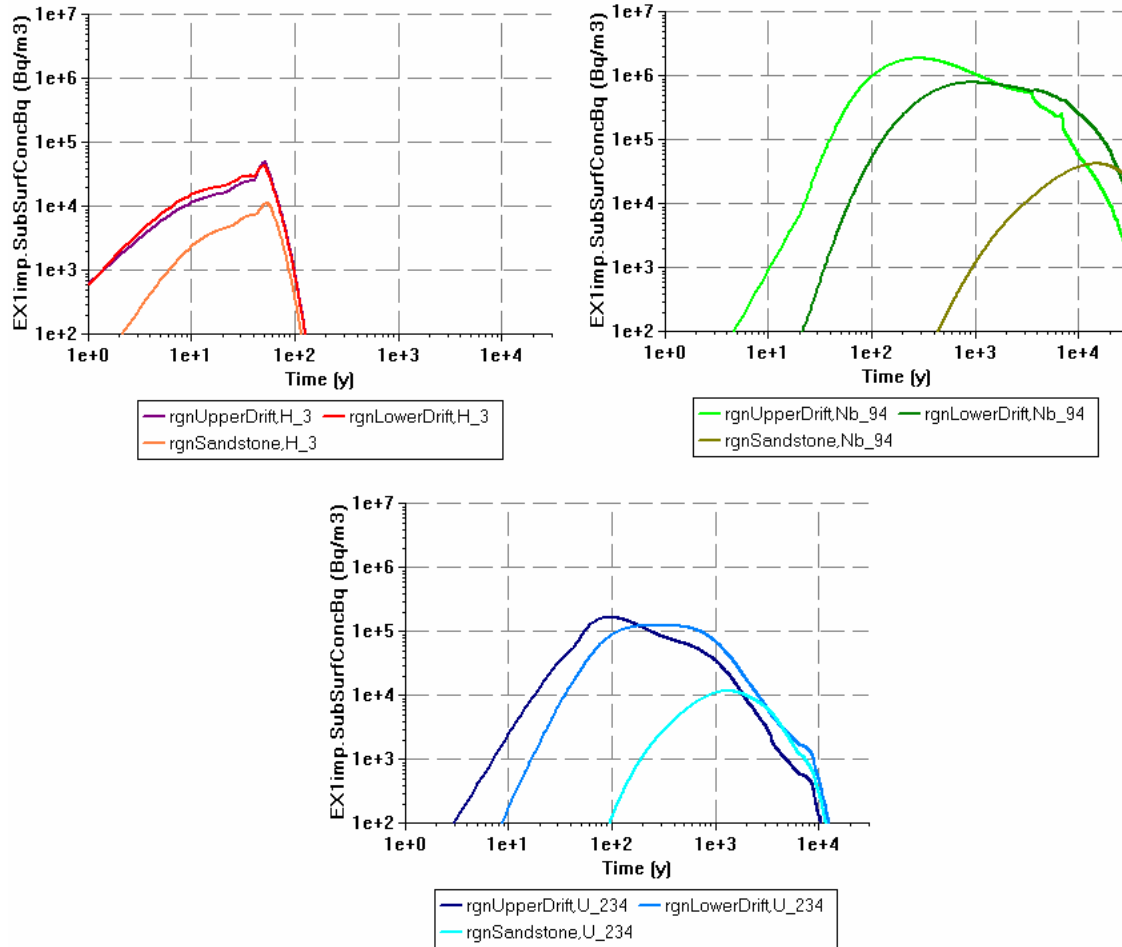
Fig. 3 Calculated Concentrations of H-3 (Top Left), Nb-94 (Top Right) and U-234 (Bottom) in Rock Strata

A limited number of illustrative exposure pathways are considered in the disposal test case, in order to show the function of the Impacts component in calculating doses for a variety of potentially exposed groups from various radionuclides and various locations. Radiation doses are assessed taking into account their occupancy and use of the land. Reference dose coefficients are used, and combined with assumed intake rates. Derived concentrations in plants and animals are calculated using equilibrium concentration factors and transfer factors.

The calculated external doses are shown in Figure 4. These figures show the results for Nb-94, disaggregated by location. The results illustrate that the Farmer's occupancy is associated with good land and the site, with relatively small amounts of time being spent on the beach and in the forest. After about 10 000 years, the farmer spends a decreasing fraction of time outdoors, staying at home on the site. This has the result that the site becomes more important as a contributor to the farmer's external irradiation.
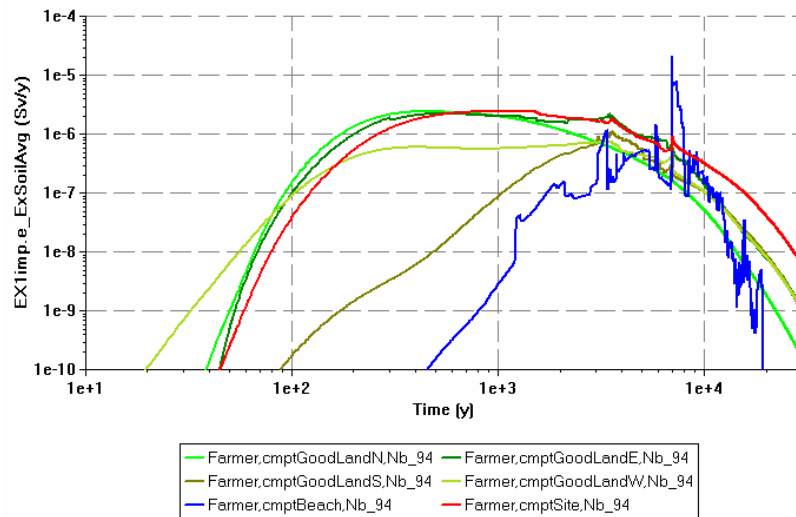
Fig. 4 External Doses from Nb-94 to a Farmer

In addition a hypothetical contaminated land integrated test represented by an example nuclear site was undertaken before (3). The test case considered comprising general contaminated land, contaminated drains, a leaking storage tank with associated contaminated soil, and a historic subterranean vault. Over a period of 60 years these facilities are remediated in various ways. SimER model results on groundwater flow, contaminant transport and radiological impacts to the PEG have been presented before (2, 3) and are not repeated here.

SAMPLE TEST CASE 2 – REMEDIATION OF URANIUM USING PRB AT THE Y-12 SITE

The Y-12 Pathway-2 Permeable Reactive Barrier (PRB) field trial experiment, conducted at the US Oak Ridge Reservation (ORR), concerning the remediation of a uranium contaminant plume was considered for the modelling study. Pathway 2 is a shallow pathway, carrying contaminants west, to the upper reaches of Bear Creek. The area around the PRB is designated as Area 2 and contains many boreholes for the monitoring of groundwater. This pathway is contaminated primarily with low levels of uranium and nitrate. Extensive field and geochemical data, with comprehensive quality assurance control, were available for this site in the public domain (10). The field trial experiment covering many aspects of typical radioactive contaminant plume remediation and thus serves as a useful test case for SimER.

Modelling at the kilometre scale has been undertaken using the SimER assessment level modelling code. SimER was used to provide a generalised representation of the regional groundwater flow to investigate the hydrogeological features of the PRB. In addition, SimER is able to model the specific time evolution and events which are essential to fully understand and compare the effect of a remediation technology. The SimER model assumes, on the basis of underpinning modelling (11), that within the remediation zone uranium is solubility limited to a concentration of 1e-4 mol m^{-3}. Elsewhere, uranium migration is affected by sorption processes which are represented by sorption coefficients typical of the soils and underlying saprolite rock.

Modelled Results

Figure 5 provides a view of the Y-12 SimER model landscape domain showing the topography, simplified geology and location of the former uranium liquor storage ponds (represented by four adjacent regions) and the location of the remediation zone, located downstream.
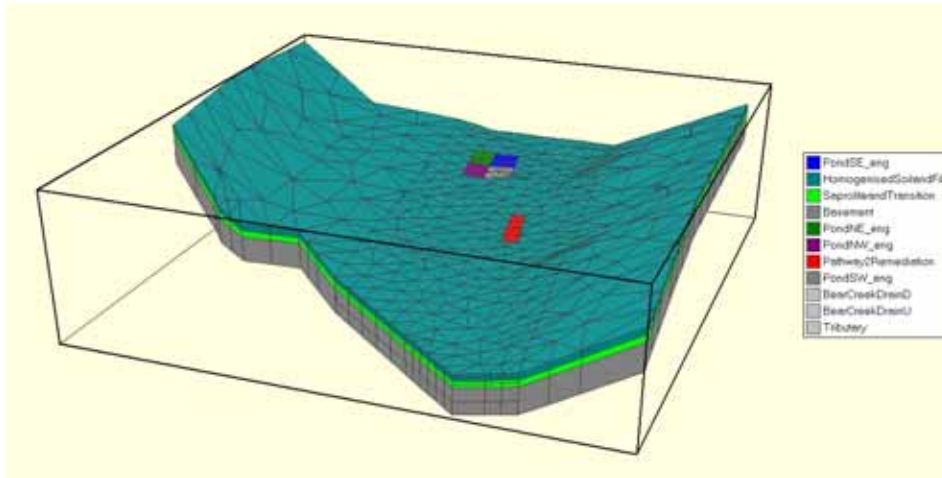
Fig. 5 View of the SimER model domain of the Y-12 site (approx. 1250m square x 3 vertical exaggeration).

Figure 6 shows the pattern of uranium concentration from the source area (red orange) and along the Old Bear Creek pathway. After 37 years, the SimER model considers the emplacement of the PRB, which results in a decrease in uranium concentration in the remediation zone (denoted in blue). At 54 years the concentration within the preferential pathway is lowered.

Figure 7 compares the uranium concentration in Bear Creek streamwater downstream of the remediation zone and shows a significant lowering of the uranium concentration. This output from SimER is an example of a direct comparison of a radiological impact representing contaminant concentration in a biosphere compartment.
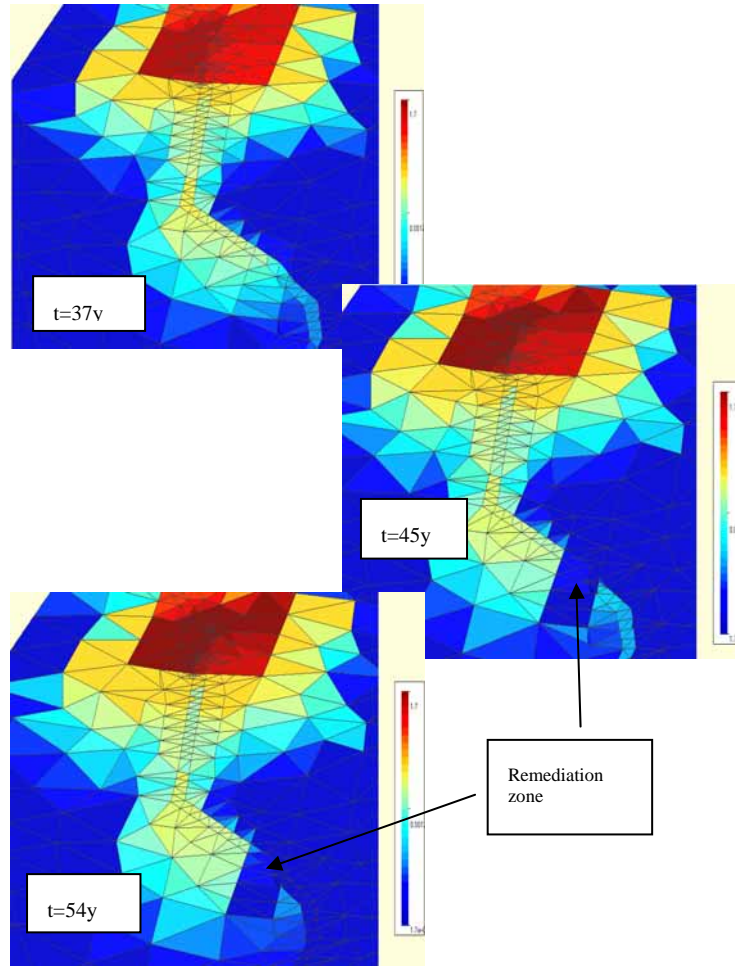
Fig. 6 Output from SimER showing the uranium concentrations in the source region and plume along the preferential pathway and lower concentrations in the remediation zone.
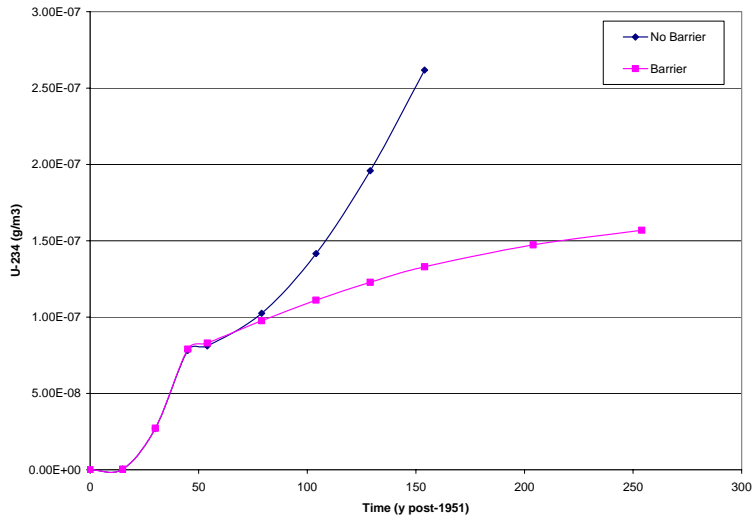

Fig. 7 Comparison of uranium concentration in Bear Creek streamwater downstream of the PRB showing the beneficial remediation effect of the gravel reactive barrier design after 45 years.

CONCLUDING REMARKS

SimER has been successfully applied to model a number of applications on contaminated land and waste disposal issues. It has demonstrated that the extensive capabilities and flexible input requirements of SimER code offer a powerful means to model the key features of the whole system (i.e. Near-field, geosphere and biosphere) in a single code for practical risk assessment problems. This avoids the need for any time consuming data transfer and the often laborious interface between the different codes, thus greatly speeds up the assessment process and has major Quality Assurance advantages. SimER thus provides a cost-effective tool for undertaking projects involving risk assessment from practical contaminated land assessments, through to full post-closure safety cases and other work supporting key site end-point decisions.

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